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Technical Commentary

Boundary condition nomenclature confusion in groundwater flow modelling

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To solve the partial differential equations of groundwater flow, the information about head (h) and/or head gradient (∇h) must be specified along the boundaries of a model domain. The descriptors of different boundary condition (BC) types are drawn from founding mathematicians mainly of the 19th century (Cheng and Cheng 2005). Mathematically, there are five different BC types, including: Dirichlet (Type 1), Neumann (Type 2), Robin (Type 3), Cauchy and Mixed (Liu 2018). These names are sometimes used in communicating the BCs of groundwater flow models, and therefore, correct association between nomenclature and the mathematical form of BCs is important for properly communicating model characteristics.

The distinction between different BC types is consistent across mathematical literature (e.g., Weisstein 2019). However, there appears to be inconsistencies in the naming of BCs of groundwater flow models, as we demonstrate later in this article. To address this issue, we firstly provide BC definitions in general mathematical forms, as given below. General BC formulae are then translated into standard groundwater flow BCs through, for example, application of Darcy's Law and using conceptualizations commonly adopted in defining BCs for groundwater problems.

<u>Dirichlet (Type 1) BC:</u>

The Dirichlet BC derives from the Dirichlet problem, which refers to a boundary problem of closed region Ω, with boundary Γ, where the BC is defined by (Cheng and Cheng 2005):

$$\phi = f\left(\mathbf{x}\right); \quad \mathbf{x} \in \Gamma \tag{1}$$

Here, ϕ is the dependent variable, $f(\mathbf{x})$ is specified as a continuous function, and $\mathbf{x}$ represents temporal and spatial dimensions.

In groundwater applications of the Dirichlet BC, the hydraulic head (or in some cases the pressure head), *h* [L], is specified. The term “specified-head condition” is used where *h* is described as a function of space and/or time, whereas *h* values that are constant (or piecewise constant) in time and space are referred to as “constant-head conditions” (Franke et al. 1987). Thus, the Dirichlet BC applied to groundwater flow problems can be written as.

$$h = \begin{cases} h_0 & \text{Constant-head boundary} \\ f(\mathbf{x}) & \text{Specified-head boundary} \end{cases} \tag{2}$$

where h_0 is a constant.

Dirichlet BCs most commonly represent the influence of surface water bodies within groundwater models, for situations where the head imposed on the groundwater system can be assumed independent of subsurface flow variations. This requires strong groundwater-surface water connectivity and sufficiently large surface water volumes and/or flow rates that are stable despite groundwater fluctuations (Bear 1979). Another common application of the Dirichlet BC to groundwater flow problems is the imposition of atmospheric pressure in locations of groundwater discharge to the land surface (e.g., a seepage face; Scudeler et al. 2017). This presumes that water does not accumulate to significant depths in surface depressions and that seepage is continuous and occurs at known locations.

<u>*Neumann (Type 2) BC:*</u>

In the Neumann BC, the normal derivative of the dependent variable is defined at the boundary, as (Cheng and Cheng 2005):

$$\frac{\partial \phi}{dn} = f(\mathbf{x}); \quad \mathbf{x} \in \mathit{\Gamma} \tag{3}$$

where *n* is the outward normal of $\mathit{\Gamma}$, and $f(\mathbf{x})$ is a continuous function. For groundwater flow problems, the normal derivative in the Neumann BC is $\partial h/\partial n$, which implies a specific discharge (or Darcy velocity, q [L/T]) of water into or out of the boundary on the basis of Darcy's Law (Franke et al. 1987). Following the terminology used to define different types of Dirichlet BC, a "specified-flux condition" refers to boundary fluxes that vary in space and/or time, while a "constant-flux condition" refers to boundary fluxes that are constant (or piecewise constant) in time and space (i.e., $\partial h/\partial n$ = constant). Setting $q = 0$ along a groundwater model boundary is a special case, referred to as a "no-flow condition". It is noteworthy that the modeller often sets the volumetric flux normal to the boundary (Q [L^3/T]) in practical applications of specified- and constant-flux conditions. For confined aquifers, setting Q as constant implies that $\partial h/\partial n$ is constant. However, in situations where the boundary conductance varies (e.g., in models of unconfined aquifers), the ratio between Q and $\partial h/\partial n$ is not constant, and rather, $h\partial h/\partial n$ is constant. Thus, setting Q to a constant value may not lead to a Neumann BC.

The assignment of no-flow conditions in groundwater models to represent low-permeability strata, geological discontinuities and hydraulic divides is commonplace. Estimates of base flow to rivers and lakes, submarine groundwater discharge to the sea, and recharge through the land surface are routinely used in setting specified- and constant-flux conditions. In practice however, it is less common to know accurately the fluxes into/out of a groundwater system compared to the knowledge of heads, which can be ascertained directly from monitoring wells, and in some cases, surface water levels and topography (e.g., Knowling and Werner 2016).

Robin (Type 3) BC:

The Robin BC is a linear combination of the Dirichlet and Neumann BCs, as (Gustafson 1999):

$$\frac{\partial \phi}{dn} + a\phi = f\left(\mathbf{x}\right); \quad \mathbf{x} \in \mathit{\Gamma} \tag{4}$$

where a [L^{-1}] is a non-zero coefficient, which might be constant or variable. Replacing ϕ with h, applying Darcy's Law, and setting a to $-1/L$ and $f(\mathbf{x})$ to $-h_{\mathrm{ref}}/L$, the follow formula is obtained that is readily applicable to flow across a model boundary:

$$Q = -\frac{KA}{L}\left(h - h_{\mathrm{ref}}\right) \tag{5}$$

where K [L/T] is aquifer hydraulic conductivity, A is the cross-sectional area of the boundary through which groundwater flows, h_{ref} is a reference head representing an externality to the model domain, and L is the length over which the head drop $h - h_{\mathrm{ref}}$ occurs. The common name in hydrogeological literature for BCs of the form given in equation (5) is "head-dependent flux condition" (e.g., Harbaugh 2005). This description refers to the reliance of Q on h at the boundary. It is commonplace to refer to KA/L as the "boundary conductance", C [L^2/T]. Both C and h_{ref} may vary in space and time.

The Robin BC can be applied in groundwater modelling to represent the truncation of aquifers, whereby regions of aquifer that fall outside of the model domain are approximated by C and h_{ref}. Additionally, flow to/from a river (in situations where the groundwater level is higher that the river bed) is often represented using equation (5), with impedance to flow caused by the river bed included in the parameterization of C (e.g., Werner and Laattoe 2016).

As mentioned above, setting Q to a constant value for an unconfined aquifer situation implies that $h\partial h/\partial n$ is constant. This can be written as $\partial h/\partial n - a/h = 0$, and therefore, $\partial h/\partial n$ and h are inversely related. Strictly speaking, this falls outside of BC forms that are defined in the current article.

Cauchy BC:

In the Cauchy BC, both the dependant variable and its normal derivative must be specified along the boundary. This corresponds to the imposition of both Dirichlet and Neumann BCs (Arfken and Weber 2005; Liu 2018). The Cauchy BC can be expressed as:

$$\begin{cases} \phi = f(\mathbf{x}); \\ \dfrac{\partial \phi}{dn} = g(\mathbf{x}); \end{cases} \quad \mathbf{x} \in \mathit{\Gamma} \qquad (6)$$

where, $g(\mathbf{x})$ is a continuous function.

Application of equation (6) to groundwater models implies knowledge of both q (via Darcy's Law) and h at the boundary. Practical groundwater problems for which both q and h are known are rare, to the degree that we were unable to find examples where equation (6) has been applied to a real-world groundwater modelling case.

Mixed BC:

The Mixed BC refers to the case in which the boundary consists of non-overlapping segments, each having different BC types (Griffiths et al. 2015). For example, if the boundary ($\mathit{\Gamma}$) consists of two disjoint parts: $\mathit{\Gamma}_{\mathrm{D}}$ with a Dirichlet BC and $\mathit{\Gamma}_{\mathrm{N}}$ with a Neumann BC, this is considered as a Mixed BC, given by (Cheng and Cheng 2005; Liu 2018):

$$\begin{cases} \phi = f(\mathbf{x}); & \mathbf{x} \in \mathit{\Gamma}_{\mathrm{D}} \\ \dfrac{\partial \phi}{dn} = g(\mathbf{x}); & \mathbf{x} \in \mathit{\Gamma}_{\mathrm{N}} \end{cases} \quad \text{where } \mathit{\Gamma}_{\mathrm{D}} \cup \mathit{\Gamma}_{\mathrm{N}} = \mathit{\Gamma} \qquad (7)$$

The vast majority of groundwater models applied to practical situations comprise multiple BC types, because various combinations of recharge, pumping, surface water controls, geological boundaries, groundwater divides (i.e., lines connecting high points in a potentiometric surface thereby acting as a no-flow boundary from which water flows in opposite directions), streamlines (i.e., advective pathways of water particles) and evapotranspiration (e.g., in 2D vertical cross-section models) are used to define external stresses acting on model domain. Therefore, using the standard definition given above, it could be said that almost all practical groundwater models have Mixed BCs, which thus does not differentiate in a meaningful way one groundwater model from another.

Inconsistencies in BC definitions

Mathematical literature is consistent in describing equation (4) as the Robin BC, which is also referred to as a Type 3 (or “third-type”) BC (e.g., Gustafson and Abe 1998). Equation (5), obtained by substitution of groundwater parameters into equation (4), defines a relationship where Q is dependent on h, and therefore the term “head-dependent flux” is a logical description of the Robin BC in groundwater applications. A review of prominent groundwater references finds, however, significant inconsistencies in the description of BCs that adopt equation (4), or that refer to “Robin BC”, “type 3” (or “third type”) or “head-dependent flux” conditions, as summarized in Table 1.

Table 1. Terminology used in describing BCs in the form of equation (4) (i.e., Robin BC).

Reference	**Referenced description of Robin BC**
Bear (1972), p252	"third, or Cauchy boundary value problem"
Bear (1979), p98, 220	"mixed boundary condition (boundary condition of third type; Cauchy boundary condition)"
Bear and Verruijt (1987), p72, 152	"mixed boundary condition, boundary condition of the third kind, or a Cauchy condition"
Franke et al. (1987), p6	"head-dependent flux, Type 3 (mixed boundary condition), Cauchy"
Guo and Langevin (2002), p15, 16, 17	"Cauchy (head-dependent flux or mixed boundary condition; Type III)"
COMSOL (2005), p16, 18, 19, 24, 89, 90, 105	"Mixed, Cauchy condition"
Holzbecher (2007), p62, 81	"3rd type, Cauchy - or Robin boundary condition"
Bear and Cheng (2010), p189, 198, 313, 439	"boundary condition of the third type, or a Robin boundary condition"
Barnett et al. (2012), p54, 169	"Type 3, Cauchy or specified head and gradient boundary condition; Type 3 (Cauchy, or mixed)"
Diersch (2014), p196	"Cauchy-Type (3rd Kind) BC"
Anderson et al. (2015), p77	"Type 3. Head-dependent boundary (Cauchy condition)"
Thangarajan and Singh (2016), p239	"Mixed type boundary condition or Cauchy-type boundary condition or head dependent flow boundary; Robin type boundary condition"
De Smedt and Zijl (2017), p21	"third-type boundary condition (Robin boundary condition)"
DHI (2017)	"Cauchy-type BCs; Fluid-transfer BCs; 'general head' boundaries"
USGS (2018)	"Head-Dependent Flux (Robin or mixed boundary condition)"

Inconsistencies in the description of the Robin BC include prominent references widely used by the groundwater community. For example, Bear (1972; 1979) and Bear and Verruijt (1987) refer to Robin BCs as "Cauchy" and "Mixed" BCs, although Bear and Cheng (2010) correctly define BCs in the form of equation (4) as the Robin BC. Bear (1972; 1979), Bear and Verruijt (1987) and Bear and Cheng (2010) consistently refer to the same form of BC equation as "third" type. The Australian Groundwater Modelling Guideline (Barnett 2012) refers to "head-dependent BC" as "Type 3", but labels these as "Cauchy", rather than "Robin" BCs. User manuals for widely used groundwater models (e.g., Guo and Langevin 2002; COMSOL 2005; DHI 2017) refer to the Robin BC as "Cauchy" (and sometimes "Mixed"), whereas USGS (2018) correctly identify the Robin BC, although they consider it also to be a “Mixed” BC. Of the references in Table 1, only Bear and Cheng (2010) and de Smedt and Zijl (2017) correctly describe the Robin BC.

Given MODFLOW’s widespread use, packages commonly applied to represent BCs should be correctly labelled according to the previous BC definitions. In attempting to do this, we find that there are BCs that switch between different BC types, usually Neumann and Robin BCs. This is demonstrated in Table 2, which outlines the mathematical constructs of several popular packages.

Table 2. MODFLOW packages defined according to standard BC types.

Application	Mathematical representation (Harbaugh 2005)	Type of BC
GHB package (general-head boundary)	$q = C(h_{\text{ref}} - h)$ h_{ref}: external source head	Robin
RIV package (river)	$q = \begin{cases} C(h_{\text{ref}} - h) & h > h_{\text{bot}} \\ C(h_{\text{ref}} - h_{\text{bot}}) & h \le h_{\text{bot}} \end{cases}$ h_{ref}: river water level (stage) h_{bot}: river bottom bed elevation	Robin Neumann
DRN package (drain)	$q = \begin{cases} C(h - h_{\text{ref}}) & h > h_{\text{ref}} \\ 0 & h \le h_{\text{ref}} \end{cases}$ h_{ref}: drain bed elevation	Robin Neumann
EVT package (evapotranspiration)	$q = \begin{cases} q_{\max} & h > h_{\text{sur}} \\ q_{\max} \dfrac{h - (h_{\text{sur}} - h_{\text{ext}})}{h_{\text{ext}}} & (h_{\text{sur}} - h_{\text{ext}}) \le h \le h_{\text{sur}} \\ 0 & h < (h_{\text{sur}} - h_{\text{ext}}) \end{cases}$ $q_{\max}$: maximum possible value of q h_{sur}: surface elevation h_{ext}: extinction depth	Neumann Robin Neumann

The switching of BC types relying on the dependent variable (h) has not been labelled in previous mathematical literature, although BCs of this type are sometimes referred to as “Mixed BCs” (see Table 1). Therefore, we recommend the term “switching condition”, followed by an explanation of the BC types that switch within this condition (in the case of Table 2, the Robin and Neumann BC types). Another example of a switching BC (using the definition herein) is described by Shoushtari et al. (2015), whereby the seepage face exit point shifts along the beach slope under tidal forcing, causing switching between Dirichlet and Neumann BC types.

It is clear from our review of the groundwater literature that correction and revision to the descriptions of groundwater flow BCs are needed, even though errors in mathematical definitions of BCs were not encountered per se. Most groundwater references appear to misname the Robin BC as “Cauchy” and/or “Mixed”. In Barnett et al. (2012), the Cauchy BC is correctly defined for solute transport, but then “Cauchy” is adopted for head-dependent flow BCs, for which Robin BC is the correct description. While we have not considered the nomenclature of solute transport BCs in groundwater literature, a review of these is likely warranted given the issues with groundwater flow BC descriptions.

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