Chapter 6
Initial, Boundary and Constraint Conditions

6.1 Introduction

The governing model equations derived in Chaps. 3 and 4, which are summarized in Table 3.7 for general variably saturated porous media, in Table 3.9 for fully saturated porous media (groundwater), in Table 3.10 for 2D unconfined aquifers and in Table 3.11 for 2D confined aquifers as well as in Tables 4.5–4.7 for variable-density flow, mass and heat transport of discrete features, have to be supplemented by initial, boundary and constraint conditions. The solutions for the flow, mass and heat transport equations are generally sought within a domain $\Omega \subset \Re^D$ closed by its boundary $\Gamma \subset \Re^D$ $(D = 1, 2, 3)$ in the $D-$dimensional Euclidean space (cf. Sect. 2.2.2). By definition, the boundary Γ is separated from the domain Ω. On the other hand, by $\bar{\Omega}$ we denote the (closure) domain, which completely joins the boundary

$$\bar{\Omega} = \Omega \cup \Gamma \tag{6.1}$$

On $\bar{\Omega}$ and Γ initial conditions (IC's) and boundary conditions (BC's) have to be specified, respectively. The boundary Γ consists of disjoint nonoverlapping portions Γ_i $(i = 1, 2, \ldots)$ bounding the domain Ω both outside and inside, which can be suitably subdivided according to the types of BC's. BC's are always required for both transient and steady-state problems, while IC's are always needed for transient problems. An exception possesses nonlinear steady-state problems, where an IC of the solution initializes an iterative procedure.

In addition, singular point conditions (SPC's) are of interest for specifying pumping (discharging) or injection (recharging) wells, which are assigned to separate points of the domain Ω. Due to the nature of singularities well-type SPC's must be treated in a singular (discrete) manner which is different to the treatment of BC's, where fluxes are continuous and integrable over a boundary section. It is interesting to note that the effect by a flux-type BC can be similar or even identical

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to a SPC specification applied to a numerical model for cases, where all connected points forming the discretized boundary are imposed by a respective SPC.

6.2 Initial Conditions (IC's)

In the domain $\bar{\Omega}$ the following IC's are valid for the flow, species mass and heat transport processes, respectively:
Flow

$$h(\boldsymbol{x}, t_0) = h_0(\boldsymbol{x}) \quad \text{in} \quad \bar{\Omega} \tag{6.2}$$

Mass transport of species k

$$C_k(\boldsymbol{x}, t_0) = C_{k0}(\boldsymbol{x}) \quad \text{in} \quad \bar{\Omega} \tag{6.3}$$

Heat transport

$$T(\boldsymbol{x}, t_0) = T_0(\boldsymbol{x}) \quad \text{in} \quad \bar{\Omega} \tag{6.4}$$

where h_0, C_{k0} and T_0 are known spatially varying functions of initial distribution at initial time t_0.

6.3 Standard Boundary Conditions (BC's) and Well-Type Singular Point Conditions (SPC's)

On the boundary Γ closing the domain Ω disjoint portions are appropriately defined as Γ_i $(i = 1, 2, \ldots)$ for which different types of BC can be separately specified. Dirichlet-type (1st kind or *essential*) BC's on Γ_1, Γ_4 and Γ_7, Neumann-type (2nd kind) BC's on Γ_2, Γ_5 and Γ_8 as well as Cauchy (Robin)-type (3rd kind) BC's on Γ_3, Γ_6 and Γ_9 will represent standard formulations (cf. Sect. 2.2.2) for flow, mass and heat, respectively, so that for standard BC's: $\Gamma = \Gamma_1 \cup \Gamma_2 \cup \Gamma_3 = \Gamma_4 \cup \Gamma_5 \cup \Gamma_6 = \Gamma_7 \cup \Gamma_8 \cup \Gamma_9$. Additionally, well-type SPC's are included providing specific sink/source conditions which have to be assigned to separate points of the domain Ω idealized as wells. Furthermore, integrated formulations of Neumann-type and Cauchy-type BC's are desired. BC's of 1st, 2nd and 3rd will be symbolized by $\bigcirc$, $\times$ and $\otimes$, respectively. A well-type SPC will be symbolized by $\Rsh$. Special formulations of BC's are necessary in various applications which will be introduced in Sect. 6.5 further below.

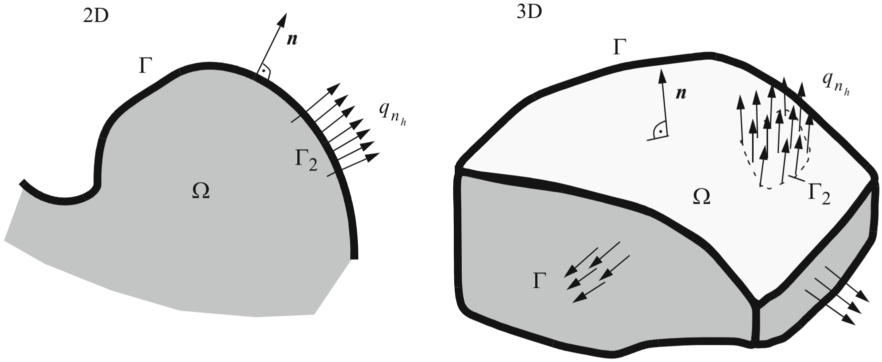

Fig. 6.1 Normal Neumann-type fluxes for 2D and 3D boundary geometries

6.3.1 Flow BC

6.3.1.1 ○ Dirichlet-Type (1st Kind) BC

$$h(\boldsymbol{x}, t) = h_D(t) \quad \text{on} \quad \Gamma_1 \times t[t_0, \infty) \tag{6.5}$$

where h_D are prescribed values of hydraulic head on $\Gamma_1 \subset \Gamma$. Note that for steady-state flow problems Dirichlet-type BC's (6.5) are usually required, i.e., $\Gamma_1 \neq \emptyset$, unless Cauchy-type BC's occur.

6.3.1.2 × Neumann-Type (2nd Kind) BC

$$\left.\begin{aligned} q_{n_h}(\boldsymbol{x}, t) &= \underbrace{-\left[k_r \boldsymbol{K} f_\mu \cdot (\nabla h + \chi \boldsymbol{e})\right] \cdot \boldsymbol{n}}_{\text{for 3D and 2D vertical \& unconfined}} = q_h(t) \\ \bar{q}_{n_h}(\boldsymbol{x}, t) &= \underbrace{-(\boldsymbol{T} f_\mu \cdot \nabla h) \cdot \boldsymbol{n}}_{\text{for 2D horizontal, confined}} = \bar{q}_h(t) \end{aligned}\right\} \quad \text{on} \quad \Gamma_2 \times t[t_0, \infty) \tag{6.6}$$

where $\boldsymbol{n}$ is the positive outward-directed unit normal to Γ_2, $q_{n_h} = \boldsymbol{q} \cdot \boldsymbol{n}$ and $\bar{q}_{n_h} = \bar{\boldsymbol{q}} \cdot \boldsymbol{n}$ represent normal fluxes (positive outward-directed) across the boundary Γ_2 and q_h and $\bar{q}_h$ are the prescribed Neumann fluxes on $\Gamma_2 \subset \Gamma$ as illustrated in Fig. 6.1. If $q_h = 0$ and $\bar{q}_h = 0$ the Neumann-type BC reduces to a *natural* (no-flux) BC associated with $\nabla h + \chi \boldsymbol{e} = \boldsymbol{0}$ and $\nabla h = \boldsymbol{0}$, respectively. Note that for saturated porous media $k_r = 1$, for density-uncoupled problems $\chi = 0$ and for constant liquid viscosity, equal to the reference viscosity, $f_\mu = 1$. For 2D horizontal unconfined aquifer problems with $k_r = 1$ and $\chi = 0$, the prescribed Neumann flux q_h has to be vertically integrated in accordance with the unknown water table h.

6.3.1.3 ⊗ Cauchy-Type (3rd Kind) BC

$$\left.\begin{aligned} q_{n_h}(\boldsymbol{x},t) &= -\big[k_r \boldsymbol{K} f_\mu \cdot (\nabla h + \chi \boldsymbol{e})\big]\cdot \boldsymbol{n} = -\Phi_h(h_C - h) \\ &\qquad \text{for 3D and 2D vertical \& unconfined} \\ \bar{q}_{n_h}(\boldsymbol{x},t) &= -(\boldsymbol{T} f_\mu \cdot \nabla h)\cdot \boldsymbol{n} \qquad\qquad = -\bar{\Phi}_h(h_C - h) \\ &\qquad \text{for 2D horizontal, confined} \end{aligned}\right\} \text{on} \quad \Gamma_3 \times t[t_0,\infty) \tag{6.7}$$

where h_C are prescribed values of hydraulic head on $\Gamma_3 \subset \Gamma$. The signs of $q_{n_h} = \boldsymbol{q}\cdot\boldsymbol{n}$ and $\bar{q}_{n_h} = \bar{\boldsymbol{q}} \cdot \boldsymbol{n}$ are chosen that the boundary fluxes are positive outward-directed if $h > h_C$. In (6.7) the *transfer coefficients* Φ_h and $\bar{\Phi}_h$ represent *dual* directional functions in form of:

$$\Phi_h = \begin{cases} \Phi_h^{\text{in}}(\boldsymbol{x},t) & \text{for} \quad h_C > h \\ \Phi_h^{\text{out}}(\boldsymbol{x},t) & \text{for} \quad h_C \leq h \end{cases} \tag{6.8}$$

$$\bar{\Phi}_h = \begin{cases} \bar{\Phi}_h^{\text{in}}(\boldsymbol{x},t) & \text{for} \quad h_C > h \\ \bar{\Phi}_h^{\text{out}}(\boldsymbol{x},t) & \text{for} \quad h_C \leq h \end{cases} \tag{6.9}$$

which are in general functions of space $\boldsymbol{x}$ and time t. Accordingly, in specifying two alternate (if necessary temporal) transfer coefficients different transfer conditions can be input to distinguish between inflow conditions ($q_{n_h} < 0$, e.g., infiltration from a surface water into the aquifer) and outflow conditions ($q_{n_h} > 0$, e.g., exfiltrating the aquifer into the surface water). Their usefulness for river-aquifer interactions is discussed further below. The special case $\Phi_h = \Phi_h^{\text{in}} = \Phi_h^{\text{out}}$ or $\bar{\Phi}_h = \bar{\Phi}_h^{\text{in}} = \bar{\Phi}_h^{\text{out}}$ does not differ between inward and outward boundary flux, so it becomes directionally independent.

The formulation of 3rd kind BC's is based on a general transfer relation between the reference value h_C on the boundary portion Γ_3 and the hydraulic head h to be computed at the same place. The reference hydraulic head h_C can also be time-dependent $h_C = h_C(t)$. The dual transfer coefficient Φ_h possesses the property of a resistance coefficient which constrains the discharge through the boundary and, additionally, differs between inflow and outflow conditions by means of Φ_h^{in} and Φ_h^{out}, respectively, according to (6.8) and (6.9). If $\Phi_h \equiv 0$ the boundary becomes impervious. On the other hand, using a very large value $\Phi_h \to \infty$ the BC of 3rd kind is reduced to a Dirichlet-type (1st kind) BC approaching to $h = h_C$ on Γ_3.

For flow problems the transfer coefficient Φ_h can be identified as a specific *colmation* (or *leakage*) coefficient as outlined in Fig. 6.2 for inflow (infiltration) conditions ($\Phi_h \to \Phi_h^{\text{in}}$ $(h_C > h)$). An adjacent river bed is clogged ('colmated') by a layer of thickness d and a hydraulic conductivity of K_o^{in}. Commonly, the layer conductivity K_o^{in} is much smaller than the conductivity K_1 of the aquifer to be modeled. Thereby the model boundary Γ represents the inner boundary of the 'colmation' layer Γ_3, where the model domain Ω ends.

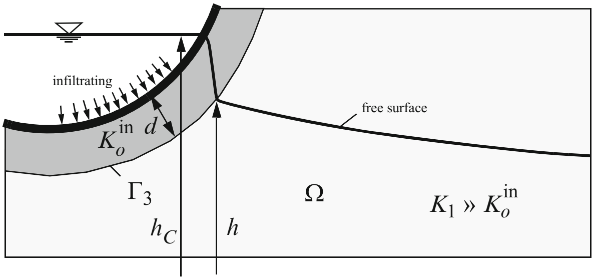

Fig. 6.2 Transfer coefficient $\Phi_h (= \Phi_h^{\text{in}})$ as 'colmation' parameter of a clogged river bed

The flux through such a 'colmation' layer can be estimated from the Darcy equation (see Fig. 6.2), viz.,

$$q_{n_h} \approx -K_o^{\text{in}} \frac{\Delta h}{\Delta s} = -K_o^{\text{in}} \frac{h_C - h}{d} \tag{6.10}$$

where s and Δs identify the arc length and line distance in direction of flow, respectively. Setting (6.7) equal to (6.10) a simple relationship results for the transfer coefficient Φ_h^{in} in 3D and 2D (vertical, horizontal unconfined) cases:

$$\Phi_h^{\text{in}} = \frac{K_o^{\text{in}}}{d} \tag{6.11}$$

For horizontal confined flow problems an inherent vertical averaging becomes necessary (in the aquifer all fluxes are integrated over the depth) resulting in a depth-integrated transfer coefficient $\bar{\Phi}_h^{\text{in}}$ as:

$$\bar{\Phi}_h^{\text{in}} = B\Phi_h^{\text{in}} = B\frac{K_o^{\text{in}}}{d} \tag{6.12}$$

For outward directed (exfiltrating) boundary fluxes according to Fig. 6.3 the following relationships for Φ_h^{out} and $\bar{\Phi}_h^{\text{out}}$ can be derived, analogously to the above, viz.,

$$\Phi_h^{\text{out}} = \frac{K_o^{\text{out}}}{d} \tag{6.13}$$

$$\bar{\Phi}_h^{\text{out}} = B\Phi_h^{\text{out}} = B\frac{K_o^{\text{out}}}{d} \tag{6.14}$$

The coefficients Φ_h^{in} and Φ_h^{out} (also $\bar{\Phi}_h^{\text{in}}$ and $\bar{\Phi}_h^{\text{out}}$) differ if in case of infiltration the conductivities of the 'colmation' layer become depart from that of the exfiltration $K_o^{\text{in}} \neq K_o^{\text{out}}$.

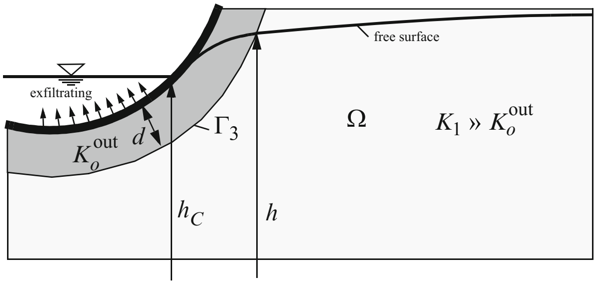

Fig. 6.3 Transfer coefficient $\Phi_h (= \Phi_h^{out})$ as 'colmation' parameter of a clogged river bed

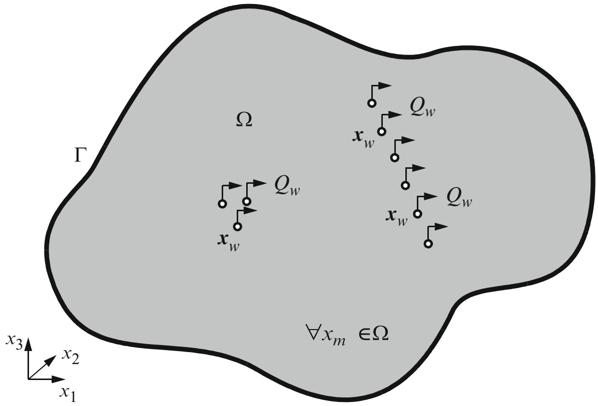

Fig. 6.4 Number of well-type SPC's on singular points $\forall \boldsymbol{x}_m \in \Omega$

6.3.1.4 Well-Type SPC

A number of pumping (or injecting) wells are idealized as singular point sinks (or sources) at locations $\boldsymbol{x}_w \in \Omega$ (Fig. 6.4):

$$Q_{hw}(\boldsymbol{x}, t) = -\sum_{w=1}^{N_W} Q_w(t)\delta(\boldsymbol{x} - \boldsymbol{x}_w) \quad \text{on} \quad \boldsymbol{x}_w \in \Omega \times t[t_0, \infty) \tag{6.15}$$

where Q_{hw} is the specific sink/source function of wells, N_W is the number of wells, $Q_w(t)$ is the prescribed volume per unit time discharge (pumping rate) of single well w at location $\boldsymbol{x}_w$ and $\delta(\boldsymbol{x} - \boldsymbol{x}_w) = \prod_{i=1}^{D} \delta(x_i - x_{iw})$ is the Dirac delta function associated with location $\boldsymbol{x}_w$. The Dirac delta $\delta(\boldsymbol{x} - \boldsymbol{x}_w)$ is zero at all points except $\boldsymbol{x} = \boldsymbol{x}_w$ and satisfies

$$\int_{\Omega} \delta(\boldsymbol{x} - \boldsymbol{x}_w) d\Omega = 1 \tag{6.16}$$

and accordingly

$$\int_{\Omega} \sum_{w=1}^{N_W} Q_w(t)\delta(\boldsymbol{x} - \boldsymbol{x}_w) d\Omega = \sum_{w=1}^{N_W} Q_w(t) \tag{6.17}$$

6.3.2 Mass Transport BC

6.3.2.1 ○ Dirichlet-Type (1st Kind) BC

$$C_k(\boldsymbol{x},t) = C_{kD}(t) \quad \text{on} \quad \Gamma_4 \times t[t_0,\infty) \tag{6.18}$$

where C_{kD} are prescribed values of concentration of species k on $\Gamma_4 \subset \Gamma$. Note that for steady-state mass transport problems Dirichlet-type BC's (6.18) are usually required, i.e., $\Gamma_4 \neq \emptyset$, unless Cauchy-type BC's occur.

6.3.2.2 × Neumann-Type (2nd Kind) BC

For 3D and 2D (vertical and axisymmetric):

$$\left.\begin{array}{ll} \text{convective form} & \\ q_{n_{kC}}(\boldsymbol{x},t) = \underbrace{-(\boldsymbol{D}_k \cdot \nabla C_k)\cdot \boldsymbol{n}}_{\text{dispersive flux}} & = q_{kC}(t) \\ \text{divergence form} & \\ q_{n_{kC}}(\boldsymbol{x},t) = \underbrace{C_k\, q_{n_h} - (\boldsymbol{D}_k \cdot \nabla C_k)\cdot \boldsymbol{n}}_{\text{total flux}} & = q^{\dagger}_{kC}(t) \end{array}\right\} \quad \text{on} \quad \Gamma_5 \times t[t_0,\infty) \tag{6.19}$$

and for 2D horizontal (confined and unconfined):

$$\left.\begin{array}{ll} \text{convective form} & \\ \bar{q}_{n_{kC}}(\boldsymbol{x},t) = \underbrace{-(\bar{\boldsymbol{D}}_k \cdot \nabla C_k)\cdot \boldsymbol{n}}_{\text{dispersive flux}} & = \bar{q}_{kC}(t) \\ \text{divergence form} & \\ \bar{q}_{n_{kC}}(\boldsymbol{x},t) = \underbrace{C_k\, \bar{q}_{n_h} - (\bar{\boldsymbol{D}}_k \cdot \nabla C_k)\cdot \boldsymbol{n}}_{\text{total flux}} & = \bar{q}^{\dagger}_{kC}(t) \end{array}\right\} \quad \text{on} \quad \Gamma_5 \times t[t_0,\infty) \tag{6.20}$$

where $q_{n_{kC}}$ and $\bar{q}_{n_{kC}}$ represent normal mass fluxes of species k (positive outward-directed) across the boundary Γ_5 and q_{kC}, $q^{\dagger}_{kC}$, $\bar{q}_{kC}$ and $\bar{q}^{\dagger}_{kC}$ are the prescribed Neumann mass fluxes of species k on $\Gamma_5 \subset \Gamma$. If $q_{kC} = 0$ and $\bar{q}_{kC} = 0$ the Neumann-type BC reduces to a *natural* (no-mass flux) BC associated with a zero concentration gradient $\nabla C_k = \mathbf{0}$ for the convective form of the mass transport equation, sometimes called as *Danckwerts condition* [111]. Alternatively, however, for the divergence form of the mass transport equation, if $q^{\dagger}_{kC} = 0$ and $\bar{q}^{\dagger}_{kC} = 0$ the Neumann-type BC reduces to a *natural* (no-mass flux) BC which forces the total (advective plus dispersive) mass flux to zero on Γ_5. Both variants of BC have their advantages. While the Neumann-type BC for the convective form is easier to implement and more flexible, their counterparts for the divergence form provide a stronger formulation in terms of mass convervation, however, possess difficulties at outflow boundaries on which the total mass flux is unknown (see Sect. 6.5.7).

The divergence form is capable of prescribing the total mass flux along a boundary portion resulting from the advective (convective) part $C_k\, q_{n_h}$ (load of concentration C_k in the liquid flow $q_{n_h} = \boldsymbol{q} \cdot \boldsymbol{n}$) and the dispersive part $-(\boldsymbol{D}_k \cdot \nabla C_k) \cdot \boldsymbol{n}$. However, regarding this formulation all boundaries have to be specified with such type of BC, which can cause a specific handling of such formulations in the case of unknown mass concentration C_k on outflow boundaries (rather, C_k is here to be solved). Such boundaries require a specific treatment. This is done by evaluating the liquid flux via a budget analysis in a postprocessing step of computation which is then involved in modifying the BC of the mass flux at such portions of boundaries, for more see discussion in Sect. 6.5.7.

On the other hand, the default convective form does not require a specific handling associated with formulations on outflow boundaries and is usually preferred. Assigning $q_{kC} = -(\boldsymbol{D}_k \cdot \nabla C_k) \cdot \boldsymbol{n} \approx 0$ as a natural BC, the mass flux freely passes through an advectively open boundary section and the concentration on the boundary automatically results. Note here, a boundary source of mass, as far as it should not be modeled via a 1st kind BC, in form of a mass boundary flux $q_{kC} \neq 0$ includes only the dispersive part, i.e., the magnitude of the flux will result from the gradient of concentration at the boundary. Thus in general, the convective form will necessarily produce a higher concentration gradient to realize the same mass load through a boundary.

However, there is a way to formulate mass flux BC providing an advective load of mass in form of Cauchy-type BC even for the convective form of mass transport. Indeed, we need not to resort to the divergence form in order to achieve suited mass load conditions on boundaries. It is easy to see that the Neumann-type BC for the divergence form, e.g., (6.19), is equivalent to Cauchy-type BC written as

$$
\begin{aligned}
-(\boldsymbol{D}_k \cdot \nabla C_k) \cdot \boldsymbol{n} &= q_{kC}^{\dagger} - C_k\, q_{n_h} \\
&= q_{n_h} (C_{kC} - C_k)
\end{aligned}
\tag{6.21}
$$

with known q_{n_h} and $q_{kC}^{\dagger} \approx q_{n_h} C_{kC}$ approximated as an input advective mass flux with prescribed boundary concentration C_{kC} for the convective form as further discussed in Sect. 6.3.2.3.

6.3.2.3 ⊗ Cauchy-Type and Robin-Type (3rd Kind) BC

For 3D and 2D (vertical and axisymmetric):

$$\left.\begin{array}{ll}\text{convective form} & \\ q_{n_{kC}}(\boldsymbol{x},t) = -(\boldsymbol{D}_k \cdot \nabla C_k)\cdot \boldsymbol{n} & = -\Phi_{kC}(C_{kC}-C_k) \\ \text{divergence form} & \\ q_{n_{kC}}(\boldsymbol{x},t) = C_k\, q_{n_h} - (\boldsymbol{D}_k \cdot \nabla C_k)\cdot \boldsymbol{n} & = -\Phi^{\dagger}_{kC}(C_{kC}-C_k)\end{array}\right\} \quad \text{on} \quad \Gamma_6 \times t[t_0,\infty) \tag{6.22}$$

and for 2D horizontal (confined and unconfined):

$$\left.\begin{array}{ll}\text{convective form} & \\ \bar{q}_{n_{kC}}(\boldsymbol{x},t) = -(\bar{\boldsymbol{D}}_k \cdot \nabla C_k)\cdot \boldsymbol{n} & = -\bar{\Phi}_{kC}(C_{kC}-C_k) \\ \text{divergence form} & \\ \bar{q}_{n_{kC}}(\boldsymbol{x},t) = C_k\, \bar{q}_{n_h} - (\bar{\boldsymbol{D}}_k \cdot \nabla C_k)\cdot \boldsymbol{n} & = -\bar{\Phi}^{\dagger}_{kC}(C_{kC}-C_k)\end{array}\right\} \quad \text{on} \quad \Gamma_6 \times t[t_0,\infty) \tag{6.23}$$

where C_{kC} are prescribed values of species k concentration on $\Gamma_6 \subset \Gamma$. The signs of $q_{n_{kC}}$ and $\bar{q}_{n_{kC}}$ are chosen that the boundary mass fluxes are positive outward-directed if $C_k > C_{kC}$. In (6.22) and (6.23) the *mass transfer coefficients* Φ_{kC}, $\bar{\Phi}_{kC}$, $\Phi^{\dagger}_{kC}$ and $\bar{\Phi}^{\dagger}_{kC}$ represent *dual* directional functions in form of:

$$\Phi_{kC} = \begin{cases} \Phi^{\text{in}}_{kC}(\boldsymbol{x},t) & \text{for} \quad C_{kC} > C_k \\ \Phi^{\text{out}}_{kC}(\boldsymbol{x},t) & \text{for} \quad C_{kC} \le C_k \end{cases} \tag{6.24}$$

$$\bar{\Phi}_{kC} = \begin{cases} \bar{\Phi}^{\text{in}}_{kC}(\boldsymbol{x},t) & \text{for} \quad C_{kC} > C_k \\ \bar{\Phi}^{\text{out}}_{kC}(\boldsymbol{x},t) & \text{for} \quad C_{kC} \le C_k \end{cases} \tag{6.25}$$

and similar for $\Phi^{\dagger}_{kC}$ and $\bar{\Phi}^{\dagger}_{kC}$, which are in general functions of space $\boldsymbol{x}$ and time t. Accordingly, in specifying two alternate (if necessary temporal) transfer coefficients different transfer conditions can be input to distinguish between inflow conditions ($q_{n_{kC}} < 0$) and outflow conditions ($q_{n_{kC}} > 0$). The special case, e.g., $\Phi_{kC} = \Phi^{\text{in}}_{kC} = \Phi^{\text{out}}_{kC}$ (and similar for $\bar{\Phi}_{kC}$, $\Phi^{\dagger}_{kC}$ and $\bar{\Phi}^{\dagger}_{kC}$) does not differ between inward and outward mass boundary flux.

As already discussed in Sect. 2.2.2 the 3rd kind BC of the convective forms of (6.22) and (6.23) can be identified as Cauchy-type BC, while the 3rd kind BC of the divergence form represents a Robin-type (mixed) BC, which is most general. It has been shown by (6.21) that Neumann-type BC of the divergence form is equivalent to Cauchy-type BC of the convective form if we simply set

$$\Phi_{kC} = -q_{n_h} \tag{6.26}$$

where $q_{n_h} = \boldsymbol{q} \cdot \boldsymbol{n}$ is a known (positive outward directed) flux of liquid on Γ_6. A typical application of such type of BC is a leaky deposit, from where a mass flux intrudes into an aquifer with a given (advective) rate as schematized in Fig. 6.5. It is assumed that the deposit having a known concentration C_{kC} leaks by a given *load* and intrudes into the domain Ω through Γ_6 via

$$q^{\text{load}}_{kC} = q^{\text{out}}_{h}\, C_{kC} \tag{6.27}$$

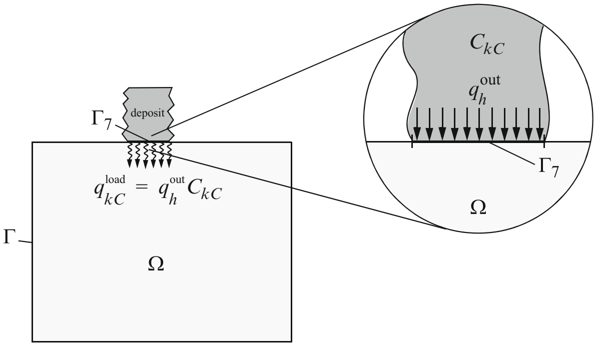

Fig. 6.5 Leak of a deposit: BC formulation of species mass load q_{kC}^{load} on $\Gamma_6 \subset \Gamma$

where q_{kC}^{load} is the load of species k on Γ_6 and q_h^{out} is the inward-directed flux of liquid leaving the deposit with concentration C_{kC}. Since $q_h^{out} = -q_{n_h}$ (negative due to the inward direction on Γ_6) we obtain with (6.26), i.e., $\Phi_{kC} = q_h^{out}$, the following Cauchy-type BC for the load of mass

$$q_{n_{kC}}(\boldsymbol{x}, t) = -(\boldsymbol{D}_k \cdot \nabla C_k) \cdot \boldsymbol{n} = -q_h^{out}(C_{kC} - C_k) \quad \text{on} \quad \Gamma_6 \times t[t_0, \infty) \tag{6.28}$$

applied to the convective form of mass transport.

The transfer coefficients, e.g., Φ_{kC}, associated with BC's of 3rd kind (6.22) can be regarded as *leaching* parameters which constrain the mass flux through the boundary. If $\Phi_{kC} = 0$ the boundary becomes impervious. On the other hand, using a very large value $\Phi_{kC} \to \infty$ the BC of 3rd kind is reduced to a Dirichlet-type (1st kind) BC with $C_k = C_{kC}$ on Γ_6. Such a leaching process is displayed in Fig. 6.6 for the example of a flow over a salt dome modeled with a diffusive input condition ($C_{kC} > C_k$). Considering a thickness d for the leaching body and applying the Fick's law (4.67) written in 1D in form of

$$q_{n_{kC}} \approx -D_{ko}^{in} \frac{\Delta C_k}{\Delta s} = -D_{ko}^{in} \frac{C_{kC} - C_k}{d} \tag{6.29}$$

the mass transfer coefficient Φ_{kC}^{in} can be assessed as

$$\Phi_{kC}^{in} = \frac{D_{ko}^{in}}{d} \tag{6.30}$$

and analogously to a horizontal problem as

$$\bar{\Phi}_{kC}^{in} = B\Phi_{kC}^{in} = B\frac{D_{ko}^{in}}{d} \tag{6.31}$$

Analogous assessments for Φ_{kC}^{out} and $\bar{\Phi}_{kC}^{out}$ result if the transition resistance differs between inflow (leaching) and outflow (releasing) conditions: $\Phi_{kC}^{in} \neq \Phi_{kC}^{out}$ ($\bar{\Phi}_{kC}^{in} \neq \bar{\Phi}_{kC}^{out}$).

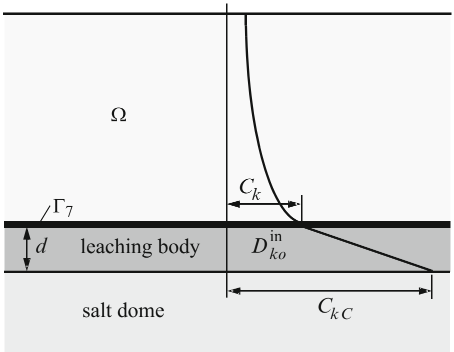

Fig. 6.6 Transfer coefficient Φ_{kC} $(= \Phi_{kC}^{\text{in}})$ as leaching parameter of a salt dome

6.3.2.4 ↱ Well-Type SPC

$$Q_{kw}(\boldsymbol{x}, t) = -\sum_{w=1}^{N_W} C_{kw} Q_w(t) \delta(\boldsymbol{x} - \boldsymbol{x}_w) \quad \text{on} \quad \boldsymbol{x}_w \in \Omega \times t[t_0, \infty) \tag{6.32}$$

and

$$\int_\Omega Q_{kw} d\Omega = -\sum_{w=1}^{N_W} C_{kw} Q_w(t) \tag{6.33}$$

where Q_{kw} is the specific kth-species mass sink/source function of wells, $Q_w(t)$ is the prescribed volume per unit time discharge (pumping rate) of single well w pumped with a known concentration of C_{kw} at location $\boldsymbol{x}_w$ and $\delta(\boldsymbol{x} - \boldsymbol{x}_w) = \prod_{i=1}^{D} \delta(x_i - x_{iw})$ is the Dirac delta function associated with location $\boldsymbol{x}_w$. The well function Q_{kw} is assigned to a point sink of mass for the divergence form of mass transport equation.

In contrast, the convective form of mass transport has to be related to a well-point sink function in the following form (cf. mass transport equations of Table 3.7):

$$\begin{aligned} Q_{kw}(\boldsymbol{x}, t) &= -\textstyle\sum_{w=1}^{N_W} C_{kw}(\boldsymbol{x}_w) Q_w(t) \delta(\boldsymbol{x} - \boldsymbol{x}_w) + C_k \textstyle\sum_{w=1}^{N_W} Q_w(t) \delta(\boldsymbol{x} - \boldsymbol{x}_w) \\ &= -\textstyle\sum_{w=1}^{N_W} Q_w(t) \delta(\boldsymbol{x} - \boldsymbol{x}_w) \big(C_{kw} - C_k(\boldsymbol{x}_w)\big) \end{aligned} \tag{6.34}$$

and

$$\int_\Omega Q_{kw} d\Omega = -\sum_{w=1}^{N_W} Q_w(t) \big(C_{kw} - C_k(\boldsymbol{x}_w)\big) \tag{6.35}$$

which reveals a similarity to a Cauchy-like, however, point-related mass transfer relation as described above. Note that the pumping rate Q_w is positive for a sink (pump) and negative for a source (recharge/injection) at well point $\boldsymbol{x}_w$. These types of SPC in form of (6.32) and (6.34) are usually applied to cases, where a mass flux given by a flow rate of $Q_w < 0$ and known concentration C_{kw} is injected through wells w.

6.3.3 Heat Transport BC

6.3.3.1 ○ Dirichlet-Type (1st Kind) BC

$$T(\boldsymbol{x}, t) = T_D(t) \quad \text{on} \quad \Gamma_7 \times t[t_0, \infty) \tag{6.36}$$

where T_D are prescribed values of temperature on $\Gamma_7 \subset \Gamma$. For steady-state heat transport problems Dirichlet-type BC's (6.36) are usually required, i.e., $\Gamma_7 \neq \emptyset$, unless Cauchy-type BC's occur.

6.3.3.2 × Neumann-Type (2nd Kind) BC

For 3D and 2D (vertical and axisymmetric):

$$\left.\begin{aligned} &\text{convective form} \\ &q_{n_T}(\boldsymbol{x}, t) = \underbrace{-(\boldsymbol{\Lambda} \cdot \nabla T) \cdot \boldsymbol{n}}_{\text{conductive flux}} = q_T(t) \\ &\text{divergence form} \\ &q_{n_T}(\boldsymbol{x}, t) = \underbrace{\rho c (T - T_0)\, q_{n_h} - (\boldsymbol{\Lambda} \cdot \nabla T) \cdot \boldsymbol{n}}_{\text{total flux}} = q_T^{\dagger}(t) \end{aligned}\right\} \quad \text{on} \quad \Gamma_8 \times t[t_0, \infty) \tag{6.37}$$

and for 2D horizontal (confined and unconfined):

$$\left.\begin{aligned} &\text{convective form} \\ &\bar{q}_{n_T}(\boldsymbol{x}, t) = \underbrace{-(\bar{\boldsymbol{\Lambda}} \cdot \nabla T) \cdot \boldsymbol{n}}_{\text{conductive flux}} = \bar{q}_T(t) \\ &\text{divergence form} \\ &\bar{q}_{n_T}(\boldsymbol{x}, t) = \underbrace{\rho c (T - T_0)\, \bar{q}_{n_h} - (\bar{\boldsymbol{\Lambda}} \cdot \nabla T) \cdot \boldsymbol{n}}_{\text{total flux}} = \bar{q}_T^{\dagger}(t) \end{aligned}\right\} \quad \text{on} \quad \Gamma_8 \times t[t_0, \infty) \tag{6.38}$$

where q_{n_T} and $\bar{q}_{n_T}$ represent normal heat fluxes (positive outward-directed) across the boundary Γ_8, T_0 is a reference temperature and q_T, $q_T^{\dagger}$, $\bar{q}_T$ and $\bar{q}_T^{\dagger}$ are the prescribed Neumann heat fluxes on $\varGamma_8 \subset \varGamma$. If $q_T = 0$ and $\bar{q}_T = 0$ the Neumann-type BC reduces to a *natural* (no-heat flux) *adiabatic BC* associated with a zero temperature gradient $\nabla T = \mathbf{0}$ for the convective form of the heat transport equation. Alternatively, however, for the divergence form of the heat transport equation, if $q_T^{\dagger} = 0$ and $\bar{q}_T^{\dagger} = 0$ the Neumann-type BC reduces to a *natural* (no-heat flux) BC which forces the total (advective plus conductive) heat flux to zero on $\varGamma_8$. The advantages of both variants of Neumann-type BC are already discussed in Sect. 6.3.2.2 in the context of mass transport. Similarly, the equivalence of the Neumann-type BC for the divergence form to the Cauchy-type BC for the convective form of the heat transport equation leads to the formulation of a heat load condition

$$\begin{aligned} -(\boldsymbol{\Lambda} \cdot \nabla T) \cdot \boldsymbol{n} &= q_T^{\dagger} - \rho c (T - T_0)\, q_{n_h} \\ &= \rho c q_{n_h} (T_C - T) \end{aligned} \tag{6.39}$$

with known $q_{n_h} = \boldsymbol{q} \cdot \boldsymbol{n}$ and $q_T^{\dagger} \approx \rho c q_{n_h} (T_C - T_0)$ approximated as an input advective heat flux with prescribed boundary temperature difference $T_C - T_0$ for the convective form as further discussed in Sect. 6.3.3.3.

6.3.3.3 ⊗ Cauchy-Type and Robin-Type (3rd Kind) BC

For 3D and 2D (vertical and axisymmetric):

$$\left.\begin{aligned} &\text{convective form} \\ &q_{n_T}(\boldsymbol{x}, t) = -(\boldsymbol{\Lambda} \cdot \nabla T) \cdot \boldsymbol{n} \qquad\qquad = -\Phi_T (T_C - T) \\ &\text{divergence form} \\ &q_{n_T}(\boldsymbol{x}, t) = \rho c (T - T_0)\, q_{n_h} - (\boldsymbol{\Lambda} \cdot \nabla T) \cdot \boldsymbol{n} = -\Phi_T^{\dagger} (T_C - T) \end{aligned}\right\} \quad \text{on} \quad \varGamma_9 \times t[t_0, \infty) \tag{6.40}$$

and for 2D horizontal (confined and unconfined):

$$\left.\begin{aligned} &\text{convective form} \\ &\bar{q}_{n_T}(\boldsymbol{x}, t) = -(\bar{\boldsymbol{\Lambda}} \cdot \nabla T) \cdot \boldsymbol{n} \qquad\qquad = -\bar{\Phi}_T (T_C - T) \\ &\text{divergence form} \\ &\bar{q}_{n_T}(\boldsymbol{x}, t) = \rho c (T - T_0)\, \bar{q}_{n_h} - (\bar{\boldsymbol{\Lambda}} \cdot \nabla T) \cdot \boldsymbol{n} = -\bar{\Phi}_T^{\dagger} (T_C - T) \end{aligned}\right\} \quad \text{on} \quad \varGamma_9 \times t[t_0, \infty) \tag{6.41}$$

where T_C are prescribed values of temperature on $\varGamma_9 \subset \varGamma$. The signs of q_{n_T} and $\bar{q}_{n_T}$ are chosen that the boundary heat fluxes are positive outward-directed if $T > T_C$. In (6.40) and (6.41) the *heat transfer coefficients* Φ_T, $\bar{\Phi}_T$, $\Phi_T^{\dagger}$ and $\bar{\Phi}_T^{\dagger}$ represent *dual* directional functions in form of:

$$\Phi_T = \begin{cases} \Phi_T^{\text{in}}(\boldsymbol{x}, t) & \text{for} \quad T_C > T \\ \Phi_T^{\text{out}}(\boldsymbol{x}, t) & \text{for} \quad T_C \leq T \end{cases} \tag{6.42}$$

$$\bar{\Phi}_T = \begin{cases} \bar{\Phi}_T^{\text{in}}(\boldsymbol{x}, t) & \text{for} \quad T_C > T \\ \bar{\Phi}_T^{\text{out}}(\boldsymbol{x}, t) & \text{for} \quad T_C \leq T \end{cases} \tag{6.43}$$

and similar for $\Phi_T^\dagger$ and $\bar{\Phi}_T^\dagger$, which are in general functions of space $\boldsymbol{x}$ and time t. Accordingly, in specifying two alternate (if necessary temporal) transfer coefficients different transfer conditions can be input to distinguish between inflow conditions ($q_{n_T} < 0$) and outflow conditions ($q_{n_T} > 0$). The special case, e.g., $\Phi_T = \Phi_T^{\text{in}} = \Phi_T^{\text{out}}$ (and similar for $\bar{\Phi}_T$, $\Phi_T^\dagger$ and $\bar{\Phi}_T^\dagger$) does not differ between inward and outward heat boundary flux.

The 3rd kind BC of the convective forms of (6.40) and (6.41) can be identified as Cauchy-type BC, while the 3rd kind BC of the divergence form represents a Robin-type (mixed) BC, which is most general (cf. Sect. 2.2.2). It has been shown by (6.39) that Neumann-type BC of the divergence form is equivalent to Cauchy-type BC of the convective form if we simply set $\Phi_T = -\rho c q_{n_h}$, where $q_{n_h} = \boldsymbol{q} \cdot \boldsymbol{n}$ is a known (positive outward directed) flux of liquid on Γ_9. This allows to prescribe (similar to the mass transport in Sect. 6.3.2.3) a heat load BC, viz.,

$$q_{n_T}(\boldsymbol{x}, t) = -(\boldsymbol{\Lambda} \cdot \nabla T) \cdot \boldsymbol{n} = -\rho c q_h^{\text{out}}(T_C - T) \quad \text{on} \quad \Gamma_9 \times t[t_0, \infty) \tag{6.44}$$

applied to the convective form of heat transport, where the heat load $q_T^{\text{load}} = q_h^{\text{out}} \rho c (T_C - T_0)$ on Γ_9 is forced by the inward-directed flux of liquid $q_h^{\text{out}} = -q_{n_h}$ entering with a boundary temperature T_C.

The heat transfer coefficients, e.g., Φ_T, associated with BC's of 3rd kind (6.40) represent *heat transition* parameters. If $\Phi_T = 0$ the boundary becomes adiabatic (insulated). On the other hand, using a very large value $\Phi_T \to \infty$ the BC of 3rd kind is reduced to a Dirichlet-type (1st kind) BC with $T = T_C$ on Γ_9. The heat transfer coefficients can be estimated analogously to the above transfer coefficients for mass flux of Sect. 6.3.2.3. Considering a thickness d for a heat transition layer and applying Fourier's law (4.76) for input condition ($T_C > T$) in form of:

$$q_{n_T} \approx -\Lambda_o^{\text{in}} \frac{\Delta T}{\Delta s} = -\Lambda_o^{\text{in}} \frac{T_C - T}{d} \tag{6.45}$$

the heat transfer coefficient Φ_T^{in} can be obtained as

$$\Phi_T^{\text{in}} = \frac{\Lambda_o^{\text{in}}}{d} \tag{6.46}$$

and similarly to a horizontal problem as

$$\bar{\Phi}_T^{\text{in}} = B \Phi_T^{\text{in}} = B \frac{\Lambda_o^{\text{in}}}{d} \tag{6.47}$$

where Λ_o^{in} represents the heat conduction coefficient of the transition layer. Analogous assessments for Φ_T^{out} and $\bar{\Phi}_T^{\text{out}}$ result if the heat transition resistance differs between inflow (leaching) and outflow (releasing) conditions: $\Phi_T^{\text{in}} \neq \Phi_T^{\text{out}}$ ($\bar{\Phi}_T^{\text{in}} \neq \bar{\Phi}_T^{\text{out}}$).

More general heat transfer coefficients and related thermal resistances of transition layers are described in Appendix E for single and composite plane wall and circular pipe wall configurations. It results in heat transfer coefficients exemplified in the form

$$\Phi_T = \frac{1}{S \sum_i R_i} \tag{6.48}$$

with the *specific thermal resistance* R_i of solid material i given as

$$R_i = \begin{cases} \dfrac{d_i}{S\, \Lambda_i^s} & \text{plane wall} \\ \dfrac{\ln(r_{i+1}/r_i)}{2\pi\ \Lambda_i^s} & \text{circular pipe wall} \end{cases} \tag{6.49}$$

where S is the specific exchange area and Λ_i^s is the thermal conductivity of solid material i. Note that for pipe wall geometry $S = 2\pi r$, where r is the radius of the boundary surface at Γ_9.

6.3.3.4 ↱ Well-Type SPC

$$Q_{Tw}(\boldsymbol{x}, t) = -\sum_{w=1}^{N_W} (T_w - T_0)\, \rho c\, Q_w(t) \delta(\boldsymbol{x} - \boldsymbol{x}_w) \quad \text{on} \quad \boldsymbol{x}_w \in \Omega \times t[t_0, \infty) \tag{6.50}$$

and

$$\int_\Omega Q_{Tw} d\Omega = -\sum_{w=1}^{N_W} (T_w - T_0)\, \rho c\, Q_w(t) \tag{6.51}$$

where Q_{Tw} is the specific heat sink/source function of wells, $Q_w(t)$ is the prescribed volume per unit time discharge (pumping rate) of single well w pumped with a known temperature of T_w at location $\boldsymbol{x}_w$, $\delta(\boldsymbol{x} - \boldsymbol{x}_w) = \prod_{i=1}^{D} \delta(x_i - x_{iw})$ is the Dirac delta function associated with location $\boldsymbol{x}_w$ and T_0 is the reference temperature. The well function Q_{Tw} is assigned to a point sink of heat for the divergence form of heat transport equation.

In contrast, the convective form of heat transport has to be related to a well-point sink function in the following form (cf. heat transport equations of Table 3.7):

$$\begin{aligned} Q_{Tw}(\boldsymbol{x},t) &= -\textstyle\sum_{w=1}^{N_W}\big(T_w(\boldsymbol{x}_w)-T_0\big)\rho c\, Q_w(t)\delta(\boldsymbol{x}-\boldsymbol{x}_w)+ \\ &\quad \rho c(T-T_0)\ \textstyle\sum_{w=1}^{N_W} Q_w(t)\delta(\boldsymbol{x}-\boldsymbol{x}_w) \\ &= -\textstyle\sum_{w=1}^{N_W}\rho c\, Q_w(t)\delta(\boldsymbol{x}-\boldsymbol{x}_w)\big(T_w-T(\boldsymbol{x}_w)\big) \end{aligned} \tag{6.52}$$

and

$$\int_\Omega Q_{Tw}\, d\Omega = -\sum_{w=1}^{N_W}\rho c\, Q_w(t)\big(T_w - T(\boldsymbol{x}_w)\big) \tag{6.53}$$

which reveals a similarity to a Cauchy-like, however, point-related heat transfer relation as described above. Note that the pumping rate Q_w is positive for a sink (pump) and negative for a source (recharge/injection) at well point $\boldsymbol{x}_w$. These types of SPC in form of (6.50) and (6.52) are usually applied to cases, where a heat flux given by a flow rate of $Q_w < 0$ and known temperature T_w is injected through wells w.

6.4 BC Constraints (BCC's) and SPC Constraints (SPCC's)

Constraints are limitations for all types of BC's and SPC's. They can be written for BC's in the following form:

$$\text{value of BC is valid } \textit{if} \begin{cases} < \text{Max bound(s) } \textit{else} \text{ replace BC by Max bound} \\ \text{and} \\ > \text{Min bound(s) } \textit{else} \text{ replace BC by Min bound} \end{cases} \tag{6.54}$$

They result from the requirement that BC should only be valid as long as minimum and maximum bounds are satisfied. If during a simulation run the conditions are violated, the constraints are to be assigned as new intermediate BC. The same procedure is applied to SPC's.

The formulation of constraints is commonly based on the formalism of *complementary conditions* for a type of BC and SPC. Accordingly, value-type (1st kind and 3rd kind) BC's (hydraulic head, species concentration or temperature) are constrained by maximum and minimum flux relations (liquid, mass and heat fluxes, respectively). On the other hand, flux-type (2nd kind) BC's and well-type SPC's are constrained by complementary limits of boundary values, i.e., the liquid flux is constrained by maximum-minimum hydraulic heads, the mass flux by minimum-maximum species concentrations and the heat flux by minimum-maximum temperatures. Following formulations are available for flow, mass and heat conditions.

6.4.1 Flow BCC and SPCC

$$
\begin{array}{llll}
\bigcirc & \text{1st kind} & h_D(t) & \textit{if} \begin{cases} \text{Max: } Q_{n_h} < Q_{n_h}^{\max_1}(t) \; \textit{else} \; Q_{n_h} = Q_{n_h}^{\max_1}(t) \\ \text{Min: } Q_{n_h} > Q_{n_h}^{\min_1}(t) \; \textit{else} \; Q_{n_h} = Q_{n_h}^{\min_1}(t) \end{cases} \\
\times & \text{2nd kind} & q_h(t) & \textit{if} \begin{cases} \text{Max: } h < h^{\max_2}(t) \quad \textit{else} \; h = h^{\max_2}(t) \\ \text{Min: } h > h^{\min_2}(t) \quad \textit{else} \; h = h^{\min_2}(t) \end{cases} \\
\otimes & \text{3rd kind} & h_C(t) & \textit{if} \begin{cases} \text{Max: } Q_{n_h} < Q_{n_h}^{\max_3}(t) \; \textit{else} \; Q_{n_h} = Q_{n_h}^{\max_3}(t) \\ \text{Min: } Q_{n_h} > Q_{n_h}^{\min_3}(t) \; \textit{else} \; Q_{n_h} = Q_{n_h}^{\min_3}(t) \end{cases} \\
\Rsh & \text{well type} & Q_{hw}(t) & \textit{if} \begin{cases} \text{Max: } h < h^{\max_4}(t) \quad \textit{else} \; h = h^{\max_4}(t) \\ \text{Min: } h > h^{\min_4}(t) \quad \textit{else} \; h = h^{\min_4}(t) \end{cases}
\end{array}
\tag{6.55}
$$

where

$$
Q_{n_h} = -\int q_{n_h} d\Gamma \tag{6.56}
$$

represents the integral boundary balance flux of liquid summed-up at discrete (nodal) points to which the corresponding boundary values are related. Note, due to compatibility reasons with SPC's the pointwise balance quantity is defined negative outward (because a positive SPC acts as a sink). The flux Q_{n_h} has to be computed in a balance analysis during the simulation (cf. Sect. 8.19.2). The minimum-maximum bounds $Q_{n_h}^{\min_1}$, $Q_{n_h}^{\max_1}$, $h^{\min_2}$, $h^{\max_2}$, $Q_{n_h}^{\min_3}$, $Q_{n_h}^{\max_3}$, $h^{\min_4}$ and $h^{\max_4}$ are optional input parameters and can be even time-dependent functions. Accordingly, it is possible to consider time-dependent variations in the existence and influence of boundary and constraint conditions. For instance, these temporary capabilities of constraints are very useful in modeling the temporarily varying occurrence of sealing or drainage activities over a restricted time period, or in simulating time-constrained BC's (e.g., 1st kind) which are associated with certain construction or remedial actions arising only at given times. Typical applications of constraint conditions formulated by (6.55) are shown in sketches of Fig. 6.7.

In the first example (Fig. 6.7a) a single well operation is constrained by minimum and maximum head conditions. A well-type SPC with a given recharging or extracting discharge Q_{hw} is applied. The computation results a hydraulic head h at the borehole. Only if the resulting head is between the bounds $h^{\min_4}$ and $h^{\max_4}$ the computation is accepted, otherwise if the head h is smaller than $h^{\min_4}$ the SPC is replaced by $h = h^{\min_4}$ at the point, which represents a (pointwise) Dirichlet-type BC, and the computation has to be repeated for the changed BC. Similarly, if the resulting head h is larger than $h^{\max_4}$ the SPC is replaced by the $h = h^{\max_4}$ Dirichlet-type BC at the point and the solution has to be restarted again.

The second example (Fig. 6.7b) is regarded to a flux-limited infiltration through a river bed. A 3rd kind BC with a hydraulic head h_C of the river is applied and constrained by a maximum flux $Q_{n_h}^{\max_3}$. If the groundwater table decreases below the

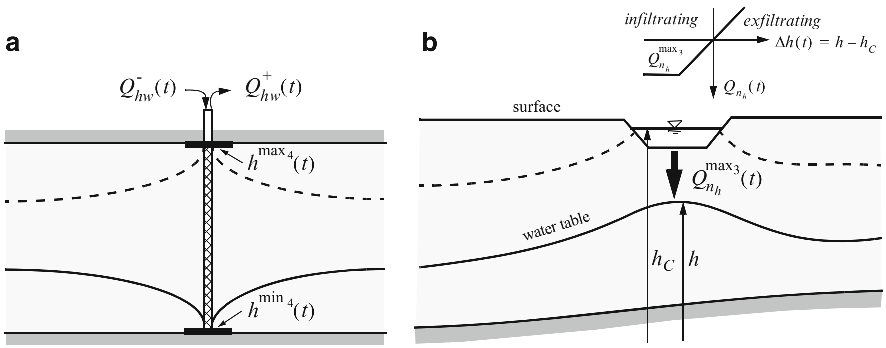

Fig. 6.7 Examples of using constraints for flow problems: (**a**) constraining a single well by an allowable drawdown in form of a minimum well head and by an allowable injection water level in form of a maximum well head, (**b**) flow separation in infiltration from surface water due to constraining the maximum seepage through the river bed

location of the river bed a specific situation in form of a 'flow separation' occurs. Physically, the zone between the river bed and the water table becomes unsaturated and the linear relationship of a flow transfer in form of (6.7) for the infiltrating water as a function of the difference $\Delta h = h - h_C$ between the groundwater head h and the reference (river) head h_C cannot be maintained anymore. It requires the prescription of the maximum bound $Q^{max_3}_{n_h}$. The formulation is termed as *flux-constrained transfer* BC. In this case the computation is started with the given 3rd kind BC. After the computation balance fluxes Q_{n_h} at the boundary are evaluated. If Q_{n_h} violates the maximum bound $Q^{max_3}_{n_h}$ (or the minimum bound $Q^{min_3}_{n_h}$) the computation has to be repeated with changed BC in form of $Q_{hw} = Q_{n_h} = Q^{max_3}_{n_h}$ (or $Q_{hw} = Q_{n_h} = Q^{min_3}_{n_h}$), which represent a well-type SPC.

Although flux-constrained transfer BC's are quite general formulations, their specification is sometimes cumbersome because the determination of the constraint fluxes requires geometric information of the boundaries (e.g., transfer areas). A more convenient and alternative formulation of constraints for 3rd kind BC's is in the form of the so-called *head-constrained transfer* BC as exemplified in Fig. 6.8 for a flux-limiting infiltration through a river bed. Instead of a direct input of constraint fluxes according to (6.55), maximum and minimum head values h^{max}_C and h^{min}_C, respectively, are prescribed, which are used to derive the constrained min-max fluxes for Cauchy-type BC's. It reads as follows:

$$\underline{\overline{\otimes}} \quad \text{3rd kind} \quad h_C(t) \quad \textit{if} \begin{cases} \text{Max:} \;\; h < h^{max}_C(t) \;\; \textit{else} \\ \qquad q_{n_h} = q^{min}_h = -\Phi_h(h_C - h^{max}_C) \;\; \textit{if} \; h_C \le h^{max}_C \\ \text{Min:} \;\; h > h^{min}_C(t) \;\; \textit{else} \\ \qquad q_{n_h} = q^{max}_h = -\Phi_h(h_C - h^{min}_C) \;\; \textit{if} \; h_C \ge h^{min}_C \end{cases} \tag{6.57}$$

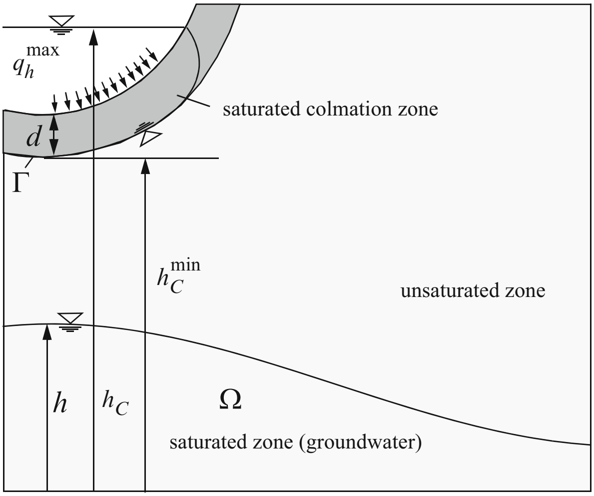

Fig. 6.8 Head-constrained transfer BC for a flux-limiting infiltration through a river bed

Note that the effects of the constraints in (6.55) and (6.57) are different. It is apparent that the minimum head bound h_C^{min} determines the maximum flux rate q_h^{max} and the maximum head bound h_C^{max} yields the minimum flux rate q_h^{min}.

The advantage of head-based constraint formulation is that the limiting (constraint) fluxes are rates and no more integral balance fluxes, which makes the computation more efficient. The transfer coefficient Φ_h in (6.57) can be determined from the layer parameters of the clogged river bed as discussed in Sect. 6.3.1.2. Time-dependent head-constraints are appropriate to prescribe intermediate flux conditions along a boundary (e.g., at certain times no flux conditions should occur as applied to temporarily moving BC's). Since $h_C = h_C(t)$ a temporal no flux condition is automatically satisfied if the reference head h_C becomes identical to the constrained head h_C^{min} (or h_C^{max}) in time. It means written for the minimum constraint

$$\begin{aligned} q_{n_h} &= q_h^{max} \equiv 0 \quad \text{for} \\ h_C(t) &= h_C^{min}(t) \quad \text{and} \quad h(t) < h_C^{min} \end{aligned} \tag{6.58}$$

To force a temporal no flux condition independent of the groundwater head $h = h(t)$, the maximum head constraint has to be set additionally to the reference head. It requires

$$\begin{aligned} q_{n_h} &= q_h^{max} \equiv 0 \quad \text{for} \\ h_C(t) &= h_C^{min}(t) = h_C^{max}(t) \quad \text{and arbitrary} \quad h(t) \end{aligned} \tag{6.59}$$

6.4.2 Mass Transport BCC and SPCC

$$
\begin{array}{llll}
\underline{\overline{\bigcirc}} & \text{1st kind} & C_{kD}(t) & \textit{if} \left\{
\begin{array}{l}
\text{Max:} \\
\left\{\begin{array}{c} Q_{n_{kC}} < Q_{n_{kC}}^{\max_1}(t) \\ \textit{and} \\ h^{\min_1} \le h \le h^{\max_1} \end{array}\right\} \textit{else} \left\{\begin{array}{c} Q_{n_{kC}} = Q_{n_{kC}}^{\max_1}(t) \\ \textit{as long as } h^{\min_1} \le h \le h^{\max_1}; \\ Q_{n_{kC}} = 0 \textit{ if } h < h^{\min_1} \textit{ or } h > h^{\max_1} \end{array}\right\} \\
\text{Min:} \\
\left\{\begin{array}{c} Q_{n_{kC}} > Q_{n_{kC}}^{\min_1}(t) \\ \textit{and} \\ h^{\min_1} \le h \le h^{\max_1} \end{array}\right\} \textit{else} \left\{\begin{array}{c} Q_{n_{kC}} = Q_{n_{kC}}^{\min_1}(t) \\ \textit{as long as } h^{\min_1} \le h \le h^{\max_1}; \\ Q_{n_{kC}} = 0 \textit{ if } h < h^{\min_1} \textit{ or } h > h^{\max_1} \end{array}\right\}
\end{array}\right. \\
\underline{\overline{\times}} & \text{2nd kind} & q_{kC}(t) & \textit{if} \left\{
\begin{array}{l}
\text{Max:} \\
\left\{\begin{array}{c} C_k < C_k^{\max_2}(t) \\ \textit{and} \\ h^{\min_2} \le h \le h^{\max_2} \end{array}\right\} \textit{else} \left\{\begin{array}{c} C_k = C_k^{\max_2}(t) \\ \textit{as long as } h^{\min_2} \le h \le h^{\max_2}; \\ Q_{n_{kC}} = 0 \textit{ if } h < h^{\min_2} \textit{ or } h > h^{\max_2} \end{array}\right\} \\
\text{Min:} \\
\left\{\begin{array}{c} C_k > C_k^{\min_2}(t) \\ \textit{and} \\ h^{\min_2} \le h \le h^{\max_2} \end{array}\right\} \textit{else} \left\{\begin{array}{c} C_k = C_k^{\min_2}(t) \\ \textit{as long as } h^{\min_2} \le h \le h^{\max_2}; \\ Q_{n_{kC}} = 0 \textit{ if } h < h^{\min_2} \textit{ or } h > h^{\max_2} \end{array}\right\}
\end{array}\right. \\
\underline{\overline{\otimes}} & \text{3rd kind} & C_{kC}(t) & \textit{if} \left\{
\begin{array}{l}
\text{Max:} \\
\left\{\begin{array}{c} Q_{n_{kC}} < Q_{n_{kC}}^{\max_3}(t) \\ \textit{and} \\ h^{\min_3} \le h \le h^{\max_3} \end{array}\right\} \textit{else} \left\{\begin{array}{c} Q_{n_{kC}} = Q_{n_{kC}}^{\max_3}(t) \\ \textit{as long as } h^{\min_3} \le h \le h^{\max_3}; \\ Q_{n_{kC}} = 0 \textit{ if } h < h^{\min_3} \textit{ or } h > h^{\max_3} \end{array}\right\} \\
\text{Min:} \\
\left\{\begin{array}{c} Q_{n_{kC}} > Q_{n_{kC}}^{\min_3}(t) \\ \textit{and} \\ h^{\min_3} \le h \le h^{\max_3} \end{array}\right\} \textit{else} \left\{\begin{array}{c} Q_{n_{kC}} = Q_{n_{kC}}^{\min_3}(t) \\ \textit{as long as } h^{\min_3} \le h \le h^{\max_3}; \\ Q_{n_{kC}} = 0 \textit{ if } h < h^{\min_3} \textit{ or } h > h^{\max_3} \end{array}\right\}
\end{array}\right. \\
\underline{\overline{\vdash}} & \text{well type} & Q_{kw}(t) & \textit{if} \left\{
\begin{array}{l}
\text{Max:} \\
\left\{\begin{array}{c} C_k < C_k^{\max_4}(t) \\ \textit{and} \\ h^{\min_4} \le h \le h^{\max_4} \end{array}\right\} \textit{else} \left\{\begin{array}{c} C_k = C_k^{\max_4}(t) \\ \textit{as long as } h^{\min_4} \le h \le h^{\max_4}; \\ Q_{n_{kC}} = 0 \textit{ if } h < h^{\min_4} \textit{ or } h > h^{\max_4} \end{array}\right\} \\
\text{Min:} \\
\left\{\begin{array}{c} C_k > C_k^{\min_4}(t) \\ \textit{and} \\ h^{\min_4} \le h \le h^{\max_4} \end{array}\right\} \textit{else} \left\{\begin{array}{c} C_k = C_k^{\min_4}(t) \\ \textit{as long as } h^{\min_4} \le h \le h^{\max_4}; \\ Q_{n_{kC}} = 0 \textit{ if } h < h^{\min_4} \textit{ or } h > h^{\max_4} \end{array}\right\}
\end{array}\right.
\end{array}
\tag{6.60}
$$

where

$$Q_{n_{kC}} = -\int q_{n_{kC}} \, d\Gamma \tag{6.61}$$

represents the integral boundary balance mass flux of species k summed-up at discrete (nodal) points to which the corresponding boundary values are related (cf. Sect. 8.19.2), $(\ldots)^{\max_i}$ and $(\ldots)^{\min_i}$ denote the prescribed maximum and minimum bounds, respectively, for the corresponding type of BC and SPC, and C_k and h in (6.60) are the concentration of species k and the hydraulic head, respectively, computed on the boundary or the singular point. The min-max bounds for the flux

$Q_{n_{kC}}$, the concentration C_k and the hydraulic head h can be again time-dependent functions allowing very comfortable rules for constraints.

Naturally, the specific balance mass flux $q_{n_{kC}}$ used in (6.61) is composed of the advective and dispersive parts according to

$$q_{n_{kC}} = \underbrace{C_k\, q_{n_h}}_{\text{advective}} - \underbrace{(\boldsymbol{D}_k \cdot \nabla C_k) \cdot \boldsymbol{n}}_{\text{dispersive}} \tag{6.62}$$

In practice, it has shown to be inappropriate to include the total (advective plus dispersive) flux into the procedure of controlling the constraint conditions (6.60) because the direction of the dispersive fluxes is ambiguous (e.g., the dispersive spreading also occurs against the advective flow direction). Accordingly, the balance-based evaluation of fluxes has to be exclusively related to the advective mass fluxes, viz.,

$$Q_{n_{kC}} = -\int q_{n_{kC}} d\Gamma \approx -\int (C_k\, q_{n_h}) d\Gamma \tag{6.63}$$

presenting unambiguously directional balance quantities.

The transport constraints (6.60) essentially consist of two parts for the individual types of BC's and SPC's:

1. A min-max bound complementary for the type of BC and SPC is imposed, i.e., a concentration boundary (1st or 3rd kind) is controlled by an allowable min-max boundary mass flux, and a mass flux boundary magnitude (2nd kind or well type) is controlled by an allowable min-max boundary concentration.
2. Optionally, a permitted range for BC and SPC within tolerable limits of hydraulic head h (ranging between $h^{\min_i}$ and $h^{\max_i}$) is imposed. If the simulated water table h lies outside this range, the BC's (all types, 1st to 3th kind) and SPC's are suppressed. This can easily be realized by assigning intermediately a zero flux $Q_{n_{kC}} = 0$, i.e., no mass flux then occurs and the BC's and SPC's are switched off.

Typical applications of mass transport constraints are outlined in Fig. 6.9. Figure 6.9a describes the case of a density-coupled saltwater intrusion problem (flow over a salt dome) having a boundary on which alternate boundary concentrations appear in dependence on the dynamic process: As long as water enters the domain it should have a prescribed concentration of freshwater. However, if the water releases the domain (along the same boundary) the concentration on the boundary is unknown and should be automatically computed. Such a description can be easily realized if the entire boundary section is assigned by a freshwater BC of 1st kind $C_k = C_{kD}$, and at the same time, the boundary will be imposed by a constraint condition in form of a null minimum mass flux $Q_{n_{kC}}^{\min_1} = 0$ (more constraints are not necessarily to be specified). Such an arrangement provides that the freshwater condition remains valid as long as the advective (convective) flux points into the

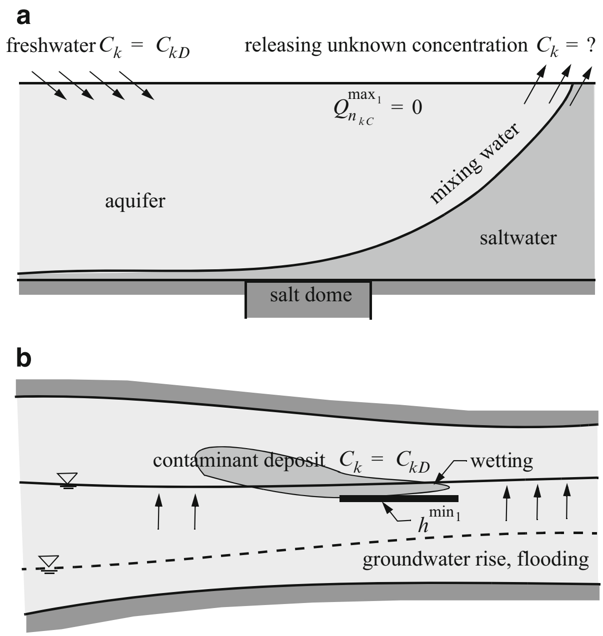

Fig. 6.9 Application of mass transport constraints: (**a**) Saltwater intrusion by flowing groundwater over a salt dome and (**b**) wetting and activating a contaminant deposit during a groundwater rise (flooding)

domain[1]:

$$Q_{n_{kC}} = -\int (C_k\, q_{n_h})\, d\Gamma \;>\; Q_{n_{kC}}^{\min_1} = 0 \quad \text{since } q_{n_h} < 0 \text{ for inflow} \tag{6.64}$$

The second example shown in Fig. 6.9b describes an application in modeling a contaminant spreading process from a deposit associated with rising groundwater in a phreatic aquifer (referred to as flooding problem). The contaminant BC (e.g., modeled as a 1st kind type) should be active only when the water table reaches the contaminant deposit (wetting case), i.e., a constraint in form of $h^{\min_1}$ is prescribed representing the bottom of the contaminant deposit. More constraints are not necessarily required in such a case.

[1]Note that a freshwater condition identical to zero ($C_{kD} = 0$) is inappropriate in the present balance-based computation to differ between inward and outward directed advective (convective) fluxes. It can fail because the directional magnitude of $Q_{n_{kC}}$ according to (6.64) is no more identifiable since $Q_{n_{kC}} = 0 \equiv Q_{n_{kC}}^{\min_1} = 0$! Accordingly, instead of zero it is recommended to use a numerically very small value for C_{kD}.

6.4.3 Heat Transport BCC and SPCC

$$
\begin{array}{lll}
\underline{\overline{\bigcirc}}\ \text{1st kind} & T_D(t) & \textit{if} \left\{\begin{array}{l}
\text{Max:}\\
\left\{\begin{array}{c} Q_{n_T} < Q_{n_T}^{\max_1}(t)\\ \textit{and}\\ h^{\min_1} \leq h \leq h^{\max_1}\end{array}\right\} \textit{else} \left\{\begin{array}{c} Q_{n_T} = Q_{n_T}^{\max_1}(t)\\ \textit{as long as } h^{\min_1} \leq h \leq h^{\max_1};\\ Q_{n_T} = 0 \textit{ if } h < h^{\min_1} \textit{ or } h > h^{\max_1}\end{array}\right\}\\
\text{Min:}\\
\left\{\begin{array}{c} Q_{n_T} > Q_{n_T}^{\min_1}(t)\\ \textit{and}\\ h^{\min_1} \leq h \leq h^{\max_1}\end{array}\right\} \textit{else} \left\{\begin{array}{c} Q_{n_T} = Q_{n_T}^{\min_1}(t)\\ \textit{as long as } h^{\min_1} \leq h \leq h^{\max_1};\\ Q_{n_T} = 0 \textit{ if } h < h^{\min_1} \textit{ or } h > h^{\max_1}\end{array}\right\}
\end{array}\right.\\
\underline{\overline{\times}}\ \text{2nd kind} & q_T(t) & \textit{if} \left\{\begin{array}{l}
\text{Max:}\\
\left\{\begin{array}{c} T < T^{\max_2}(t)\\ \textit{and}\\ h^{\min_2} \leq h \leq h^{\max_2}\end{array}\right\} \textit{else} \left\{\begin{array}{c} T = T^{\max_2}(t)\\ \textit{as long as } h^{\min_2} \leq h \leq h^{\max_2};\\ Q_{n_T} = 0 \textit{ if } h < h^{\min_2} \textit{ or } h > h^{\max_2}\end{array}\right\}\\
\text{Min:}\\
\left\{\begin{array}{c} T > T^{\min_2}(t)\\ \textit{and}\\ h^{\min_2} \leq h \leq h^{\max_2}\end{array}\right\} \textit{else} \left\{\begin{array}{c} T = T^{\min_2}(t)\\ \textit{as long as } h^{\min_2} \leq h \leq h^{\max_2};\\ Q_{n_T} = 0 \textit{ if } h < h^{\min_2} \textit{ or } h > h^{\max_2}\end{array}\right\}
\end{array}\right.\\
\underline{\overline{\otimes}}\ \text{3rd kind} & T_C(t) & \textit{if} \left\{\begin{array}{l}
\text{Max:}\\
\left\{\begin{array}{c} Q_{n_T} < Q_{n_T}^{\max_3}(t)\\ \textit{and}\\ h^{\min_3} \leq h \leq h^{\max_3}\end{array}\right\} \textit{else} \left\{\begin{array}{c} Q_{n_T} = Q_{n_T}^{\max_3}(t)\\ \textit{as long as } h^{\min_3} \leq h \leq h^{\max_3};\\ Q_{n_T} = 0 \textit{ if } h < h^{\min_3} \textit{ or } h > h^{\max_3}\end{array}\right\}\\
\text{Min:}\\
\left\{\begin{array}{c} Q_{n_T} > Q_{n_T}^{\min_3}(t)\\ \textit{and}\\ h^{\min_3} \leq h \leq h^{\max_3}\end{array}\right\} \textit{else} \left\{\begin{array}{c} Q_{n_T} = Q_{n_T}^{\min_3}(t)\\ \textit{as long as } h^{\min_3} \leq h \leq h^{\max_3};\\ Q_{n_T} = 0 \textit{ if } h < h^{\min_3} \textit{ or } h > h^{\max_3}\end{array}\right\}
\end{array}\right.\\
\underline{\overline{\vdash}}\ \text{well type} & Q_{Tw}(t) & \textit{if} \left\{\begin{array}{l}
\text{Max:}\\
\left\{\begin{array}{c} T < T^{\max_4}(t)\\ \textit{and}\\ h^{\min_4} \leq h \leq h^{\max_4}\end{array}\right\} \textit{else} \left\{\begin{array}{c} T = T^{\max_4}(t)\\ \textit{as long as } h^{\min_4} \leq h \leq h^{\max_4};\\ Q_{n_T} = 0 \textit{ if } h < h^{\min_4} \textit{ or } h > h^{\max_4}\end{array}\right\}\\
\text{Min:}\\
\left\{\begin{array}{c} T > T^{\min_4}(t)\\ \textit{and}\\ h^{\min_4} \leq h \leq h^{\max_4}\end{array}\right\} \textit{else} \left\{\begin{array}{c} T = T^{\min_4}(t)\\ \textit{as long as } h^{\min_4} \leq h \leq h^{\max_4};\\ Q_{n_T} = 0 \textit{ if } h < h^{\min_4} \textit{ or } h > h^{\max_4}\end{array}\right\}
\end{array}\right.
\end{array}
\tag{6.65}
$$

where

$$
Q_{n_T} = -\int q_{n_T}\, d\Gamma \tag{6.66}
$$

represents the integral boundary balance heat flux summed-up at discrete (nodal) points to which the corresponding boundary values are related (cf. Sect. 8.19.2), $(\ldots)^{\max_i}$ and $(\ldots)^{\min_i}$ denote the prescribed maximum and minimum bounds, respectively, for the corresponding type of BC and SPC, and T and h in (6.65) are the temperature and the hydraulic head, respectively, computed on the boundary or the singular point. The min-max bounds for the heat flux Q_{n_T}, the temperature T and the hydraulic head h can be again time-dependent functions.

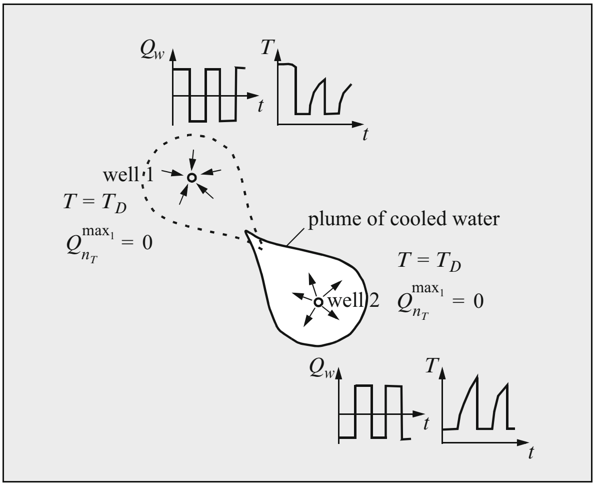

Fig. 6.10 Intermittent pumping regime of a well doublet system for heat extraction and re-injection (*horizontal view*)

Similar to the mass flux constraints in Sect. 6.4.2 the balance-based evaluation of heat fluxes must be exclusively related to the advective (convective) part

$$Q_{n_T} \approx -\int (T\, q_{n_h}) d\Gamma \tag{6.67}$$

to assure unambiguously directional balance quantities. An example of using BCC's and SPCC's for heat transport is schematized in Fig. 6.10 for a well doublet system under an intermittent pumping regime. The wells extract water from a heated aquifer in a time-given pumping operation $Q_w > 0$ for which the temperature at the wells has to be determined and re-inject cooled water with given temperature $T = T_D(t)$ as long as a recharging pumpage occurs $Q_w < 0$. Both wells comprise a temperature BC of 1st kind with $T = T_D(t)$ and a minimum heat flux constraint of zero $Q_{n_T}^{\min_1} = 0$.

6.5 Special BC's

6.5.1 Free (Phreatic) Surface BC

Free surface and phreatic surface are used as a synonym for porous-media problems describing the upper bound of a saturated zone (see Fig. 6.11 and definitions introduced in Sects. 2.2.1 and 2.2.2). A free (phreatic) surface is a moving boundary and subjected to two conditions: (1) a constant liquid pressure, usually taken to be $p = 0$ as the atmospheric pressure, and (2) a given mass conservation of flux across the macroscopic surface of discontinuity. The first pressure condition $p = \psi = 0$ is equivalent to $h = x_j$ expressed by the hydraulic head h, cf. (3.260), where x_j

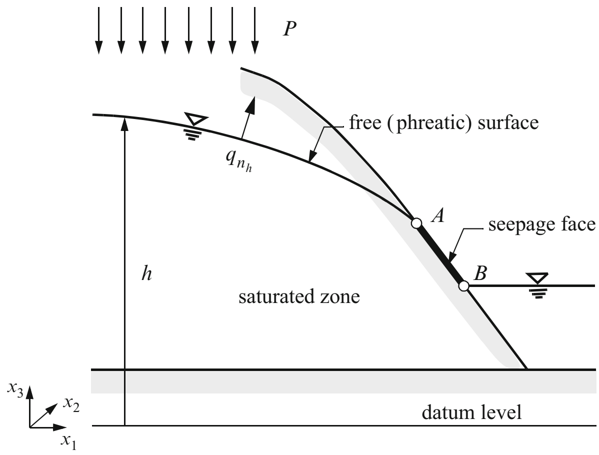

Fig. 6.11 Free (phreatic) surface and seepage face, $\widehat{AB}$

is the coordinate aligned to the gravity direction (e.g., vertical coordinate $x_3 = z$). The second condition is derived in Sect. 3.10.7 in form of (3.295). Both conditions finally lead to the following formulation of a free (phreatic) surface:

$$\left.\begin{aligned} q_{n_h} &= \varepsilon_e \frac{\partial h}{\partial t} - P \\ h &= x_j \end{aligned}\right\} \tag{6.68}$$

where ε_e is the specific yield (3.296) and P is the rate of infiltration (groundwater recharge). Note that for a pure (non-porous) liquid flow $\varepsilon_e = 1$. According to (6.68) the two BC's imposed on a free (phreatic) surface are to be satisfied simultaneously, viz.,

- A prescribed flux rate (as an infiltration or, if equal to zero, then impervious) as Neumann-type BC and
- The location corresponds to the hydraulic head, the water table (constant pressure level) as Dirichlet-type BC

which leads to a nonlinear boundary-value problem because the location (shape) of a free surface is initially unknown.

6.5.2 Seepage Face BC

It is possible that a free surface approaches a rigid boundary of known geometry on which the flow can freely drain out the saturated porous-medium domain. Such a boundary is called a *seepage face* as illustrated in Fig. 6.11 for the boundary segment $\widehat{AB}$. The shape of the seepage face is known, except for the location of its end point A, which represents the point, where the *a priori* unknown free surface is terminated. Accordingly, the extent of a seepage face is initially unknown and its solution also leads to a nonlinear task.

Since a seepage face is exposed to the atmosphere, the condition $p = 0$ or equivalently $h = x_j$ must be imposed. Additionally, a seepage face only allows drainage, i.e., through it the liquid seeps *out*. This can be enforced by applying a constraint condition, where it is required that the balanced flux Q_{n_h} (6.56) on the boundary is only directed outward, i.e., $Q_{n_h} < 0$ (note that a negative Q_{n_h} means outflow). Thus, a seepage face is formulated by the following two conditions:

$$\left.\begin{aligned} h &= x_j \\ Q_{n_h} &< Q_{n_h}^{\max_1} = 0 \end{aligned}\right\} \tag{6.69}$$

Mathematically, a seepage face corresponds to a Dirichlet-type BC with $h = h_D = x_j$ which is combined with a maximum flux constraint $Q_{n_h}^{\max_1}$ equal to zero according to (6.55).

Alternatively, instead of a Dirichlet-type BC allowing a free drainage through the boundary, the pressure condition of the seepage face can be prescribed by a Cauchy-type BC, which provides a *limited* drainage. It reads

$$\left.\begin{aligned} q_{n_h} &= -\Phi(x_j - h) \\ Q_{n_h} &< Q_{n_h}^{\max_1} = 0 \end{aligned}\right\} \tag{6.70}$$

where the transfer coefficient Φ mimics a flow 'resistance' to limit the outflow through the seepage face (e.g., at a dam covering).

6.5.3 Surface Ponding BC

Surface ponding denotes a 'surface reservoir' BC to describe the storage of liquid (water) at the ground surface as illustrated in Fig. 6.12. This occurs when the liquid's pressure at ground surface satisfies the condition $p > 0$ (or $h > x_j = h^{\min_2}$). Usually, ponding is only allowed up to a maximum head, i.e., $h < h^{\max_2}$, where $h^{\max_2}(t)$ is a given maximum limit. Furthermore, mass conservation at the ponding boundary has to be imposed. Thus, the following formulation at a surface ponding boundary is required:

$$\left.\begin{aligned} q_{n_h} &= \frac{\partial h}{\partial t} - P \\ h^{\min_2} = x_j &< h < h^{\max_2} \end{aligned}\right\} \tag{6.71}$$

which is easily performed by a Neumann-type BC combined with min-max head constraints according to (6.55). Note that the first condition of (6.71) represents the interfacial mass conservation (3.295) for which the specific yield ε_e becomes unity (assuming that ponding on the ground surface occurs in an 'air layer'). Condition (6.71) can be recognized a specific free surface condition (6.68) which permits liquid to store on top of the ground.

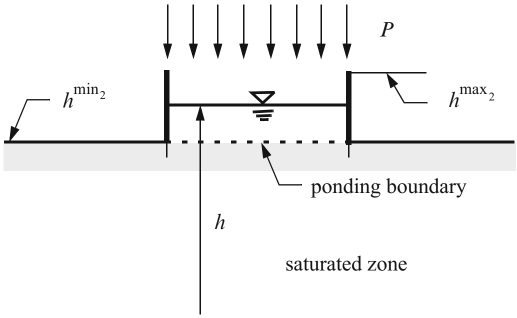

Fig. 6.12 Surface ponding boundary

6.5.4 Integral BC

With respect to BC's of 2nd and 3rd kind special BC's are available for problems with free (phreatic) surface(s). They are referred to as *integral BC's* and are defined as follows:

$\int\times$ *2nd kind integral BC (integral Neumann type):*

$$\left.\begin{array}{l}
\text{Flow:}\\
q_{n_h}(\boldsymbol{x},t) = \begin{cases} q_h(t) & \text{for 3D related to the initial stratigraphic structure} \\ \bar{q}_h(t) & \text{for 2D horizontal-unconfined as depth-integrated flux} \end{cases}\\
\text{Mass:}\\
q_{n_{kC}}(\boldsymbol{x},t) = \begin{cases} q_{kC}(t) & \text{for 3D related to the initial stratigraphic structure} \\ \bar{q}_{kC}(t) & \text{for 2D horizontal-unconfined as depth-integrated flux} \end{cases}\\
\text{Heat:}\\
q_{n_T}(\boldsymbol{x},t) = \begin{cases} q_T(t) & \text{for 3D related to the initial stratigraphic structure} \\ \bar{q}_T(t) & \text{for 2D horizontal-unconfined as depth-integrated flux} \end{cases}
\end{array}\right\} \tag{6.72}$$

$\int\otimes$ *3rd kind integral BC (integral Cauchy type):*

$$\left.\begin{array}{l}
\text{Flow:}\\
q_{n_h}(\boldsymbol{x},t) = \begin{cases} -\Phi_h(h_C - h) & \text{for 3D related to the initial stratigraphic structure} \\ -\bar{\Phi}_h(h_C - h) & \text{for 2D horizontal-unconfined as depth-integrated flux} \end{cases}\\
\text{Mass:}\\
q_{n_{kC}}(\boldsymbol{x},t) = \begin{cases} -\Phi_{kC}(C_{kC} - C_k) & \text{for 3D related to the initial stratigraphic structure} \\ -\bar{\Phi}_{kC}(C_{kC} - C_k) & \text{for 2D horizontal-unconfined as depth-integrated flux} \end{cases}\\
\text{Heat:}\\
q_{n_T}(\boldsymbol{x},t) = \begin{cases} -\Phi_T(T_C - T) & \text{for 3D related to the initial stratigraphic structure} \\ -\bar{\Phi}_T(T_C - T) & \text{for 2D horizontal-unconfined as depth-integrated flux} \end{cases}
\end{array}\right\} \tag{6.73}$$

Using these integral formulations of flux BC's it is ensured that a given flux rate on their boundary portions becomes independent of the actually discharging aquifer thickness and the location of free surface. This is unlike a default nonintegral BC where a flux rate is integrated along the effective aquifer thickness, which depends on the actual (computed) free-surface position, and accordingly, varying (gross-) discharges may occur through such boundaries. As a result, it may happen that the total discharge through such varying boundaries constantly decreases at a descending water table. Consequently, such a flow region can inevitably fall dry and possibly the problem can 'collapse' with a zero inflow. Integral BC's prevent such situations since the gross discharges are not influenced by the location of free surface. The relation of fluxes, however, is distinguished in 2D and 3D applications due to reasons of implementation:

1. For 2D problems the fluxes have to be assigned as already depth-integrated. The dimension of these fluxes is then L^2T^{-1}, similar to a horizontal confined condition.
2. For 3D problems the aquifer system is compiled as an initial stratigraphic layer structure. BC's of the integral type are related to this initial structure and accordingly, the integrated gross discharges remain independent of the free-surface location during the computation with the BASD technique (see Sect. 9.5.3). Notice, the dimension of these boundary fluxes is LT^{-1} (not L^2T^{-1}).

Integral boundary flux conditions have only a distinct meaning for problems with free (movable) surface(s). If no free surfaces exist, they are totally equivalent to the nonintegral BC's of 2nd and 3rd kind, in accordance with (6.6), (6.19), (6.20), (6.37), (6.38) and (6.7), (6.22), (6.23), (6.40), (6.41), respectively.

6.5.5 Gradient-Type BC

Applied to unsaturated problems a Neumann flux-type BC (6.6) in the form

$$-\left[k_r(s)\boldsymbol{K} f_\mu \cdot (\nabla h + \chi \boldsymbol{e})\right] \cdot \boldsymbol{n} = q_h \tag{6.74}$$

can be sometimes inappropriate, for instance if modeling a drainage boundary in the vadose zone with a bottom outflow BC for situations where the water table is located far below the domain of interest (Fig. 6.13). Here, a *gradient-type BC* is often to be preferred [362] written as

$$-\left\{\boldsymbol{K} f_\mu \cdot [\nabla\psi + (1+\chi)\boldsymbol{e}]\right\} \cdot \boldsymbol{n} = q_h^\nabla \tag{6.75}$$

On such a boundary it can be assumed that the pressure gradient diminishes $\nabla\psi \approx \mathbf{0}$ and (6.75) can be practically applied in the following form:

$$-\left\{\boldsymbol{K} f_\mu \cdot [(1+\chi)\boldsymbol{e}]\right\} \cdot \boldsymbol{n} = q_h^\nabla \tag{6.76}$$

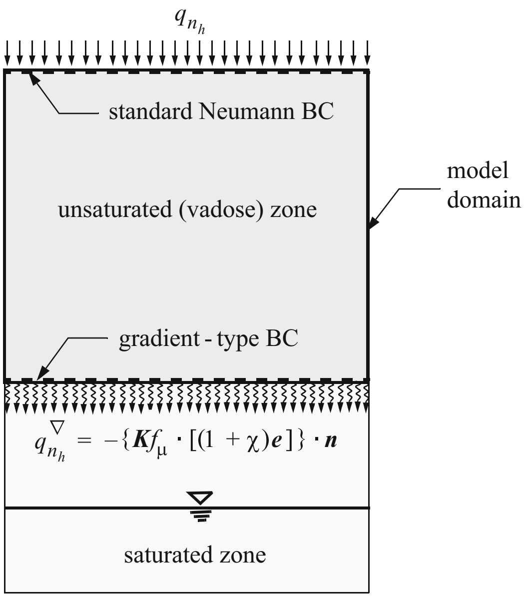

Fig. 6.13 Gradient-type BC for free bottom outflow from a vadose zone with deep water table

Once $(1 + \chi)\boldsymbol{e} \cdot \boldsymbol{n} \neq 0$ the boundary freely drains the flow domain due to the influence of gravity.

6.5.6 Multilayer Well BC

The prescription of well-type BC in 3D heterogeneous aquifers under confined or unconfined conditions requires a more general formulation to model the effects of well bore storage and the vertical gradients of variables (hydraulic head, concentrations, temperature) along the well bore and well screens in a more realistic way. The standard well-type SPC's in form of (6.15), (6.32) and (6.50) are only applicable to singular points in the domain. Those points are per se not linked among each other and could not suitably present a well bore and well screen, where a relatively uniform distribution of a priori unknown head (or concentration and temperature) results from the high conductivity of the conduit that transmits flow, species mass and energy between different locations. Conventionally, iterative procedures (e.g., [384]) are used to adapt a uniform distribution of variables (e.g., hydraulic head h) at a series of points forming a well or well screen when mimicked via standard well-type SPC's. But, this technique is cumbersome and rather inefficient.

In contrast, the present *multilayer well BC* is a noniterative, straightforward, efficient and accurate method for handling well bore conditions in 3D aquifer systems which can consist of different layers or heterogeneous formations. Even in a 3D homogeneous aquifer, where a partially penetrating pumping well has to be

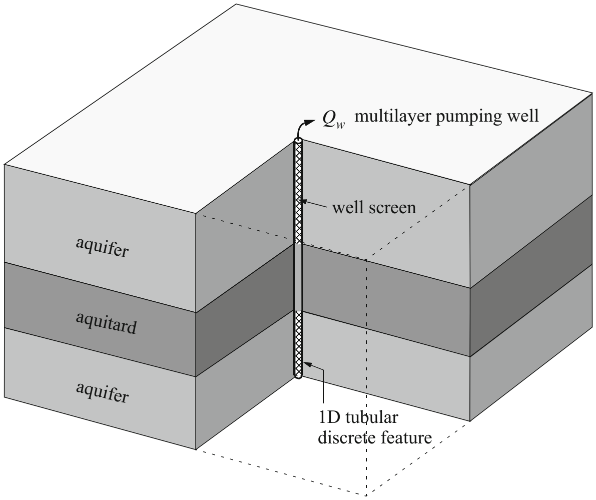

Fig. 6.14 Aquifer system containing a multilayer pumping well

imposed, the multilayer well BC is superior because the depth-variable inflow to the well is naturally accommodated.

The multilayer well BC involves a method, which superimposes high-conductivity 1D tubular discrete features (see Chap. 4) representing the well bore and well screens (Fig. 6.14). It was firstly introduced by Sudicky et al. [502] for aquifer flow problems and extended to contaminant transport by Lacombe et al. [328]. The use of high-conductivity 1D discrete features to represent a well ensures a uniform head (or concentration and temperature) along the well bore and well screens, with slight vertical gradients in the well toward the point where the well discharges. Storage in the well casing can also be accommodated by the superposition of the 1D discreate features. This effect can be significant at early times due to a rapid withdrawal of liquid from these features.

Assuming that the flow in the well along its axis is laminar and that the effect of storage in the well casing can be uniformly distributed along the length of the well bore, the 1D discrete feature equation describing transient liquid flow along the axis of the well bore is given according to Table 4.5, case TP, pure liquid:

$$\pi R^2\Big(\frac{1}{L_w} + \rho_0 g \gamma\Big)\frac{\partial h}{\partial t} - \pi R^2 K_w \frac{\partial}{\partial s}\Big[f_\mu\Big(\frac{\partial h}{\partial s} + \chi \boldsymbol{e}\Big)\Big] = -Q_w \delta(s - s_w) \qquad (6.77)$$

in which

$$K_w = \frac{R^2 \rho_0 g}{8\mu_0} \qquad (6.78)$$

by using the Hagen-Poiseuille law (4.51), where Q_w is the total pumping rate of the well, s is the arc length along the well bore (for vertical boreholes s is identical to vertical coordinate $x_3 = z$), s_w is the location of the point that is assigned to discharge (or recharge) the well bore, h is the hydraulic head in the well, L_w is the total length of the liquid-filled well bore, R is the radius of the well casing and screen(s), assuming to be equal, $\delta()$ is the Dirac delta function in 1D, γ is the compressibility of liquid, f_μ is the viscosity relation function of liquid (3.264), χ is the buoyancy coefficient (3.265), $\boldsymbol{e}$ is gravitational unit vector (3.261), g is the gravitational acceleration, ρ_0 is the reference density of liquid and μ_0 is the reference viscosity of liquid. Equation (6.77) is written for a well in which the casing is open (unconfined) to the atmosphere so that the storage in the well occurs due to a change in the water table and effects by compressibility of liquid.

Analogously, based on the derivations done in Chap. 4 and summarized in Tables 4.6 and 4.7, 1D discrete feature equations of the well bore can be formulated for species mass transport (Table 4.6, case TP, pure liquid)

$$\pi R^2 \frac{\partial C_k}{\partial t} + \pi R^2 v \frac{\partial C_k}{\partial s} - \pi R^2 \frac{\partial}{\partial s}\Big[\big(D_k + D_{(k)\mathrm{mech}}\big)\frac{\partial C_k}{\partial s}\Big] + \pi R^2 \vartheta_k C_k = -(C_{kw} - C_k) Q_w \delta(s - s_w) \tag{6.79}$$

using Taylor's relation (4.69) of mechanical dispersion in a liquid-filled tube under laminar conditions as

$$D_{(k)\mathrm{mech}} = \frac{R^2 v^2}{48 D_k} \tag{6.80}$$

where C_k is the concentration of species k in the well, v is the velocity of liquid in the well bore, D_k is the free-solution diffusion coefficient of species k, ϑ_k is the decay rate of species k and C_{kw} is the prescribed concentration of species k at well point s_w,

and for heat transport (Table 4.7, case TP, pure liquid)

$$\pi R^2 \rho c \frac{\partial T}{\partial t} + \pi R^2 \rho c v \frac{\partial T}{\partial s} - \pi R^2 \frac{\partial}{\partial s}\Big[\big(\Lambda + \rho c D_{\mathrm{mech}}\big)\frac{\partial T}{\partial s}\Big] = -(T_w - T)\rho c Q_w \delta(s - s_w) \tag{6.81}$$

using solute-analogous Taylor's relation (4.69) for thermal mechanical dispersion in a liquid-filled tube under laminar conditions according to

$$D_{\mathrm{mech}} = \frac{R^2 v^2 \rho c}{48 \Lambda} \tag{6.82}$$

where T is the temperature in the well, ρ is the density of liquid, c is the specific heat capacity of liquid, Λ is the coefficient of thermal conductivity of liquid and T_w is the prescribed temperature at well point s_w.

The governing equations (6.77), (6.79) and (6.81) for flow, species mass transport and heat transport, respectively, are formulated for a liquid-filled well bore tube. However, in cases, where the borehole is filled (or partially filled) with aquifer sediments (e.g., abandoned borehole), the well bore equations could be applied to porous-medium flow and transport conditions, which can be taken from Tables 4.5–4.7. Then, the K_w of (6.78) has to be replaced by Darcy's hydraulic conductivity and D_{mech} of (6.80) and (6.82) by the Scheidegger-Bear dispersion relation (4.68). More complex situations occur in heat transport for borehole heat exchanger (BHE), where different individual pipes and grout components are placed into a cylindrical borehole. The concept of multilayer BC must then be extended as further described in Sect. 13.5.

6.5.7 Outflow BC (OBC)

Often in mass and heat transport the liquid flows *through* (i.e., both into and out of) the computational domain Ω and advects transport quantities (concentration C_k, temperature T). This situation is necessitated by the fact that the true physical domain of interest is much too large to even be considered in a numerical simulation. Particularly, we have to consider outflow conditions in which the computational domain is *truncated* and suited BC's have to be necessarily applied at these 'artifical boundaries' of the truncated domain.

An outflow boundary of a truncated domain is often delicate to handle because the advective (convective) and dispersive quantities cannot be specified *a priori*. The goal of an outflow BC (OBC) is then to allow the transport quantities to leave freely with a minimal influence on the upstream solution. In practice, outflow boundaries are often subject to the assumption that the gradient of the transport quantity is zero (i.e., a common natural BC of Neumann type with $\nabla C_k = \mathbf{0}$ and/or $\nabla T = \mathbf{0}$), viz.,

$$\begin{aligned} -(\boldsymbol{D}_k \cdot \nabla C_k) \cdot \boldsymbol{n} &= 0 \\ -(\boldsymbol{\Lambda} \cdot \nabla T) \cdot \boldsymbol{n} &= 0 \end{aligned} \tag{6.83}$$

with the consequence that the boundary is impermeable to the normal diffusive (dispersive/conductive) fluxes. The question arises how such a common natural BC does influence the solution upstream on the effluent boundary. To enlighten the situation let us consider a domain, which becomes truncated by a transition zone of infinitesimal thickness $\delta \to 0$ representing an outflow boundary Γ_+ as shown in Fig. 6.15 for heat transport. Providing the OBC in form of the transition zone has no conserved property, heat balance requires that the temperature T varies continuously and should not be changed by the presence of the boundary compared to the untruncated domain. Apparently, the boundary permeable to both the advective (convective) part $\rho c T \boldsymbol{q}$ and the conductive (dispersive) part $-\boldsymbol{\Lambda} \cdot \nabla T$ of the total heat flux $\boldsymbol{j}_T^\dagger$ permits upgradient heat movement by conduction. However, if the temperature gradient at the boundary is forced to zero, the conductive component of the heat flux is dropped at the boundary and the temperature profile differs over a certain distance upstream from the boundary as evidenced in Fig. 6.15. The

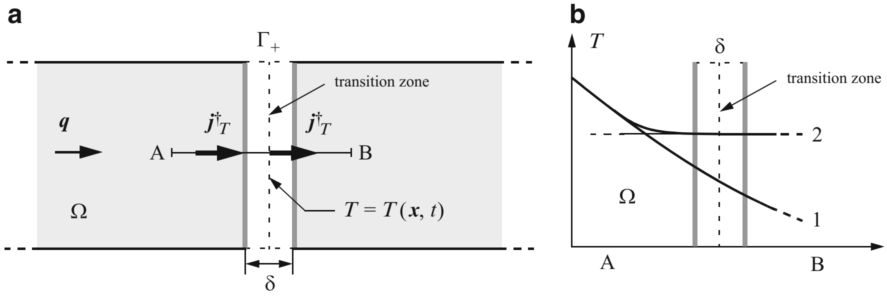

Fig. 6.15 Finite transition zone representation of outflow boundary $\varGamma_+$ of domain $\varOmega$: (**a**) continuity of total heat flux $\boldsymbol{j}_T^\dagger = \rho c T \boldsymbol{q} - \boldsymbol{\varLambda} \cdot \nabla T$ within the transition zone of infinitesimal thickness δ, where inside the temperature $T = T(\boldsymbol{x}, t)$ may vary continuously, (**b**) profile showing the behavior of temperature T when it varies continuously (1) and when temperature gradient is forced to zero (2) (Modified from [103])

measure of this upstreaming alteration in the temperature profile is controlled by the ratio between advection (convection) and conduction (dispersion). If advection dominates this alteration effect is usually small. On the other hand, if heat transport is dominated by thermal conduction, which possesses upstream conduction at the outflow boundary to a greater extent, a zero-gradient condition could not be a good choice. The situation can be mitigated if we can choose a more appropriate location of the outflow boundary far enough, where the gradients are small or negligible during the simulation. Moreover, there are applications, where the zero-gradient condition is useful. For instance, the outlet into a big reservoir, where the temperature is perfectly mixed out.

We have to ask what is a better OBC than the common natural BC of Neumann type in form of (6.83). Alternative formulations have been analyzed by Gresho and Sani [209] in a numerical context. A promising OBC treatment is proposed by Frind [175] and Cornaton et al. [103] termed as *free exit BC* and *implicit Neumann condition*, respectively. It consists in the following: Instead of explicitly prescribing the Neumann-type BC's for mass and heat transport written in the convective form

$$\begin{aligned} q_{n_{kC}} &= -(\boldsymbol{D}_k \cdot \nabla C_k) \cdot \boldsymbol{n} \\ q_{nT} &= -(\boldsymbol{\varLambda} \cdot \nabla T) \cdot \boldsymbol{n} \end{aligned} \tag{6.84}$$

and in the divergence form

$$\begin{aligned} q_{n_{kC}} &= C_k q_{nh} - (\boldsymbol{D}_k \cdot \nabla C_k) \cdot \boldsymbol{n} \\ q_{nT} &= \rho c (T - T_0) q_{nh} - (\boldsymbol{\varLambda} \cdot \nabla T) \cdot \boldsymbol{n} \end{aligned} \tag{6.85}$$

the boundary terms of (6.84) and (6.85) are treated as unknown quantities and put back onto the LHS for the numerical solution. In this way, no assumptions must be made anymore for the gradients of the concentration or temperature. This form of OBC ensures that mass and heat fluxes become freely permeable at the boundary both to the advective (convective) and dispersive (conductive) components of transport. For the divergence forms of transport the OBC needs the knowledge of the advective flux $q_{nh} = \boldsymbol{q} \cdot \boldsymbol{n}$ at the outflow boundary. In general, q_{nh} is a prior unknown and must be determined from the flow equation via a postprocessing balance analysis. The numerical treatment of OBC's is described in Sects. 8.5.3 and 8.9.