Recent Advances in Laplace Transform Analytic Element Method (LT-AEM) Theory and Application to Transient Groundwater Flow

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Furman and Neuman (2003) proposed a Laplace Transform Analytic Element Method (LT-AEM) for transient groundwater flow. The LT-AEM solves the modified Helmholtz equation in Laplace space and back-transforms it to the time domain using a Fourier series numerical inverse Laplace transform method (de Hoog *et al.,* 1982). We have extended the method to compute hydraulic head and flow velocity distributions due to any two-dimensional combination and arrangement of point and circular area sinks and sources, nested circular regions having different hydraulic parameters, and circular regions with specified head or flux. The strengths of all sinks and sources, and the specified head and flux values, can vary with time in an independent and arbitrary fashion. Initial conditions may vary from one circular element to another. We obtain a solution by matching heads and normal fluxes inside and outside each circular element. The effect of each circular element on flow is expressed in terms of a generalized Fourier series that converges rapidly (≤ 10 terms) in most cases. As there are more matching points than Fourier terms, the matching is accomplished in Laplace space by least-squares. We illustrate the method by calculating head for a distribution of circular inhomogeneities and transient sources. The results are compared to a MODFLOW simulation. Further study will extend the method to ellipses in two dimensions and spheroids in three dimension.

1 INTRODUCTION

The analytic element method (AEM) simulates groundwater flow in an aquifer through superposition of individual flow feature contributions (e.g., wells, rivers, lakes); each flow feature, or element, is represented either as an analytic or high-precision solution to the governing flow equation. The AEM was developed for 2D steady-state aquifers by Strack and his students in the 1980s (Strack & Haitjema, 1981; Strack, 1989), and subsequently was extended to include many types of elements for different types of flow problems (3D, multi-aquifer, transient and unsaturated); see Strack's review papers (1999, 2003) for a more complete AEM bibliography.

Several researchers have extended the AEM to transient problems. In one of the first approaches, Zaadnoordijk and Strack (1993) used a mixture of steady and transient elements, where the net transient effect must be zero; this method has limited flexibility and accuracy. Bakker (2004) developed transient elements using Fourier series to represent time variability; this method was much more accurate, but does not allow for specifying initial conditions. Most recently, Strack (2006) outlined the development of transient elements which create localized divergence. He showed a transient solution using finite differences in time superimposed on a background steady-state solution. These divergence elements are simpler than previous methods, but they are confined to problems with uniform initial conditions and transient effects are restricted to regions specified by the user.

In contrast to other transient AEM schemes, the Laplace transform AEM (LT-AEM) solves the Laplace-transformed transient groundwater flow equation; AEM techniques are applied in the Laplace domain, and therefore the time-convolution properties of the Laplace transform can be leveraged to simplify the problem. Final transient solutions are obtained from solutions in Laplace-space using a robust Fourier series inverse Laplace transform method (de Hoog *et al.*, 1982). LT-AEM elements initially developed by Furman and Neuman (2003, 2004) are expanded and generalized here to allow for finite domains with prescribed boundary conditions and non-zero initial conditions.

2 MATHEMATICAL REPRESENTATION

The diffusion equation describes the transient flow of saturated groundwater through a porous medium; for 2D polar coordinates it is

$$\frac{\partial^2 \Phi}{\partial r^2} + \frac{1}{r}\frac{\partial \Phi}{\partial r} + \frac{1}{r^2}\frac{\partial^2 \Phi}{\partial \theta^2} = \frac{1}{\alpha}\frac{\partial \Phi}{\partial t}, \tag{1}$$

where Φ is the discharge potential ($\Phi = K\,h$), α is hydraulic diffusivity ($\alpha = K/S_s$), S_s is specific storage, and h is hydraulic head (aquifer thickness being unity). We take the Laplace transform of the diffusion equation (1) to arrive at the groundwater flow equation in Laplace space,

$$\frac{\partial^2 \bar{\Phi}}{\partial r^2} + \frac{1}{r}\frac{\partial \bar{\Phi}}{\partial r} + \frac{1}{r^2}\frac{\partial^2 \bar{\Phi}}{\partial \theta^2} = \frac{1}{\alpha}(p\,\bar{\Phi} - \Phi_0), \tag{2}$$

where $\bar{\Phi} = \mathcal{L}\{\Phi\}$, p is the Laplace parameter, and Φ_0 is the initial discharge potential. Most LT-AEM elements require an initial condition of zero, but we accommodate a non-zero starting condition through a distribution of instantaneous area sources at $t=0$. With an assumed initial condition of zero, (2) simplifies to the modified Helmholtz equation

$$\frac{\partial^2 \bar{\Phi}}{\partial r^2} + \frac{1}{r}\frac{\partial \bar{\Phi}}{\partial r} + \frac{1}{r^2}\frac{\partial^2 \bar{\Phi}}{\partial \theta^2} - \frac{p}{\alpha}\,\bar{\Phi} = 0. \tag{3}$$

LT-AEM elements are developed using one of two strategies. Either the element can be derived in the time domain (as a solution to (1)), and the Laplace transform used to arrive at this element's analog in the Laplace domain, or elements may be derived directly in the Laplace domain (as a solution to (3)). Both methods are utilized in the derivation of the fundamental elements of the LT-AEM.

2.1 Point Elements

Taking the Laplace transform of a 2D instantaneous point source (Carslaw & Jaeger, 2003), the Laplace domain point source element is found directly as

$$\mathcal{L}\{\Phi_{\mathrm{pt}}(r,t)\} = \bar{\Phi}_{\mathrm{pt}}(r,p) = \frac{Q_{\mathrm{pt}}}{2\pi\alpha}\mathrm{K}_0\!\left(r\sqrt{\frac{p}{\alpha}}\right), \tag{4}$$

where t is elapsed time since the instantaneous source was activated, r is radial distance, Q_{pt} is the strength of the source, and $\mathrm{K}_0(z)$ is modified Bessel function of the second kind. We present a generalization of the LT-AEM point source which uses the convolution of a transfer function (instantaneous source) and an input function (time behavior) to produce a more general time behavior. A general point source is simply

$$\bar{\Phi}_{\text{pt}} = \bar{f}\,(p)\frac{Q_{\text{pt}}}{2\pi\alpha}\mathrm{K}_0(r\,q), \tag{5}$$

where $q = \sqrt{p/\alpha}$, and $\bar{f}\,(p)$ is the Laplace transform of the desired time input function. For example, a source with constant strength in time would have a constant as a time input function, $\mathcal{L}\{c\} = 1/p$; when this is substituted into (5), the result is the Theis solution in Laplace space (Lee, 1999). Laplace transforms of most commonly encountered time input functions (e.g., a step, pulse, sawtooth wave, square wave or stair-step) are available in published tables, for example (Prudnikov *et al.,* 1992) or (Abramowitz & Stegun, 1964).

The point source is typically a passive element (strength is specified by the user), but it can be an active element by specifying $h(t)$ at the point and solving for the strength. The active solution depends on the behavior of the other elements in the domain.

2.2 Circular Elements

Non-intersecting circular elements are derived directly in Laplace space through separation of variables in 2D polar coordinates. Furman and Neuman developed the active circular matching element; we now present some extensions to this element. The new features introduced here are specified boundary conditions along the circumference of the element, or specified flux distributed over the area of the element (which can be used to represent non-zero initial conditions). Generalizing the matching element of Furman and Neuman, circular elements are used to divide the domain into two related or unrelated sub-domains, inside and outside.

2.2.1 Matching using circular elements (active)

The discharge potential inside and outside the circles is obtained through separation of variables in 2D radial coordinates; following the previous derivation (Furman & Neuman, 2003), the expression for the inside of the circle is

$$\bar{\Phi}_c^- = \sum_{v=0}^{N-1} \frac{\mathrm{I}_v(r\,q^-)}{\mathrm{I}_v(r_0 q^-)}[c_v \cos(v\theta) + d_v \sin(v\theta)], \tag{6}$$

where $\mathrm{I}_v(z)$ is the modified Bessel function of the first kind, a superscript minus indicates a parameter related to the inside of the circle, and r_0 is the radius of the current circle. Similarly, the expression for discharge potential outside the circle is

$$\bar{\Phi}_c^+ = \sum_{v=0}^{N-1} \frac{\mathrm{K}_v(r\,q^+)}{\mathrm{K}_v(r_0 q^+)}[a_v \cos(v\theta) + b_v \sin(v\theta)], \tag{7}$$

where analogously, the superscript plus indicates a quantity related to the outside of the circle. For the active circular matching element, the two expressions for $\bar{\Phi}_c$ inside and outside the circle are matched at points along each circle's circumference to satisfy the continuity of head and normal flux conditions there. In the matching case, the number of unknowns (here $4N-2$) can be cut in half by expressing the head matching conditions in terms of the normal flux matching conditions (Furman & Neuman, 2004, eqns 14-17). The generalized Fourier series coefficients (a_v, b_v, c_d and d_v) in the resulting matching equations are solved for by least squares along the circumference of the circles, since the equations are posed at more locations than there are unknowns.

2.2.2 Specified boundary conditions using circular elements (active)

A simple extension to the circular matching elements derived by Furman and Neuman is the specification of the total head or total normal flux along the circumference of a circular element. For example, this can be used to make the boundary of a circle impermeable (setting $\partial\Phi^{\pm}_{\text{total}}/\partial r=0$) without having to set the hydraulic conductivity inside the element to zero. In general, $\bar{h}$ or $\partial\bar{\Phi}/\partial r$ can be set at a specified (not necessarily constant in space) value along the circumference of a circular element which may be constant or variable in time (via time-convolution).

Specifying the head or normal flux (as opposed to matching) along the circumference of a circular element has the effect of splitting the traditionally infinite AEM domain into two disconnected domains (e.g., hatched and gray regions of Figure 1). Therefore, a finite circular domain can be simulated inside a circle by specifying a boundary condition along the circumference of the circle; nothing outside this circle need be calculated or considered.

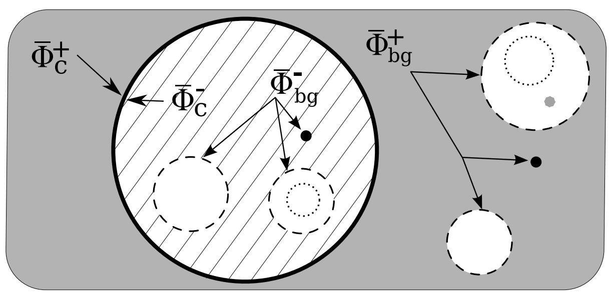

FIGURE 1. Specification of backgound elements with respect to large circle

For a specified head element, the continuity of head condition used to derive the matching equations simply becomes a specification of head along the circle's circumference, namely

$$\mathcal{L}\{h^{\pm}(\theta,t)\}K^{\pm}=\left[\bar{\Phi}^{\pm}_{c}+\sum\bar{\Phi}^{\pm}_{\text{bg}}\right]_{r_0}, \tag{8}$$

where $h^{\pm}(\theta,t)$ is desired total head along the element edge and $\sum\bar{\Phi}^{\pm}_{\text{bg}}$ is the net discharge potential due to all elements in the background of the current element (see Figure 1). Similarly, the normal flux matching equation becomes

$$\mathcal{L}\{Q^{\pm}(\theta,t)\}=\left[\frac{\partial\left(\bar{\Phi}^{\pm}_{c}+\sum\bar{\Phi}^{\pm}_{\text{bg}}\right)}{\partial r}\right]_{r_0}, \tag{9}$$

where $Q^{\pm}(\theta,t)$ is specified total normal flux along the circumference, potentially a function of both space and time. Both these expressions state that the required effects of the circular element of interest ($\bar{\Phi}^{\pm}_{c}$) is simply the difference between the specified value and the net effect of the background inclusions ($\sum\bar{\Phi}^{\pm}_{\text{bg}}$) at that point on the circumference.

Substituting (6) and (7) into (8) and (9) provides the relationships for finding the generalized Fourier coefficients of a specified total head circular element,

$$\sum_{v=0}^{N-1}\frac{\mathrm{K}_v(rq^+)}{\mathrm{K}_v(r_0q^+)}[a_v\cos(v\theta)+b_v\sin(v\theta)]=h^+(\theta)\bar{f}\,(p)K^+-\left[\sum\bar{\Phi}^+_{\mathrm{bg}}\right]_{r_0}, \tag{10}$$

$$\sum_{v=0}^{N-1}\frac{\mathrm{I}_v(rq^-)}{\mathrm{I}_v(r_0q^-)}[c_v\cos(v\theta)+d_v\sin(v\theta)]=h^-(\theta)\bar{f}\,(p)K^--\left[\sum\bar{\Phi}^-_{\mathrm{bg}}\right]_{r_0}. \tag{11}$$

The time behavior of $h^{\pm}(\theta,t)$ is represented by the general time input function, $\bar{f}\,(p)$, while $h^{\pm}(\theta)$ represents the spatial distribution of specified head in Laplace space, in terms of a truncated Fourier series.

Each of these equations has $2N-1$ unknown coefficients, and since the head is being specified, there is no set of normal flux matching equations; the number of unknowns cannot be reduced as Furman and Neuman did in the case of matching elements. Analogous to this, the equations for determining the generalized Fourier coefficients outside and inside a specified flux circular element are,

$$q^+\left\{\sum_{v=0}^{N-1}\left[\frac{\partial\mathrm{K}_v(rq^+)}{\partial r}\right]_{r_0}\left[\frac{a_n\cos(v\theta)+b_v\sin(v\theta)}{\mathrm{K}_v(r_0q^+)}\right]\right\}=Q^+(\theta)\bar{f}\,(p)-\left[\sum\frac{\partial\bar{\Phi}^+_{\mathrm{bg}}}{\partial r}\right]_{r_0}, \tag{12}$$

$$q^-\left\{\sum_{v=0}^{N-1}\left[\frac{\partial\mathrm{I}_v(rq^-)}{\partial r}\right]_{r_0}\left[\frac{c_n\cos(v\theta)+d_v\sin(v\theta)}{\mathrm{I}_v(r_0q^-)}\right]\right\}=Q^-(\theta)\bar{f}\,(p)-\left[\sum\frac{\partial\bar{\Phi}^-_{\mathrm{bg}}}{\partial r}\right]_{r_0}. \tag{13}$$

The derivatives of modified Bessel functions can be expressed in terms of modified Bessel function of the same kind but different order using recursion relationships (Abramowitz & Stegun, 1964, §9.6). The derivatives of $\bar{\Phi}^{\pm}_{\mathrm{bg}}$ in (12) and (13) are with respect to the radius of the current element (r_0). Each of these equations contains $2N-1$ unknown coefficients, and there are no corresponding head matching equations.

A linear (or potentially non-linear) combination of head and normal flux can also be specified along the boundary of the circle, to simulate mixed (type 3) boundary conditions.

Since the active specified head and normal flux elements effectively isolate the two sides of a circular element from each other, different conditions could be applied on each side. For example, a circular element could be set at a specified value of head on its outside, and have zero normal flux (no-flow) on its inside. Alternatively, a different value of $h(\theta,t)$ or $Q(\theta,t)$ could be ascribed to each side of the element.

2.2.3 Specified flux along circular elements (passive)

Briefly, another type of circular element is a circle or ring of specified normal flux (a ring source), which does not partition the domain into an "inside" and "outside"; it does not have a total head or total normal flux matching condition as do the active elements.

These elements are the same as specified total flux elements derived in the previous section (12 and 13), except that they lack the $\bar{\Phi}^{\pm}_{\mathrm{bg}}$ terms; therefore, their strength does not depend on other elements.

2.2.4 Specified area flux and non-zero initial condition (passive)

A final extension of the previously developed matching circular elements is the circular element with time-variable specified area flux. An instantaneous area source, applied at $t=0$, can be used to represent a non-zero initial condition.

Adapting the method outlined by Strack (1989) for steady-state analytic elements, the specified area flux elements are derived in Laplace space by decomposing $\bar{\Phi}$ into two functions, and separately dealing with the inside and outside of the circular element,

$$\begin{array}{ll} \nabla^2\bar{\Phi} - q^2\,\bar{\Phi} = \bar{\gamma}\,(r,\theta,p) & \text{inside circular element,} \\ \nabla^2\bar{\Phi} - q^2\,\bar{\Phi} = 0 & \text{outside circular element,} \end{array} \tag{14}$$

where $\bar{\gamma}$ is the strength of the area flux that, in general, can be a function of both space and time. The partial differential equation (PDE) used inside the circle has the same form as the Laplace transformed diffusion equation, before the simplification of zero initial condition (2), with $\bar{\gamma} = -\,\Phi_0/\alpha$. The total discharge potential is defined as a sum of two functions, $\bar{\Phi} = \bar{\Phi}_p + \bar{\Phi}_h$. The function $\bar{\Phi}_p$ is set to zero outside the circular element, and satisfies the above PDE inside the element; it is any suitable particular solution. The function $\bar{\Phi}_h$ is that solved for elsewhere in the domain (the homogeneous solution, where Φ_0 is set to zero). The combination of these two functions is used to make $\bar{\Phi}$ match correctly at element boundaries (there may be a jump in $\bar{\Phi}$ if there is a change in properties).

To ensure continuity in $\bar{\Phi}$, the jump in $\bar{\Phi}_h$ across the circumference of the circle is equal to the jump in $\bar{\Phi}_p$, or $\bar{\Phi}_p^- = -\bar{\Phi}_h^- + \bar{\Phi}_h^+$. The homogeneous solution ($\bar{\Phi}_h^{\pm}$) is the total discharge potential ($\bar{\Phi}_h^{\pm} = \bar{\Phi}_c^{\pm} + \sum \Phi_{\text{bg}}^{\pm}$). The modified form of the head matching condition for elements with a passive area flux is then

$$\left[\frac{\bar{\Phi}_c^+ + \sum \bar{\Phi}_{\text{bg}}^+}{K^+}\right]_{r_0} = \left[\frac{\bar{\Phi}_c^- + \sum \bar{\Phi}_{\text{bg}}^- + \bar{\Phi}_p^-}{K^-}\right]_{r_0}; \tag{15}$$

similarly, the modified form of the normal flux matching condition would be

$$\left[\frac{\partial(\bar{\Phi}_c^+ + \sum \bar{\Phi}_{\text{bg}}^+)}{\partial r}\right]_{r_0} = \left[\frac{\partial(\bar{\Phi}_c^- + \sum \bar{\Phi}_{\text{bg}}^- + \bar{\Phi}_p^-)}{\partial r}\right]_{r_0}. \tag{16}$$

Particular solutions can be found using Green's functions inside a circle; for some simpler distributions of areal flux the particular solution may be found by inspection. The simplest non-trivial form which $\bar{\Phi}_p^-$ can take, so that $\bar{\Phi}$ still satisfies (14), is that of a recharge rate which is constant in space but variable in time. The particular solution for constant areal flux is simply

$$\bar{\Phi}_p^- = -\,\bar{f}\,(p)\frac{\bar{\gamma}}{q^2},$$

where $\bar{\gamma}$ is a constant, and $\bar{f}\,(p)$ represents time variability. In this simple case, since $\bar{\Phi}_p^-$ is constant in space, the modified normal flux matching equation (16) reverts to its original form, and one only needs to modify the head matching equation.

Area flux elements have wide potential application. They can be used for simulating hydrologic processes such as infiltration, evapotranspiration, or leakage from lakes or from adjacent aquifers, potentially providing a means to approximate transient multi-aquifer systems with the LT-AEM.

3 NUMERICAL IMPLEMENTATION

The elements described in the previous sections, and those developed previously, are implemented in a Fortran program. Two illustrative scenarios using consistent units are shown and compared with space-time finite difference model output (McDonald & Harbaugh, 1988). First, the head from a finite circular domain with a no-flux boundary and variable non-zero initial conditions is shown; the second case illustrates results from a finite circular domain with a constant head boundary, nested inclusions of different aquifer properties, and a pumping well.

3.1 Finite no-flow domain with non-constant Φ_0

The domain is bounded by a no-flow circle of unit radius; the area inside the large circle has unit initial condition ($h_0 = 1$), while in the smaller nested circles $h_0 = 5$. The domain has uniform aquifer properties ($K = 1$, $S_s = 0.001$). Figure 2a is a cross-sectional plot showing the time evolution of head along the section indicated in Figure 2b, where the circular elements are in red. In Figure 2c, LT-AEM (dark) and MODFLOW (light) results at $t = 1.25 \times 10^{-4}$ in the NE circular element (contour interval $= 0.25$) are seen to virtually coincide. The LT-AEM results were calculated on the same 200×200 spatial grid as the MODFLOW results, the latter using 100 time steps. This example illustrates the ability of the LT-AEM to simulate both finite domains and non-zero initial conditions.

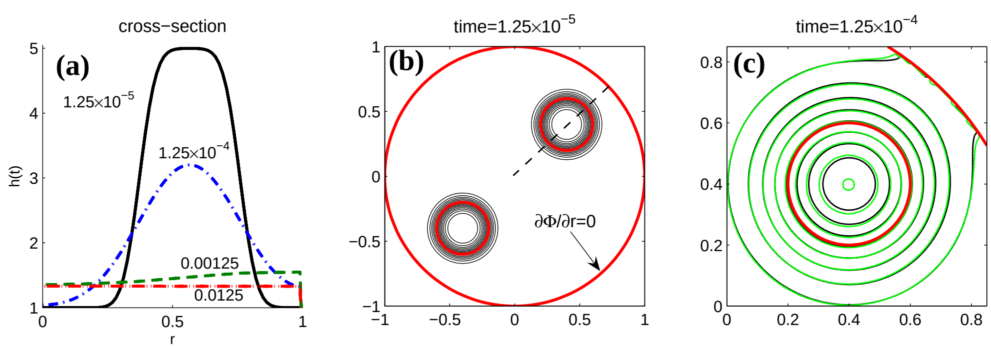

FIGURE 2. Results for a finite circular domain with variable non-zero initial conditions.

3.2 Finite constant head domain with nested elements

The domain is bounded by a constant head ($h_c = 2$) circle of unit radius, with a uniform unit initial condition (see Figure 3). There are two sub-regions (NE and SW) of contrasting permeability ($K_{\mathrm{NE}} = K_{\mathrm{bg}}/10$; $K_{\mathrm{SW}} = 10\,K_{\mathrm{bg}}$), an interior circle (NW) of constant head ($h_c = 2$), an internal no-flux boundary (SE), and an injection well ($Q_{\mathrm{pt}} = 2.0$) in the center of the domain which is activated at $t = 2 \times 10^{-4}$ ($\bar{f}\,(p) = \frac{1}{p}\,e^{-0.0002p}$).

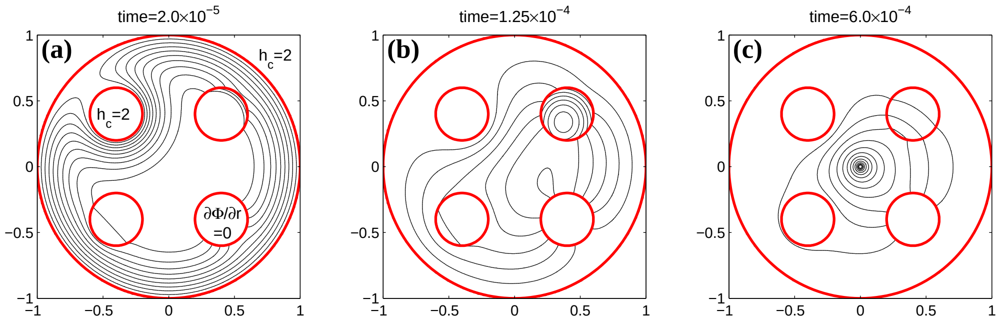

FIGURE 3. LT-AEM results with constant head circles, a well, and nested circular elements.

In Figure 3a head changes propagate differently through the two circles of different permeability, while the center of the domain is still at $h=1$ (contour interval = 0.1). In Figure 3b head continues to rise to the constant boundary values. In Figure 3c, after the injection well is activated, head at the center of the domain rises above that at the constant head boundaries.

4 CONCLUSIONS

We have presented several extensions to the LT-AEM that broaden its applicability to realistic transient groundwater flow conditions. Circular elements are extended to include specified boundary conditions along their circumference or specified flux distributed over their area. The instantaneous area source solution overcomes the previous limitation of a zero initial condition.

There are three main classifications of LT-AEM elements; one is based on the dimensionality of the element (point, line, or area), the second on how the element interacts with other elements (active or passive), and the third relates to the element's time behavior.

The strength of a passive element is specified by the user. Active elements have some condition other than their strength specified (head, flux or a combination of the two), which depends on the effects of the other elements in the domain; their use requires solving a system of equations. Circular elements can take an active role, for example, where $\partial(\bar{\Phi}_c+\sum\bar{\Phi}_{\mathrm{bg}})/\partial r=0$ is specified; here the element must respond to the net effect the background elements have along its boundary, to maintain the no-flux condition. In a passive role, an element contributes normal flux to the overall domain independent of other elements.

To allow for flexible time behavior, we used Laplace space convolution to combine simple known functions; in the Laplace domain convolution is equivalent to multiplication (Carslaw & Jaeger, 2003). This solution technique alleviates many of the difficulties encountered when even constant or linearly variable time behaviors are developed directly in the time domain (Zaadnoordijk & Strack, 1993).

In the LT-AEM, circular elements are used to partition the domain into finite parts. In the AEM, polygons constructed of line doublets are similarly used to cut the flow domain into sub-domains (Strack, 1989), although using separation of variables produces more intuitive results (however, the approach is restricted to separable geometries). The methods outlined here extends to 2D elliptical coordinates, or in general any of the various coordinate systems (both 2D and 3D) where the Helmholtz equation is separable (Moon & Spencer, 1961); however, numerical evaluation of the resulting special functions in Laplace space may be difficult.

The simple examples illustrated here are not exhaustive of the current capabilities of the LT-AEM; we are developing additional elements to create a general transient groundwater modeling environment. Different approaches to developing suitable line elements (both source and doublet) are being investigated, as well as elliptical and ellipsoidal elements as analogs to the circular elements illustrated here.

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