Analytical Solutions of Moisture Flow Equations and Their Numerical Evaluation

A. G. Gibbs

April 1981

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ABSTRACT

The role of analytical solutions of idealized moisture flow problems is discussed. Some different formulations of the moisture flow problem are reviewed. A number of different analytical solutions are summarized, including the case of idealized coupled moisture and heat flow. The evaluation of special functions which commonly arise in analytical solutions is discussed, including some pitfalls in the evaluation of expressions involving combinations of special functions. Finally, perturbation theory methods are summarized which can be used to obtain good approximate analytical solutions to problems which are too complicated to solve exactly, but which are close to an analytically solvable problem.

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1.0 INTRODUCTION

The most general formulations of the moisture flow problem lead to partial differential equations which are nonlinear and which have variable coefficients. These equations are not solvable by known analytical methods, but must be treated numerically, using finite differences, finite elements, collocation methods, etc. It is only with considerable simplification that transport problems sufficiently idealized to be analytically tractable are obtained.

Different philosophies can be advanced to justify the seeking of such solutions. Clearly, whatever their physical shortcomings, analytical solutions can provide important test cases for more general numerical methods. In a given application, to the extent that essential physics is retained, the form of analytical solutions may also provide important insights into the behavior of solutions of real-world problems, and may thus help in the design of numerical methods. Also if, in a particular application, only small changes in a solution from its initial values are anticipated, then a linearization of the general equations about those initial values may lead to a realistic set of equations which are simple enough to treat analytically. Finally, some problems too difficult to solve exactly are "close enough" to solvable problems so that approximate analytical solutions may be obtained by perturbation methods.

2.0 FORMULATIONS OF THE MOISTURE TRANSPORT PROBLEM

Various levels of generality are possible in formulating moisture flow problems. Quite generally, the moisture content θ satisfies the equation:

$$\frac{\partial \theta}{\partial t} = -\nabla \cdot \mathbf{q}_\theta + S_\theta \quad (2.1)$$

where $\mathbf{q}_\theta$ denotes the moisture flux and S_θ any local sources of moisture. For the case of isotropic soils, assuming Darcy's law to be valid, the flux $\mathbf{q}_\theta$ can be written as:

$$\mathbf{q}_\theta = -K(\nabla \Psi - \hat{z}) \quad (2.2)$$

where K is the hydraulic conductivity, Ψ the moisture potential, and $\hat{z}$ a unit vector in the downward direction (representing the effect of gravity). Using (2.2) in (2.1) gives:

$$\frac{\partial \theta}{\partial t} = \nabla \cdot K \nabla \Psi - \frac{\partial K}{\partial z} + S_\theta \quad (2.3)$$

If Ψ is determined as a unique function of θ (empirically), then by defining the soil water diffusivity:

$$D(\theta) = K \frac{d\Psi(\theta)}{d\theta}, \quad (2.4)$$

Equation (2.3) can be rewritten as:

$$\frac{\partial \theta}{\partial t} = \nabla \cdot D(\theta) \nabla \theta - \frac{dK(\theta)}{d\theta} \frac{\partial \theta}{\partial z} + S_\theta \quad (2.5)$$

In general, $D(\theta)$ and $K(\theta)$ are complicated functions of θ .

Alternatively, the moisture potential ψ may be treated as the dependent variable rather than θ . Then, defining:

$$C(\psi) = \frac{d\theta}{d\psi} = \frac{1}{d\psi/d\theta} \quad (2.6)$$

allows (2.3) to be written as:

$$C(\psi) \frac{\partial \psi}{\partial t} = \nabla \cdot K(\psi) \nabla \psi - \frac{dK(\psi)}{d\psi} \frac{\partial \psi}{\partial z} + S_{\theta} \quad (2.7)$$

A third variant is obtained by applying a Kirchoff transformation to Equation (2.7). Define a new independent variable $\phi(\psi)$ by:

$$\phi(\psi) = \int_{\psi_0}^{\psi} K(\psi') d\psi' \quad (2.8)$$

where ψ_0 is some constant. (The function ϕ is known as the matric flux potential.) Then, clearly:

$$\nabla \phi = \frac{d\phi}{d\psi} \nabla \psi = K(\psi) \nabla \psi \quad (2.9)$$

Thus, Equation (2.7) becomes:

$$S_{\theta} + \nabla^2 \phi - \frac{dK}{d\psi} \frac{\partial \psi}{\partial z} = C(\psi) \frac{\partial \psi}{\partial t} \quad (2.10)$$

and by defining:

$$\frac{d\theta}{d\phi} = B(\phi) = C(\psi) \frac{d\psi}{d\phi} = \frac{C(\psi)}{d\phi/d\psi} = \frac{C(\psi)}{K(\psi)} \quad (2.11)$$

Equation (2.10) becomes:

$$B(\phi) \frac{\partial \phi}{\partial t} = \nabla^2 \phi - \frac{dK(\phi)}{d\phi} \frac{\partial \phi}{\partial z} + S_{\theta} \quad (2.12)$$

In order to obtain an analytical solution to any of the above equations, some simple forms must be assumed for $D(\theta)$ and $K(\theta)$, $C(\psi)$ and $K(\psi)$, or $B(\phi)$ and $K(\phi)$. Also, an elementary geometry and simple boundary conditions are required.

Boundary conditions usually state that either θ or ψ is known on part of the boundary, and that the moisture flux q_{θ} is known on the remaining part of the boundary. If the ϕ -formulation of Equation (2.12) is being used, then specifying ψ on the boundary is equivalent, via Equation (2.8), to specifying ϕ , while specifying q_{θ} is, via Equations (2.2) and (2.9), equivalent to specifying $\nabla \phi$, since:

$$q_{\theta} = \nabla \phi + K \hat{z} \quad (2.13)$$

3.0 SOME ANALYTICAL SOLUTIONS

The most elementary solutions of the equations of the previous section are obtained by assuming that coefficients, such as $D(\theta)$, are constant, and prescribing constant initial and boundary conditions. Solutions of the resulting constant-coefficient partial differential equations may be obtained by a variety of methods. When boundary and initial conditions are compatible, similarity solutions may exist (Hansen 1964). These are solutions in which the independent variables occur only in particular combinations so the solution actually depends on a smaller number of variables. One such example occurs when $\theta(z,t) = \theta(z/\sqrt{t})$. The transformation to the new variable $z/\sqrt{t}$ is known as Boltzmann's transformation, and leads to a simpler equation for θ . However, such similarity solutions are rather special and occur only for certain combinations of initial and boundary conditions. More generally, the partial differential equations must be solved by the method of separation of variables (Rainville 1958), or by using integral transforms (Tranter 1974). The simplest problem of all is the "horizontal infiltration problem" in which the z -variation does not occur. Then, with a constant D and no sources, Equation (2.5) reduces to:

$$\frac{\partial \theta}{\partial t} = D \frac{\partial^2 \theta}{\partial x^2} \quad (0 < x < \infty) \quad (3.1)$$

With the elementary boundary and initial conditions:

$$\begin{aligned} \theta(x,0) &= \theta_i & x > 0 \\ \theta(0,t) &= \theta_u & t > 0 \end{aligned} \quad (3.2)$$

the solution, due to Philip (1966), is:

$$\theta = \theta_i + (\theta_u - \theta_i) \operatorname{erfc} \frac{x}{2\sqrt{Dt}} \quad (3.3)$$

(The above problem is, of course, an exact analog of a problem in heat conduction. Many other heat conduction problems are mathematically equivalent to idealized forms of one of the formulations of the moisture equations of the previous section. Thus, references such as Carslaw and Jaeger (1948) can be browsed for analytical solutions of problems that may also be of use in moisture flow applications.)

Another idealized problem is the "vertical infiltration problem" in which the solution depends only on the z -coordinate. Then, Equation (2.5), with D and $dK/d\theta = K_\theta$ assumed constant, becomes:

$$\frac{\partial \theta}{\partial t} = D \frac{\partial^2 \theta}{\partial z^2} - K_\theta \frac{\partial \theta}{\partial z} \quad (3.4)$$

Subject to the conditions:

$$\begin{aligned} \theta(z, 0) &= \theta_i & z > 0 \\ \theta(0, t) &= \theta_u & t > 0 \end{aligned} \quad (3.5)$$

the solution obtained by Philip (1966), is:

$$\begin{aligned} \theta = \theta_i + \frac{\theta_u - \theta_i}{2} & \left[\operatorname{erfc} \left(\frac{z - K_\theta t}{2\sqrt{Dt}} \right) \right. \\ & \left. + \exp(K_\theta z/D) \operatorname{erfc} \left(\frac{z + K_\theta t}{2\sqrt{Dt}} \right) \right] \end{aligned} \quad (3.6)$$

An analogous solution was obtained by Philip for the case of a spherically symmetric problem with infiltration from a spherical cavity, but neglecting the gravity term (Philip 1969).

In a series of papers by Warrick and his coworkers (1974, 1976, 1978), analytical solutions are obtained for some simplified forms of the ϕ -equation, i.e., Equation (2.12). They consider the hydraulic conductivity K to be an exponential function of the moisture potential Ψ , i.e.:

$$K(\psi) = K_0 e^{\alpha\psi} \quad (3.7)$$

with K_0 and α constant. Then, with the constant ψ_0 taken to be $-\infty$, Equation (2.8) gives:

$$\phi(\psi) = \frac{K_0}{\alpha} e^{\alpha\psi} = \frac{1}{\alpha} K(\psi) \quad (3.8)$$

Thus, for this model, the function ϕ is a constant multiple of K . In addition, the function $B(\phi)$, Equation (2.11), is taken to be a constant. (Since $B(\phi) = d\theta/d\phi$, and since ϕ and K are linearly related in the present case, then this is equivalent to assuming that $d\theta/dK$ is constant, or that K is linear as a function of θ). Using Equations (3.7) and (3.8) in Equation (2.12) simplifies it to:

$$B \frac{\partial \phi}{\partial t} = \nabla^2 \phi - \alpha \frac{\partial \phi}{\partial z} + S \quad (3.9)$$

Solutions have been obtained for a number of different geometries and source/sink distributions.

Warrick (1974) considered the case of a point source located at the origin on the surface of the ground. An initial condition:

$$\phi(r, z=0) = 0 \quad (3.10)$$

was assumed, along with a boundary condition corresponding to no flow across the surface $z=0$ except at the origin. From Equations (2.13) and (3.7), this implies that:

$$-\frac{\partial \phi}{\partial z} + \alpha \phi = 0 \quad z=0, r \neq 0, t > 0 \quad (3.11)$$

The solution was obtained by superposing the solutions for point sources in an infinite medium. Dimensionless variables are defined by:

$$R = \frac{\alpha r}{2}, \quad Z = \frac{\alpha z}{2}, \quad T = \frac{\alpha k t}{4} \quad (3.12)$$

with:

$$k = \frac{\alpha}{B} \quad (3.13)$$

Also, let:

$$\rho = \sqrt{R^2 + Z^2} \quad (3.14)$$

Define the function:

$$\begin{aligned} \phi_B(R, Z, T) = \frac{e^Z}{2\rho} & \left\{ e^{\rho} \operatorname{erfc} \left(\frac{\rho}{2\sqrt{T}} + \sqrt{T} \right) \right. \\ & \left. + e^{-\rho} \operatorname{erfc} \left(\frac{\rho}{2\sqrt{T}} - \sqrt{T} \right) \right\} \end{aligned} \quad (3.15)$$

Then the solution of Equation (3.9), subject to (3.10) and (3.11), can be written as:

$$\begin{aligned} \phi = \frac{8\pi}{\alpha q} \phi = 2 & \left\{ \phi_B(R, Z, T) \right. \\ & \left. - \int_Z^\infty e^{-2(Z'-Z)} \phi_B(R, Z, T) \, dZ' \right\} \end{aligned} \quad (3.16)$$

(The integral must be evaluated numerically.) Here, q is the strength of the point source.

Similar solutions were reported for line disk, and strip sources by Loman and Warrick (1974, 1976).

Solutions were obtained, also by Lomen and Warrick (1978), for the case of Z, t dependence only, but with an initial condition and a sink both dependent on depth, and for a time-dependent surface flux. In terms of the dimensionless variables, Z, T , this problem is stated as:

$$\frac{\partial \phi}{\partial T} = \frac{\partial^2 \phi}{\partial Z^2} - 2 \frac{\partial \phi}{\partial Z} - \frac{4}{\alpha} S(Z) \quad (3.17)$$

with:

$$\begin{aligned} \phi(Z, 0) &= g(Z) + \phi_{\infty}, & T=0, Z>0 \\ -\frac{\partial \phi}{\partial Z} + 2\phi &= \frac{2}{\alpha} v(T), & T>0, Z=0 \end{aligned} \quad (3.18)$$

Here, $g(Z)$ and $v(T)$ are given functions, and ϕ_{∞} is a given constant.

The solution is written as:

$$\phi(Z, T) = \phi_{\infty} + \phi_S(Z) + \phi_T(Z, T) \quad (3.19)$$

where:

$$\phi_S(Z) = \frac{U}{\alpha} - \frac{4}{\alpha^2} \int_Z^{\infty} dZ' e^{2(Z-Z')} \int_0^{Z'} S(\xi) d\xi \quad (3.20)$$

with:

$$U = \frac{2}{\alpha} \int_0^{\infty} S(Z) dZ \quad (3.21)$$

Also:

$$\begin{aligned} \phi_T(Z, T) = & 2 \exp(Z-T) \int_0^T [\exp \left\{ -Z^2/4(T-\tau) \right\} \left\{ \pi(T-\tau) \right\}^{-1/2} \\ & - \exp(T-\tau+Z) \operatorname{erfc} \left\{ Z/2(T-\tau)^{1/2} + (T-\tau)^{1/2} \right\}] \\ & [\left\{ v(\tau) - u \right\} / \alpha - \phi_\infty] \exp(\tau) d\tau + R(Z, T, g(Z) - \phi_S(Z)) \end{aligned} \quad (3.22)$$

with:

$$\begin{aligned} R(Z, T, f) = & \exp(Z-T) \int_0^\infty (4\pi T)^{-1/2} [\exp \left\{ -(Z-Z')^2/4T \right\} + \\ & \exp \left\{ -(Z+Z')^2/4T \right\} - \exp(T+Z+Z) \operatorname{erfc} \left\{ (Z+Z')/2T^{1/2} \right. \\ & \left. + T^{1/2} \right\}] f(Z') \exp(-Z') dZ' \end{aligned} \quad (3.23)$$

4.0 COMBINED MOISTURE AND HEAT FLOW

Some analytical solutions are available for simplified forms of the coupled heat and moisture flow equations. One of these is due to Hauk (1971). He worked with equations for the temperature T and the moisture potential ψ . By appealing to the principles of irreversible thermodynamics he suggested that the appropriate form of the coupled equations is:

$$C \frac{\partial T}{\partial t} = K_a \frac{\partial^2 T}{\partial x^2} + w \frac{\partial^2 \psi}{\partial x^2} \quad (4.1)$$

$$C_m \frac{\partial \psi}{\partial t} = v \frac{\partial^2 T}{\partial x^2} + k_a \frac{\partial^2 \psi}{\partial x^2} (\psi - gx) \quad (4.2)$$

Here C , C_m , K_a , k_a , v , w , and g are treated by Hauk as appropriate constants.

Hauk considered the problem of the above equations subject to the (constant) initial conditions:

$$\left. \begin{aligned} T(x,0) &= T_0 \\ \psi(x,0) &= 0 \end{aligned} \right\} \quad (4.3)$$

and boundary conditions corresponding to diffusion-limited moisture uptake by the atmosphere and a constant net heat flux at the ground surface:

$$\left. \begin{aligned} k \frac{\partial \psi}{\partial x} &= A_v (\psi - \psi_a), \text{ at } x=0 \\ -K \frac{\partial T}{\partial x} &= R_n, \text{ at } x=0 \end{aligned} \right\} \quad (4.4)$$

This problem was solved by Hauk using Laplace transforms with respect to the time variable. The solutions are expressed in terms of dimensionless ratios:

$$\begin{aligned}
T_1 &= (T-T_0)/T_0 \\
\Psi_1 &= \Psi/\Psi_a \\
\left. \begin{aligned} \xi &= x/L_1 \\ \tau &= t/t_1 \end{aligned} \right\} \quad L_1, t_1 \text{ arbitrary}
\end{aligned} \tag{4.5}$$

The results are:

$$\begin{aligned}
\Psi_1(\xi, \tau) &= \frac{1}{(a_1-b_1) \sqrt{a^2-b^2}} \left\{ (HR_a a_1 b_1) F_2(\sqrt{a+b} \xi, d, \tau) \right. \\
&\quad - F_2(\sqrt{a-b} \xi, d, \tau) \\
&\quad + a_1 (R_a b_1 + H) \sqrt{a-b} F_1(\sqrt{a+b} \xi, d, \tau) \\
&\quad \left. - b_1 (R_a a_1 + H) \sqrt{a+b} F_1(\sqrt{a-b} \xi, d, \tau) \right\}
\end{aligned} \tag{4.6}$$

$$\begin{aligned}
T_1(\xi, \tau) &= \frac{1}{(b_1-a_1) \sqrt{a^2-b^2}} \left\{ HR_a [b_1 F_2(\sqrt{a+b} \xi, d, \tau) \right. \\
&\quad - a_1 F_2(\sqrt{a-b} \xi, d, \tau)] \\
&\quad + (R_a b_1 + H) \sqrt{a-b} F_1(\sqrt{a+b} \xi, d, \tau) \\
&\quad \left. - (R_a a_1 + H) \sqrt{a+b} F_1(\sqrt{a-b} \xi, d, \tau) \right\}
\end{aligned} \tag{4.7}$$

Here, the functions F_1 and F_2 are given by:

$$F_1(x, d, t) = \frac{1}{d} \left\{ \operatorname{erfc} \left(\frac{x}{2\sqrt{t}} \right) - e^{dx+d^2t} \operatorname{erfc} \left(\frac{x}{2\sqrt{t}} + d\sqrt{t} \right) \right\} \tag{4.8}$$

$$F_2(x, d, t) = \left\{ \frac{2}{d} \sqrt{\frac{t}{\pi}} e^{-x^2/4t} - \frac{(1+dx)}{d^2} \operatorname{erfc} \left(\frac{x}{2\sqrt{t}} \right) \right. \\ \left. + \frac{1}{d^2} e^{xd+d^2t} \operatorname{erfc} \left(\frac{x}{2\sqrt{t}} + d\sqrt{t} \right) \right\} \quad (4.9)$$

The various constants appearing in Equations (4.6 through 4.9) are given by:

$$a_1 = \frac{\kappa(a+b)-1}{\kappa\eta(a+b)}$$

$$b_1 = \frac{\kappa(a-b)-1}{\kappa\eta(a-b)}$$

$$a = \frac{\lambda + \kappa}{2\lambda\kappa(1-\delta\eta)}$$

$$b = \left[a^2 - \frac{1}{\lambda\kappa(1-\delta\eta)} \right]^{1/2}$$

$$d = H \frac{a_1 \sqrt{a-b} - b_1 \sqrt{a+b}}{(a_1 - b_1) \sqrt{a^2 - b^2}}$$

$$\kappa = K_a t_1 / CL_1^2$$

$$\eta = \frac{w\psi_a}{K_a T_0}$$

$$\delta = \frac{v T_0}{K_a \psi_a}$$

$$\lambda = \frac{k_a t_1}{C_m L_1^2}$$

$$g' = gL/\psi_a$$

$$H = A_v L/k$$

$$R_a = R_n L / K T_0$$

An alternative model for coupled moisture and heat flow was suggested by Nicholaichuk (1974) who began with rather general expressions for the moisture flux due to Philip and deVries (1957):

$$q_{\theta} = -K \frac{\partial}{\partial x} (\psi - x) - D_T \frac{\partial T}{\partial x} \quad (4.10)$$

This expression is linear in the gradients of moisture potential, gravitational potential, and temperature. By defining the soil water diffusivity:

$$D_{\theta} = K \frac{d\psi}{d\theta} \quad (\text{cm}^2/\text{sec}) \quad (4.11)$$

this expression takes the more symmetrical form:

$$q_{\theta} = K - D_{\theta} \frac{\partial \theta}{\partial x} - D_T \frac{\partial T}{\partial x} \quad (4.12)$$

The moisture flow equation then becomes:

$$\frac{\partial \theta}{\partial t} = - \frac{\partial}{\partial x} q_{\theta} = \frac{\partial K}{\partial x} + \frac{\partial}{\partial x} \left(D_{\theta} \frac{\partial \theta}{\partial x} \right) + \frac{\partial}{\partial x} \left(D_T \frac{\partial T}{\partial x} \right) \quad (4.13)$$

Treating K as a function of T and θ , and defining:

$$\left. \begin{aligned} M &= \frac{\partial K}{\partial \theta} \\ N &= \frac{\partial K}{\partial T} \end{aligned} \right\} \quad (4.14)$$

then leads to:

$$\frac{\partial \theta}{\partial t} = \frac{\partial}{\partial x} \left(D_{\theta} \frac{\partial \theta}{\partial x} \right) + \frac{\partial}{\partial x} \left(D_T \frac{\partial T}{\partial x} \right) - M \frac{\partial \theta}{\partial x} - N \frac{\partial T}{\partial x} \quad (4.15)$$

The coefficients D_θ , D_T , M and N are, in general, functions of T and θ . For purposes of obtaining an analytical solution, Nicholaichuk treated them as constants.

A corresponding equation for $\partial T/\partial t$ was obtained by Nicholaichuk in somewhat less satisfying way. By expressing the heat flux q_h as a linear combination of thermal conduction, vapor convection and liquid convection, he was lead to an equation for $\partial T/\partial t$ in which a number of highly nonlinear terms occur, e.g., $\partial\theta/\partial x \partial T/\partial x$, $T\partial\theta/\partial t$, etc. In order to obtain an equation tractable for analytical solutions, he simply ignored the troublesome terms, setting them to zero. It is not clear whether the resulting equation contains all the essential physics, but it has the simple form:

$$\frac{\partial T}{\partial t} = F_1 \frac{\partial^2 T}{\partial x^2} - F_4 \frac{\partial T}{\partial t} \quad (4.16)$$

Here, F_1 and F_4 are appropriate constants.

Nicholaichuk suggested boundary conditions of the form:

$$\left. \begin{aligned} \frac{\partial T}{\partial x} + K_2 T &= K_1 \\ \frac{\partial \theta}{\partial x} &= K_3 + K_4 T \end{aligned} \right\} \quad \text{at } x=0 \quad (4.17)$$

It was later suggested by Gibbs (1981) that a more consistent model is obtained with the boundary conditions:

$$\left. \begin{aligned} \frac{\partial T}{\partial x} + K_2 T &= K_1 \\ \frac{\partial \theta}{\partial x} - \frac{M}{D_\theta} \theta &= K_3 + K_4 T \end{aligned} \right\} \quad \text{at } x=0 \quad (4.18)$$

Finally, initial conditions:

$$\left. \begin{array}{l} T = T_0 \\ \theta = \theta_0 \end{array} \right\} \quad \text{at } t=0 \quad (4.19)$$

were proposed.

Nicholaichuk obtained analytical solutions of the above problem, using Laplace transforms with respect to t , first solving Equation (4.6) for T , then using that result in Equation (4.15) and solving it for θ . His results have never been published in a journal, but are available as a thesis (Nicholaichuk (1974)). Unfortunately, the thesis appears to contain a very large number of typographical errors, making it an unreliable source of mathematical results. Because of this, the results were rederived by Gibbs (1981), including the case of the alternative boundary condition, Equation (4.18). These results are given in the report RHO-LP-48 (1981). The expression for T is:

$$\frac{T-T_0}{T_0} = \left(\frac{K_1}{\alpha T_0} - \frac{K_2}{\alpha} \right) g_0(x_0, t_0, R_1) \quad (4.20)$$

Here:

$$\begin{aligned} \alpha &= F_4/2F_1 \\ x_0 &= \alpha x \\ t_0 &= t/\tau \\ R_1 &= -K_2/\alpha \\ \tau &= 1/\alpha^2 F_1 \end{aligned} \quad (4.21)$$

and:

$$g_0(x_0, t_0, R_1) = \left\{ \frac{1}{2(2-R_1)} e^{2x_0} \operatorname{erfc} \left(\frac{x_0}{2\sqrt{t_0}} + \sqrt{t_0} \right) \right\} \quad (4.22)$$

$$\begin{aligned}
& - \frac{1}{2R_i} \operatorname{erfc} \left(\frac{x_0}{2\sqrt{t_0}} - \sqrt{t_0} \right) \\
& - \frac{(1-R_i)}{R_i(R_i-2)} e^{R_i(R_i-2)t_0 + R_i x_0} \\
& \operatorname{erfc} \left(\frac{x_0}{2\sqrt{t_0}} + (R_i-1)\sqrt{t_0} \right) \Bigg\}
\end{aligned}$$

The expression for θ is rather lengthy:

$$\theta = \theta_0 + V_p(x_0, t_0) + V_h(x_0, t_0) \quad (4.23)$$

Here:

$$V_p(x_0, t_0) = C_1 \sum_{i=1}^2 B_i g_0(x_0, t_0, R_i) \quad (4.24)$$

with:

$$\left. \begin{aligned}
C_1 &= \left(\frac{K_1}{\alpha T_0} - \frac{K_2}{\alpha} \right) / (\tau D_\theta \alpha^2 - 1) \\
B_1 &= \frac{P_1 - P_2 R_1}{R_1 - R_2} \\
B_2 &= -B_1 - P_2 \\
P_1 &= N \alpha T_0 \tau \\
P_2 &= D_T T_0 \tau \alpha^2 \\
R_2 &= \frac{M \alpha \tau - 2}{\tau D_\theta \alpha^2 - 1}
\end{aligned} \right\} \quad (4.25)$$

Also:

$$v_h(x_0, t_0) = C_1 f_1(x_0, t_0) + f_2(x_0, t_0) \quad (4.26)$$

where:

$$\begin{aligned} f_1(x_0, t_0) = & \left\{ \left(\frac{x_0}{2} + \frac{1}{4\beta} + \frac{\beta\tau}{n} t_0 \right) e^{2\beta x_0} \right. \\ & \operatorname{erfc} \left(\frac{1}{2} \sqrt{\frac{n}{\tau}} \frac{x_0}{\sqrt{t_0}} + \beta \sqrt{\frac{\tau}{n}} \sqrt{t_0} \right) \\ & - \frac{1}{4\beta} \operatorname{erfc} \left(\frac{1}{2} \sqrt{\frac{n}{\tau}} \frac{x_0}{\sqrt{t_0}} - \beta \sqrt{\frac{\tau}{n}} \sqrt{t_0} \right) \\ & \left. - \sqrt{\frac{\tau}{\pi\beta}} \frac{1}{\sqrt{t_0}} \exp(\beta x_0) - \left(\frac{n}{4} \frac{x_0^2}{t_0} + \frac{\beta^2 \tau}{n} t_0 \right) \right\} \end{aligned} \quad (4.27)$$

with:

$$\left. \begin{aligned} \beta &= M/2\alpha D_\theta \\ n &= 1/\alpha^2 D_\theta \end{aligned} \right\} \quad (4.28)$$

Also:

$$f_2(x_0, t_0) = \int_0^t h_{10}(t'_0) h_{20}(x_0, t_0 - t'_0) dt'_0 \quad (4.29)$$

with:

$$h_{10}(t_0) = -\frac{\tau}{n} \sum_{i=1}^2 d_i g_0(0, t_0, R_i) \quad (4.30)$$

$$\left. \begin{aligned} d_1 &= \frac{K_4}{a^2} (K_1 - K_2 T_0) - C_1 B_1 (R_1 - 2\beta) \\ d_2 &= -C_1 B_2 (R_2 - 2\beta) \end{aligned} \right\} \quad (4.31)$$

and:

$$\begin{aligned} h_2(x_0, t_0) &= \left\{ \sqrt{\frac{n}{\pi\tau}} \frac{1}{\sqrt{t_0}} \exp - \left(\frac{1}{2} \sqrt{\frac{n}{\tau}} \frac{x_0}{\sqrt{t_0}} - \beta \sqrt{\frac{\tau}{n}} \sqrt{t_0} \right)^2 \right. \\ &\quad \left. - \beta e^{2\beta x_0} \operatorname{erfc} \left(\frac{1}{2} \sqrt{\frac{n}{\tau}} \frac{x_0}{\sqrt{t_0}} + \beta \sqrt{\frac{\tau}{n}} \sqrt{t_0} \right)^2 \right\} \quad (4.32) \end{aligned}$$

A computer program "MOIST" has been written by Gibbs (1980) to evaluate the above expressions. Limited comparisons with finite element numerical solutions of the same equations have been reported (1980).

5.0 NUMERICAL EVALUATION OF SPECIAL FUNCTIONS

Analytical solutions of moisture flow problems often involve certain special functions such as Bessel functions, exponential integrals, or error functions. Highly accurate numerical methods exist for evaluating these functions. Modern routines can be obtained from the Argonne National Laboratory FUNPACK Library, the International Mathematical and Statistical Library (IMSL) available on the BCSR UNIVAC 1100 and the Battelle OEC VAX-11, or from specific papers in the literature. These routines are usually based on rational approximations, i.e., expressions for the desired special function as a quotient of polynomials. Often, different polynomials are used, depending on whether the argument of the function is large or small. A slightly less efficient, but equally accurate, approach is to use the series expansions, continued fractions, and asymptotic expansions given, e.g., in the NBS Handbook of Mathematical Functions, AMS-55 (1964). Either of the above approaches leads to accurate numerical values for the common special functions.

It is easy to assume that having accurate values of special functions will guarantee an accurate evaluation of analytical solutions of moisture flow problems. This attitude can be overly optimistic, since analytical solutions often involve lengthy expressions containing differences or products of special functions. Round-off errors can be large, and products of large numbers with small numbers can easily degenerate, in a computational environment, to the indeterminate form "underflow x overflow."

The above problems can be particularly pronounced when combinations of exponentials and error functions are involved. For example, the function:

$$f(x,y) = e^{\alpha x} \operatorname{erfc}(\beta y) \quad (5.1)$$

easily reduces to $\infty \times 0$ if αx and βy are both very large. However, for large arguments:

$$\operatorname{erfc}(\beta y) = \frac{1}{\sqrt{\pi}} e^{-\beta^2 y^2} \left(\frac{1}{x + \frac{1}{2x + \dots}} \right) \quad (5.2)$$

and thus:

$$f(x,y) = \frac{1}{\sqrt{\pi}} e^{ax-by^2} \left(\frac{1}{x + \frac{1}{2x + \dots}} \right) \quad (5.3)$$

By combining the exponents before calling the exp routine the problem of $\infty \times 0$ is avoided.

Similarly, the function:

$$g(x,y,z) = e^x (\text{erf } y - \text{erf } z) \quad (5.4)$$

can reduce to $\infty \times 0$ if all three arguments are very large. In addition, considerable round-off error can occur in evaluating the difference of the erf's if y and z both exceed about 2.0. Here, a possible approach is to use the definition:

$$\text{erf } y = \frac{2}{\sqrt{\pi}} \int_0^y e^{-t^2} dt \quad (5.5)$$

to write:

$$\begin{aligned} \text{erf } y - \text{erf } z &= \frac{2}{\sqrt{\pi}} \int_z^y e^{-t^2} dt \\ &= \frac{2}{\sqrt{\pi}} e^{-z^2} \int_0^{y-z} e^{-\tau^2 - 2z\tau} d\tau \end{aligned} \quad (5.6)$$

where the change of variable $\tau = t-z$ has been used. The exponential in the last integral is the generating function for the Hermite polynomials (Sneddon 1956), i.e.:

$$e^{-\tau^2 - 2z\tau} = \sum_{n=0}^{\infty} \frac{(-1)^n}{n!} H_n(z) \tau^n \quad (5.7)$$

Thus:

$$\operatorname{erf} y - \operatorname{erf} z = \frac{2}{\sqrt{\pi}} e^{-z^2} \sum_{n=0}^{\infty} \frac{(-1)^n}{n!} H_n(z) \int_0^{y-z} \tau^n dt \quad (5.8)$$

The integrals are elementary, giving:

$$\operatorname{erf} y - \operatorname{erf} z = \frac{2}{\sqrt{\pi}} e^{-z^2} \sum_{n=0}^{\infty} \frac{(-1)^n H_n(z)}{(n+1)!} (y-z)^{n+1} \quad (5.9)$$

Thus, multiplying by e^x gives:

$$g(x, y, z) = \frac{2}{\sqrt{\pi}} e^{x-z^2} \sum_{n=0}^{\infty} \frac{(-1)^n H_n(z)}{(n+1)!} (y-z)^{n+1} \quad (5.10)$$

If $y-z$ is not too large, the series may converge rapidly requiring only a few terms. Even if x, y and z are all large, the problem of loss of significant figures is minimized by computing the difference $y-z$ rather than $\operatorname{erf} y - \operatorname{erf} z$, and the problem of $\infty \times 0$ is minimized by combining the $x-z^2$ terms before calling the exp routine.

In the above example, if the difference $y-z$ is too large, then it is better to use the expansion:

$$\operatorname{erf} y = 1 - \operatorname{erfc} y \approx \frac{1}{\sqrt{\pi}} e^{-y^2} \left(\frac{1}{y + \frac{1}{2y} + \dots} \right) \quad (5.11)$$

and similarly for $\operatorname{erf} z$, to obtain:

$$g(x,y,z) = \frac{1}{\sqrt{\pi}} \left\{ e^{x-y^2} \left(\frac{1}{y + \frac{1}{2y + \dots}} \right) \right. \\ \left. - e^{x-z^2} \left(\frac{1}{z + \frac{1}{2z + \dots}} \right) \right\} \quad (5.12)$$

Clearly, depending on the values of x, y , and z , the function $g(x,y,z)$ may be evaluated either directly using Equation (5.4) or by using the Hermite expansion as in Equation (5.10), or by using the asymptotic expansion of Equation (5.12).

The above example should indicate that the evaluation of expressions involving certain special functions can be demanding, even when the individual functions are available to high accuracy. The development and testing of a function routine to evaluate a function, such as $g(x,y,z)$ in the example above, for all conceivable values of the arguments can be challenging and time-consuming. If the particular application requires only arguments in a certain limited range, then considerable time may be saved by developing a method which works well for that range. The only pitfall is that the original limitations must be remembered if the same routine is to be used in a later application.

As illustrations of how some of the above special functions and their combinations may be computed, FORTRAN listings of programs to compute $\text{erf}(x)$, $\text{erfc}(x)$, $e^x \text{erfc}(y)$, and $e^x [\text{erf}(y) - \text{erf}(z)]$ appear in Appendix I.

6.0 EXTENSIONS OF ANALYTICAL SOLUTIONS BY PERTURBATION THEORY

As noted above, analytical solutions of the moisture flow equations are obtained only with simplifying assumptions, such as that certain coefficients in the equations are constants, or at least are very elementary functions.

These solutions often can be extended, using perturbation theory, to obtain solutions of problems whose coefficients are not elementary, but which differ only by small quantities from being elementary. Of course, just as there are functions in calculus which do not have a derivative, or which have discontinuous derivatives, so too there are physical problems in which a small change in the equations leads to a large change in the solutions. These cases cannot be treated by elementary perturbation theory. But in many physical problems, small changes in the equations do lead to small changes in the solutions, and the treatment of these is summarized here (Lewins 1965 and Cacuci et al. 1980).

Suppose that an analytical solution has been obtained to an idealized linear moisture flow problem whose basic differential equation is abbreviated as:

$$L\theta = S \quad (6.1)$$

Here, L denotes the linear differential operator and S denotes any source terms. The symbol θ denotes the dependent variable (either θ , $\psi(\theta)$, $\phi(\psi)$, etc).

Now, consider a problem with variable coefficients which is "close" to this problem, i.e., we replace the operator L by $L+\delta L$, where δL denotes the (small) change in the operator. For generality, suppose that the source S is also replaced by $S+\delta S$. Because of the perturbations in L and S , the solution θ is replaced by $\theta+\delta\theta$, where:

$$(L+\delta L) (\theta+\delta\theta) = S+\delta S \quad (6.2)$$

If $L+\delta L$ is also linear then:

$$L\theta + L\delta\theta + \delta L\theta + \delta L\delta\theta = S + \delta S \quad (6.3)$$

Since the quantities involving δ are small, we make the approximation that $\delta L\delta\theta$ can be neglected as a second order term. Then subtracting (6.1) from (6.3) yields:

$$L\delta\theta = \delta S - \delta L\theta$$

Thus, formally:

$$\delta\theta = L^{-1} (\delta S - \delta L\theta) \quad (6.4)$$

Here, L^{-1} is the inverse of the differential operator for which we have the analytical solution, and it is understood that $\delta\theta$ satisfies appropriate boundary or initial conditions. (Actually, we don't need to calculate L^{-1} ; see below!)

Suppose now that some particular result of the calculation is needed; one which can be written as an integral over the solution, i.e., the result R has the form:

$$R = \int S^+(x) \theta(x) dx \quad (6.5)$$

Here, $S^+(x)$ denotes some weight function, and dx is shorthand notation for integrating over all the independent variables, i.e., " $\int dx$ " = $\int dx \int dy \int dt$, or whatever your problem has in it. If the result of interest is the value of θ at a particular "point" $x=x_0$, then take $S^+(x)=\delta(x-x_0)$ so that:

$$R \Rightarrow \int \delta(x-x_0) \theta(x) dx = \theta(x_0) \quad (6.6)$$

If the result is the total moisture in a subregion G , then $S^+=1$ if $x \in G$ and $S^+=0$ if $x \notin G$, i.e., then:

$$R \rightarrow \int_{x \in G} \theta(x) dx \quad (6.7)$$

(These examples are meant to show that a variety of types of results can be written in the form (6.5) by an appropriate choice of the function $S^+(x)$.)

Now, if R is obtained from the analytical solution of the original problem (6.1), and if the perturbed problem is considered, then R is replaced by:

$$R + \delta R = \int S^+(x) [\theta(x) + \delta \theta(x)] dx \quad (6.8)$$

or, subtracting (6.5), the change in R is:

$$\delta R = \int S^+(x) \delta \theta(x) dx \quad (6.9)$$

Substituting $\delta \theta$ from (6.4) gives:

$$\delta R = \int S^+(x) L^{-1} [\delta S(x) - \delta L \theta(x)] dx \quad (6.10)$$

Now, recall the definition of the adjoint operator L^+ : if $f(x)$ and $g(x)$ are any two functions in the proper domains, then L^+ is defined so that:

$$\int f(x) L g(x) dx = \int [L^+ f(x)] g(x) dx \quad (6.11)$$

Now, let $\theta^+(x)$ be a function satisfying the equation:

$$L^+ \theta^+(x) = S^+(x) \quad (6.12)$$

Then, Equation (6.10) becomes:

$$\delta R = \int [L^+ \theta^+(x)] L^{-1} [\delta S(x) - \delta L \theta(x)] dx \quad (6.13)$$

By the property of the adjoint operator, Equation (6.11), this can be written as:

$$\delta R = \int \theta^+(x) L L^{-1} [\delta S(x) - \delta L \theta(x)] dx + \text{"boundary terms"} \quad (6.14)$$

Since $L L^{-1} = I$, the operators cancel. The "boundary terms" arise since going from (6.13) to (6.14) usually requires integration by parts, Green's theorem, et al. The trick is to pick the boundary and initial conditions on $\theta^+(x)$ to make the "boundary terms" vanish. (It's usually obvious how to do this in any particular case.) Suppose this has been done. Then, Equation (6.14) reduces to:

$$\delta R = \int \theta^+(x) [\delta S(x) - \delta L \theta(x)] dx \quad (6.15)$$

If, in particular, $S^+(x)$ had been chosen to be $\delta(x-x_0)$, then R is $\theta(x_0)$ and δR would represent the change in θ at x_0 due to the perturbations δL and δS .

Let's summarize how this expression can be used:

1. An analytical solution is obtained to the simple problem $L\theta=S$.
2. The operator L^+ is determined from the identity $\int \theta^+ L \theta dx = \int (L^+ \theta^+) \theta dx$, and boundary and initial conditions for θ^+ are chosen to get rid of any "boundary terms" that appear here.
3. The adjoint equation $L^+ \theta^+ = S^+$ must be solved, subject to these conditions. This is usually the same degree of difficulty as the original equation $L\theta=S$; thus, this can probably be done analytically too.
4. Now, any problem which is "close" to the original problem (i.e., it differs by a small δS and δL) will have a solution $\theta + \delta \theta$, leading to a change in the result R by an amount δR given by Equation (6.15). It may be possible to do the integral in closed form, but at least everything under the integral is known.

Note: this is an approximate method, since second order terms $\delta L \delta \theta$ were ignored. But if the δ terms are, say, 10% of the original terms, then δ^2 may be $\approx 1\%$, which may be negligible.

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APPENDIX I

FORTRAN PROGRAMS FOR THE FUNCTIONS

APPENDIX I

FORTRAN PROGRAMS FOR THE FUNCTIONS

(A. G. Gibbs)

$\text{erf}(x)$

$\text{erfc}(x)$

$e^x \text{erfc}(y)$

$e^x [\text{erf}(y) - \text{erf}(z)]$


```

FUNCTION ERF(Z)
C  EVALUATES ERF(Z) BY KUKI CONTINUED FRACTION EXPANSIONS
C  AG GIBBS ADAPTATION
  IF(Z)2,1,2
1  CALC=0.0
  GO TO 9
2  V=ABS(Z)
  IF(V-4.17)4,4,3
3  CALC=1.0
  GO TO 7
4  S=V*V
  IF(V-1.51)6,6,5
5  CFL=0.56418958*V/((S+0.5-0.5/(S+2.5-3.0/(S+4.5-7.5/(S+6.5
  A-10.803134/(S+4.2690240))))))
  CALC=1.0-CFL*EXP(-S)
  GO TO 7
6  CFS=1.1283792-1.1600697*S/(S+10.215980-167.17295/(S+9.8102679+
  B201.38669/(S+11.569899 +31.227929/(S-1.7730436 +64.244197
  C/(S+5.5781859))))))
  CALC=V*CFS
7  IF(Z)8,8,9
8  CALC=-CALC
9  ERF =CALC
10 RETURN
  END
C

```

```

FUNCTION ERFC(Z)
C  AG GIBBS VERSION
C  COMPUTES COMP ERROR FUNCTION VIA SERIES OR ASYMPTOTIC EXPANSION
  IF(Z)2,1,2
1  CALC=1.0
  GO TO 9
2  V=ABS(Z)
  IF (V-10.)4,4,3
3  CALC=0.0
  GO TO 7
4  S=V*V
  IF (V-1.51)6,6,5
5  CFL=0.56418958*V/((S+0.5-0.5/((S+2.5-3.0/((S+4.5-7.5/((S+6.5
  A-10.803134/((S+4.2690240))))))
  CALC=CFL*EXP(-S)
  GO TO 7
6  CALC=1.0-V*(1.1283792-1.1600697*S/((S+10.215980-167.17295/((S+
  B9.8102679+201.38669/((S+11.569899+31.227929/((S-1.7730436+64.244197
  C/((S+5.5781859))))))
7  IF(Z)8,8,9
8  CALC=2.0-CALC
9  ERFC=CALC
10 RETURN
  END

```

C

```

C      FUNCTION EXERFC(X,Y)
C      AG GIBBS VERSION
C      EVALUATES EXP(X) * ERFC(Y)
C      CALLS ERFC FOR Y .LT. 1.51
C      OTHERWISE COMBINES EXPONENTS USING ASYMPTOTIC REPRN FOR ERFC
      CALC = 0.0
      IF (Y.LT.1.51) GO TO 100
      S=Y*Y
      EP = X-S
      IF (EP.LT.-100.) GO TO 200
      CFL=0.56413958*Y/((S+0.5-0.5/(S+2.5-3.0/(S+4.5-7.5/(S+6.5
A-10.803134/(S+4.2690240))))))
      CALC = EXP(EP)*CFL
      GO TO 200
100 IF(X.LT.-100.) GO TO 200
      CALC = EXP(X)*ERFC(Y)
200 EXERFC = CALC
      RETURN
      END
C

```

```

      FUNCTION DELERF(XX,YY,ZZ)
C EVALUATES EXP(X)*( ERF(Y)-ERF(Z) )
C   AG GIBBS BATTELLE-NORTHWEST
      X=XX
      Y=YY
      Z=ZZ
C FIRST TEST FOR SIMPLE CASES Y=0 OR Z=0
      IF (Y) 20,10,20
10 DEL=-ERF(Z)
      GO TO 120
20 IF (Z) 40,30,40
30 DEL=ERF(Y)
      GO TO 120
C NOW SEE WHETHER THE ARGUMENTS HAVE SAME OR DIFFERENT SIGN
40 IF (ABS(Y+Z).GT.ABS(Y-Z)) GO TO 50
C ERFS ARE ACTUALLY ADDED, SO THERE IS NO PROBLEM
      GO TO 65
C ERFS ARE SUBTRACTED... CHECK IF SIGNIFICANCE WOULD BE LOST
50 U=ABS(Y)
      V=ABS(Z)
      UU=AMAX1(U,V)
      DL=ABS(U-V)
      IF (UU.LT.1.51) GO TO 55
      TEST=UU-1.163+.277/(UU*UU)
      IF(DL.GT.TEST) GO TO 65
      IF(DL.LT.(.5/UU) ) GO TO 68
C MUST USE ASYMPTOTIC EXPANSIONS
C   CHECK FOR LARGE NEGATIVE EXPONENTIALS AND SET TO ZERO.
      DRLF=0.
      S=Z*Z
      ARG=X-S
      IF(ARG.LT.-88.) GO TO 52
      CFL=0.56418958*Z/(S+0.5-0.5/(S+2.5-3.0/(S+4.5-7.5/(S+6.5
      A=14./(S+8.5-14.738599/(S+4.1687335))))))
      DRLF=CFL*EXP(ARG)
52 T=Y*Y
      ARG=X-T
      IF(ARG.LT.-88.) GO TO 54
      CFL=0.56418958*Y/(T+0.5-0.5/(T+2.5-3.0/(T+4.5-7.5/(T+6.5
      A=14./(T+8.5-14.738599/(T+4.1687335))))))
      DRLF=DRLF-CFL*EXP(ARG)
54 DELERF=DRLF
      RETURN
55 IF(UU.LT.0.5) GO TO 60
      TEST=.1-.11333333*UU*(1.-2.117647*UU)
      IF(DL.LT.TEST) GO TO 68
      GO TO 65
60 IF(DL.LT.(.11) ) GO TO 68
C CAN DO DIRECTLY
65 DEL=ERF(Y)-ERF(Z)
      GO TO 120

```

C MUST USE SERIES...CHOOSE EXPANSION WHICH MINIMIZES SIZE OF EXPONENT

```
68 A=X-Y*Y
   B=X-Z*Z
   IF (ABS(A).LT.ABS(B) ) GO TO 70
   EP=EXP (B)
   ATX=-Z-Z
   GO TO 80
70 EP=EXP (A)
   ATX=Y+Y
```

C BEGIN HERMITE EXPANSION

```
80 DL=Y-Z
   T=ATX*DL*.5
   TMM1=0.0
   F=0.5*DL
   H=ATX
   HMM1=1.0
   N=1
   NP1=2
   S=0.0
85 S=S+T
   TT=ABS(T)+ABS(TMM1)
   IF (TT-1.E-8) 100,100,90
90 MM1=N
   N=NP1
   NP1=NP1+1
   HMM2=HMM1
   HMM1=H
   H=ATX*HMM1-FLOAT(NM1+NM1)*HMM2
   F=(DL*F)/FLOAT(NP1)
   TMM1=T
   T=F*H
   GO TO 85
100 DEL=(1.1283792)*DL*(1.0+S)
   GO TO 130
120 EP=EXP (X)
130 DELERF=EP*DEL
   RETURN
   END
```

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