Chapter 7

Appendices

7.1 Boundary conditions

7.1.1 Flow equation

This is the generic flow equation solved by TRANSIN:

\[ \frac{\partial \theta}{\partial h} \frac{\partial h}{\partial t} = \nabla (K \nabla h) + q \]  

(7.1)

where:

- \( h \) [L] piezometric head \( (h = p/\gamma + z = \psi + z) \)
- \( p \) [F/L^2] water pressure
- \( \gamma \) [F/L^3] specific weight
- \( \psi \) [L] pressure head
- \( z \) [L] vertical position from a reference level
- \( K \) hydraulic conductivity tensor
- \( q \) [T^{-1}, L/T, L^2/T] instantaneous recharge per element size (length for 1-D elements, area for 2-D elements and volume for 3-D elements)
- \( \theta \) volumetric water content

\[ \theta = \phi S_w f \]  

(7.2)

where:

- \( \phi \) porosity
- \( S_w \) saturation degree
- \( f \) factor that depends upon the dimensionality and type of the problem. In our case, a 2-D confined problem, the factor \( f \) will be the saturated thickness of the aquifer.
Prescribed head

Prescribed head is a Dirichlet boundary condition since we are setting a fixed head and this is the main variable of the differential equation.

$$h = h_{ext} \quad (7.3)$$

Prescribed flow

Prescribed flow is a Neumann boundary condition since we are setting a fixed flow and this is the derivative of the main variable of the differential equation.

Leakage condition

Leakage condition is a Robin boundary condition since we are establishing a relation between the flow and the head. It is a linear combination of the Dirichlet and Neumann conditions.

$$Q = A.K.\frac{\Delta h}{L}; \quad Q = \frac{A.K}{L}(h - H_{ext}); \quad Q = \alpha(h - H_{ext}); \quad \alpha = \frac{A.K}{L} \quad (7.4)$$

7.1.2 Solute transport equation

The generic solute transport equation including saturated or unsaturated flow state, diffusion processes, dispersion, advection, first order reactions, retardation and matrix diffusion may be written as:

$$\theta R \frac{\partial c}{\partial t} = \nabla(D \nabla c) - q \nabla c + q_r(c - c') - \theta \lambda R c - \sigma_m \phi_m D_m \frac{\partial c_m}{\partial z} \quad (7.5)$$

where:

- $\theta$ volumetric water content
- $\phi$ aquifer’s porosity
- $c[M/L^3]$ solute concentration
- $t$ time
- $q[L/T]$ Darcy’s flow
- $c'$ external solute concentration
- $\lambda[T^{-1}]$ first order reactions parameter
- $\phi_m$ matrix porosity
- $D_m[L^2/T]$ matrix molecular diffusion
- $\sigma_m[L^{-1}]$ matrix specific surface
- $R$ retardation coefficient due to adsorption phenomena

Note: All the equivalencies between the heat and solute transport equations have been explained in the 3rd chapter of this work.
7.2. Dimensionless parameters

7.1.3 Prescribed temperature

Prescribed temperature is a Dirichlet boundary condition since we are setting a fixed temperature and this is the main variable of the differential equation.

7.1.4 Heat flow

The heat flow is a boundary condition that tries to quantify the energy flux through a contour. Depending on the sign of the energy flux (whether it enters the system or it rather leaves it), this will be either a Robin condition or a Neumann condition.

When the energy enters the system, it has an external temperature prescribed:

\[ F_E = q \rho w c_w T - (\lambda + \rho w c_w \alpha q) \nabla T = q \rho w c_w T_{ext} \iff -D_T \nabla T = q \rho c_w (T_{ext} - T) \]  

(7.6)

where:

\[ D_T = \lambda + \rho w c_w \alpha q \]

Then, as it can be seen above, this will turn out to be a Robin boundary condition since the variable \( T \) and its derivative are taking part in the condition.

Otherwise, when the energy leaves the system, the energy flux is quantified with the actual temperature of the system:

\[ F_E = q \rho w c_w T - (\lambda + \rho w c_w \alpha q) \nabla T = q \rho w c_w T \iff \nabla T = 0 \]  

(7.7)

This is a condition on the derivative of the temperature thus, this will be a Neumann boundary condition.

7.2 Dimensionless parameters

First of all, we will consider heat transport equation:

\[ \rho' c' \frac{\partial T}{\partial t} = \nabla ((\alpha \rho w c_w q + \lambda) \nabla T) - \rho w c_w q \nabla T \]  

(7.8)

From now on, dispersion will be neglected since as it has been seen in this thesis, it is not a relevant heat transport process for small scales.

\[ \rho' c' \frac{\partial T}{\partial t} = \lambda \nabla^2 T - \rho w c_w q \nabla T \]  

(7.9)

Some dimensionless parameter are defined below so as to proceed:[7]

\[ T_D = \frac{T}{T_c} \quad t_D = \frac{t}{t_c} \quad \nabla_D = L \nabla \quad \nabla_D^2 = L^2 \nabla^2 \]  

(7.10)

where subindex D denotes dimensionless parameter and the subindex c denotes characteristic parameter. Then, replacing each parameter by its dimensionless equivalent we get:
\[ \rho' c' \frac{\partial T_D T_c}{\partial t_D} \frac{\partial T_D}{\partial t} = \left[ \lambda \frac{\nabla^2}{L^2} T_D T_c \right] - \rho_w c_w q \frac{\nabla_D T_D}{L} T_c \] (7.11)

Dividing each term of the equation by \( T_c \):

\[ \frac{\rho' c' T_D}{T_c} \frac{\partial T_D}{\partial t_D} = \left[ \lambda \frac{\nabla^2}{L^2} T_D \right] - \rho_w c_w q \frac{\nabla_D T_D}{L} \] (7.12)

Now, multiplying all the equation by \( L^2 \) we obtain:

\[ \frac{\rho' c' L^2}{T_c} \frac{\partial T_D}{\partial t_D} = \left[ \lambda \nabla^2 T_D \right] - \rho_w c_w q L \nabla_D T_D \] (7.13)

**Diffusive-conductive term** On the one hand, we can divide all the equation by \( \lambda \) in order to obtain a dimensionless diffusive-conductive term:

\[ \frac{\rho' c' L^2}{\lambda T_c} \frac{\partial T_D}{\partial t_D} = \left[ \nabla^2 T_D \right] - \rho_w c_w q L \frac{\nabla_D T_D}{\lambda} \] (7.14)

The coefficient that accompanies the temporal term is the so-called Fourier number for the heat transport problem.

\[ N_{FO} = \frac{\rho' c' L^2}{\lambda t_c} \] (7.15)

Taking into consideration that this is a dimensionless parameter, we can obtain a characteristic diffusive-conductive time:

\[ t_{dif}^* = \left( \frac{\rho' c'}{\lambda} L^2 \right) \rightarrow N_{FO} = \frac{t_{dif}^*}{t_c} \] (7.16)

Thus, if the time discretization of the problem \( t_c \leq t_{dif} \), the problem will be transient \( (N_{FO} << 1) \). On the other hand, the thermal problem will be in steady state if \( t_c \geq t_{dif} \) \( (N_{FO} >> 1) \).

**Advective term** Instead of analyzing the characteristic diffusive-conductive term, we can do the same with the advective term:

\[ \frac{\rho' c' L}{\rho_w c_w q t_c} \frac{\partial T_D}{\partial t_D} = \frac{\lambda}{\rho_w c_w q L} (\nabla^2_D T_D) - \nabla_D T_D \] (7.17)

The coefficient that accompanies the temporal variation of the temperature is:

\[ \frac{\rho' c' L}{q \rho_w c_w t_c} \] (7.18)

where we can deduce a characteristic advective time:

\[ T_{adv}^* = \frac{\rho' c' L}{q \rho_w c_w} \] (7.19)

In order to check whether the problem is in transient or steady state is equivalent to the one made for the Fourier number.
7.3 Numerical Stability

Now, if we divide the characteristic diffusive-conductive term and the characteristic advective term, we get the Peclet number for the heat transport problem:

\[ N_{PE} = \frac{t_{dif}^*}{t_{adev}^*} = \frac{\rho_w c_w q L}{\lambda} \quad (7.20) \]

This is an important number because it expresses the relative importance of heat transport by means of advection in comparison with conduction. So, high \( N_{PE} \) numbers indicate that the main heat transport process is advection.

7.3 Numerical stability

As it has been stated in the former section, the Peclet number establishes a relation between the conductive and the advective transport \[ \text{ If we assume the characteristic length of the media (L) to be the dimension of the domain discretization, we get the Peclet number of the mesh:} \]

\[ N_{PE} = \frac{\rho_w c_w q \Delta X}{\lambda} \quad (7.21) \]

Then, the Peclet number may be controlled by means of the element size of the mesh.

Furthermore, the Courant number establishes a relation between the advective transport and a characteristic length. As it was done before, this characteristic length (L) is taken as the spatial discretization. Consequently, the Courant number may be understood as the number of mesh elements counted in one time step.

\[ N_{CO} = \frac{\rho_w c_w q \Delta t}{\rho_c \ell c \Delta X} \quad (7.22) \]

Then, so as to guarantee numerical stability of the model, two conditions must be satisfied:

\[ N_{PE} = \frac{\rho_w c_w q \Delta X}{\lambda} < 2 \Leftrightarrow \Delta X < \frac{2 \lambda}{\rho_w c_w q} \]
\[ N_{CO} = \frac{\rho_w c_w q \Delta t}{\rho_c \ell c \Delta X} < 1 \Leftrightarrow \Delta t < \frac{\rho_c \ell c \Delta X}{\rho_w c_w q} \quad (7.23) \]

In general, the Courant condition is easy to be accomplished reducing the time step. However, the Peclet condition is harder to be guaranteed. The mesh dimension cannot be drastically reduced because the number of nodes increases and so it does the CPU cost.