

# Theory of Modeling Inhomogeneity Domains in GFLOW

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April 4, 2005

## Inhomogeneity domains in GFLOW

Inhomogeneity domains in GFLOW allow for discontinuities in hydraulic conductivity, porosity, aquifer base and recharge rate due to precipitation. Discontinuities in the porosity do not influence the groundwater flow solution, they are only used for calculation of average groundwater flow velocities, e.g. during particle tracking (pathline tracing). Discontinuities in the areal recharge rate due to precipitation cause the inhomogeneity domains to serve as areal sinks (with negative sink density). A discussion on areal sinks is found in Haitjema (1995), see page 220 through 223, and more extensively in Strack (1989), see pages 426 through 434. Discontinuities in the hydraulic conductivity lead to jumps in the discharge potential across the domain boundary, which is modeled by use of second order line-doublets, see Strack and Haitjema (1981), Strack (1989), pages 411 and 412, and Haitjema (1995), pages 215 through 220. Changes in the aquifer base elevation also lead to jumps in the discharge potential across the domain boundary, see Strack (1989), pages 412 through 414. The mathematical details of the implementation of inhomogeneity domains in GFLOW are summarized below.

### Jump in hydraulic conductivity and aquifer base elevation

With reference to Figure 1 the following parameters are defined: Hydraulic conductivity  $k_i$  and  $k_o$ , inside and outside the domain, respectively. Aquifer base elevation  $b_i$  and  $b_o$ , inside and outside the domain, respectively. The aquifer top elevation is  $h_t$ , which is the same inside and outside the domain. The discharge potential at a point on the domain boundary, just inside and outside the domain, is  $\Phi_i$  and  $\Phi_o$ , respectively. The line-doublet strength at some point on the boundary is denoted by  $s$ , which varies parabolically along the straight line-doublet:

$$s(x) = -s_j \frac{(x-1)}{2} + s_{j+1} \frac{(x+1)}{2} - \mu_j (x^2 - 1) \quad (1)$$

where  $s_j$  and  $s_{j+1}$  are the real line-doublet strengths at the beginning and end node of the  $j^{th}$  line-doublet and where  $\mu_j$  is a parabolic strength component

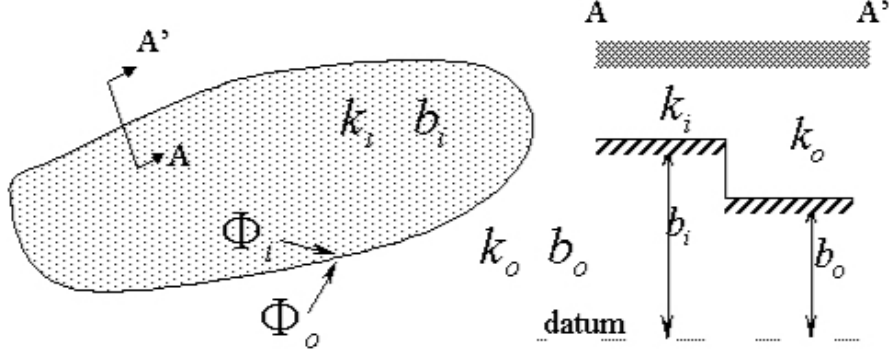


Figure 1: Closed domain with a jump in hydraulic conductivity and aquifer base elevation across its boundary.

at the center of the  $j^{\text{th}}$  line-doublet, see Strack and Haitjema (1981). The parameter  $x$  defines a point on the line-doublet between the beginning node ( $x = -1$ ) and the end node ( $x = +1$ ). The line-doublet strength  $s$  equals the jump in the discharge potential across the line-doublet as follows:

$$s = \Phi_i - \Phi_o \quad (2)$$

For *unconfined flow* conditions expression (2) may be expanded as,

$$s = \frac{1}{2}k_i(\phi - b_i)^2 - \frac{1}{2}k_o(\phi - b_o)^2 \quad (3)$$

where  $\phi$  is the head at the point on the boundary. Equation (3) can be rewritten in terms of the transmissivities  $T_i$  and  $T_o$ , which are defined as:

$$T_i = k_i h_i \quad ; \quad T_o = k_o h_o \quad (4)$$

where for unconfined flow conditions:

$$h_i = \phi - b_i \quad ; \quad h_o = \phi - b_o \quad \phi \leq h_t \quad (5)$$

or for confined flow conditions:

$$h_i = h_t - b_i \quad ; \quad h_o = h_t - b_o \quad \phi > h_t \quad (6)$$

With (6) the jump condition (2) can be written for *confined flow* conditions as

$$s = k_i h_i (\phi - b_i) - \frac{1}{2} k_i h_i^2 - (k_o h_o (\phi - b_o) - \frac{1}{2} k_o h_o^2) \quad (7)$$

Both (3) and (7) may be written in terms of  $\Phi_i$  as:

$$s = \frac{T_i - T_o}{T_i} \Phi_i + \frac{1}{2} T_o (b_o - b_i) \quad (8)$$

or alternatively in terms of  $\Phi_o$  as:

$$s = \frac{T_i - T_o}{T_o} \Phi_o + \frac{1}{2} T_i (b_o - b_i) \quad (9)$$

In writing (3) and (7) it has been tacitly assumed that the head  $\phi$  is the same just inside and outside the domain boundary. In other words, the head is continuous. This is true as long as the head is larger than the largest aquifer base elevation. If not, either  $\Phi_i$  or  $\Phi_o$  is zero because the head is at the aquifer base inside or outside the domain, depending on which aquifer base is the highest. It follows from (8) that the jump  $s$  is equal to the inside potential in case the head is below the outside aquifer base:

$$s = \lim_{T_o \rightarrow 0} \left( \frac{T_i - T_o}{T_i} \Phi_i + \frac{1}{2} T_o (b_o - b_i) \right) = \Phi_i \quad (10)$$

Similarly, it follows from (9) that the jump  $s$  is equal to minus the outside potential in case the head is below the inside aquifer base:

$$s = \lim_{T_i \rightarrow 0} \left( \frac{T_i - T_o}{T_o} \Phi_o + \frac{1}{2} T_i (b_o - b_i) \right) = -\Phi_o \quad (11)$$

The jump condition may be satisfied at a discrete number of collocation points distributed along the inhomogeneity boundary. At the  $j^{th}$  collocation point the inside potential may be written as:

$$(\Phi_i)_j = s_1 F_{1j} + s_2 F_{2j} + \dots + s_j F_{jj} + \dots + \sum \text{other functions} \quad (12)$$

Where the terms  $F_{ij}$  represent the influence functions of the line-doublets associated with the strength parameters  $s_i$ , and where the last term in (12) represents the sum of the strength parameters times influence functions for the remainder of the line-doublets and all other analytic elements in the flow problem. Combining (8) with (12) yields:

$$-\frac{1}{2} \frac{T_o T_i}{T_i - T_o} (b_o - b_i) = s_1 F_{1j} + s_2 F_{2j} + \dots + s_j \left( F_{jj} - \frac{T_i}{T_i - T_o} \right) + \dots + \sum \text{other functions} \quad (13)$$

In GFLOW the equations are formulated as the difference between two successive iterations (*iterative refinement*), as follows:

$$-\frac{1}{2} \frac{T_o T_i}{T_i - T_o} (b_o - b_i) - \overset{old}{\Phi_i} + \overset{old}{s_j} \frac{T_i}{T_i - T_o} = (s_1 - \overset{old}{s_1}) F_{1j} + (s_2 - \overset{old}{s_2}) F_{2j} + \dots \\ (s_j - \overset{old}{s_j}) \left( F_{jj} - \frac{T_i}{T_i - T_o} \right) + \dots + \sum \text{other functions} \quad (14)$$

By use of (2),

$$s_j = (\Phi_i)_j - (\Phi_o)_j \quad (15)$$

it may be shown that when using (9) instead of (8) the same matrix equation (13) or (14) will result.

As written the matrix coefficient for  $s_j$  depends on the head for the case of unconfined flow, since the transmissivities  $T_i$  and  $T_o$  depend on the head, see (4) and (5). Consequently, the matrix equations are non-linear in that some of its coefficients depend on the solution. It may be seen that in case the aquifer base elevation does not jump, hence only the hydraulic conductivity jumps, the matrix coefficient of  $s_j$  reduces to  $k_i/(k_i - k_o)$ , which is independent of the solution. Hence, hydraulic conductivity inhomogeneities are easier to solve than inhomogeneities in the aquifer base elevation.

## Implementation of common inhomogeneity boundaries

The inhomogeneity domains in GFLOW have been designed as isolated or nested domains only. This implies that for each inhomogeneity there exists only one jump condition for the aquifer properties (hydraulic conductivity or aquifer base). In March 2005 the GFLOW inhomogeneity domains have been reformulated to allow for common inhomogeneity boundaries, which implies that different boundary segments of a domain may exhibit different jump conditions (depending on its own properties and that of the bounding domain). In addition, part of an inhomogeneity domain may coincide with that of one or more other domains, while there exist only one jump condition for one domain segment (line-doublet). This has been implemented by making the following design modifications to the GFLOW solver code:

1. Inside and outside properties are stored for each line-doublet separately, rather than for each domain. These properties are obtained by considering the properties associated with the domain itself (inside properties) and by requesting the properties at a point just outside the center of the line-doublet (outside properties). Since the latter procedure involves finding properties at a finite distance from the line-doublet (domain in question) it is possible to find an incorrect value if two domains are very close together, but do (just) not have common boundaries. This situation is assumed not to occur.
2. Control points are placed at line-doublet centers regardless whether the line-doublet is part of a single or a multiple domain boundary.
3. Control points are placed at line-doublet vertices if the two adjacent line-doublets are part of a single domain boundary or if the two adjacent line-doublets share the same two domains.
4. Control points are shifted away from the vertices if the condition in the previous item is not met.
5. Line-doublets that coincide with another line-doublet (of another domain boundary) that is already included in the matrix is skipped during matrix construction, it does not add control points to the matrix.

### Note on the design

The above design changes are complex and the result of the earlier nested domain design. A simpler design would have been to have the GUI provide only one line-doublet per domain boundary segment and to define the properties inside domains by line-elements that are independent of the line-doublets. In addition, each line-doublet would have received its own control points, which would have been one at the center and two near, *not on*, the line-doublet end points (vertices). Such a design, while much simpler, would have required a complete redesign of the inhomogeneity logic in both the Solver and the GUI. Moreover, it would have added extra control points (no savings by placing control points on vertices). On the other hand, placing two control points on either side of a vertex has two advantages: (1) by avoiding the singular vertex (singular in the specific discharge) a better solution is obtained, and (2) no-flow or resistance boundaries that cross inhomogeneity boundaries create a jump in the potential jump (line-doublet strength). This jump can be accounted for when the no-flow or resistance boundary intersects an inhomogeneity boundary at a node with control points on either side of the node. The current design, however has the advantage of minimizing the total number of control points and thus equations, possibly at the expense of some reduction of accuracy.

### Cases of control point placement

Vertices may occur alone, be shared by another domain, or be the starting vertex of a line-doublet that is ignored in the matrix construction. If a vertex is not shared by another vertex it will be used as a control point location. A vertex that coincides with a vertex on an other domain may be treated in several different ways, as explained below.

There are seven different cases that may be associated with a vertex that is shared by another domain. These cases are numbered from 0 to 6, whereby case 0 indicates the situation where the vertex coincides with the vertex of another domain, but the associated line-doublets do not. All other cases have at least one line-doublet in common, as illustrated in Figure 2. The vertices CZ1, CZ2, and CZ3 occur on the "current" domain boundary into the direction of the boundary line-element (such that when traversing the boundary the domain is on the left-hand side). The vertices C1, C2, and C3 occur on the domain boundary of the adjacent domain. A code "idbcode" is set for both CZ2 and C2 (the coinciding vertices under consideration) to manage the control point allocation during matrix construction. These codes are as follows:

- idbcode=0 The line-doublet that follows is not in the matrix.
- idbcode=1 Both the previous and the following line-doublets are in the matrix. Place one control point on this vertex.
- idbcode=2 Place a control point that is offset from the vertex along the line-doublet. Note: Matrix construction is done per line-doublet. If the starting vertex has a code 2 the control point is shifted away from the starting vertex.

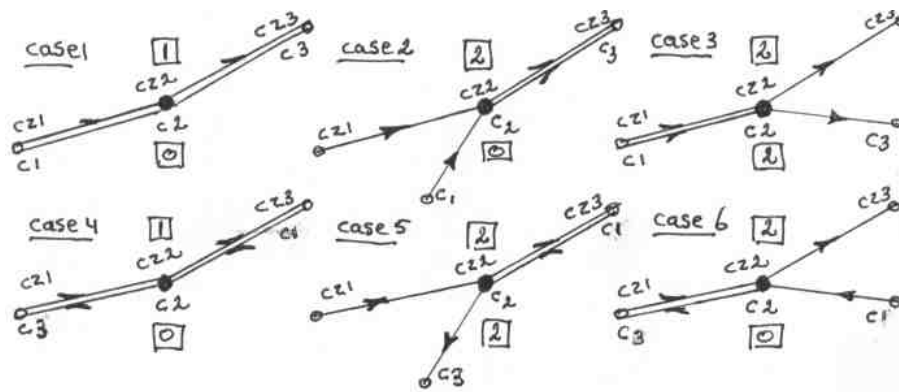


Figure 2: Cases 1 through 6 for a common domain boundary.

The center of the line-doublet always gets a control point (unless not in the matrix (starting code is zero). If the ending vertex has a code 2 a third control point is added shifted away from that vertex.

All vertices for a domain are visited to set their "idbcode" values, but once a vertex has an idbcode=0 (excluded from the matrix) it will not be reset. The values of "idbcode" for the vertices CZ2 and C2 are indicated in Figure 2 in square boxes.

### Presence of interface flow

The jump conditions become more complicated in the presence of a freshwater - salt water interface. A detailed analysis for the jump conditions at collocation points along inhomogeneity boundaries for this case is provided in the document: "Freshwater and Salt Water Interface Flow in GFLOW", July 22, 2002, by Henk Haitjema.

### Jump in the recharge rate

The inhomogeneity domain may be given an areal source or sink distribution to add or subtract recharge due to precipitation. In GFLOW all withdrawals of water are defined as positive, hence a jump in recharge rate is implemented by adding an areal sink distribution to the inside of the inhomogeneity domain. The theory of area sinks is presented in detail in Strack (1989), see section 37 page 426 through 442. The idea is to add a solution to Poisson's equation inside the boundary of the inhomogeneity (omitting it on the outside) and apply both line-doublets and line-dipoles along the boundary to eliminate the resulting jumps in the potential and flow across the boundary, respectively. The inhomogeneity domains in GFLOW already have line-doublets along their boundary to model the jump in the potential associated with the jump in hydraulic conductivity

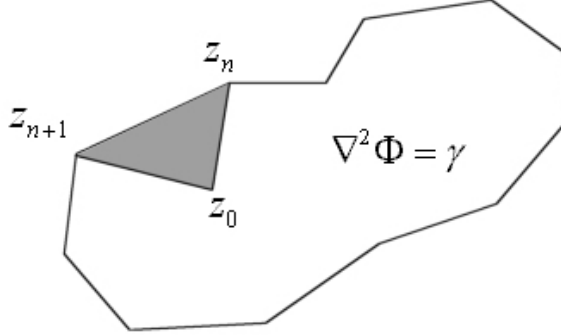


Figure 3: Adding recharge to an inhomogeneity domain.

and aquifer bottom. By adding a complex strength parameter to these line-doublets the desired line-doublet (real part of the strength parameter) and line-dipole (imaginary part of the strength parameter) distribution can be created for the added recharge in the inhomogeneity domain. In GFLOW the following potential is added to the inside of the inhomogeneity:

$$\Phi = \frac{\gamma}{4}(r^2 - R^2) \quad (16)$$

The Laplacian of (16) is  $\gamma$ , which is the sink density (exfiltration rate) of the inhomogeneity. The implementation in GFLOW is carried out as follows.

With reference to Figure 3 the potential added to the inside of the polygon (inhomogeneity) is:

$$\Phi = \frac{\gamma}{4} (|z - z_0|^2 - R^2) \quad (17)$$

where  $z_0$  is the average of all complex vertices  $z_n$  of the polygon:

$$z_0 = \frac{\sum_{n=1}^N z_n}{N} \quad (18)$$

The distance  $R$  in (17) is chosen such that the area of the circle with radius  $R$  equals that of the polygon:

$$R^2 = \frac{\sum_{n=1}^N A_n}{\pi} \quad (19)$$

where  $A_n$  is the area of the triangle formed by the line elements  $z_0 - z_n$ ,  $z_0 - z_{n+1}$  and  $z_n - z_{n+1}$ , see Figure 3. The area  $A_n$  is calculated by evaluating the vector product of the two vectors  $u_i$  and  $v_i$  that span the shaded triangle in Figure 3:

$$A_n = \frac{1}{2}(u_1 v_2 - u_2 v_1) \quad (20)$$

where  $u_i$  and  $v_i$  are defined as:

$$u_i = (\Re\{z_n - z_0\}, \Im\{z_n - z_0\}) \quad (21)$$

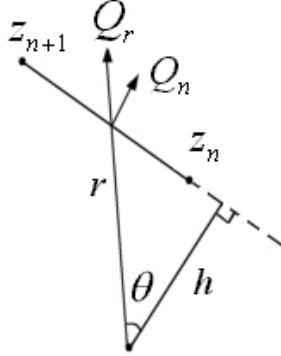


Figure 4: The discharge  $Q_n$  across the polygon side is constant.

and

$$v_i = (\Re\{z_{n+1} - z_0\}, \Im\{z_{n+1} - z_0\}) \quad (22)$$

The flow across a polygon side, due to the added potential (17) is constant along the side, as may be seen as follows. The discharge  $Q_r$  due to (17) is radially toward  $z_0$ , hence with (16):

$$Q_r = -\frac{d\Phi}{dr} = -\frac{\gamma}{2}r \quad (23)$$

In Figure 4  $Q_r$  is shown as positive and thus pointing away from  $z_0$ . The component  $Q_n$  normal to the polygon side is:

$$Q_n = Q_r \cos \theta = -\frac{\gamma}{2}r \cos \theta \quad (24)$$

With  $h = r \cos \theta$  equation (24) becomes:

$$Q_n = -\frac{\gamma}{2}h \quad (25)$$

which is indeed constant for the polygon side. The minus signs in equations (23) through (25) indicate that the directions of flow due to the sink distribution inside the polygon are inward, opposite the direction shown in Figure 4.

In GFLOW line-doublet functions are used with a parabolic strength distribution, which is composed of a linear component with strength  $s_n$  and  $s_{n+1}$  at the vertices  $z_n$  and  $z_{n+1}$ , respectively, and a parabolic component with strength  $\mu_n$  at the line-doublet center and zero at the vertices, see (1). In order to eliminate the jump in both the potential and the normal flow across the polygon sides, which are caused by adding (17) to the inside of the domain, complex strength parameters are added at the vertices ( $c_n$ ) and at the line-doublet centers ( $d_n$ ):

$$c_n = s_n^* + it_n^* \quad (26)$$



and

$$d_n = \mu_n^* + i\nu_n^* \quad (27)$$

Since the potential (17) is only added to the inside of the domain, the jump across the polygon side equals (17) evaluated at that side. Hence, the real part of  $c_n$  and  $d_n$  must be minus the inside potential in order to eliminate the jump:

$$s_n^* = -\frac{\gamma}{4} (|z_n - z_0|^2 - R^2) \quad (28)$$

and

$$\mu_n^* = -\frac{\gamma}{4} \left( \left| \frac{z_n + z_{n+1}}{2} - z_0 \right|^2 - R^2 \right) - \frac{s_n^* + s_{n+1}^*}{2} \quad (29)$$

The imaginary parts of the strength parameters provide a line-dipole distribution, which increase in strength represents the inflow in the line-dipole, see Strack, 1989 page 291 - 297. A constant inflow rate is obtained by a linearly varying line-dipole strength. Hence, in view of (25) the parabolic strength component  $\nu_n^*$  vanishes:

$$\nu_n^* = 0 \quad (30)$$

The linear strength component  $t_n^*$  at each successive vertex increases with the amount of flow that crosses the polygon side, which is equal to the area of the shaded triangle in Figure 3 times the recharge rate  $\gamma$ :

$$t_{n+1}^* = t_n^* - \gamma A_n \quad (31)$$

where  $t_1^*$  at the first vertex is zero. The minus sign in (31) compensates the minus sign generated by  $it_n^*$  times the line-doublet function, which is  $-t_n^*$  times a line-dipole function. Note, that the last vertex is also the first vertex in a closed domain. Consequently, at that vertex there is both an imaginary strength component of zero and an imaginary strength component equal to the total withdrawal of groundwater by the inhomogeneity domain. This jump in the line-dipole strength at the first (and last) vertex is realized by adding another potential function to both the inside and outside domain:

$$\Phi = \frac{\gamma \sum_{n=1}^N A_n}{2\pi} \ln(z - z_1) \quad (32)$$

which represents a well with a total discharge equal to the total withdrawal of groundwater by the inhomogeneity domain, see also Strack, 1989 page 433 equation (37.51).

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