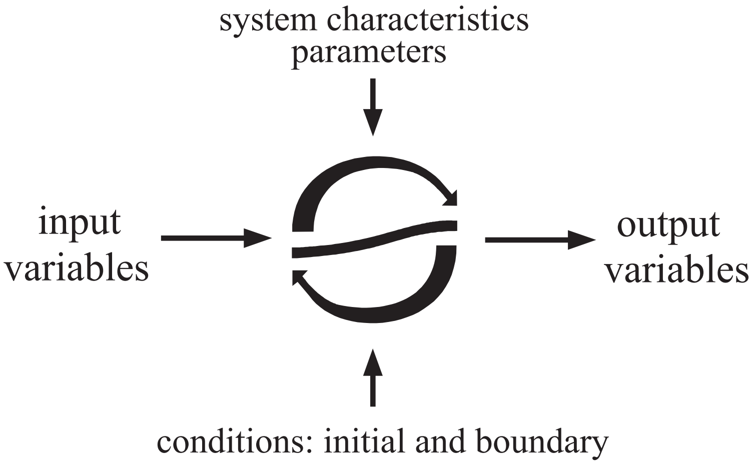
L4018/GWM I

Groundwater Modelling

September 2000 G.H.P. Oude Essink



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Contents

Chapter 8

Numerical aspects of groundwater models

Whatever numerical approach is chosen, always inaccuracies or errors are induced. They can be subdivided into [Spaans, 1992]:

- *physical system errors*, due to an wrong concept, an inadequate simplification or an incorrect schematisation of the hydrologic system, variables, parameters and boundary conditions,
- *mathematical errors*, due to wrong or incomplete expressions of the differential equations,
- *numerical errors*, due to an incorrect transformation of differential into difference equations (e.g. order of approximation is too low, faults in the computer code, numerical dispersion),
- *computational errors*, due to convergence and computer inaccuracies (e.g. machine truncation).

In this chapter, the interest is focussed on the numerical errors. The numerical approximations, that define the derivatives of the groundwater flow and solute transport equations, may introduce errors in the numerical solution. These errors limit the techniques that solve partial equations.

Artificial *numerical dispersion* occurs in the solution as a result of numerical approximation of the nonlinear solute transport equation (see figure 8.1). It depends on the applied discretisation scheme of the advective term in the solute transport equation whether or not a *truncation error* arises. This truncation error has the appearance of an additional dispersion-like term. It may dominate the numerical accuracy of the solution (see section 8.1).

In addition, over and undershooting of the solute concentration values, which is called *oscillation* (see figure 8.1), may lead to *oscillation errors* in the solution of the solute concentration. If the oscillation reaches unacceptable values, the solution may even become unstable.

There exists a close relation between numerical accuracy (numerical dispersion) and stability (oscillation) [Peaceman, 1977; Pinder & Gray, 1977]. In fact, numerical dispersion acts to stabilize the solution of the equation. Numerical dispersion spreads the sharp front by generating a solution which applies a greater dispersion than the hydrodynamic dispersion. In order to suppress the numerical dispersion, the numerical scheme (spatial as well as temporal) can be adapted. Meanwhile, this scheme may lead to over and undershooting,

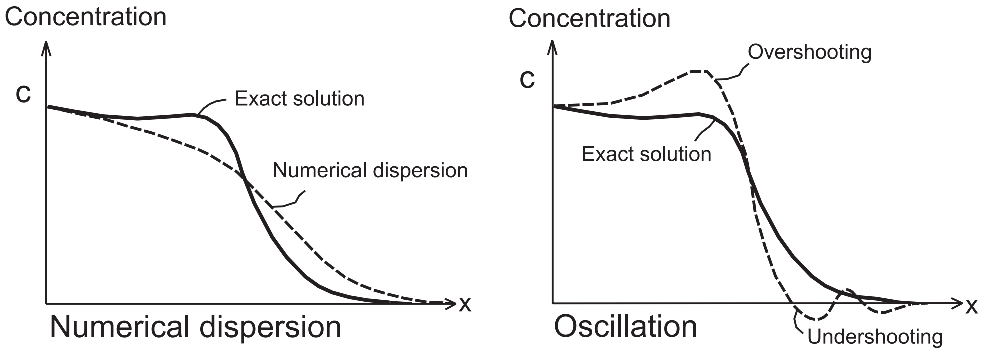

Figure 8.1: *Schematisation of numerical dispersion and oscillation (after Kinzelbach, 1987a).*

and subsequently, oscillation can be amplified. For these reasons, the discretisation scheme should be chosen carefully in order to control both numerical accuracy and stability.

8.1 Numerical dispersion

Standard finite difference methods may generate significant truncation errors. In this section, an one-dimensional schematisation is applied to demonstrate in a simple way the principle of assessing truncation errors. The standard (one-dimensional) advection-dispersion equation is defined as follows:

$$D\frac{\partial^2 C}{\partial x^2} - V\frac{\partial C}{\partial x} = \frac{\partial C}{\partial t} \tag{8.1}$$

where

- V = real velocity of groundwater $[L\,T^{-1}]$,
- D = hydrodynamic dispersion $[L^2\,T^{-1}]$.

In most examples, this equation is discretised as (backwards in space and time: implicit):

$$D\frac{C_{i+1}^k - 2C_i^k + C_{i-1}^k}{\Delta x^2} - V\frac{C_i^k - C_{i-1}^k}{\Delta x} = \frac{C_i^k - C_i^{k-1}}{\Delta t} \tag{8.2}$$

Here, the interest is focussed on the truncation errors, made in the Taylor series development of the partials (see the equations 7.71 to 7.76 for the Taylor series expansions), in order to detect the numerical errors caused by the discretisation:

Backwards in space (implicit):

$$\frac{\partial C}{\partial x} = \frac{C_i - C_{i-1}}{\Delta x} + \frac{\Delta x}{2}\frac{\partial^2 C}{\partial x^2} - \frac{\Delta x^2}{6}\frac{\partial^3 C}{\partial x^3} + O(\Delta x^3) \tag{8.3}$$

Central in space (Crank-Nicolson):

$$\frac{\partial C}{\partial x} = \frac{C_{i+1} - C_{i-1}}{2\Delta x} - \frac{\Delta x^2}{6}\frac{\partial^3 C}{\partial x^3} + O(\Delta x^4) \tag{8.4}$$

$$\frac{\partial^2 C}{\partial x^2} = \frac{C_{i+1} - 2C_i + C_{i-1}}{\Delta x^2} - \frac{\Delta x^2}{12}\frac{\partial^4 C}{\partial x^4} + O(\Delta x^4) \tag{8.5}$$

Forwards in time (explicit):

$$\frac{\partial C}{\partial t} = \frac{C_i^{k+1} - C_i^k}{\Delta t} - \frac{\Delta t}{2}\frac{\partial^2 C}{\partial t^2} - \frac{\Delta t^2}{6}\frac{\partial^3 C}{\partial t^3} + O(\Delta t^3) \tag{8.6}$$

Backwards in time (implicit):

$$\frac{\partial C}{\partial t} = \frac{C_i^{k} - C_i^{k-1}}{\Delta t} + \frac{\Delta t}{2}\frac{\partial^2 C}{\partial t^2} - \frac{\Delta t^2}{6}\frac{\partial^3 C}{\partial t^3} + O(\Delta t^3) \tag{8.7}$$

Central in time (Crank-Nicolson):

$$\frac{\partial C}{\partial t} = \frac{C_i^{k+1} - C_i^k}{\Delta t} - \frac{\Delta t^2}{24}\frac{\partial^3 C}{\partial t^3} + O(\Delta t^4) \tag{8.8}$$

Inserting the three upper above-mentioned expressions in the discretised advection-dispersion equation 8.2 gives:

$$D\left(\frac{\partial^2 C}{\partial x^2} + \frac{\Delta x^2}{12}\frac{\partial^4 C}{\partial x^4}\right) - V\left(\frac{\partial C}{\partial x} - \frac{\Delta x}{2}\frac{\partial^2 C}{\partial x^2} + \frac{\Delta x^2}{6}\frac{\partial^3 C}{\partial x^3}\right) = \frac{\partial C}{\partial t} - \frac{\Delta t}{2}\frac{\partial^3 C}{\partial t^3} \tag{8.9}$$

Neglecting third and fourth order terms gives:

$$D\frac{\partial^2 C}{\partial x^2} - V\left(\frac{\partial C}{\partial x} - \frac{\Delta x}{2}\frac{\partial^2 C}{\partial x^2}\right) = \frac{\partial C}{\partial t} - \frac{\Delta t}{2}\frac{\partial^2 C}{\partial t^2} \tag{8.10}$$

Rewriting the term $\frac{\partial^2 C}{\partial t^2}$ gives:

$$\frac{\partial^2 C}{\partial t^2} = \frac{\partial}{\partial t}\left(\frac{\partial C}{\partial t}\right) = \frac{\partial}{\partial t}\left(D\frac{\partial^2 C}{\partial x^2} - V\frac{\partial C}{\partial x}\right) = D\frac{\partial^2}{\partial x^2}\left(\frac{\partial C}{\partial t}\right) - V\frac{\partial}{\partial x}\left(\frac{\partial C}{\partial t}\right) \tag{8.11}$$

$$\frac{\partial^2 C}{\partial t^2} = D\frac{\partial^2}{\partial x^2}\left(D\frac{\partial^2 C}{\partial x^2} - V\frac{\partial C}{\partial x}\right) - V\frac{\partial}{\partial x}\left(D\frac{\partial^2 C}{\partial x^2} - V\frac{\partial C}{\partial x}\right) \tag{8.12}$$

$$\frac{\partial^2 C}{\partial t^2} = D^2\frac{\partial^4 C}{\partial x^4} - VD\frac{\partial^3 C}{\partial x^3} - VD\frac{\partial^3 C}{\partial x^3} + V^2\frac{\partial^2 C}{\partial x^2} \tag{8.13}$$

$$\frac{\partial^2 C}{\partial t^2} \approx V^2\frac{\partial^2 C}{\partial x^2} \tag{8.14}$$

Combining this result with equation 8.10 gives:

$$D\frac{\partial^2 C}{\partial x^2} - V\left(\frac{\partial C}{\partial x} - \frac{\Delta x}{2}\frac{\partial^2 C}{\partial x^2}\right) = \frac{\partial C}{\partial t} - V^2\frac{\Delta t}{2}\frac{\partial^2 C}{\partial x^2} \tag{8.15}$$

$$\left(D + V\frac{\Delta x}{2} + V^2\frac{\Delta t}{2}\right)\frac{\partial^2 C}{\partial x^2} - V\frac{\partial C}{\partial x} = \frac{\partial C}{\partial t} \tag{8.16}$$

Here an interesting appearance occurs: approximations of the first-order derivatives generates errors in the order of second-order derivatives. Two extra terms have been added to the real hydrodynamic dispersion coefficient D: $V\frac{\Delta x}{2} + V^2\frac{\Delta t}{2}$. These terms are called the numerical dispersion terms:

backwards in space and time (implicit):

$$D_{apparent} = D + D_{num} = D + V\frac{\Delta x}{2} + V^2\frac{\Delta t}{2} \tag{8.17}$$

Similar equations can be found for:

central in space (Crank-Nicolson) and backwards in time (implicit):

$$D_{num} = V^2\frac{\Delta t}{2} \tag{8.18}$$

backwards in space (implicit) and forwards in time (explicit):

$$D_{num} = V\frac{\Delta x}{2} - V^2\frac{\Delta t}{2} \tag{8.19}$$

Suppose your discretised model has the following parameters: D=1.2 m^2/d V=1 m/d, Δt=0.4 d and Δx=1 m. In this situation, the value of the dispersion coefficient (for the backwards in space and time discretisation) used in the model is equal to:

$$D_{apparent} = D + D_{num} = 1.2 + 1\frac{1}{2} + 1^2\frac{0.4}{2} = 1.9\, m^2/d \tag{8.20}$$

Thus, the dispersion coefficient is larger and your computational results for the solute transport will deviate significantly for what you would expect with a smaller dispersion coefficient. Remedy to reduce the effect of numerical dispersion:

- make Δt and Δx smaller,
- use central in space and time discretisations: however, these solutions can easily create oscillations of the solution,
- use another hydrodynamic dispersion coefficient D: e.g.: use D=0.7 m^2/d instead of D=1.2 m^2/d in order to account for the numerical dispersion: now $D_{apparent}$=1.2 m^2/d.

In summary, the truncation errors depends on the chosen numerical approximation [Bear & Verruijt, 1987]:

- Backward difference in space (upstream weighting)
  The finite difference approximations in space also introduce truncation errors. It is well-known that a backward difference in space approximation gives the following equation for the term $\frac{\partial C}{\partial x}$:

  $$\frac{\partial C}{\partial x} = \frac{C_i - C_{i-1}}{\Delta x} + \frac{\Delta x}{2}\frac{\partial^2 C}{\partial x^2} + \ldots \tag{8.21}$$

  The term $\frac{\partial C}{\partial x}$ should be multiplied with $-V$ to be inserted properly in equation 8.1. Thus, the approximation results in an additional truncation error term of the dispersion-term: $-\frac{1}{2}V\Delta x$. Focusing on only the backward spatial approximation, the numerical dispersion D_{num} due to the truncation error in space will be:

  $$D_{num} = +\frac{\Delta x}{2}V \tag{8.22}$$

Approximation scheme		Numerical dispersion
Time	Spatial	Truncation error
FIT: forward in time (explicit)	BIS (upstream)	$\frac{1}{2}V\Delta x - \frac{1}{2}V^2\Delta t$
	CIS (centered)	$-\frac{1}{2}V^2\Delta t$
BIT: backward in time (implicit)	BIS (upstream)	$\frac{1}{2}V\Delta x + \frac{1}{2}V^2\Delta t$
	CIS (centered)	$\frac{1}{2}V^2\Delta t$
CIT: centered in time (Crank-Nicolson)	BIS (upstream)	$\frac{1}{2}V\Delta x$
	CIS (centered)	none

Table 8.1: *Summary of numerical dispersion for the one-dimensional equation [modified from Lantz, 1971; INTERCOMP, 1976; Bear & Verruijt, 1987].*

Table 8.1 summarizes the truncation error forms for the one-dimensional equation.

- Central difference in space

  As the central finite difference in space does not generate a space truncation error of the second-order derivative, no numerical dispersion due to this approximation occurs.

$$\frac{\partial C}{\partial x} = \frac{C_{i+1} - C_{i-1}}{2\Delta x} + \mathrm{O}\left((\Delta x)^2, \frac{\partial^3 C}{\partial x^3}\right) \tag{8.23}$$

- Forward difference in space

  Forward difference in space also results in a truncation error term, as the derivation for the term $\frac{\partial C}{\partial x}$ gives:

$$\frac{\partial C}{\partial x} = \frac{C_{i+1} - C_i}{\Delta x} - \frac{\Delta x}{2}\frac{\partial^2 C}{\partial x^2} + \ldots \tag{8.24}$$

  As this spatial difference approximation is not commonly used for the advective term, this truncation error is not be displayed in table 8.1.

- Forward difference in time (explicit)

  A truncation error in the time derivative may cause numerical dispersion for the finite difference approximation in time:

$$\frac{\partial C}{\partial t} = \frac{C^{k+1} - C^k}{\Delta t} - \frac{\Delta t}{2}\frac{\partial^2 C}{\partial t^2} + \ldots \tag{8.25}$$

  By applying the original equation 8.1, this expression can be rewritten as [Lantz, 1971]:

$$\frac{\partial C}{\partial t} = \frac{C^{k+1} - C^k}{\Delta t} - \frac{\Delta t}{2}V^2\frac{\partial^2 C}{\partial x^2} + \ldots \tag{8.26}$$

  Accordingly, the term which contributes to the numerical dispersion is $-\frac{1}{2}V^2\Delta t$ (see also table 8.1).

- Backward difference in time (implicit)
  Analogous to the forward difference in time, the backward difference in time induces an equivalent error in numerical dispersion, though now the sign is opposite: $+\frac{1}{2}V^2\Delta t$ (see table 8.1).

- Central difference in time (Crank-Nicolson)

  This scheme is the most often used second-order time approximation, as the time truncation error contribution to numerical dispersion is removed. Nonetheless, oscillations in time can still occur [INTERCOMP, 1976].

8.1.1 Stability analysis of the advection-dispersion equation

The so-called von Neumann stability analysis is often applied to analyse the stability of a solution[1]. The question is asked whether or not the errors in the equation can grow uncontrolled during subsequent time steps Δt.

Backwards in space (implicit) and forwards in time (explicit)

Here follows the analysis of the advection-dispersion equation which is discretised backwards in space (implicit) and forwards in time (explicit):

$$D\frac{C_{i+1}^k - 2C_i^k + C_{i-1}^k}{\Delta x^2} - V\frac{C_i^k - C_{i-1}^k}{\Delta x} = \frac{C_i^{k+1} - C_i^k}{\Delta t} \tag{8.27}$$

It is assumed that the solution of the equation is defined as:

$$C^k = \tilde{C}^k + \varepsilon \Longleftrightarrow C^k = \tilde{C}^k + r_t \mathrm{e}^{i\beta x} \tag{8.28}$$

where:

- $\tilde{C}$=the correct solution on time k,
- ε=$r_t\mathrm{e}^{i\beta x}$=the error written as a Fourier component, where i indicates that a complex imaginary number is used.

The new solution is of the equation is:

$$C^{k+1} = \tilde{C}^{k+1} + r_{t+\Delta t}\mathrm{e}^{i\beta x} \tag{8.29}$$

Substituting these two equations in the discretised equation gives:

$$\begin{aligned} D\tfrac{\tilde{C}_{i+1}^k - 2\tilde{C}_i^k + \tilde{C}_{i-1}^k}{\Delta x^2} &+ D\tfrac{r_t\mathrm{e}^{i\beta(x+\Delta x)} - 2r_t\mathrm{e}^{i\beta x} + r_t\mathrm{e}^{i\beta(x-\Delta x)}}{\Delta x^2} \\ -V\tfrac{\tilde{C}_i^k - \tilde{C}_{i-1}^k}{\Delta x} &- V\tfrac{r_t\mathrm{e}^{i\beta x} - r_t\mathrm{e}^{i\beta(x-\Delta x)}}{\Delta x} \\ = \tfrac{\tilde{C}_i^{k+1} - \tilde{C}_i^k}{\Delta t} &+ \tfrac{r_{t+\Delta t}\mathrm{e}^{i\beta x} - r_t\mathrm{e}^{i\beta x}}{\Delta t} \end{aligned} \tag{8.30}$$

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[1] This section is based on lecture notes of A. Leijnse (LUW, RIVM).

As the following equation is valid:

$$D\frac{\tilde{C}_{i+1}^k - 2\tilde{C}_i^k + \tilde{C}_{i-1}^k}{\Delta x^2} - V\frac{\tilde{C}_i^k - \tilde{C}_{i-1}^k}{\Delta x} = \frac{\tilde{C}_i^{k+1} - \tilde{C}_i^k}{\Delta t} \tag{8.31}$$

and dividing the equation by $\mathrm{e}^{i\beta x}$, equation 8.30 becomes:

$$D\frac{r_t \mathrm{e}^{i\beta\Delta x} - 2r_t + r_t \mathrm{e}^{-i\beta\Delta x}}{\Delta x^2} - V\frac{r_t - r_t \mathrm{e}^{-i\beta\Delta x}}{\Delta x} = \frac{r_{t+\Delta t} - r_t}{\Delta t} \tag{8.32}$$

$$r_{t+\Delta t} = r_t\left[1 + \frac{D\Delta t}{\Delta x^2}\left(\mathrm{e}^{i\beta\Delta x} - 2 + \mathrm{e}^{-i\beta\Delta x}\right) - \frac{V\Delta t}{\Delta x}\left(1 - \mathrm{e}^{-i\beta\Delta x}\right)\right] \tag{8.33}$$

$$\rho = \frac{r_{t+\Delta t}}{r_t} = 1 - \frac{2D\Delta t}{\Delta x^2}\left(1 - \frac{\mathrm{e}^{i\beta\Delta x} + \mathrm{e}^{-i\beta\Delta x}}{2}\right) - \frac{V\Delta t}{\Delta x}\left(1 - \mathrm{e}^{-i\beta\Delta x}\right) \tag{8.34}$$

$$\rho = 1 - \frac{2D\Delta t}{\Delta x^2}\gamma_1 - \frac{V\Delta t}{\Delta x}\gamma_2 \tag{8.35}$$

where:

- $\rho = \frac{r_{t+\Delta t}}{r_t} =$ the amplification factor
- $\gamma_1 = 1 - \frac{\mathrm{e}^{i\beta\Delta x} + \mathrm{e}^{-i\beta\Delta x}}{2}$
- $\gamma_2 = 1 - \mathrm{e}^{-i\beta\Delta x}$

The equation is stable when the absolute value of the amplification factor ρ is smaller than or equal to one:

$$|\rho| \le 1 \tag{8.36}$$

$$-1 \le 1 - \frac{2D\Delta t}{\Delta x^2}\gamma_1 - \frac{V\Delta t}{\Delta x}\gamma_2 \le 1 \qquad \Longleftrightarrow \qquad -2 \le -\frac{2D\Delta t}{\Delta x^2}\gamma_1 - \frac{V\Delta t}{\Delta x}\gamma_2 \le 0 \tag{8.37}$$

$$0 \le \frac{2D\Delta t}{\Delta x^2}\gamma_1 + \frac{V\Delta t}{\Delta x}\gamma_2 \le 2 \tag{8.38}$$

Analysing γ_1 and γ_2 gives the following equations (making use of the theory of complex functions !):

$$\gamma_1 = 1 - \frac{\mathrm{e}^{i\beta\Delta x} + \mathrm{e}^{-i\beta\Delta x}}{2} = 1 - \cos\beta\Delta x \tag{8.39}$$

Knowing that a cosine is always between -1 en 1 gives:

$$0 \le \gamma_1 \le 2 \tag{8.40}$$

The term γ_2 is somewhat more complex:

$$\gamma_2 = 1 - e^{-i\beta\Delta x} = 1 - \cos\beta\Delta x + i\sin\beta\Delta x \tag{8.41}$$

To determine the length of this complex term γ_2, the absolute value must be calculated:

$$|\gamma_2| = |1 - \cos\beta\Delta x + i\sin\beta\Delta x| = \sqrt{(1 - \cos\beta\Delta x)^2 + (\sin\beta\Delta x)^2} \tag{8.42}$$

$$|\gamma_2| = \sqrt{1 - 2\cos\beta\Delta x + \cos\beta\Delta x^2 + \sin\beta\Delta x^2} = \sqrt{2 - 2\cos\beta\Delta x} \tag{8.43}$$

Knowing, once again, that a cosine is always between -1 en 1 gives:

$$0 \le \gamma_2 \le 2 \tag{8.44}$$

Based on the equations 8.38, 8.40 and 8.44, it can be obtained that:

$$V\frac{\Delta t}{\Delta x} + \frac{2D\Delta t}{\Delta x^2} \le 1 \tag{8.45}$$

If this equation is valid then $V\frac{\Delta t}{\Delta x} \le 1$ (V is positive) and $\frac{2D\Delta t}{\Delta x^2} \le 1$. Suppose that $V\frac{\Delta t}{\Delta x} > \frac{2D\Delta t}{\Delta x^2}$, then equation 8.38 becomes:

$$0 \le \frac{2D\Delta t}{\Delta x^2}\gamma_1 + \frac{V\Delta t}{\Delta x}\gamma_2 \le 2 \Longrightarrow 0 \le \frac{V\Delta t}{\Delta x}\left(\gamma_1 + \gamma_2\right) \le 2 \tag{8.46}$$

As $V\frac{\Delta t}{\Delta x} \le 1$, then:

$$0 \le \gamma_1 + \gamma_2 \le 2 \tag{8.47}$$

Knowing the equations 8.40 and 8.44, this equation is valid if the terms $V\frac{\Delta t}{\Delta x}$ plus $\frac{2D\Delta t}{\Delta x^2}$ is smaller/equal than 1 (check it). A similar analysis can be obtained if $\frac{2D\Delta t}{\Delta x^2} > V\frac{\Delta t}{\Delta x}$. In conclusion, based on the von Neumann stability analysis, the following criterion can be obtained for the backwards in space (implicit) and forwards in time (explicit):

$$V\frac{\Delta t}{\Delta x} + \frac{2D\Delta t}{\Delta x^2} \le 1 \tag{8.48}$$

In fact: this criterion is also used in the stability criteria of the MOC code (but then in 2D):

$$V\frac{\Delta t}{\Delta x} \le 1, \text{where } V\tfrac{\Delta t}{\Delta x} \text{is the so-called Courant number} \tag{8.49}$$

$$\frac{2D\Delta t}{\Delta x^2} \le 1 \qquad \text{or} \qquad \tfrac{D\Delta t}{\Delta x^2} \le 0.5, \text{ which is the so-called Neumann-criterion} \tag{8.50}$$

Backwards in space (implicit) and backwards in time (implicit)

When applying a backwards in time (implicit) discretisation, the discretised equation becomes:

$$D\frac{C_{i+1}^k - 2C_i^k + C_{i-1}^k}{\Delta x^2} - V\frac{C_i^k - C_{i-1}^k}{\Delta x} = \frac{C_i^k - C_i^{k-1}}{\Delta t} \tag{8.51}$$

or, if $k = k + 1$:

$$D\frac{C_{i+1}^{k+1} - 2C_i^{k+1} + C_{i-1}^{k+1}}{\Delta x^2} - V\frac{C_i^{k+1} - C_{i-1}^{k+1}}{\Delta x} = \frac{C_i^{k+1} - C_i^k}{\Delta t} \tag{8.52}$$

The von Neumann analysis gives the following equation:

$$\rho = \frac{r_{t+\Delta t}}{r_t} = \frac{1}{1 + \frac{2D\Delta t}{\Delta x^2}\gamma_1 + \frac{V\Delta t}{\Delta x}\gamma_2} \tag{8.53}$$

$$|\rho| \leq 1 \quad \text{for each} \ \Delta x, \ \Delta t \ \text{unless} \ D_{apparent} = D - V\frac{\Delta x}{2} - V^2\frac{\Delta t}{2} \tag{8.54}$$

For this situation, ρ is stable if:

$$\frac{2D_{apparant}\Delta t}{\Delta x^2}\gamma_1 + \frac{V\Delta t}{\Delta x}\gamma_2 \geq 0 \qquad \text{or} \qquad \frac{2D_{apparant}\Delta t}{\Delta x^2} + \frac{V\Delta t}{\Delta x} \geq 0 \tag{8.55}$$

$$\frac{2\left(D - V\frac{\Delta x}{2} - V^2\frac{\Delta t}{2}\right)\Delta t}{\Delta x^2} + \frac{V\Delta t}{\Delta x} \geq 0 \qquad \text{or} \qquad \frac{2D\Delta t - V^2\Delta t^2}{\Delta x^2} \geq 0 \tag{8.56}$$

$$\Delta t \leq \frac{2D}{V^2} \tag{8.57}$$

How to obtain the following central in time (Crank-Nicolson) approximation:

$$\text{Central in time (Crank-Nicolson):} \qquad \frac{\partial C}{\partial t} = \frac{C_i^{k+1} - C_i^k}{\Delta t} - \frac{\Delta t^2}{24}\frac{\partial^3 C}{\partial t^3} + O(\Delta t^4) \tag{8.58}$$

$$C_i^{k+1} = C_i^{k+1/2} + \frac{\Delta t}{2}\frac{\partial C}{\partial t} + \frac{1}{2}\left(\frac{\Delta t}{2}\right)^2\frac{\partial^2 C}{\partial t^2} + \frac{1}{6}\left(\frac{\Delta t}{2}\right)^3\frac{\partial^3 C}{\partial t^3} + \frac{1}{24}\left(\frac{\Delta t}{2}\right)^4\frac{\partial^4 C}{\partial t^4} + \frac{1}{120}\left(\frac{\Delta t}{2}\right)^5\frac{\partial^5 C}{\partial t^5}\cdots \tag{8.59}$$

$$C_i^{k} = C_i^{k+1/2} - \frac{\Delta t}{2}\frac{\partial C}{\partial t} + \frac{1}{2}\left(\frac{\Delta t}{2}\right)^2\frac{\partial^2 C}{\partial t^2} - \frac{1}{6}\left(\frac{\Delta t}{2}\right)^3\frac{\partial^3 C}{\partial t^3} + \frac{1}{24}\left(\frac{\Delta t}{2}\right)^4\frac{\partial^4 C}{\partial t^4} - \frac{1}{120}\left(\frac{\Delta t}{2}\right)^5\frac{\partial^5 C}{\partial t^5}\cdots \tag{8.60}$$

Equations 8.59-8.60 give:

$$C_i^{k+1} - C_i^k = 2\frac{\Delta t}{2}\frac{\partial C}{\partial t} + 2\frac{1}{6}\left(\frac{\Delta t}{2}\right)^3\frac{\partial^3 C}{\partial t^3} + 2\frac{1}{120}\left(\frac{\Delta t}{2}\right)^5\frac{\partial^5 C}{\partial t^5} + \ldots \tag{8.61}$$

$$\frac{\partial C}{\partial t} = \frac{C_i^{k+1} - C_i^k}{\Delta t} - \frac{\Delta t^2}{24}\frac{\partial^3 C}{\partial t^3} + O(\Delta t^4) \tag{8.62}$$

8.2 Oscillation

Oscillations may occur in case the total dispersion (that is the sum of hydrodynamic dispersion D and numerical dispersion D_{num}) is negative. Thus, the following expression should be obeyed:

$$D + D_{num} \geq 0 \tag{8.63}$$

A stability analysis indicates whether or not the approximation scheme for the solute transport equation causes an instable solution [e.g. INTERCOMP, 1976; Peaceman, 1977]. Various analyses can be applied to determine the stability criteria for each approximation scheme. Two examples of this scheme are briefly discussed in this section:

- Central difference in time (Crank Nicolson)
  No numerical dispersion occurs if a central difference in time scheme is applied in combination with central difference in space (see table 8.1). Hence, this approximation scheme seems to be ideal. There is, however, a tendency of central difference approximations to over and undershoot the maximum and minimum limits, and subsequently, oscillations in time are caused. These oscillation errors could be reduced

by limiting the time step. This criterion appears to be related to the criterion of the explicit scheme: in fact, it equals about one-half of the forward in time first-order stability criterion [INTERCOMP, 1976]:

$$\frac{V\Delta t}{\Delta x} \leq 2 \tag{8.64}$$

- Backward difference in time (implicit)
  No stability criteria exist for implicit schemes. Still, however, a so-called *spatial oscillation* may occur in the central in space approximation [Price *et al.*, 1966; INTERCOMP, 1976]. In order to limit this oscillation, the following equation should be fulfilled:
  $$\frac{V\Delta x}{2} \leq D \quad \text{or} \quad Pe_{grid} = \frac{V\Delta x}{D} \leq 2 \tag{8.65}$$
  where Pe_{grid} = grid-Peclet-number $(-)$, which determines the relative size of the advective and dispersive fluxes on the level of a discretisation element.

8.3 Analysis of truncation and oscillation errors

The solution of the solute transport equation may be faced with difficulties, since standard finite difference and finite element models may yield unreliable results if the discretisation conditions are not met. Although, in general, representation of the dispersion by the finite element method[2] is accurate if numerical dispersion is small with respect to the hydrodynamic dispersion [Bear & Verruijt, 1987], it is recommended to analyse the solute transport equation anyway.

In order to quantify numerical accuracy, an *eigenvalue analysis* of the advection-dispersion equation should be performed. Such an analysis will demonstrate the importance of mesh spacing [e.g. Frind & Pinder, 1983]. In addition, a stability analysis should determine the stability condition. For example, the von Neumann criterion for stability defines that the modulus of the amplification factor must be less than or equal to one for all the components [Peaceman, 1977; Stelling & Booij, 1996]. In order to obtain real and distinct eigenvalues, the spatial discretisation in the finite element formulations should meet the condition [Daus *et al.*, 1985]:

$$Pe_{grid} = \frac{V\Delta x}{D} \leq 2 \tag{8.66}$$

In advective-dominant solute transport, the hydrodynamic dispersion D approximates $D{=}\alpha_L\, V$, and thus, equation 8.66 becomes:

$$Pe_{grid} = \frac{\Delta x}{\alpha_L} \leq 2 \tag{8.67}$$

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[2] The analysis of (truncation and oscillation) errors due to numerical dispersion and oscillation for the finite difference method by means of central finite difference approximations is similar for the finite element method [Pinder & Gray, 1977, Kinzelbach, 1987a].

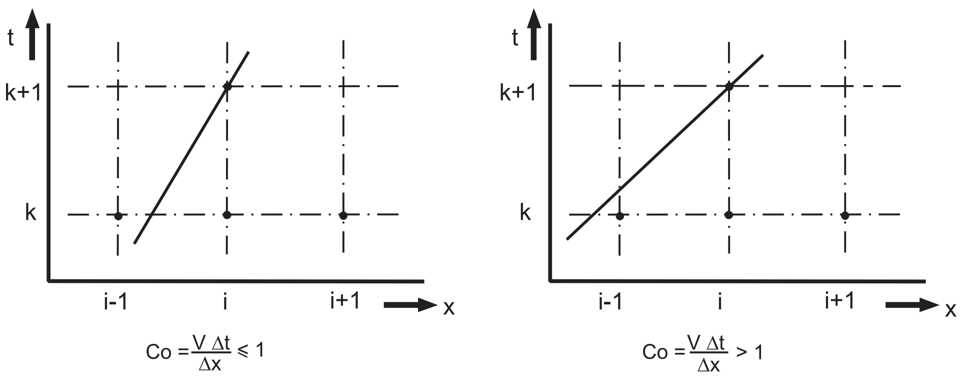

Figure 8.2: *Schematisation of the Courant condition.*

Daus *et al.* [1985] obtains for the temporal discretisation:

$$Co = \frac{V\Delta t}{\Delta x} \leq \frac{Pe_{grid}}{2} \tag{8.68}$$

where $Co =$ the Courant number $[-]$. The Courant condition Co is physically interpreted as the ratio of the advective distance during one time step to the spatial discretisation. Figure 8.2 illustrates the Courant condition in a numerical scheme. If the grid-Peclet-number Pe_{grid} is assumed to be maximum (viz. $Pe_{grid} = 2$), the Courant constraint becomes:

$$Co = \frac{V\Delta t}{\Delta x} \leq 1 \tag{8.69}$$

Grid-Peclet-numbers and Courant numbers have been mentioned in various quantitative descriptions. Whether or not the numerical dispersion is suppressed, depends on the discretisation technique applied [e.g. Jensen & Finlayson, 1978; Campbell *et al.*, 1981; Voss & Souza, 1987]. In summary, the criteria for the grid-Peclet-number are:

$$\begin{aligned} Pe_{grid} &\leq 2 && \text{Finite difference algorithm, central-in-space} \\ Pe_{grid} &\leq 2 && \text{Finite element algorithm, linear basic functions} \\ Pe_{grid} &\leq 4 && \text{Finite element algorithm, quadratic basic functions} \end{aligned} \tag{8.70}$$

If mechanical dispersion dominates over molecular diffusion, the hydrodynamic dispersion D in equation 8.65 can be expressed as $D{=}\alpha_L\,|V|$, and thus, equation 8.70 becomes:

$$\begin{aligned} \Delta x &\leq 2\;\alpha_L && \text{Finite difference algorithm, central-in-space} \\ \Delta x &\leq 2\;\alpha_L && \text{Finite element algorithm, linear basic functions} \\ \Delta x &\leq 4\;\alpha_L && \text{Finite element algorithm, quadratic basic functions} \end{aligned} \tag{8.71}$$

Note that there are acceptable solutions obtained with values up to $\Delta x < 10\,\alpha_L$[3]. As such, this restriction is not very compulsory. Under those circumstances, the solution can still be satisfactory though in some places over and undershooting (viz. oscillation) may occur.

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[3] Sudicky [1989] even obtained highly accurate solutions for grid-Peclet-numbers in excess of 30 for the finite element method, based on a Laplace transformation of the temporal derivatives.

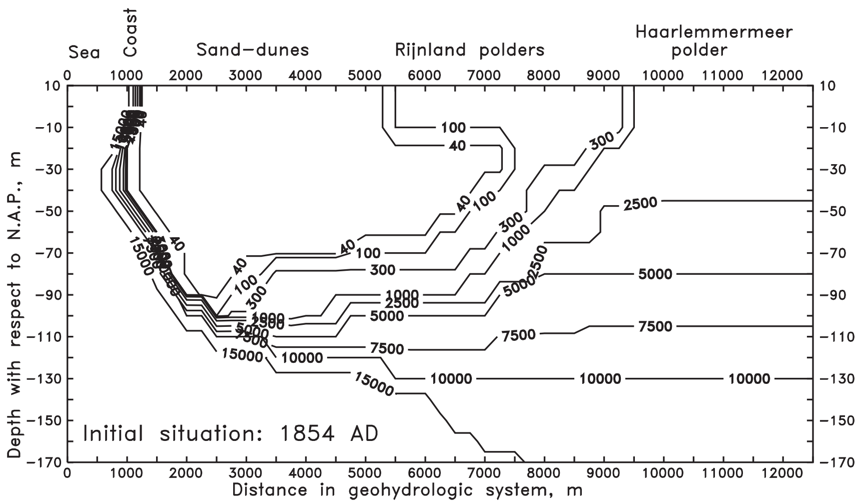

Figure 8.3: *Initial chloride distribution (values in mg Cl^-/l) at the beginning of 1854 AD, computed for 900 elements [Kooiman, 1989].*

Effect of the magnitude of α_L on the numerical solution: a case-study

The influence of longitudinal dispersivities α_L on the solution is analysed through simulation of a specific cross-section in Noord-Holland with two groundwater flow computer codes: SUTRA [Voss, 1984] (see the lecture notes of Hydrological Transport Processes/Groundwater Modelling II) based on the finite element method and the adapted MOC code [Konikow & Bredehoeft, 1978; Oude Essink, 1996] (see section 9.5) based on the method of characteristics. The cross-section through the sand-dune area of Gemeentewaterleidingen Amsterdam up to halfway the Haarlemmermeer polder is taken as the reference case.

The simulations start with an initial chloride distribution at the beginning of 1854 AD (see figure 8.3), as it is proposed by Kooiman [1989] through 'trial and error'. Each of the models computes the chloride distribution after a simulation time of 134 years, from the reclamation of the Haarlemmermeer polder till the end of 1987. The following two longitudinal dispersivities are applied: α_L=0.02 m and α_L=20.0 m. In order to compare the two models with each other, the dimension of the elements should be equal. The dimension is set to Δx=250 m and Δz=10 m. This implies for a cross-section with the dimensions 12,500 m by 180 m = 50 columns by 18 rows = 900 elements.

Figure 8.4 shows four chloride distributions in the cross-section at the end of 1987, after a simulation time of 134 years. The computed chloride distribution matches measured chloride distribution (not shown here) best if the longitudinal dispersivity α_L is small. The case with a small longitudinal dispersivity, that is α_L=0.02 m, has a freshwater lens that corresponds with measurements. For both models, the case with α_L=20.0 m does not simulate a freshwater lens any more. The aquifer system consists of only a large zone with brackish groundwater. Obviously, this situation does not match reality.

Moreover, as can be seen in the figure 8.4, the chloride distributions by the adapted MOC code are smooth. This is in contrast with the distributions by SUTRA. When lon-

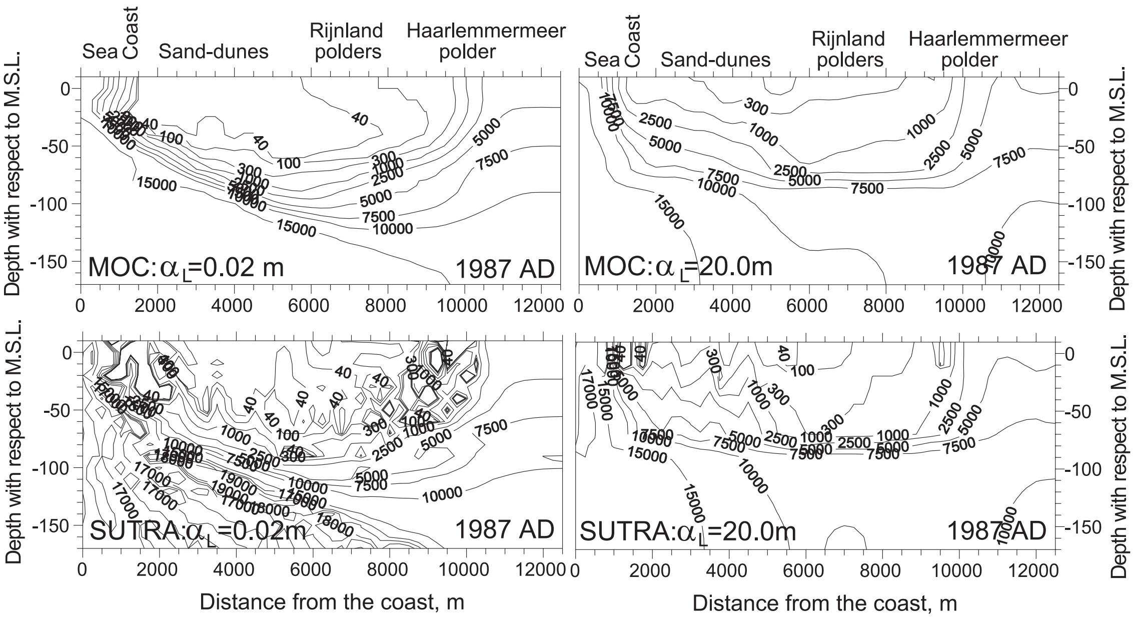

Figure 8.4: *Chloride distributions (in mg Cl^-/l) in 1987, computed for 900 elements with MOC and SUTRA for α_L=0.02 m and α_L=20.0 m. Note that here 900 elements are applied, whereas in figure 6.9 4500 elements are applied.*

Table 8.2: *Influence of the longitudinal dispersivity on the accuracy of the solution: the minimum and maximum chloride concentrations; and the number of elements undershooting a chloride concentration of 0 mg Cl^-/l and overshooting 17,000 mg Cl^-/l (the maximum chloride concentration which is inserted in the cross-section).*

SUTRA				
α_L	Minimum	Maximum	Undershoot	Overshoot
(m)	($mg\ Cl^-/l$)	($mg\ Cl^-/l$)	(elements)	(elements)
0.02	-8707	37,580	66	133
0.2	-7506	25,436	50	130
2.0	-7063	27,089	21	70
20.0	-1958	22,970	6	14

gitudinal dispersivities are small, SUTRA computes inaccurate chloride distributions, and over and undershooting of the maximum and minimum chloride concentrations frequently occur. Table 8.2 shows that in SUTRA over and undershooting occur in several elements. The smaller the longitudinal dispersivity, the more elements are subject to over and undershooting. The main reason for this phenomenon is that SUTRA applies the finite element method, whereas the adapted MOC code applies the method of characteristics to simulate solute transport. æ