**Appendix A: Mathematical Formulation of Series - AEM solution**

The 3D series solution to steady-state groundwater flow governing equation (Equation 2) at the *m*th layer is obtained using the method of separation of variables ([as was developed in Ameli and Craig 2014](#_ENREF_5)) as:

|  |  |  |
| --- | --- | --- |
|  |  | (A.1) |
|  |  |  |

In the above equation, and were obtained by applying no flow boundary conditions at four sides of the domain (Figure 1), *j* and *n* represent the coefficient index while *J* and *N* are the order of approximation in the *x* and *y* direction, respectively (in total, *N* x *J*  series terms are used). , are the unknown series coefficients associated with the *mth* layer.

The AEM solution representing the radial collector well is calculated by superimposing the analytic solutions corresponding to all segments representing the collector well as:

|  |  |  |
| --- | --- | --- |
|  |  | (A.2) |

 is the discharge potential corresponding to *i*th well segment in the global coordinate system and is the number of line segment used to emulate the presence of radial collector well. Note that subscript *w* denotes well properties in the remainder of this paper. By integrating the potential for a set of point sinks along a line segment of a length of 2, [Steward and Jin (2003](#_ENREF_25)) developed a closed form expression representing the discharge potential in local coordinate of the segment. Here, in the global coordinate system of the model, the discharge potential correspond to *i*th line segment located in *x* direction is defined as follows;

|  |  |  |
| --- | --- | --- |
|  |  | (A.3) |

where refers to the a priori *unknown* constant strength of *i*th segment, and and is the half of the segment length. , and refer to the center of *i*th segment in the global coordinate system. The method of images (Figure A.1) is here employed to enable AEM part of the solution to satisfy no-flow conditions at the sides of the domain. Therefore equation A.2 is modified as

|  |  |  |
| --- | --- | --- |
|  |  | (A.4) |

where refers to discharge potential correspond to the image of *i*th segment and is the number of image wells. Figure A.1 depicts the layout (plan view) of real and image wells, and the images of images wells used in this paper to fulfill the AEM portion of the no-flow condition at the sides of the domain. Note that the no-flow boundary conditions at the sides of the domain are only met exactly when the number of image wells at the four sides approaches infinity. In addition, to mimic no-flow condition at the bottom boundary by AEM portion of the solution, all real and image wells shown in Figure A.1 should be placed symmetrically below the bottom bedrock interface as image wells. Using the method of images, the strength associated with each image segment is identical to its real counterpart and only their locations are different. The no-flow condition along the bottom boundary for the series portion of the solution is enforced at control points using a least square numerical scheme (Appendix B).

 There are also other boundary conditions which should be applied along the radial collector wells and the boundaries of the computational domain to calculate the unknown coefficients of Equations A.1 and A.3. [Steward and Jin (2003](#_ENREF_25)) have suggested that two boundary conditions must be satisfied along the entire well screen’s length. First, the a priori unknown head along the cylindrical face of the well () must be uniform, which implies zero head loss along the well screens. This is applied by setting the head at a set of control points (located along screens surface) equal to the head at a specified but arbitrary position along this boundary.

|  |  |
| --- | --- |
|  | (A.5) |

In Equation (A.5), is conditional upon the layer where each control point is located. The uniformity of head condition is met exactly when the number of line sink segments approaches infinity. For the second boundary condition at the collector well, the summation of unknown strengths of consecutive line sink segments along all arms is set equal to the pumping rate

|  |  |  |
| --- | --- | --- |
|  |  | (A.6) |

The top of the modelled domain (Figure 1) is the surface defined as the water table surface where the water table is lower than the land surface (recharge areas), and the land surface at areas in direct contact with surface water body. The former is located using an iterative scheme, while the latter (land surface) is known a priori. The top of the modelled domain surface is subject to a specified infiltration rate (R) at recharge areas, and/or Dirichlet boundary conditions along surface water bodies (Figure 1). Continuity of flux and pressure head is required along each layer interface (). The readers are referred to [Ameli and Craig (2014](#_ENREF_5)) for a detail discussion of the boundary and continuity conditions and iterative scheme used to locate the water table surface.

The 3D semi-analytical Series-AEM solution for the interaction between groundwater, surface water bodies and a radial collector well (Equation (3)) in each layer of a stratified unconfined aquifer is completed by identifying unknown coefficients of the series solution ( in Equation (A.1)) and AEM terms ( in Equation (A.3)). These coefficients are calculated using a constrained least squares numerical algorithm to satisfy boundary and continuity conditions at a set of control points. A set of control points are located along the water table surface where is the iteration number), bottom boundary () and each layer interface () to implement the aforementioned boundary and continuity conditions using least squares algorithm. Note that here *NC* is the product of *NCx* and *NCy* which are the number of uniformly spaced control points in *x* and *y* directions, respectively. The uniformity of head boundary condition along the radial screens is satisfied by applying equation A.5 at a set of *NCw* control points located along the screen’s surface. Initially, the water table surface, , is assumed to be equal to the river or other surface water body stage, , at all control points. At each iteration, the unknown coefficients for each guess of the water table surface are calculated by minimizing the total sum of squared boundary and continuity condition errors (at control points along the mentioned interfaces and well screen surfaces) that is constrained with Equation A.6 such that the total inflow be equal to pumping rate *Q* at the radial collector well. The total sum of squared errors (TSSE) at each iteration is subdivided into the errors along mentioned evaluation curves:

|  |  |
| --- | --- |
| +  | (A.7) |

The subscript (t) refers to the sum of squares boundary condition errors along the modelled domain surface, subscript (m) refers to the sum of squares continuity errors along the layer interfaces, subscript (b) refers to the sum of squares boundary condition errors along the bedrock interface (series solution portion) and subscript (w) refers to the sum of squares error for the implementation of uniformity of head along radial collector well screens (Equation A.5). The equations for sum of squares error along these evaluation curves are included in Appendix B. The unknown series solution and AEM coefficients for each iteration (*r*), are calculated by minimizing Equation A.7. Then, the 3D Series-AEM expansion for discharge potential (Equation (3)) is fully obtained; however the zero pressure head condition along the water table surface is still not obtained exactly due to the initially incorrect location of water table. Equation (3) provides a hydraulic head distribution () in each iteration and for each control point along the location of water table surface. Due to the zero pressure head condition along the water table, in each iteration and for each control point, the following equation may be used to update the water table location:

|  |  |
| --- | --- |
| + | (A.8) |

where is an under-relaxation factor which is always between 0 and 1. The location of water table is updated in this iterative scheme until the Series-AEM solution converges and , which represents the error in zero pressure head condition along the water table, approaches zero.

**Appendix B: Sum of Squares error equations**

The component of the total sum of squares error (Equation (A.7)), i.e. sum of squares errors along the evaluation surfaces are as follows:

 (B.1)

where SSEt refers to the sum of squares error at *NC* control points in imposing the recharge infiltration flux (*R*) along the a priori unknown location of the phreatic surface (*Zwt*) and constant head () at areas in direct contact with surface water body. In addition, is the set of coordinate indices for control points in direct contact with the surface water body and is the coordinate normal to the phreatic surface.

for *m*=2 *M* (B.2)

 (B.3)

SSEm refers to the sum of squares error at *NC* control points in applying continuity of flux and head across the layer interfaces, and SSEb refers to the sum of squares error at *NC* control points located along the bottom boundary used to impose no-flow condition (series solution portion). Again, is the coordinate normal to the layer interfaces or bottom boundary.

 (B.4)

SSEw refers to the sum of squares error at *NCw* control points located along the radial collector well screens to impose uniformity of head condition (Equation A.5).

**Appendix C: Boundary and continuity errors**

The application of least squares algorithm (which minimizes the errors in the implementation of boundary or continuity conditions at the control points) is subject to numerical error. To assess if the developed least squares solution is able to accurately implement boundary or continuity conditions throughout the computational domain, we calculate the normalized error along the evaluation surfaces at points located halfway between the control points which are initially used to construct the constrained least squares solution as follows:

 for *m* = 2, …, *M* (C.1)

 for *m* = 2, …, *M* (C.2)

where and refer to normalized continuity of head and flux error across the layer interfaces.

 (C.3)

 (C.4)

 (C.5)

here and are normalized flux error along the water table surface and bottom bedrock surface, respectively. also refers to normalized head error along the land surface at areas in direct contact with surface water body.

 (C.6)

is the normalized uniformity of the head errors along well screens. In the above equations, max (flux) and min (flux) (LT-1) refer to the minimum and maximum flux across the top surface and is the water stage of the surface water body or river. The (−) and (+) signs refer to the top and bottom of each interface, respectively. The subscript () refers to the reference point at the well screens where uniformity of head along the screens is assessed with respect to the head at this point.

**Appendix D: Non-uniform Random Walk Particle Tracking**

Similar to [Delay and Bodin (2001](#_ENREF_13)) and [Salamon *et al.* (2006](#_ENREF_23)), the non-uniform random walk step of a particle is then given by :

 (D.1a)

 (D.1b)

 (D.1c)

where & &

 and [L2T-1] are longitudinal and transverse hydrodynamic dispersion coefficients, and and [L] are longitudinal and transverse dispersivities of the porous medium, respectively. and are random numbers drawn from normal distributions with zero mean and unit variance for each particle and each time step (). The asterisk denotes the correction of the implementation of non-uniformity in flow within the RWPT method. The corrected velocities (, , ) are:

 (D.2a)

 (D.2b)

 (D.2c)

where , and are mean pore water velocities in *x*, *y* and *z* directions calculated using Series-AEM solution. In the above equations, the tensor of dispersion is given by:

 (D.2d)

 (D.2e)

 (D.2f)

= () (D.2g)

= () (D.2h)

= () (D.2i)

where

The particle tracking scheme used to generate pathlines can also estimate transit time or groundwater age corresponding to each pathline and transit time distribution (TTD) of water discharged into the river and captured by the radial collector well. The simulated TTDs are the probability density function of the transit time (age) of discharging particles into the river and well. These age distributions are here fitted with a Gamma probability density function as a function of the transit time ():

*ƿ*() = (D.3)

where is the mean groundwater age of the discharged water into the river or radial collector well, *a* is the Gamma shape parameter and is the Gamma function. As the Gamma shape parameter decreases, the age variability of water captured in the river (or well) increases.

**References**

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Figure A.1. Plan view of image wells method used to emulate no-flow boundary (AEM portion) of the sides of the domain. Dashed angled-shape lines represent the original radial collector well which includes two arms while continuous angled-shape lines refer to the images and the image of images radial collector well.