Chapter 2
Foundations of Forward and Inverse Groundwater Flow Models

2.1 Basic Equations and Parameters

The equations governing groundwater flow through a porous medium are the water balance equation

$$s\frac{\partial h}{\partial t} + \nabla \cdot \mathbf{q} = 0 \tag{2.1}$$

and Darcy's law

$$\mathbf{q} = -\underline{\mathbf{k}} \cdot \nabla h \tag{2.2}$$

where s [L^{-1}] is the specific storage, h [L] is the head, $\mathbf{q}$ [L T^{-1}] is the flux density or specific discharge, $\underline{\mathbf{k}}$ [L T^{-1}] is the hydraulic conductivity tensor (in short the conductivity), t [T] is the time, ∇ [L^{-1}] is the gradient operator, [∇h is the vector with Cartesian components $(\partial h/\partial x, \partial h/\partial y, \partial h/\partial z)$], and $\nabla\cdot$ [L^{-1}] is the divergence operator ($\nabla \cdot \mathbf{q}$ is the scalar $\partial q_x/\partial x + \partial q_y/\partial y + \partial q_z/\partial z$). Equation 2.2 holds under conditions where the water density may be considered as constant. In Eq. 2.1, the specific storage term $s\,\partial h/\partial t$ accounts for the compressibility of the water and the pore space. To be precise, the terms flux and flux density have a different meaning. The flux density $q_n = \mathbf{q} \cdot \mathbf{n}$ [L T^{-1}] through a face with unit vector $\mathbf{n}$ [−] and surface area A [L^2] is equal to the flux Q [L^3 T^{-1}] through that surface area divided by the surface area of that face. However, in many texts and also in this book, the terms flux and flux density are used as synonyms, except when the difference is specified explicitly. In the literature, also the terms specific flux and specific discharge are used for flux density.

For incompressible flow, i.e., flow where compressible storage is negligibly small, the water balance (Eq. 2.1) simplifies to the continuity equation

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$$\nabla \cdot \mathbf{q} = 0 \tag{2.3}$$

In many formulations, the right-hand sides of Eqs. 2.1 and 2.3 contain a source/sink term of the form $\sum_{n=1}^{N} Q_n \delta(\mathbf{x} - \mathbf{x}_n)$ to account for wells with injection rate Q_n or production rate $-Q_n$ [L^3 T^{-1}] in the points $\mathbf{x}_n$, where $\delta(\cdot)$ represents the Dirac delta function (Butkov 1973: 223–232; Morse and Feshbach 1953: 825).

In practical modeling applications, this source/sink approach is much simpler to apply than the more exact formulation based on well boundary conditions; in the limit of small well diameters, the two formulations are mathematically equivalent (Chavent and Jaffré 1986: 70–88). However, in applications where instead of the well rate the head is imposed, a source/sink approach is not applicable; in that case, the original equations (Eqs. 2.1 and 2.3) have to be applied. The well head has then to be imposed at the boundary of the well. In discretized models (numerical models), the head in the grid volume can be imposed. For nonzero production rates, the volume-centered head may differ from the measured well head; therefore, a near-well model (generally a relatively simple algebraic model) has to be used to relate the two heads (Peaceman 1977a, 1983, 1991; Chen and Zhang 2009).

Substitution of Darcy's law (Eq. 2.2) into the water balance equations (Eqs. 2.1 and 2.3) results in the groundwater flow equations for, respectively, compressible and incompressible flow

$$\begin{array}{ll} \text{Compressible flow} & \text{Incompressible flow} \\ s\frac{\partial h}{\partial t} = \nabla \cdot (\underline{\mathbf{k}} \cdot \nabla h) & \nabla \cdot (\underline{\mathbf{k}} \cdot \nabla h) = 0 \end{array} \tag{2.4}$$

When there is nonzero groundwater flow ($\mathbf{q} \neq \mathbf{0}$, $\mathbf{e} = -\nabla h \neq \mathbf{0}$), the entropy per unit volume is increasing in time, which means that the dissipation rate $\rho g\, \mathbf{e} \cdot \mathbf{k} \cdot \mathbf{e} > 0$ (heat produced per unit volume and unit time) is positive. As a consequence, hydraulic conductivity tensor $\underline{\mathbf{k}}$ is positive definite and specific storage s is non-negative. The conductivity tensor has the nine components, k_{11}, k_{12}, k_{13}, k_{21}, k_{22}, k_{23}, k_{31}, k_{32}, k_{33}. On the scale of a representative elementary volume, this tensor is symmetric (Olmstead 1968), i.e., $k_{12} = k_{21}$, $k_{23} = k_{32}$, $k_{31} = k_{13}$. Also, on coarser scales, this tensor may often be assumed to be symmetric; symmetry is exactly the case for periodic porous media (Trykozko et al. 2001), but is not generally the case (Zijl and Nawalany 1993). In an orthogonal curvilinear coordinate system, this positive-definite symmetric matrix has three orthogonal eigendirections with non-negative eigenvalues, or principal conductivities, $k_1 = k_{11} \geq 0$, $k_2 = k_{22} \geq 0$, $k_3 = k_{33} \geq 0$, while the cross terms vanish, i.e., $k_{12} = k_{23} = k_{31} = 0$. From now on, we assume that we know the principal directions of the conductivity tensor already before calibration. A popular choice is to apply a Cartesian coordinate system in which x and y represent the two horizontal directions and z the vertical direction and to assume $k_1 = k_x$, $k_2 = k_y$, $k_3 = k_z$.

The water table, or phreatic surface, forms the top boundary of the groundwater domain. The boundary conditions on the top boundary of the model play a prominent role in the so-called flow systems analysis (Bresciani et al. 2016;

El-Rawy et al. 2016; Tóth 2009). Flow systems analysis is one of the approaches that have inspired our approach to inverse modeling. Because of its importance, we will first give a rigorous description of the exact water table conditions (Eqs. 2.5 and 2.6). Then, we present a simpler and perhaps more insightful approximation (given by Eq. 2.7).

Denoting the water table height above a horizontal reference level as $z = \zeta(x,\ y,\ t)$, the kinematics of the water table (its movements in time) are governed by the kinematic condition

$$\theta \frac{\partial \zeta}{\partial t} + q_x \frac{\partial \zeta}{\partial x} + q_y \frac{\partial \zeta}{\partial y} - q_z = r_{eff} \text{ on } z = \zeta(x, y, t) \tag{2.5}$$

where $\theta(x, y, \zeta)$ [−] is the specific yield, or effective porosity, and $r_{eff}(x, y, t)$ [L T^{-1}] is the recharge rate, or effective precipitation, arriving at the water table from the unsaturated zone above the water table. In flux models, i.e., in models where the flux is imposed on the boundaries, the recharge rate r_{eff} is imposed. (To be precise, in Eq. 2.5 it is assumed that the recharge flux density, r_{eff}, is vertical. Its component normal to the curved phreatic surface is $r_{eff}/[1 + (\partial\zeta/\partial x)^2 + (\partial\zeta/\partial y)^2]^{1/2}$.

The dynamics of the water table, i.e., the forces exerted in the water table, are governed by the fact that at the water table the water pressure is equal to the atmospheric pressure. This is equivalent to the statement that, on the water table, the head, h, is equal to the water table height, ζ, resulting in the dynamic boundary condition

$$h(x, y, \zeta(x, y, t), t) = \zeta(x, y, t) \text{ on } z = \zeta(x, y, t) \tag{2.6}$$

In "head models," i.e., in models where the head is imposed on the boundaries, head h is imposed on the water table. For instance, flow systems analysis (Tóth 2009) is based on such a head model. From the dynamic condition (2.6), it follows that $\partial h/\partial\lambda = (\partial\zeta/\partial\lambda)/(1 - \partial h/\partial z)$, $\lambda = x, y, t$, and substitution into kinematic condition (2.5) leads to an expression for the recharge rate r_{eff} as a function of the head and its derivatives with respect the horizontal coordinates x and y, vertical coordinate z, and time t (Bear 1972). For a detailed explanation of the physics underlying the water table equations (Eqs. 2.5 and 2.6), see Bear (1972), Zijl and Nawalany (1993), and De Smedt and Zijl (2018); these books present also a derivation of the well-known two-dimensional Dupuit–Forchheimer equation for flow in unconfined aquifers (water-bearing ground layers in which the periodically rising and falling water table resides).

To illustrate the essence of the above-presented water table description, we present a rough approximation to water table equations (Eqs. 2.5 and 2.6). Assuming that $|\partial h/\partial z| \ll 1$, we may replace in Eq. 2.5 water table height function $\zeta(x, y, t)$ with head function $h(x, y, z, t)$. This assumption can be justified in many practical applications, and the often-applied hydraulic approximation, or Dupuit–Forchheimer approximation, is based on this assumption (De Smedt and Zijl 2018). However, for the purpose of demonstration, we also assume that in

Eq. 2.5 the terms $q_x \partial h/\partial x$ and $q_y \partial h/\partial y$ are negligibly small with respect to q_z. This linearization leads to the simple (often too simple), but insightful expression

$$-q_z = r_{eff} - \theta \frac{\partial h}{\partial t} \text{ on the top boundary} \tag{2.7}$$

Since the vertical direction is defined positive upward, the term $-q_z$ in Eq. 2.7 is the downward directed vertical groundwater flux density. Equation 2.7 illustrates clearly the water balance on the water table. On the top boundary of the model domain, i.e., on the water table $h = z$, the downward directed vertical groundwater flux, $-q_z$, is equal to the recharge rate, r_{eff}, minus the increase in the amount of groundwater, $\theta \partial \zeta/\partial t$, flowing into the model domain. In a time interval Δt, the volume of the model domain is increased by the raised water table height $\Delta \zeta = (\partial h/\partial t)\Delta t$. Although the phreatic boundary conditions have to be applied at the phreatic surface $z = \zeta(x, y, t)$, the linearized condition (Eq. 2.7) may sometimes be applied on a fixed horizontal top boundary $z = h_0$ representing the water table height averaged over space and time. This geometric linearization can be justified for cases in which the variations and fluctuations of the water table height are relatively small with respect to the depth of the basin under consideration. Combined with Eq. 2.7, this results in a linear groundwater flow problem that can be solved by analytical methods; see, for instance, Tóth (2009: 41–46), El-Rawy et al. (2015).

In conventional "flux models," i.e., in forward models where the recharge rate r_{eff}^F is imposed on the top boundary, the solution of groundwater flow Eq. 2.4 yields head h^F and groundwater flux $\mathbf{q}^F$ in the model domain as well as on the boundaries including the top boundary (superscript F refers to the flux model). On the other hand, in Tóthian "head models," i.e., in forward models where the head, h^H, is imposed on the top boundary, the solution of groundwater flow Eq. 2.4 yields the head h^H and groundwater flux $\mathbf{q}^H$ in the model domain as well as on the boundaries including the top boundary (superscript H refers to the head model). Provided that specific yield θ is known, Eq. 2.7 then results in the recharge rate r_{eff}^H. The requirement that recharge rate r_{eff}^F imposed on the flux model matches with recharge rate r_{eff}^H obtained from the head model can be used to modify the original "old" conductivity k_z^{old} in a corrected "new" conductivity k_z^{new} by the simple correction equation $k_z^{new} = -q_z^F/(\partial h^H/\partial z) = k_z^{old}(q_z^F/q_z^H)$ based on Darcy's law. This idea has been worked out and justified in more detail in Chaps. 3 and 6, while the case studies presented in Chaps. 5 and 6—in which both flux and head models are applied in coupled mode—have generally been based on the linearized approximation (Eq. 2.7 applied on an averaged top boundary).

The four parameters, k_x, k_y, k_z, and s, are assumed to be dependent on position x, y, z, but independent from time t (as has been justified above, we neglect the six cross terms k_{xy}, k_{yz},k_{zx}, k_{yx}, k_{zy}, k_{xz} of the conductivity tensor). The fifth parameter, the specific yield θ, is only dependent on the horizontal coordinates x and y. It is

generally assumed that this parameter is time-independent, but it dependent on the timescale of the process under consideration. On timescales where $|\partial h/\partial t|$ is relatively large, θ is small, while on timescales where $|\partial h/\partial t|$ is relatively small, θ is relatively large. If the flow is incompressible (negligible term $s\,\partial h/\partial t$ in Eq. 2.1) and if in addition the phreatic storage term $s\,\theta\,\partial\zeta/\partial t$ in Eq. 2.5 is negligible, the flow is called quasi-steady (also see Chap. 4, Sect. 4.1 and Chap. 6, Sect. 6.4). Although we will pay some attention to the two storage parameters s and θ in Chap. 4, Sect. 4.1, this book focuses mainly on the hydraulic conductivity.

2.2 Introduction to Calderón's Conjecture

In a highly cited paper (1215 cites Google Scholar), Calderón conjectured that, under some smoothness conditions, the conductivity field in a model domain can be determined uniquely from the head and the normal flux imposed on the closed boundary of that model domain (Calderón 1980). To be more specific, Calderón considered equation $\nabla \cdot k\,\nabla h = 0$ for incompressible flow (see Eq. 2.4). Calderón used this equation in the context of electrical impedance tomography for geophysical and medical imaging. He considered an electricity conducting body with isotropic conductivity k and electric potential h where the potential and the normal current density (normal flux) are imposed on the boundary; see, for instance, Cheney et al. (1999), Borcea (2002, 2003), Borcea et al. (2003), Holder (2005). To be sure, in hydrogeology we cannot know both head and normal flux on the boundary; head–flux pairs are generally known only at some places on the external boundary and/or internal boundaries (wells, including monitoring wells). However, because Calderón's conjecture is inspiring for the inverse methods presented in the next chapters focusing on hydrogeological problems, we will present below an argument for the validity of Calderón's conjecture.

We consider an isotropic porous medium with heterogeneous conductivity $k = \alpha^2 \geq 0$. To avoid the occurrence of negative conductivities in the conductivity estimation procedure, we base the theories presented in this book as much as possible on the square root of the conductivity, in short denoted as the sqrt-conductivity $\alpha = \pm k^{1/2}$. The heterogeneous sqrt-conductivity may be discontinuous. However, we also pay some attention to subsurface bodies in which the sqrt-conductivity is a smooth function of space, as may, for instance, be the case within aquifers or aquitards.

Under the condition that the heterogeneous square root conductivity $\alpha = \alpha\,(x, y, z)$ has at least continuous second derivatives, it follows from straightforward mathematical manipulations that the groundwater flow equation (Eq. 2.4) is mathematically equivalent with the equation $\nabla^2 h\alpha - h\nabla^2\alpha = (s/\alpha)\,\partial h/\partial t$, which can be written in two coupled equations for the three functions α [$\mathrm{L}^{-1/2}\ \mathrm{T}^{-1/2}$], $\omega = h\alpha$ [$\mathrm{L}^{-3/2}\ \mathrm{T}^{-1/2}$], and $\tau = \alpha^{-1}\nabla^2\alpha$

$$\nabla^2\alpha - \tau\alpha = 0 \tag{2.8}$$

$$\nabla^2\omega - \tau\omega = \frac{s}{\alpha^2}\frac{\partial\omega}{\partial t} \tag{2.9}$$

In the literature on Calderón's conjecture, the analysis is generally based on Eqs. 2.8 and 2.9 (Salo 2008). Following their approach, we have to invoke the condition that $\alpha = \alpha(\mathbf{x})$ is a smooth function of position vector $\mathbf{x}$ with Cartesian components x, y, z. In realistic hydrogeological applications, the hydraulic conductivity is generally discontinuous. At faces of discontinuous conductivities, the head, h, and the normal component of the flux density, $q_n = -k\,\partial h/\partial n$, are continuous. As a consequence, the normal derivative of sqrt-conductivity α is discontinuous, which means that derivatives of α do not exist at discontinuity faces. In such cases, Eqs. 2.8 and 2.9 are not at all equivalent to the groundwater flow equation (Eq. 2.4).

However, within certain subsurface units, it is often reasonable to assume spatially correlated conductivities. For instance, zonation, in which the conductivity is assumed to be homogeneous within a number of zones, is a technique for inverse modeling (see Chap. 6). A discontinuous conductivity field cannot be fully determined from measured head and flux data on the boundaries of a model domain (wells, including monitoring wells, may be considered as internal boundaries); for a further analysis of this case, see Sect. 2.4.

Under the assumption that the conductivity field is smooth (differentiable), we are able to add a third equation to the two coupled equations (Eqs. 2.8 and 2.9); for a further analysis of this case, see Sect. 2.4. To show the way how this can be accomplished, we expand sqrt-conductivity field $\alpha(\mathbf{x})$ in a series of meaningfully chosen basis functions, or representer functions, $u_i(\mathbf{x})$; i.e.,

$$\alpha(\mathbf{x}) = \sum_{i=1}^{m} \gamma_i u_i(\mathbf{x}) \tag{2.10}$$

where γ_i is a coefficient. The m coefficients $\gamma_1, \gamma_2, \ldots, \gamma_m$ are related to the values $\alpha_1, \alpha_2, \ldots, \alpha_m$ of the sqrt-conductivity in m points $\mathbf{x}_1, \mathbf{x}_2, \ldots, \mathbf{x}_m$ on the boundaries. This results in a linear relation between $\gamma_1, \gamma_2, \ldots, \gamma_m$ and $\alpha_1, \alpha_2, \ldots, \alpha_m$.

$$\alpha_j = \alpha(\mathbf{x}_j) = \sum_{i=1}^{m} \gamma_i u_i(\mathbf{x}_j) \tag{2.11}$$

In this way, the sqrt-conductivities α within the model domain are linearly related to the m sqrt-conductivities α_j on the boundaries. Meaningful basis functions

for this approach may be exponential functions (Uhlmann 2003, 2009; Salo 2008) or powers of x, y, and z; see Sect. 2.4 for a detailed analysis.

Substitution of Eq. 2.10 into Eq. 2.8 yields $\tau = (\sum_{i=1}^{m} \alpha_i \nabla^2 u_i)/(\sum_{i=1}^{m} \alpha_i u_i)$, and considering incompressible flow (flow for which $(s/\alpha^2)\,\partial\omega/\partial t$ in Eq. 2.4 is negligible), substitution into Eq. 2.9 results in an equation for ω

$$\nabla^2\omega - \frac{\sum_{i=1}^{m} \gamma_i \nabla^2 u_i}{\sum_{i=1}^{m} \gamma_i u_i}\omega = 0 \text{ in the model domain} \tag{2.12}$$

For given α_i and ω_i on the boundary, Eq. 2.12 (or its discretized approximation) can be solved to determine ω in the whole model domain, from which also the head $h = \omega/\alpha$ is known in the whole model domain. However, instead of specifying m values of sqrt-conductivity α_i on the boundary, we may impose m normal flux values $q_{m;i} = -\alpha_i^2 \partial h/\partial n$ on the boundary. Doing so, Eq. 2.12, combined with this flux boundary condition and this head boundary condition, has been turned into a nonlinear problem to determine the m sqrt-conductivities on the boundary, as well as the heads and the sqrt-conductivities in the model domain. This problem could then be solved iteratively (also see Chap. 2, Sect. 2.4). The above-presented argument shows a way how to tackle Calderón's conjecture (in which $m \rightarrow \infty$). For more details, see Sect. 2.4. The solution exists only if the boundary conditions allow for a nonnegative conductivity field. This latter requirement is not always satisfied in hydrology, where the imposed boundary conditions may be based on too inaccurately measured data to allow for a nonnegative solution.

The above-presented original Calderón problem is inspiring, because it shows that for inverse modeling (parameter estimation) more heads and fluxes have to be imposed than required for forward modeling (specified parameters). However, in realistic groundwater flow problems, we do not know head and flux on the full boundary; we know head and flux only in a limited number of observation wells (zero flux, head measured) and, sometimes, on the water table (estimated water table height and recharge rates). Therefore, we will from now on focus on the incomplete Calderón problem, in which only a limited number of flux and head data are measured, often with rather great inaccuracy. Fluxes are imposed only at locations where fluxes are known, while heads are imposed only at locations where heads are known. In this incomplete Calderón problem, the conductivity field is not unique, but depends on the initial choice of the conductivity field. Moreover, because in hydrogeology the conductivity is generally discontinuous, $\nabla^2\alpha$ does not exist, and therefore, Eqs. 2.8, 2.9, and 2.10 cannot be applied. For that reason, we introduce in Chap. 3 a "Calderón-inspired" approach to parameter estimation that is directly based on the water balance equation (Eq. 2.1) and, to avoid negative conductivities, on Darcy's law (Eq. 2.2) formulated with sqrt-conductivity α, as well as on the imposed flux and head conditions.

2.3 Stefanescu's Alpha Centers

Stefanescu (1950) introduced the so-called alpha center method in the context of geo-electrical problems. His method is based on solutions of Eqs. 2.8 and 2.9 with $\partial\omega/\partial t = 0$. In his approach $\tau = 0$ except in a number of singular points (x_n, y_n, z_n), $n = 1, 2, \ldots, N$, the so-called alpha centers. The components α_n of the sqrt-conductivity field $\alpha = \sum_{n=1}^{N} \alpha_n = \pm k^{1/2}$ are then given as

$$\alpha_n = \frac{A_n}{\sqrt{(x - x_n)^2 + (y - y_n)^2 + (z - z_n)^2}} \tag{2.13}$$

From Eq. 2.8, it follows then that, in the limit $(x, y, z) \to (x_n, y_n, z_n)$, τ_n is equal to

$$\tau_n = -4\pi\sqrt{(x - x_n)^2 + (y - y_n)^2 + (z - z_n)^2} \times \delta(x - x_n)\delta(y - y_n)\delta(z - z_n) \tag{2.14}$$

where $\delta(\cdot)$ represents the Dirac delta function (Butkov 1973: 223–232; Morse and Feshbach 1953: 825). From the definition of the Dirac delta function, it follows that $\tau_n = 0$ and, as a consequence, $\tau = \sum_{n=1}^{N} \tau_n = 0$ outside the alpha centers (x_n, y_n, z_n) and may have any value (is undetermined) in the alpha centers.

Since Eq. 2.9 with $\partial\omega/\partial t = 0$ has the same form as Eq. 2.8, a similar solution holds for ω_n

$$\omega_n = \frac{\Omega_n}{\sqrt{(x - x_n)^2 + (y - y_n)^2 + (z - z_n)^2}} \tag{2.15}$$

From Eqs. 2.14 and 2.15, it follows that the head is

$$h = \frac{\omega}{\alpha} = \frac{\sum_{n=1}^{N} \omega_n}{\sum_{n=1}^{N} \alpha_n} \tag{2.16}$$

In the alpha centers (x_n, y_n, z_n), the head is equal to the finite value $h_n = \Omega_n/A_n$; i.e., the head is a smooth function of x, y, z without singularities.

Finally, the $2N$ constants A_n, Ω_n can be adjusted to honor both the head boundary condition and the flux boundary condition at the N alpha centers. This approximation method shows that inverse problems can be solved approximately using the two coupled equations (Eqs. 2.8 and 2.9) with both head and flux boundary conditions.

Stefanescu's approach is inspiring because of its assumption $\nabla^2\alpha = 0$. Although not directly applicable to groundwater modeling, this idea can be generalized to assuming $\nabla^{2m}\alpha = 0$ for the construction of basis functions $u_i(x, y, z)$ and coefficients γ_i in which sqrt-conductivity $\alpha(x, y, z)$ is expanded to solve the Calderón problem; see Sect. 2.4.

2.4 In Depth: A Closer Look at Calderón's Conjecture

In this section, we analyze the so-called "Calderón problem" in more detail. Calderón conjectured that from the potential equation $\nabla \cdot k \nabla h = 0$ (Eq. 2.4) with "sufficiently smooth" nonnegative conductivity field $k(x, y, z) \geq 0$, the conductivity can be determined uniquely from exact measurements of head h and normal flux $q_n = -k\, \partial h / \partial n$ on the closed boundary of the model domain. For inaccurately measured conditions, a conductivity that is nonnegative everywhere in the domain cannot always be found. The Calderón problem is then to determine what "sufficiently smooth" means to guarantee existence and uniqueness, and to find solutions.

For the estimation of conductivities in grid volumes, we apply Calderón's idea of "conductivity smoothness" to correlate the conductivities in neighboring grid blocks. In this framework, existence and uniqueness need not be considered: A "sufficiently accurate" approximate solution can always be found.

In Sect. 2.4.1, we investigate how many uncorrelated conductivities (in the grid volumes of a numerical model) can be derived from specification of a finite number of imposed flux and head conditions, and in the remaining sections (Sects. 2.4.2, 2.4.3, 2.4.4, 2.4.5, and 2.4.6), we show how we can determine many more conductivities if we correlate them by "smoothness conditions."

2.4.1 Uncorrelated Conductivity Fields

In this subsection, we investigate the following question: How many conductivities can be determined from $N + 1$ measured flux–head pairs?

Let us consider a groundwater flow domain with $N + 1$ nodes with node numbers n = 1, 2, …, $N + 1$, where we know both the flux of water Q_n [$L^3\ T^{-1}$] into each node n and the head h_n [L^3] in each node n. Only the differences in measured head play a role in groundwater flow (see Eq. 2.2), which means that all heads could be measured with respect to head h_{N+1}. That is, only the N measured head differences $h_n - h_{N+1}$, n = 1, 2, …, N, play a role. Also, for incompressible flow, only N fluxes are measured; the $N + 1$st flux follows from continuity equation $\sum_{n=1}^{N+1} Q_n = 0$ (flow in = flow out; also see Eq. 2.3).

From the point of view of the $N + 1$ nodes, the subsurface is "seen" as a network of $N(N + 1)/2$ conductors mutually connecting the $N + 1$ nodes. Each conductor has a conductance defined as flux through the conductor divided by head difference between the conductor's end nodes. As will be shown below, only N conductivities can be determined from the N measured fluxes and head differences, the other $N(N - 1)/2$ conductivities have to be obtained from additional knowledge (the soft data).

Let us consider nodes 1 and 2 with measured heads h_1 and h_2, respectively. Head difference $h_1 - h_2$ causes flow through the conductor connecting node 1 to node 2. If we know flux $Q_{1\to 2}$ from node 1 to node 2, we can determine conductance $K_{1\leftrightarrow 2} = Q_{1\to 2}/(h_1 - h_2)$ [$L^2\ T^{-1}$] (see Darcy's law, Eq. 2.2). To determine flux $Q_{1\to 2}$, we assign realistically chosen values (the soft data) to the remaining $N-1$ conductances $K_{1\leftrightarrow n}$, $n = 3, 4, \ldots, N+1$, connecting node n to node 1. From the measured head differences between all nodes, we can then determine the $N-1$ fluxes $Q_{1\to n} = K_{1\leftrightarrow n}(h_1 - h_n)$. The measured total flux of water flowing into node 1 is equal to $Q_1 = Q_{1\to 2} + \sum_{n=3}^{N+1} Q_{1\to n}$, from which we determine $Q_{1\to 2}$ resulting in $K_{1\leftrightarrow 2}$.

A similar procedure can be set up for node 2. Because we know already conductance $K_{1\leftrightarrow 2}$, we have to assign $N-2$ realistically chosen values (soft data) of the conductances $K_{2\leftrightarrow n}$, $n = 4, 5, \ldots, N+1$, to the $N-2$ remaining conductors connecting node n to node 2; only conductance $K_{2\leftrightarrow 3}$ is left unspecified. From these conductances and from the known head differences between their nodes, we calculate the $n-2$ fluxes $Q_{2\to n} = K_{2\leftrightarrow n}(h_2 - h_n)$. The measured total flux of water flowing into node 2 is equal to $Q_2 = Q_{1\to 2} + Q_{2\to 3} + \sum_{n=4}^{N+1} Q_{2\to n}$, from which we determine $Q_{2\to 3}$ resulting in $K_{2\leftrightarrow 3} = Q_{2\to 3}/(h_2 - h_3)$.

Continuation of this procedure shows that, in the end, we have to assign values (soft data) to $N(N-1)/2$ conductances to determine N conductances from the measured N flux–head pairs in the nodes.

Now, we consider a gridded numerical model. The above-presented "tubes with conductances" are now made up of the grid block conductivities in the model. Also in this case holds that from $N+1$ measured heads (i.e., N measured head differences) and N measured fluxes, the conductivities of only N grid volumes can be determined. In fact, we know more, because the soft data, i.e., the chosen $N(N-1)/2$ conductivity values, cannot be chosen arbitrarily; they have to be chosen in such a way that the calculated N conductivities are nonnegative. Smoothing, i.e., allowing only small differences between conductivity values in neighboring grid blocks, may help to avoid negative conductivities.

The above-presented conductance network procedure is an example of direct inversion as defined by Yeh (1986), from which we observe that small head gradients, as they often occur in flat deltaic regions, makes the solution unstable because of the divisions by $h_n - h_{n*}$ with $h_n \approx h_{n*}$. Smoothing will stabilize the inversion procedure (also see the discussion on Chap. 3, Sect. 3.9.2.2). For the above-mentioned reasons, Sect. 2.4.2 explores the concept of smoothness in more detail.

2.4.2 *Smoothed Conductivity Fields*

Defining sqrt-conductivity $\alpha = \pm k^{1/2}$ and assuming that α is sufficiently smooth to allow for the existence of $\nabla^2\alpha$, the groundwater flow equation (Eq. 2.4) can be written as Eqs. 2.8 and 2.9. Elimination of τ from these equations results in

$$\nabla^2 h\alpha - h\nabla^2\alpha = (s/\alpha)\,\partial h/\partial t \tag{2.17}$$

Terms like "smooth" and "sufficiently smooth" to denote some form of differentiability, as well as the mathematics to handle such notions, are used here in an intuitive way based on quantized (discretized) space. The mathematical framework in which these terms are rigorously defined and applied for continuous space can, for instance, be found in Duvaut and Lions (1976).

In a differentiable conductivity field, neighboring conductivities are related to each other by the well-known Taylor series expansion

$$\begin{aligned}\alpha(x+\Delta x) = \alpha(x) + (\partial\alpha/\partial x)_x \Delta x \\ + \frac{1}{2}(\partial^2\alpha/\partial x^2)_x \Delta x^2 + \cdots + \frac{1}{n!}(\partial^n\alpha/\partial x^n)_x \Delta x^n + \cdots\end{aligned} \tag{2.18}$$

We exemplify our approach for a two-dimensional grid with discretization lengths $\Delta x = \Delta y = \Delta$. Then, the finite difference approximations of the terms in Eq. 2.17 are

$$\begin{aligned}(\nabla^2 h\alpha)_{i,j} &\approx [(h\alpha)_{i-1,j} + (h\alpha)_{i+1,j} \\ &\quad + (h\alpha)_{i,j-1} + (h\alpha)_{i,j+1} - 4(h\alpha)_{i,j}]/\Delta^2 \\ h_{i,j}(\nabla^2\alpha)_{i,j} &\approx h_{i,j}(\alpha_{i-1,j} + \alpha_{i+1,j} \\ &\quad + \alpha_{i,j-1} + \alpha_{i,j+1} - 4\alpha_{i,j})/\Delta^2\end{aligned} \tag{2.19}$$

and substitution of Eq. 2.19 into Eq. 2.17 yields

$$\begin{aligned}&\alpha_{i+1,j}(h_{i,j} - h_{i+1,j}) - \alpha_{i-1,j}(h_{i-1,j} - h_{i,j}) \\ &\quad + \alpha_{i,j+1}(h_{i,j} - h_{i,j+1}) - \alpha_{i,j-1}(h_{i,j-1} - h_{i,j}) \\ &\quad = -(s/\alpha)\partial h/\partial t\end{aligned} \tag{2.20}$$

From now on, we simplify our presentation by considering incompressible flow (negligible term $s\,\partial h/\partial t$); generalization to compressible flow is straightforward. In the block-centered finite difference method, Darcy's law for the flux in the x-direction through the face between grid block $i+1, j$ and grid block i,j is approximated by

$$q_{x,\,i+\frac{1}{2},\,j} = -\alpha^2_{i+\frac{1}{2},\,j}(h_{i,\,j} - h_{i+1,\,j}) \tag{2.21}$$

where $\alpha^2_{i+\frac{1}{2},\,j}$, the effective conductivity at that face, is equal to the harmonic average of the conductivities in the grid blocks $i+1$, j and i,j. Similar approximations follow for the other three faces. Substitution of Eq. 2.21 into Eq. 2.20 yields

$$\frac{\alpha_{i+1,j}}{\alpha^2_{i+\frac{1}{2},j}} q_{x,i+\frac{1}{2},j} - \frac{\alpha_{i-1,j}}{\alpha^2_{i-\frac{1}{2},j}} q_{x,\,i-\frac{1}{2},j} + \frac{\alpha_{i,j+1}}{\alpha^2_{i,j+\frac{1}{2}}} q_{y,\,i,j+\frac{1}{2}} - \frac{\alpha_{i,j-1}}{\alpha^2_{i,j-\frac{1}{2}}} q_{y,\,i,j-\frac{1}{2}} = 0 \tag{2.22}$$

Thanks to the water balance (Eq. 2.1), the fluxes through the faces are continuous, and in the model domain, the fluxes change only gradually. Equation 2.22 shows then that not only the fluxes, but also the conductivities vary smoothly in the model domain. This is clearly demonstrated for one-dimensional flow, where $q_{x,\,i+\frac{1}{2},j} = q_{x,\,i-\frac{1}{2},j} = q_0$ is constant. From Eq. 2.22, it follows then that the smoothest possible solution is $\alpha_{i+1,j} = \alpha_{i+\frac{1}{2},j} = \alpha_{i-1,j} = \alpha_0$ is constant. Of course, there are infinitely more smooth solutions, but here we consider the smoothest possible solution.

Since the flux runs and head runs with a numerical model (e.g., MODFLOW) for the double constraint method are based on the conventional formulation (Eq. 2.4), the resulting sqrt-conductivity field will not be smooth. To smooth the sqrt-conductivity, we propose an additional step in the double constraint iterations.

Equation 2.17 (for incompressible flow) can also be written as $\nabla^2\alpha = (h+h_0)^{-1}\nabla^2[(h+h_0)\alpha]$ in which h_0 is a suitably chosen reference head. To avoid division by zero, we choose $h_0 > -h_{\min}$, where $h_{\min}$ is the smallest value of h in the model domain. Then, $\tilde{h} = h + h_0$ is positive everywhere in the model domain.

Now, we consider the original double constraint method, in which each grid volume (each "point") is a zone. Consider a sqrt-conductivity α obtained after an iteration step with head $\tilde{h}$ in the head run. From the α-values in the grid volume centers, we calculate $b = \tilde{h}^{-1}\nabla^2\tilde{h}\alpha$ by numerical differentiation (using an expression like Eq. 2.19). According to Eq. 2.17, b may be considered as a source term for Poisson equation $\nabla^2\alpha' = b$. Using the sqrt-conductivity obtained from the iteration step as boundary condition for this Poisson equation (i.e., applying Dirichlet boundary condition $\alpha'|_{\partial D} = \alpha|_{\partial D}$), the smoothed sqrt-conductivity α' is then obtained by solving the Poisson equation. This can simply be done by a groundwater flow model (e.g., MODFLOW). We use the thus-obtained smoothed α' as initial sqrt-conductivity for the next iteration step by the double constraint method. Repeating this procedure after every DCM iteration step will then result to converge, i.e., to $\alpha \to \alpha'$ in the grid block centers. Instead of smoothing the whole model domain, we could also select a number of zones in which we want to smooth.

2.4.3 *Smoothest Possible Sqrt-Conductivity Fields*

We consider a two- or three-dimensional domain D enclosed by boundary ∂D in which the conductivity is isotropic but heterogeneous; i.e., $k = k(x, y, z)$ is a

function of the spatial coordinates x, y, z (for a one-dimensional domain problem, see Sect. 2.4.6). We require that this heterogeneous conductivity field is "the smoothest possible" conductivity field. That is, if everywhere on boundary ∂D the conductivity has the same value, k_B, independent from its spatial position, the conductivity in domain D is homogeneous and equal to its boundary value k_B. This requirement corresponds with Calderón's aim to develop a method that can detect an internal deviation from homogeneity by voltage and current measurements on the surface. In this way we can detect a well-conducting tumor in a poorly conducting breast, or a well-conducting salt lens in a poorly conducting fresh water body (Uhlmann 2003, 2009). For hydrogeological applications, voltage is replaced by head and current by flux, for instance, to detect a poorly conducting clay lens in a well-conducting aquifer.

In Stefanescu's approach (Chap. 2, Sect. 3), the construction of an inverse solution is based on the simple assumption $\tau = 0$ leading to $\nabla^2\alpha = 0$ and $\nabla^2 h\alpha = 0$ (see Eqs. 2.8 and 2.9). Although Stefanescu's approximation may lead to acceptable conductivity estimations in simple applications, application to more comprehensive problems has to be based on more general and flexible assumptions. Instead of Stefanescu's assumption $\nabla^2\alpha = 0$ (Sect. 2.3), we base the inverse solution of sqrt-conductivity function $\alpha(x, y, z)$ on equation $\nabla^{2(L+1)}\alpha = 0$. For a sufficiently large number L, the groundwater flow equation $\nabla^2\alpha = h^{-1}\nabla^2 h\alpha$, or its more usual mathematically equivalent $\nabla \cdot \alpha^2 \nabla h = 0$, is then used to determine a sqrt-conductivity field α in domain D that approximately honors the head and flux conditions h_B and q_B on boundary ∂D. This approach implies that we have solved the equation $\nabla^{2L}(h^{-1}\nabla^2 h\alpha) = 0$ instead of Stefanescu's equation $\nabla^2 h\alpha = 0$.

In principle, the above-introduced approach can be used for model domains with an arbitrary shape. However, to illustrate the idea, we consider a rectangular or block-shaped domain D with closed boundary $0 \le x \le D_x$, $0 \le y \le D_y$, $0 \le z \le D_z$. For this domain, we construct a finite number of L polynomials $p_{L-\ell}$ ($\ell = 1, 2, \ldots, L < \infty$) in x, y, z, in such a way that the polynomials preserve their form when the coordinates are interchanged (e.g., when $x \to y$, $y \to z$, $z \to x$ or $x \to z$, $y \to x$, $z \to y$). In addition, we consider polynomials of finite degree.

To avoid nonzero solutions α for which $\alpha = 0$ on the boundary (spurious solutions), we derive conditions for function τ in the coupled equations $\nabla^2\alpha - \tau\alpha = 0$ and $\nabla^2\omega - \tau\omega = 0$ (Eqs. 2.8 and 2.9, respectively) for incompressible flow. Sqrt-conductivity α is expanded in a series of linearly independent basis functions, or representer functions, $u(x)$, $v(y)$, $w(z)$ in such a way that $\alpha = \sum_{ijk} \gamma_{ijk}\, u_i\, v_j\, w_k$, where the γ_{ijk}'s are the coefficients. For each component $\alpha_{ijk} = \gamma_{ijk} u_i v_j w_k$ in this series expansion, we find $\tau_{u_i v_j w k} = \alpha_{ijk}^{-1}\nabla^2\alpha_{ijk} = u_i^{-1}\partial^2 u_i/\partial x^2 + v_j^{-1}\partial^2 v_j/\partial y^2 +$. A boundary condition for α on the closed boundary ∂D (a Dirichlet condition for Eq. 2.8) leads to a unique solution only if at least one of the functions $\tau_{u_i} = u_i^{-1}\partial^2 u_i/\partial x^2$, $\tau_{v_j} = v_j^{-1}\partial^2 v_j/\partial y^2$, $\tau_{w_k} = w_k^{-1}\partial^2 w_k/\partial z^2$ is nonnegative. If all three functions $\tau_{u_i}, \tau_{v_j}, \tau_{w_k}$ derived from function $u_i(x)\, v_j(y)\, w_k(z)$ are negative, there exist spurious solutions, which means that the solution of $\nabla^2\alpha - \tau\alpha = 0$ is not

unique. For example, for the above-defined block-shaped domain the solution $\alpha_{ijk} = \gamma_{ijk} \sin(\kappa_x x) \sin(\kappa_y y) \sin(\kappa_z z)$ results for $\kappa_x = \pm m\pi/D_x$, $\kappa_y = \pm m\pi/D_y$, $\kappa_z = \pm m\pi/D_z$ ($m = 1, 2, 3, \ldots$) in nonzero values of α inside domain D for zero boundary values $\alpha_B = 0$. In that case, $\tau_{u_i} = -\kappa_x^2 < 0$, $\tau_{v_j} = -\kappa_y^2 < 0$, and $\tau_{w_k} = -\kappa_z^2 < 0$ are negative. On the other hand, a solution like $\alpha_{ijk} = \gamma_{ijk} \sin(\kappa_x x) \sin(\kappa_y y) \exp(\kappa_z z)$ cannot give rise to nonzero solutions for the Dirichlet boundary conditions $\alpha_B = 0$. Although $\tau_{u_i} = -\kappa_x^2 < 0$ and $\tau_{v_j} = -\kappa_y^2 < 0$ are negative, spurious solutions do not occur because $\tau_{w_k} = \kappa_z^2 > 0$ is positive. Polynomial basis functions $u_i(x) = x^i$, $v_j(y) = y^j$, $w_k(z) = z^k$, $i, j, k = 0, 1, 2, 3, \ldots$, do not result in spurious solutions, as well as exponential basis functions [upon which "complex geometrical optics" is based (Salo 2008: 18)].

2.4.4 Polynomial Construction

To simplify the presentation, we consider a two-dimensional rectangular domain; the extension to the above-introduced three-dimensional rectangular domain is straightforward.

For the ease of presentation, we assume that the domain is a square with center $(x_1, y_1) = (\delta, \delta)$, where $2\delta = D_x = D_y = D_z$. The polynomial solution of Poisson equation $\nabla^2 p_L = c_L$, where c_L is a constant, is $p_L = (a_x x^2 + b_x x) + (a_y y^2 + b_y y) + c$, from which it follows that $c_L = \nabla^2 p_L = 2(a_x + a_y)$. Specifying the four boundary conditions, the four polynomial values $p_{L;0,1}, p_{L;2,1}, p_{L;1,0}, p_{L;1,2}$ result in the following four equations for the four polynomial constants: $a_y\delta^2 + b_y\delta = p'_{L;0,1}$, $a_x\delta^2 + b_x\delta = p'_{L;1,0}$, $4a_x\delta^2 + 2a_x\delta + a_y\delta^2 + b_x\delta = p'_{L;2,1}$, and $a_x\delta^2 + b_x\delta + 4a_y\delta^2 + 2b_y\delta = p'_{L;1,2}$, where $p'_{L;i,j} = p_{L;i,j} - (b_x + b_y)$. Solving this system yields the four polynomial constants a_x, b_x, a_y, b_y, from which the constant $c_L = 2(a_x + a_y)$ can be determined. Constant $c = p_{L;\,0,\,0}$ is chosen equal to the average of the boundary conditions specified near the origin (0,0); i.e., $c = (p_{L;\,0,\,1} + p_{L;\,1,\,0})/2$. Thanks to this choice, a conductivity that is homogeneous on the boundary (i.e., $p_{L;\,0,\,1} = p_{L;\,2,\,1} = = p_{L;\,1,\,2} = \alpha_B$) results in a conductivity that is homogeneous in the model domain (i.e., $a_x = a_y = 0$, $b_x = b_y = 0$, $c = \alpha_B$).

Because of the extremely coarse discretization, the above-presented approximation is very poor. However, we can systematically derive better approximations. For that purpose, we partition the model domain in four grid blocks, which means that we can honor eight boundary conditions. For this grid-refined domain, we solve Poisson equation $\nabla^2 p_{L-1} = p_L + c_{L-1}$ with the eight boundary conditions for p_{L-1}. To be sure, we do not use the polynomial constants calculated for the one-grid block domain; they will be recalculated. Since function p_L is a polynomial of degree 2, function p_{L-1} is a polynomial of degree 4: $p_{L-1} = (a'_x x^4 + b'_x x^3 + c'_x x^2 + d'_x x)$ plus a similar polynomial in y plus a constant, e. Honoring the eight boundary

conditions for A_{L-1} results in a system of eight linear algebraic equations that can be solved to find the eight polynomial constants $a'_x, b'_x, c'_x, d'_x, a'_x, b'_x, c'_x, d'_x$. Function p_L is then $p_L = \nabla^2 p_{L-1} = 12a'_x x^2 + 6b'_x x + c'_x$ plus a similar polynomial in y, while constant e is equal to $e = p_{L-1;\,0,\,0} = (p_{L-1;\,0,\,1} + p_{L-1;\,1,\,0})/2$. Again, thanks to this choice, we find a conductivity field that is homogeneous in the domain if the conductivities on the boundary are homogeneous (i.e., all polynomial constants are equal to zero, except for $e = \alpha_B$).

Continuing this procedure, we introduce polynomials of degree $2L$ (for which we recalculate the polynomial constants obtained for the previous 4th degree polynomial example). For that number of L grid blocks, we consider the sequence of Poisson equations $\nabla^2 p_{L-\ell} = p_{L-\ell+1} + c_{L-\ell}$ for $\ell = 2,\ 3,\ \ldots,\ L-3,\ L-1$.

For $\ell = L-1$, we have to solve Poisson equation $\nabla^2 p_1 = p_2 + c_1$, which means that polynomial p_1 has degree $2L$. The $4L$ polynomial constants can be determined from the $4L$ boundary conditions for p_1 specified in the $4L$ boundary points, while the additional constant $p_{1;\,0,\,0} = (p_{1;\,0,\,1} + p_{1;\,1,\,0})/2$ is chosen equal to the average of the two boundary values specified near the origin.

2.4.5 A Double Constraint Methodology

Now, we equate sqrt-conductivity α to the above-determined polynomial p_1; i.e., generalizing to three dimensions we set $\alpha(x, y, z) = p_1(x, y, z)$. From the above-presented polynomial construction, it follows that for given $\alpha_B = \alpha(x_B, y_B, z_B)$ on the boundary with coordinates x_B, y_B, z_B sqrt-conductivity $\alpha(x, y, z)$ is known in the whole model domain. For imposed head boundary condition $h_B = h(x_B, y_B, z_B)$, head $h(x, y, z)$ can then be determined in the whole model domain from groundwater flow equation $\nabla \cdot \alpha^2 \nabla h = 0$.

However, instead of specifying boundary values of the sqrt-conductivity, we may impose normal boundary fluxes $q_B = q_n(x_B, y_B, z_B)$. Doing so, groundwater flow equation $\nabla^2 h\alpha - h\nabla^2 \alpha = 0$, or its mathematical equivalent $\nabla \cdot \alpha^2 \nabla h = 0$ (Eq. 2.4), with both this flux boundary condition and this head boundary condition, results in a partial differential problem from which the boundary sqrt-conductivity $\alpha_B = \alpha(x_B, y_B, z_B)$ as well as the sqrt-conductivities, heads and fluxes in the model domain can be determined. More specifically, assume that boundary condition h_B for head h has been determined from measurements. As a consequence, the normal head gradients $\partial h(\alpha_B)/\partial n$ on the boundary can be determined as a function of function $\alpha_B(x_B, y_B, z_B)$, where argument α in $h(\alpha)$ denotes the dependency of head h on sqrt-conductivity field α (a "function of a function" is a functional; see Sect. 3.4). Also, the normal head gradient $[\partial h(\alpha_B)/\partial n]_B$ on the boundary can be determined as a function of function $\alpha(x, y, z)$. To match this normal head gradient to the measured normal boundary flux $q_B(\alpha_B)$, we apply Darcy's law (Eq. 2.2) to obtain the $q_B(\alpha_B) + \alpha_B^2 [\partial h(\alpha_B)/\partial n]_B = 0$. In other

words, we have to find the function $\alpha_B = \alpha(x_B, y_B, z_B)$ that makes the functional $q_B(\alpha_B) + \alpha_B^2[\partial h(\alpha_B)/\partial n]_B$ equal to zero, thus honoring Darcy's law. Thanks to the polynomial construction presented in Sect. 2.4.4, this formulation results in a system of nonlinear algebraic equations for the N_B values of α_B in the N_B boundary points, where $N_B = 2nL$ for n-dimensional flow with $n \geq 2$; see Sect. 2.4.4. Finally, sqrt-conductivity $\alpha(x, y, z)$, head $h(x, y, z)$, and flux density $\mathbf{q}(x, y, z)$ follow from the polynomial expansions.

As an introduction to the double constraint method presented in Chap. 3, we extend the above-presented argument to a constructive iterative approach to find a solution. For an estimated initial sqrt-conductivity $\alpha_{B;i} = \alpha_i(x_B, y_B, z_B)$, the sqrt-conductivity $\alpha_i(x, y, z)$ can be determined from the polynomial construction. Head boundary condition $h_B = h(x_B, y_B, z_B)$ is determined by measurements, and given the estimated initial sqrt-conductivity $\alpha_i(x, y, z)$, head $h_i(x, y, z)$ can be calculated in the whole model domain from groundwater flow equation $\nabla \cdot \alpha_i^2 \nabla h_i = 0$ (Eq. 2.4). As a consequence, the normal head derivative $(\partial h_i/\partial n)_B$ on the boundary can be determined, while the normal boundary flux follows from Darcy's law (Eq. 2.2) yielding $q_{B;i} = -\alpha_{B;i}^2(\partial h_i/\partial n)_B$. The thus-determined normal boundary flux does not generally match the measured normal boundary flux q_B. To determine a new normal boundary flux $q_{B;\,i+1}$ that better matches the measured normal flux, we introduce a new sqrt-conductivity, α_{i+1} by applying Darcy's law in the form $q_B = -\alpha_{B;\,i+1}^2 (\partial h_i/\partial n)_B$. Substitution of the above-presented expression for $q_{B;i}$ leads then to the update rule $k_{B;\,i+1} = k_{B;\,i}\, q_B/q_{B;\,i}$ for the conductivity on the boundary. The updated $\alpha_{i+1} = \pm k_{i+1}^{1/2}$ in the whole model domain follows then from the above-derived polynomial construction. After starting the procedure for $i = 0$, we repeat this procedure for $i = 1,\ 2,\ 3,\ \ldots$ until α_{i+1} has converged sufficiently close to α_i.

Until now, we have supposed that the system is well posed (existence of stable unique solution). However, in practical applications, the step $\alpha_{i+1} = \pm k_{i+1}^{1/2}$, which is required for the polynomial construction, may turn out to fail. During the iteration process, k_{i+1} may become negative in a number of boundary points, which means that, even if α_i was a real number, α_{i+1} is no longer real (is an imaginary number). Negative conductivity updates may be caused by measurement errors and also by a poor initial guess of the initial conductivities. To handle such cases, the update rule has to be modified to $k_{B;i+1} = k_{B;i}\left|q_B/q_{B;i}\right|$, as will be explained in Chap. 3, Sect. 3.4. Using this modified update rule, negative conductivities caused by a poor initial guess may gradually disappear during the iteration process, but negative conductivities caused by measurement errors cannot be removed.

The above-presented iterative approach may be considered as a simple example of the double constraint methodology presented in Chap. 3. The introduction of smoothness (differentiable polynomials) has resulted in a simplified double constraint methodology in which the update rule is only applied to the boundary conductivities. Moreover, in this case, the groundwater flow equation is only used to determine the head, while in the general approach this equation has also to be solved for the flux. For a detailed explanation, see Chap. 3.

2.4.6 The One-Dimensional Case

In one dimension, for example, flow through a tube of length L_{tube} filled with porous material, the situation is different. Since there are only two boundary points $(N_B = 2)$, only two polynomial coefficients can be determined, which means that the smoothest possible polynomial is $\alpha = bx + c$. From groundwater flow equation $h\nabla^2\alpha = \nabla^2 h\alpha$, it follows that $d^2h\alpha/dx^2 = 0$, i.e., $h\alpha = b'x + c'$, $h = (b'x + c')/(bx + c)$, $dh/dx = [b'(bx + c) - b(b'x + c')]/(bx + c)^2$, and $q = -\alpha^2 dh/dx = b(b'x + c') - b'(bx + c)$. Continuity equation $dq/dx = 0$ requires that q is constant, which means that $b' = 0$ or $b = 0$. Solution $b' = 0$ means that there is no head gradient and, as a consequence, no flow, which contradicts our requirement that there should be at least one point in which the flux is nonzero. Hence, the solution is $b = 0$, which means that conductivity $\alpha^2 = k$ is constant. Darcy's law then results in $k = qL_{tube}/(h_{+L_{tube}/2} - h_{-L_{tube}/2})$.

One of the aspects of the Calderón problem is to determine the smoothness requirements in such a way that there exists a unique conductivity field determined by the head–flux boundary conditions (another aspect is to find solutions). Requiring, in addition, that the smoothness condition is as simple as possible, the above-presented example shows that the required smoothness for a one-dimensional Calderón problem is a constant conductivity.

In Sects. 2.4.3, 2.4.4, and 2.4.5, we have shown that for n-dimensional problems with $n \geq 2$ a solution exists. The above-presented "discrete analytical" construction may be considered as an argument for the validity of Calderón's conjecture. In our example, where the N_B boundary points are evenly distributed over the boundary, the continuum limit $N_B \to \infty$ could be considered as a strong argument for the validity of Calderón's conjecture. However, it is not a general proof for all types of bounded continuous space; the smoothness conditions, the distribution of boundary points, and the way of approaching the continuum limit may be specified in different ways. For instance, Kenig et al. (2007) present a three-dimensional problem in which on some parts of the boundary no head–flux data are specified. For more details on the general continuous problem, see, for instance, Barber and Brown (1984, 1986), Sylvester and Uhlmann (1987), Nachman (1996), Brown (1996), Brown and Uhlmann (1997), Siltanen et al. (2000), Bukhgeim and Uhlmann (2002), Uhlmann (2003, 2009), Borcea (2002, 2003), Borcea et al. (2003), Bukhgeim and Uhlmann (2002).

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