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## Numerical Modelling of Streams

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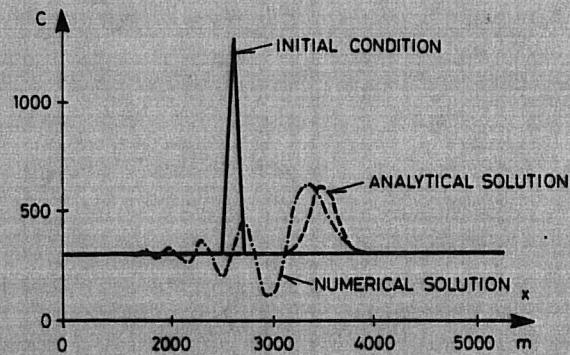
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## Numerical Modelling of Streams

**Hydrodynamic models and models for transport  
and spreading of pollutants**



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University of Aalborg**

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Hydrodynamic models and models for  
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by

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June 1989

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## Preface

The present report is submitted as one of the requirements for the degree of Ph.D. according to the notice no. 627 of October 17th, 1988 from the Danish Ministry of Education.

The study was carried out at the Department of Civil Engineering, University of Aalborg under supervision of Torben Larsen, and was financially supported from the Danish Technical Research Council.

I wish to thank the whole staff at the Hydraulics & Coastal Engineering Laboratory without whose help and guidance this book would never have been completed. Especially I wish to thank Birte Torstveit for invaluable help in typing the book and for showing great patience in correcting my written English. Furthermore, I wish to thank Lizzi Levin and Charlotte Kronholm for carefully performance of the drawings.

Aalborg, 1. June, 1989

Kristian Vestergaard

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## LIST OF SYMBOLS

The following list includes the the most oftenly used symbols. The list may not be complete, and in some sections another meaning of the symbols may be found, but for these occasions the actual meaning will be explained in the text.

$a_i$	a coefficient in a system of equations
$A$	cross section area
$A_d$	cross section area of the dead zone
$b$	cross section width at the surface
$b_i$	a coefficient in a system of equations
$C$	Chezy number
$C$	concentration of a dissolved pollutant
$C_d$	concentration of a pollutant in a dead zone
$C_k$	kinematic wave celerity
$C_j^n$	concentration at node no. $(n, j)$
$Cr_c$	the convective Courant number
$Cr_d$	the dispersive Courant number
$D$	mean depth
$f$	a function
$F$	flux of a pollutant through a cross section
$Fr$	Froude number
$g$	gravity
$h$	local water depth
$h_c$	critical depth
$I$	friction slope
$I_0$	bottom slope
$j$	index for space, number of space level
$j_m$	index for lower boundary, maximum valu of $j$
$K_2$	numerical dispersion coefficient
$K_3$	numerical skewness coefficient
$K_x$	longitudinal dispersion coefficient

$m$	source term, input per unit length
$m$	mass of a pollutant
$M$	Manning number
$M_k$	the $k$ 'th moment of a distribution
$n$	index for time, number of time level
$P$	wetted perimeter
$Pe$	the Peclet number
$q$	lateral inflow per unit length
$q_d$	exchange flow per unit length
$Q$	flow through a cross section
$R$	hydraulic radius or resistance radius
$t$	time coordinate
$tt$	travel time
$T_d$	residence time in the dead zone
$u$	average flow velocity
$u_q$	velocity in the x-direction of lateral inflow
$V$	average flow velocity
$V$	volume of flowing zone
$V_d$	volume of the dead zone
$x$	longitudinal space coordinate
$y$	water stage
$z$	vertical space coordinate
$\alpha$	velocity distribution coefficient
$\alpha$	a coefficient for time dicretization
$\beta$	a coefficient for space discretization
$\Delta x$	step in space
$\Delta t$	step in time
$\varepsilon$	volume fraction dead zone
$\Theta$	a coefficient for time centering
$\mu$	mean value
$\sigma^2$	variance

# Chapter 1

## Introduction

### 1.1 Numerical modelling

“Very much as the steam engine was the principal physical instrument of the industrial revolution, so the digital computer is the principal physical instrument of our current informational revolution”, Mike Abbott (Abbott, 1979).

The development of the digital computer has also been of great importance for the hydraulic engineer. Through many centuries hydraulic engineering was based on practical know-how, obtained through many hundred years of experience. Gradually mathematical theories were introduced and accepted among the engineers, but as the scale and the complexity of the hydraulic works increased, the mathematical models became so complex that a mathematical solution could not be obtained. This created a demand for new methods and again the experimental investigation became popular, but this time as measurements on small-scale models. But still the scale and complexity of hydraulic works were increasing, and soon even small-scale models reached a natural limit for some applications. In the mean time the modern computer was developed, and it became possible to solve complex mathematical models by use of computer-based numerical methods.

The development of numerical methods in hydraulics or fluid dynamics, – often called computational hydraulics, began for nearly one hundred years ago, but engineering applications awaited the development of the electronic computer. Since then, during the latest 30-40 years, numerical modelling has

become a more and more common used tool, and a lot of efforts has been used in developing sufficient numerical models. A brief historical outline of "Computational Fluid Dynamics" can be found in Roache (1976).

Many examples can be mentioned on applications of numerical models in hydraulics. They have been used for design of nuclear reactors, offshore installations and for simulation of flow in the non-saturated soil zone, in sewers network and in open channels.

The use of numerical models for simulation of flow in open channels has been rapidly increasing during the recent twenty years, and several modelling systems have been developed and used for practical engineering. An example is the microcomputer-based MIKE 11 from the Danish Hydraulic Institute. Though it seems that the study of the subject "Computational River Hydraulics" has been intensive, – hundreds of authors have published other hundreds of articles on this subject, a need for further development is still present.

Before river modelling is treated further, it could be necessary to clarify some basic concepts. The use of the word "model" is intensive and the meaning is often not clear, which perhaps is illustrated in the lines above. A model can be a mathematical formulation of a physical relationship, it can be a physical model built in a laboratory, it can be a numerical model, or it can be a nice girl showing the newest fashion. In this work two different types of models appear – the mathematical model and the numerical model.

The mathematical model is a discription of some physical or chemical relations expressed in mathematical terms, e.g. the Saint Venant equations, in which the movement of water in a one-dimensional open channel are expressed in two partial differential equations. The mathematical formulation can be based on causal or on empirical relationships, or both in combination. Often the equations are so complicated that analytical solutions only can be found for a limited number of occasions, often after extensive simplification.

Instead a numerical method is introduced. By use of the numerical method the governing equations are not solved, but approximated with a numerical solution. The numerical model is characterized by repetition of many calculations, and is therefore very often closely connected to a computer.

In the following the word "model" denotes a mathematical model, but created with the purpose of being solved by use of a numerical method implemented on a computer.

## 1.2 Numerical models for open channels

The flow in rivers has always been studied with great interest, and many efforts have been used for developing methods, which could describe the movement of water in a proper manner.

Mathematical models for unsteady flow conditions in open channels find their origin in the 19th century, where de Saint Venant on the basis of two fundamental physical laws, – continuity for mass and the 2nd law of Newton, formulated his classical mathematical model for one-dimensional unsteady flow – the Saint Venant equations. Still these equations are the most commonly used model for description of flow conditions in open channels.

Phenomena as flood waves and tidal motions can be described using the Saint Venant equations, from which the two variables, the flow through a cross section and the water stage, can be determined as functions of time and space. An analytical solution can only be obtained for some specific boundary conditions, and only for a simplified version of the model. For practical purpose numerical methods must be applied.

An early attempt to solve the Saint Venant equations were published in 1889 by Massau, but it took more than 60 years before the first engineering application were seen, which was closely connected to the development of the electronic computer. In 1952-53 Isaacson, Stoker and Troesch constructed and ran a mathematical model for some portion of the Ohio and Mississippi rivers. Since then the use of the Saint Venant equations for engineering purpose has accelerated, and during the last 10-15 years the growth in use has been almost exponential.

But while the application of the Saint Venant equations awaited the development of the computer, other models for unsteady flow were born. One of the perhaps best known and widely used is the Muskingum method, which was developed in 1934-35 for the Muskingum River Basin in Ohio. This method is based on continuity for mass and some empirical expressions of the storage of water on a reach of the river. Even though the mathematical description is relative weak, this "storage" or "channel routing" method still is widely used for river modelling.

River modelling includes more than hydrodynamic modelling, as described above. Also the erosion of, and the deposition on the river bed and banks have been studied with great interest, and several models for sediment transport have been developed. The model can be based on either a description

of the total sediment load, or a divided description of bed load and suspended load. The basic equations in both models are based on continuity considerations, often combined with more or less empirical relationships.

These equations make it possible to create and maintain a sediment budget for a river reach when the hydrodynamic features are known, e.g. found by use of a hydrodynamic model. But the hydrodynamic modelling is dependent of a knowledge to the river bed form, which is determined by the sediment transport model. For some situations this interaction is very important, which means that the two models must be solved simultaneously.

Another type of river model, which is also based on a hydrodynamic model, is the water quality model. But in opposition to the sediment transport model the water quality model does not affect the hydrodynamics, unless for some very special occasions. During the latest 10-20 years the water quality model has become more and more important, and today many hydrodynamic models have been built with the primary purpose to support a water quality model.

Water quality modelling can be divided into two classes, namely modelling of events of short duration, e.g. a sudden release of poison into a river, and long time models for determination of e.g. mass transport, algae growth etc. Again, continuity considerations forms the mathematical model. This can include several physical, chemical and biological processes, such as convective and dispersive transport, sedimentation, resuspension, adsorption, chemical and biological consumption and production etc. Often several substances and interaction between these are considered, which forms a set of coupled differential equations to be solved simultaneously.

Often the mathematical description of chemical and biological relationships is poorly developed and mostly empirical expressions are present. The mathematical description of transport and dispersion is based on the well-known heat-flow equation, which can be solved analytical for some simplified flow and boundary conditions. But for unsteady flow conditions and for a non-conservative matter numerical methods must be applied.

As a general rule one-dimensional river modelling can be divided into four groups of models:

- Hydrodynamic models for determination of the flow and the water stage (or depth).

- Sediment transport models for determination of the sediment transport rate and the bed level.
- Transport-dispersion models for determination of the concentration of a dissolved conservative matter.
- Water quality models for determination of the concentration of non-conservative matter.

Each group contains more than one mathematical model and for each of those several numerical methods can be applied. This means that the possible number of numerical models is very large, and it can be very difficult to survey this subject. But nevertheless this is necessary if the improvement of river modelling shall continue.

### 1.3 Scope of this work

Even though the area of mathematical, numerical computer based models has been investigated for many years, still a lot of work has to be done.

For some of the models the mathematical formulation of the physical, chemical and biological processes is weak and incomplete. So some basic investigations have to be done in this area, but this will not be the subject for further discussion in this work.

Knowing the mathematical model the next problem is to choose a proper numerical method. For this choice concepts as stability, numerical errors and demands for computer speed and store are essential. In this work the main discussion will be concerned about this choice, – which numerical methods can be used, how are they applied and which properties are related to them?

Because of the limited time for the preparation of this work not all four classes of models have been considered. The hydrodynamic models have been used for several years and the numerical aspect are well investigated, so for this class of models the description will tend to be a view, while the Transport/Dispersion models will be discussed in a more detailed manner. Water quality and sediment transport models will not be discussed directly, but in a way indirectly, as a lot of numerical aspects are common for all numerical models.

It is not the purpose with this work to identify the best numerical model for open channel modelling. Such a model does not exist. Some numerical models can be found excellent for a specific task, but in other connections the model may not be usable. The aim with this report is to help a new modeller to obtain a general view over this subject, which will improve his possibility for a proper choice of a numerical model.

As mentioned a lot of concepts are very like each other for many types of models, e.g. the terminologi. This and other generel concepts are treated in chapter 2, followed by a brief description of the most commonly used numerical methods for river modelling.

In chapter 3 hydrodynamic modelling is treated. The mathematical models for steady and for unsteady flow are described, and different simplifications of the Saint Venant equations are mentioned. This is followed by a description of numerical models for steady and unsteady flow, and finally some considerations are made upon the choice of the hydrodynamic model.

Chapter 4 is the main chapter in this report. Three different mathemat-

ical models for transport and spreading of a dissolved conservative matter are described and considered by mean of physical properties. A classification of numerical schemes are made, and a number of schemes are described in some details. The numerical properties, divided into stability and numerical errors, are considered with the purpose to extract some general properties for numerical models for transport and spreading of pollutants.



# Chapter 2

## Numerical Methods

### 2.1 Introduction

In the past several numerical methods have been used in numerical modelling of open channels, and even though they seem to be different, they have many properties in common. Numerical modelling of open channels is a very extensive subject and in this work it is impossible to discuss all the methods which have been used. Instead the methods will be divided into a number of classes and the characteristic elements in the methods will be described and discussed.

It is obvious that the choice of numerical method depends on the governing mathematical equations, but in this chapter, where the purpose is to describe different types of numerical methods, it is not of vital importance which example to use.

Since the Transport/Dispersion model is the most carefully treated model later on in this work, it is natural to choose this model as an example in this general chapter. If the flow is assumed to be steady and uniform the Transport/Dispersion equation can be written as:

$$\frac{\partial C}{\partial t} + u \frac{\partial C}{\partial x} = K_x \frac{\partial^2 C}{\partial x^2} \quad (2.1)$$

where  $C$  : concentration of a dissolved matter ( $gr/m^3$ )  
 $u$  : average flow velocity ( $m/sec$ )  
 $K_x$  : longitudinal dispersion coefficient ( $m^2/sec$ )  
 $x$  : space-coordinate ( $m$ )  
 $t$  : time-coordinate ( $sec$ )

Three classes of methods will be treated in the following sections, namely:

- the Control Volume approach
- the Method of Characteristics
- the Finite Difference technique

Even though these methods seem to be quite different, it will show up that they are basically equal.

## 2.2 General concepts

### Variables

In numerical models two different types of variables occur. From the Transport/Dispersion model (eq. 2.1) we want to calculate the concentration  $C$  as a function of the space  $x$  and the time  $t$ . The variable  $C$  is called a dependent variable, while  $x$  and  $t$  are called independent variables.

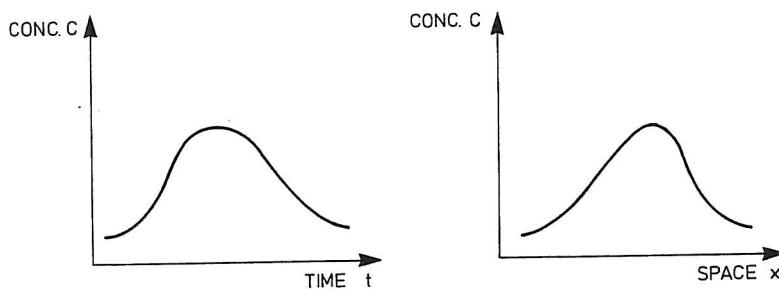


Fig. 2.1. Dependent variable as function of independent variables.

Normally the dependent variables are determined as functions of the independent variables, but in some numerical models the opposite is performed. This means that the time and place for a specific concentration is calculated through the numerical model. These models are called inverse models, and will not be treated directly as a class in this work, but indirectly as the method of characteristics contains a lot of the properties for the inverse models.

### The numerical grid

A mathematical model – a mathematical expression, is formulated in the continuous domain, while a numerical model is formulated in the discrete domain. In the mathematical model the variables are expressed at every place ( $x$ ) and every time ( $t$ ), but in the numerical model the variables can be determined only at a limited number of places and times. So when a numerical method is applied on a mathematical model, it simply means that the continuous domain is exchanged with the discrete domain, and then a number of points, where the variables can be calculated, have to be defined.

This is normally done and written through the numerical grid, where the dependent variable (the concentration) can be evaluated at the gridpoints (or nodes), as shown at Fig. 2.2.

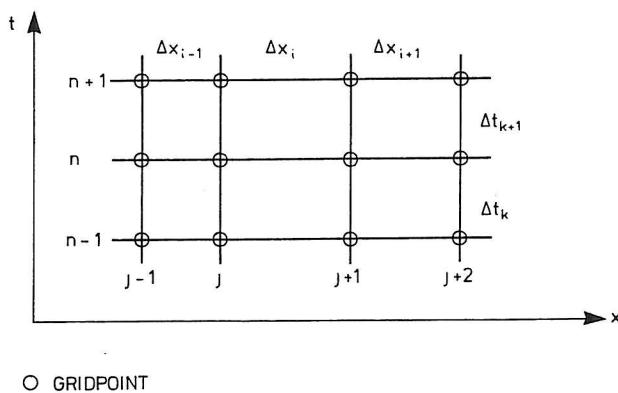


Fig. 2.2. Numerical grid.

In a one-dimensional model this grid is determined of the two independent variables, the space  $x$  and the time  $t$ . The grid size is expressed through the space step  $\Delta x$  and the time step  $\Delta t$ . In many numerical models a uniform grid is used, which means that  $\Delta x$  and  $\Delta t$  are constants, but in other models a non-uniform grid is used. The grid in Fig. 2.2 is a non-uniform grid where  $\Delta x$  varies with  $x$ , while  $\Delta t$  is constant. Normally  $\Delta x$  only varies with  $x$  and  $\Delta t$  with  $t$ , but in rare occasions other combinations may occur.

#### Direction of calculation

A numerical model is a step by step method, which by use of known values of the dependent variables at some nodes and some relations expressed through the mathematical model makes it possible to calculate the dependent variables at other nodes.

Normally the calculation is progressing in time, which means that the dependent variables are determined at all nodes at a lower time level before the calculation starts at a higher time level. But in rare occasions it could be suitable to let the calculation make progress in space, and then the dependent variable is determined for all time levels at the first space level, before the calculation starts at the next space level. These two situations are illustrated

in Fig. 2.3. In the following sections only calculations which make progress in time will be considered.

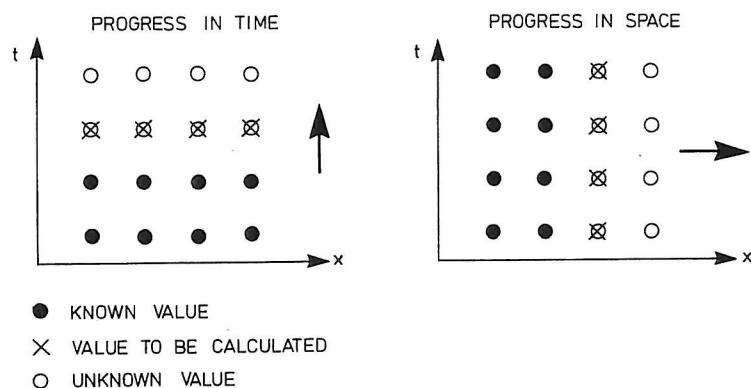


Fig. 2.3. Direction of numerical calculations.

### Explicit/implicit formulation

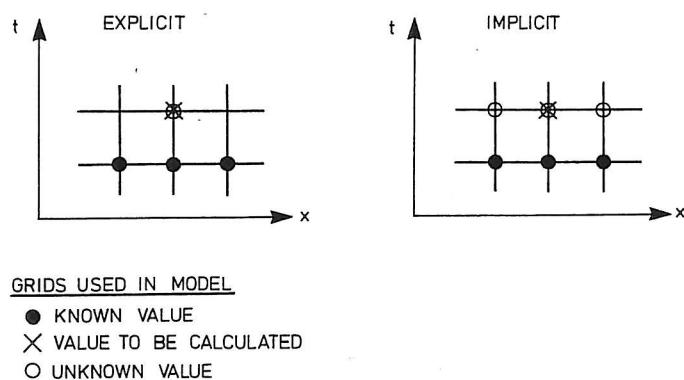


Fig. 2.4. Explicit and implicit numerical method.

If only known values from a lower time level are used in the numerical determination of a dependent variable, then the numerical model is explicit and we are able to determine the variable directly from the equations, as only one unknown variable is present.

The numerical model is called implicit if more than one unknown value of the dependent variable occurs in the equations. Then a system of equations has to be drawn up, and solved by use of a solution technique for systems of equations, which will be described in section 2.6.

### Initial conditions

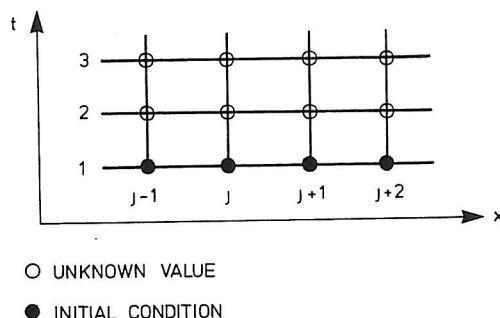


Fig. 2.5. Initial conditions.

Before the numerical calculation can start, we have to know the value of the dependent variables or a way to calculate these at the lowest time level. This is called the initial conditions.

### Boundary conditions

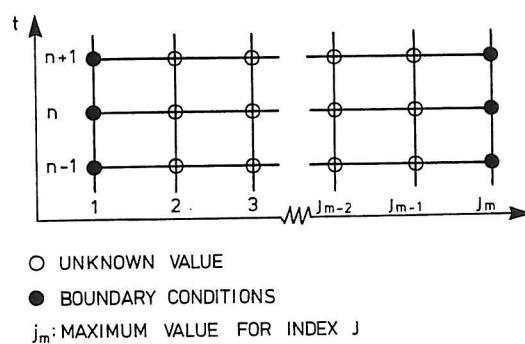


Fig. 2.6. Boundary conditions.

To start and to finish the calculation at one time level, normally two boundary conditions are needed, i.e. a condition at the upper boundary located at the first space level and a condition at the lower boundary located at the last space level. The boundary conditions can consist of known values of the dependent variable for all time levels or of a specific way to calculate the dependent variable at the boundary.

### Stability conditions and numerical errors

As mentioned before the numerical model only provides an approximation to the true solution of the mathematical model. This means that the calculation is encumbered with errors. These numerical errors can be divided into two classes:

- round off errors created by the computer, which only works with a limited number of digits
- truncation errors provided by the numerical model, in which the continuous mathematical model is approximated with a discrete formulation.

Normally only the last type of error is important for practical numerical modelling.

Each step in the numerical calculation is affected by the truncation error, and if the error accumulates, it might result in absurd results, often violent oscillations and computer "crash". In this case the numerical model is unstable. But it is important to remember that all numerical models are encumbered with errors, and even if these errors do not accumulate, – the model is stable, then the magnitude of the numerical errors can make the achieved results useless.

In Fig. 2.7 a typical unstable calculation of a Transport/Dispersion model is shown.

Later on in chapter 4 some methods to predict under which conditions a numerical model is stable will be described. Also some methods for estimating the truncation error will be discussed.

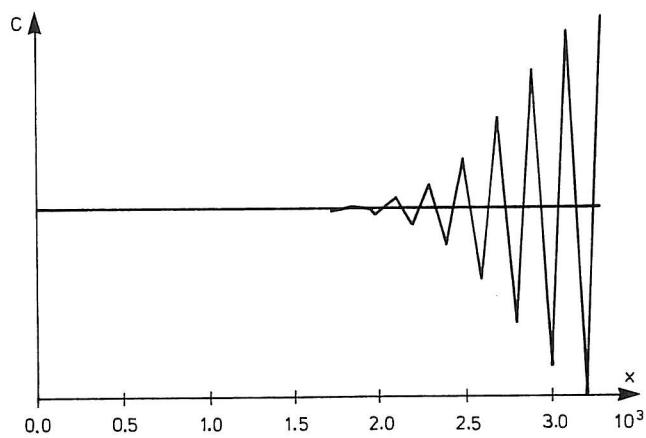


Fig. 2.7. Unstable numerical calculation.

## 2.3 The Control Volume approach

The Control Volume approach is a very straightforward method, where the numerical scheme is obtained directly from the grid and the mathematical expressions for the present physical phenomena.

Equation (2.1) can be found from a continuity on a infinite small element, or a control volume, of water. If exactly the same approach is used on a finite element of water, of the length  $\Delta x$ , then the numerical scheme can be written directly. Many different schemes can be obtained, explicit or implicit, but in this section only one of each type will be developed. A parallel development will be performed, where explicit expressions are labelled *a* and implicit expressions *b*.

A control volume with the length  $\Delta x$  is considered, Fig. 2.8. The grid-points are related to the middle of the element, and the dependent variable  $C$  is the average concentration in the element or control volume (CV).

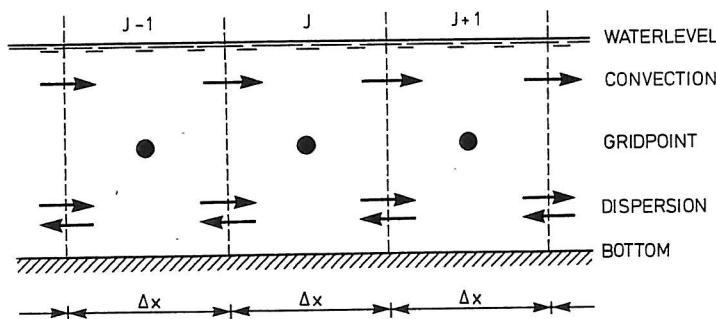


Fig. 2.8. Definition sketch for a control volume.

At the time  $t$  (index  $n$ ) the total amount of matter in the control volume (index  $j$ ) can be expressed as:

$$C_j^n \cdot A \cdot \Delta x \quad (2.2)$$

where  $A$  is the cross section area. During the time  $\Delta t$  a change in the concentration occurs, and at the time  $t + \Delta t$  (index  $n + 1$ ) the total amount of matter is:

$$C_j^{n+1} \cdot A \cdot \Delta x \quad (2.3)$$

These two equations are identical whether the scheme is explicit or implicit. But for the convective and the dispersive transport across the limits of the CV, different expressions are used for an explicit and an implicit model.

During the time  $\Delta t$  some matter are transported into the CV by convection from control volume no.  $j - 1$ . If the concentration in the convected water is expressed as the average between the concentration in CV no.  $j - 1$  and CV no.  $j$  at time level  $n$ , then the total amount of matter convected into CV no.  $j$  can be written as:

$$Q \cdot \Delta t \frac{C_{j-1}^n + C_j^n}{2} \quad (2.4 \text{ a})$$

where  $Q$  is the flow. But since this process takes place between time  $n$  and  $n + 1$ , instead the average of the concentrations at time  $n$  and  $n + 1$  could be used. This would form an implicit expression:

$$Q \frac{\Delta t}{2} \left( \frac{C_{j-1}^n + C_{j-1}^{n+1}}{2} + \frac{C_j^n + C_j^{n+1}}{2} \right) \quad (2.4 \text{ b})$$

In exactly the same way the convection out of CV no.  $j$  during the time  $\Delta t$  can be expressed explicit

$$Q \cdot \Delta t \frac{C_j^n + C_{j+1}^n}{2} \quad (2.5 \text{ a})$$

or implicit

$$Q \frac{\Delta t}{2} \left( \frac{C_j^n + C_j^{n+1}}{2} + \frac{C_{j+1}^n + C_{j+1}^{n+1}}{2} \right) \quad (2.5 \text{ b})$$

But during  $\Delta t$  also dispersion occurs. If the dispersion is assumed to be a Fickian diffusion process, then the transport of matter into CV no.  $j$  from CV no.  $j - 1$  can be written explicit as:

$$-K_x \cdot A \cdot \Delta t \frac{\partial C}{\partial x} \sim -K_x \cdot A \cdot \Delta t \frac{C_j^n - C_{j-1}^n}{\Delta x} \quad (2.6 \text{ a})$$

and implicit as:

$$-K_x \cdot A \cdot \Delta t \frac{\partial C}{\partial x} \sim -K_x \cdot A \frac{\Delta t}{2} \left( \frac{C_j^n - C_{j-1}^n}{\Delta x} + \frac{C_j^{n+1} - C_{j-1}^{n+1}}{\Delta x} \right) \quad (2.6 \text{ b})$$

where  $K_x$  is the one-dimensional longitudinal dispersion coefficient. Notice the way of expressing the first derivative in space. This will be treated further in section 2.5.

Finally the dispersion from CV no.  $j$  into CV no.  $j + 1$  can be written as:

$$-K_x \cdot A \cdot \Delta t \frac{\partial C}{\partial x} \sim -K_x \cdot A \cdot \Delta t \frac{C_{j+1}^n - C_j^n}{\Delta x} \quad (2.7 \text{ a})$$

or

$$-K_x \cdot A \cdot \Delta t \frac{\partial C}{\partial x} \sim -K_x \cdot A \frac{\Delta t}{2} \left( \frac{C_{j+1}^n - C_j^n}{\Delta x} + \frac{C_{j+1}^{n+1} - C_j^{n+1}}{\Delta x} \right) \quad (2.7 \text{ b})$$

By use of all these expressions a continuity for the CV no.  $j$  during the time  $\Delta t$  can be written, knowing that:

$$\begin{array}{lcl} \text{storage} & = & \text{inflow} - \text{outflow} \\ (2.3 - 2.2) & & (2.4 + 2.6) - (2.5 + 2.7) \end{array}$$

which yields:

$$\begin{aligned} C_j^{n+1} \cdot A \cdot \Delta x - C_j^n \cdot A \cdot \Delta x &= \\ Q \cdot \Delta t \frac{C_{j-1}^n + C_j^n}{2} - K_x \cdot A \cdot \Delta t \frac{C_j^n - C_{j-1}^n}{\Delta x} - \\ Q \cdot \Delta t \frac{C_j^n + C_{j+1}^n}{2} + K_x \cdot A \cdot \Delta t \frac{C_{j+1}^n - C_j^n}{\Delta x} \\ \Downarrow \\ C_j^{n+1} &= u \frac{\Delta t}{\Delta x} \frac{C_{j-1}^n - C_{j+1}^n}{2} + \\ K_x \frac{\Delta t}{\Delta x^2} (C_{j-1}^n - 2 \cdot C_j^n + C_{j+1}^n) + C_j^n \end{aligned} \quad (2.8 \text{ a})$$

for the explicit model, while the implicit model yields:

$$\begin{aligned} C_j^{n+1} \cdot A \cdot \Delta x - C_j^n \cdot A \cdot \Delta x &= \\ Q \frac{\Delta t}{2} \left( \frac{C_{j-1}^n + C_{j-1}^{n+1}}{2} + \frac{C_j^n + C_j^{n+1}}{2} \right) - \end{aligned}$$

$$\begin{aligned}
& K_x \cdot A \frac{\Delta t}{2} \left( \frac{C_j^n - C_{j-1}^n}{\Delta x} + \frac{C_j^{n+1} - C_{j-1}^{n+1}}{\Delta x} \right) - \\
& Q \frac{\Delta t}{2} \left( \frac{C_j^n + C_j^{n+1}}{2} + \frac{C_{j+1}^n + C_{j+1}^{n+1}}{2} \right) + \\
& K_x \cdot A \frac{\Delta t}{2} \left( \frac{C_{j+1}^n - C_j^n}{\Delta x} + \frac{C_{j+1}^{n+1} - C_j^{n+1}}{\Delta x} \right) \\
& \Downarrow \\
& \left( -\frac{1}{4} u \frac{\Delta t}{\Delta x} - \frac{1}{2} K_x \frac{\Delta t}{\Delta x^2} \right) C_{j-1}^{n+1} + \\
& \left( 1 + K_x \frac{\Delta t}{\Delta x^2} \right) C_j^{n+1} + \\
& \left( \frac{1}{4} u \frac{\Delta t}{\Delta x} - \frac{1}{2} K_x \frac{\Delta t}{\Delta x^2} \right) C_{j+1}^{n+1} = \\
& \left( \frac{1}{4} u \frac{\Delta t}{\Delta x} + \frac{1}{2} K_x \frac{\Delta t}{\Delta x^2} \right) C_{j-1}^n + \\
& \left( 1 - K_x \frac{\Delta t}{\Delta x^2} \right) C_j^n + \\
& \left( -\frac{1}{4} u \frac{\Delta t}{\Delta x} + \frac{1}{2} K_x \frac{\Delta t}{\Delta x^2} \right) C_{j+1}^n
\end{aligned} \tag{2.8 b}$$

Now the difference between explicit and implicit schemes are easily seen. From eq. (2.8 a) the unknown concentration in CV no.  $j$  at time level  $n + 1$  can be evaluated directly, since only one unknown variable is present, while the implicit expression contains three unknown variables.

But if equation (2.8 b) is used for every CV on time level  $n + 1$  and suitable boundary conditions are made, then a linear system of equations appears. In vector and matrix notation this can be written as:

$$\bar{\bar{A}} \cdot \bar{C} = \bar{b} \tag{2.9}$$

where the coefficient matrix  $A$  is a tridiagonal matrix. By solving this linear system of equations the concentrations at timelevel  $n + 1$  can be determined. How to solve the system is described in section 2.6.

## 2.4 The Method of Characteristics

The Method of Characteristics has not been used so often in modelling of open channels, except when dealing with special problems as sudden release of a large amount of water, e.g. in connection with dambreaks etc. Examples can be found in Abbott (1979) and Sjöberg (1976). But when dealing with flow in pipes under pressure, the method have been widely applied.

The main idea in the method is to rewrite the governing differential equations, using that some specific features are present along the characteristics, which are some specific conditions. Under these conditions the rewritten equations can be solved, often quite easily.

Even though the method has not been applied very often for open channel modelling, it is well worth to spend some time and space for describing the method. Many elements are common with other types of numerical methods, and the method is very valuable for the understanding of some aspects in numerical modelling. Furthermore some physical phenomena are easily explained by use of the characteristics.

When dealing with the Transport/Dispersion model the rewriting of the governing equation is easily done. If the original equation:

$$\frac{\partial C}{\partial t} + u \frac{\partial C}{\partial x} = K_x \frac{\partial^2 C}{\partial x^2} \quad (2.10)$$

is multiplied with  $dt$ :

$$\frac{\partial C}{\partial t} dt + u \cdot dt \frac{\partial C}{\partial x} = K_x \frac{\partial^2 C}{\partial x^2} dt \quad (2.11)$$

This equation can be rewritten under the following condition:

$$dx = u \cdot dt \quad (2.12)$$

and we get:

$$\frac{\partial C}{\partial t} dt + \frac{\partial C}{\partial x} dx = K_x \frac{\partial^2 C}{\partial x^2} dt \quad (2.13)$$

↓

$$dC = K_x \frac{\partial^2 C}{\partial x^2} dt \quad \text{for} \quad dx = u \cdot dt \quad (2.14)$$

An integration of this expression yields:

$$\Delta C = \int_0^{\Delta t} K_x \frac{\partial^2 C}{\partial x^2} dt \quad (2.15)$$

If it is assumed that the dispersion can be neglected, then a very simple expression occurs:

$$\Delta C = 0 \quad \text{for} \quad dx = u \cdot dt \quad (2.16)$$

This means that the concentration will not change if the condition in expression (2.12) is fulfilled. This can be illustrated in a graphical way, Fig 2.9. If the numerical calculation proceeds along the characteristic, determined of expression (2.12), which forms a straight line with the slope  $1/u$ , then the concentration will not change. If dispersion cannot be neglected, then the concentration will change, but only as a result of dispersion (eq. 2.15).

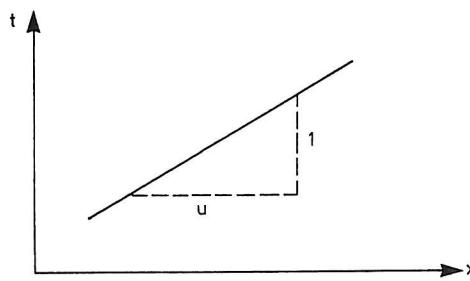


Fig. 2.9. The characteristic for a Transport model.

This quality can be used when choosing the numerical grid, Fig. 2.10. If the grid is determined from expression (2.12), which in a discrete manner can be written as:

$$\Delta x = u \cdot \Delta t \quad (2.17)$$

then the numerical scheme for the pure convective transport model becomes very simple:

$$C_{j+1}^{n+1} = C_j^n \quad (2.18)$$

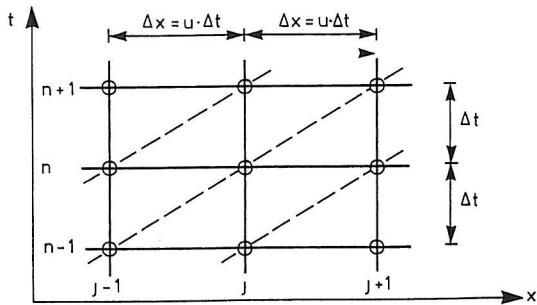


Fig. 2.10. Numerical grid for the Transport equation.

Another way for achieving this result would be to use a movable coordinate system - a system moving downstream with the speed of  $u$  (Fischer, 1979). This would result in identical equations as above. Using this approach a model for the Transport/Dispersion equation is easily obtained. Referring to the notation at Fig. 2.11 and using an explicit formulation of the dispersion term, a numerical scheme could be:

$$C_j^{n+1} = C_j^n + K_x \cdot \Delta t \frac{C_{j+1}^n - 2 \cdot C_j^n + C_{j-1}^n}{\Delta x^2} \quad (2.19)$$

It can be seen that this expression is very like the one achieved using the traditional Control Volume approach, except that using the movable coordinate system (or The Method of Characteristics) eliminates the convective transport term.

When the flow is assumed to be steady and uniform, then the Method of Characteristics provides very simple numerical schemes as seen above. If the flow is non-uniform and/or unsteady, then the expressions become much more complicated, and then other methods seem to be more attractive.

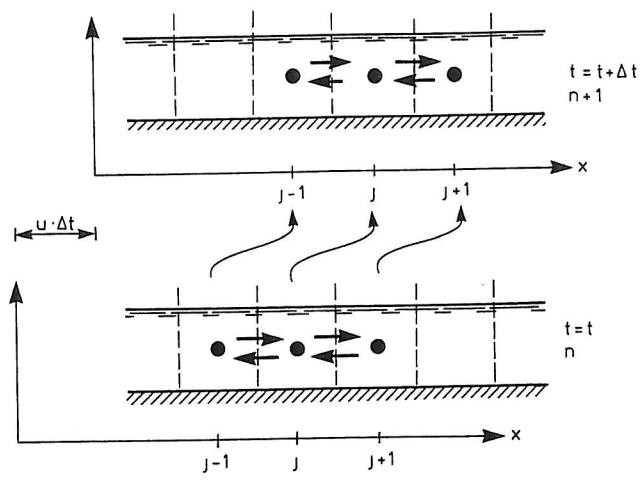


Fig. 2.11. Movable coordinate system.

## 2.5 Finite Differences

Finite differences is the most commonly used numerical method for open channel modelling, and many different numerical schemes have been developed and applied.

The method is based directly on the governing differential equations. These are transformed into difference equations through a discretization, – a transformation from a continuous domain into a discrete domain.

Discretization of a first derivative can be performed in three different ways. Referring to the function  $f$  in Fig. 2.12 the derivative at point  $b$  can be approximated either by use of values of  $f$  at  $a$  and  $b$ ,  $b$  and  $c$ , or  $a$  and  $c$ .

Backward difference ( $a$  &  $b$ ):

$$\left. \frac{\partial f}{\partial \Theta} \right|_b \sim \frac{f(\Theta_b) - f(\Theta_a)}{\Theta_b - \Theta_a} \quad (2.20)$$

Forward difference ( $b$  &  $c$ ):

$$\left. \frac{\partial f}{\partial \Theta} \right|_b \sim \frac{f(\Theta_c) - f(\Theta_b)}{\Theta_c - \Theta_b} \quad (2.21)$$

Central difference ( $a$  &  $c$ ):

$$\left. \frac{\partial f}{\partial \Theta} \right|_b \sim \frac{f(\Theta_c) - f(\Theta_a)}{\Theta_c - \Theta_a} \quad (2.22)$$

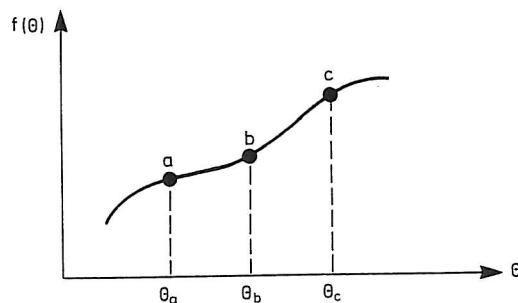


Fig. 2.12. Sketch of a function  $f$ .

A discretization of a second derivative at point  $b$  is normally performed as a central difference:

$$\frac{\partial^2 f}{\partial \Theta^2} = \frac{\partial}{\partial \Theta} \left( \frac{\partial f}{\partial \Theta} \right) \sim \frac{\frac{f(\Theta_c) - f(\Theta_b)}{\Theta_c - \Theta_b} - \frac{f(\Theta_b) - f(\Theta_a)}{\Theta_b - \Theta_a}}{\frac{1}{2} (\Theta_c - \Theta_a)} \quad (2.23)$$

If the governing equation is partial, – the numerical calculation proceeds in time as well in space, e.g. the Transport/Dispersion model, then several combinations of time and space derivatives can be used in the discretization.

Using a forward time derivative and central space derivatives for the Transport/Dispersion model, we get:

$$\begin{aligned} \frac{\partial C}{\partial t} + u \frac{\partial C}{\partial x} &= K_x \frac{\partial^2 C}{\partial x^2} \quad \rightsquigarrow \\ \frac{C_j^{n+1} - C_j^n}{\Delta t} + u \frac{C_{j+1}^n - C_{j-1}^n}{2 \cdot \Delta x} &= K_x \frac{\frac{C_{j+1}^n - C_j^n}{\Delta x} - \frac{C_j^n - C_{j-1}^n}{\Delta x}}{\Delta x} \\ \Downarrow \\ C_j^{n+1} &= C_j^n - u \frac{\Delta t}{\Delta x} \frac{C_{j+1}^n - C_{j-1}^n}{2} + \\ &\quad K_x \frac{\Delta t}{\Delta x^2} (C_{j+1}^n - 2 \cdot C_j^n + C_{j-1}^n) \end{aligned} \quad (2.24)$$

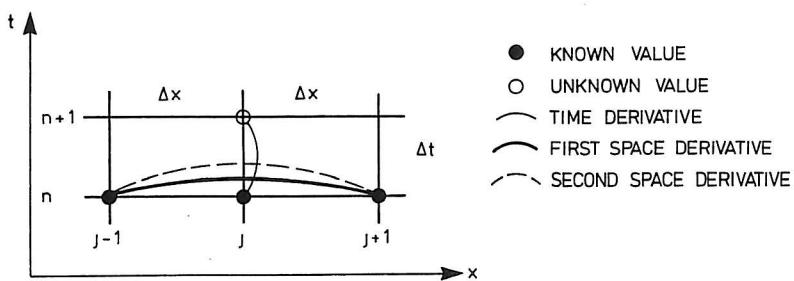


Fig. 2.13. The forward time central space scheme (FTCS).

This numerical scheme is called FTCS (Forward Time Central Space) and is illustrated in Fig. 2.13. Since only one unknown value occurs in the

difference equation, this scheme is explicit, and since central differences are used for the space derivatives, the scheme is centered in space, but not in time.

A fully centered scheme can be developed by use of a slightly different formulation of the space derivatives. If these are expressed as average values of the derivatives at time level  $n$  and  $n + 1$ , Fig. 2.14, then another scheme turns up:

$$\frac{\partial C}{\partial t} + u \frac{\partial C}{\partial x} = K_x \frac{\partial^2 C}{\partial x^2} \quad \sim$$

$$\frac{C_j^{n+1} - C_j^n}{\Delta t} + u \frac{1}{2} \left( \frac{C_{j+1}^{n+1} - C_{j-1}^{n+1}}{2 \cdot \Delta x} + \frac{C_{j+1}^n - C_{j-1}^n}{2 \cdot \Delta x} \right) = \\ K_x \frac{1}{2} \left( \frac{C_{j+1}^{n+1} - 2 \cdot C_j^{n+1} + C_{j-1}^{n+1}}{\Delta x^2} + \frac{C_{j+1}^n - 2 \cdot C_j^n + C_{j-1}^n}{\Delta x^2} \right)$$

↓

$$\left( -\frac{1}{4} u \frac{\Delta t}{\Delta x} - \frac{1}{2} K_x \frac{\Delta t}{\Delta x^2} \right) C_{j-1}^{n+1} + \\ \left( 1 + K_x \frac{\Delta t}{\Delta x^2} \right) C_j^{n+1} + \\ \left( \frac{1}{4} u \frac{\Delta t}{\Delta x} - \frac{1}{2} K_x \frac{\Delta t}{\Delta x^2} \right) C_{j+1}^{n+1} = \\ \left( \frac{1}{4} u \frac{\Delta t}{\Delta x} + \frac{1}{2} K_x \frac{\Delta t}{\Delta x^2} \right) C_{j-1}^n + \\ \left( 1 - K_x \frac{\Delta t}{\Delta x^2} \right) C_j^n + \\ \left( -\frac{1}{4} u \frac{\Delta t}{\Delta x} + \frac{1}{2} K_x \frac{\Delta t}{\Delta x^2} \right) C_{j+1}^n \quad (2.25)$$

Since more than one unknown concentration is present, this is an implicit scheme and in the following this will be called the Crank & Nicholson scheme, since the way of expressing the second derivative in eq. (2.25) was suggested by Crank and Nicholson.

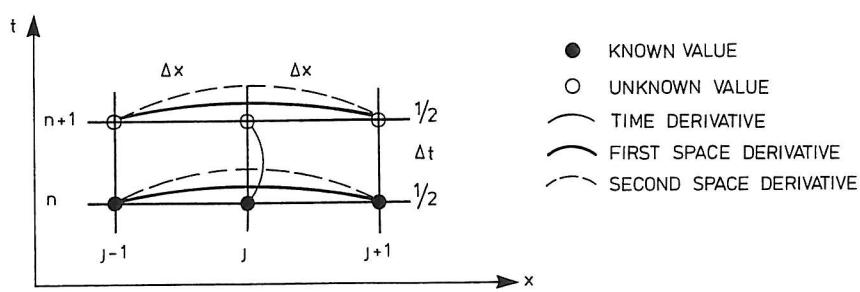


Fig. 2.14. The Crank & Nicholson scheme.

If the two schemes above, – the FTCS scheme and the Crank & Nicholson scheme, are compared with the two schemes obtained by use of the Control Volume approach in sec. 2.3, then we discover that the schemes are identical. The only difference is the way of obtaining the schemes. Boundary conditions and solution techniques can be applied in an equal manner, and often the two methods are mixed, especially for expressing the boundary conditions in the finite difference schemes.

## 2.6 Solution of large systems of equations

Very often large systems of equations are developed in numerical modelling, e.g. when using implicit schemes. These systems of equations must be solved in an accurate and quick way. Mostly the equations are linear, as e.g. the equations determined in the Crank & Nicholson scheme, sec. 2.5, but also non-linear equations can be present. Normally non-linear mathematical models should provide non-linear systems of equations, but often the discretization is performed in a special way providing a linear system of equations. An example of this can be seen in chapter 3.

Large systems of equations can be solved in several ways, which roughly can be divided into two classes, – methods of iteration and methods of elimination. Five different methods will be mentioned briefly in the following. For a more complete description the reader should consult the references.

The most simple method to apply is iteration directly in the system of equations. This method can be applied on as well linear as non-linear systems. Having  $n$  equations with  $n$  variables, each variable can be isolated from one of the equations, and in this rewritten system an iteration can be performed. Often many iterations are needed to obtain an accurate solution, and in the worst case the iteration may not converge against a solution at all.

Another iterative method is the Newton-Raphson iteration, which also can be applied on non-linear equations. Still the iteration may not converge, but if it does then it will converge much quicker than the direct iteration. The method is much more complicated to apply since the first derivatives of the functions describing the variables must be known, by use of either an analytical expression or a numerical approximation. A complete mathematical description of iteration methods can be found in e.g. Kreyzig (1979), and examples of application in e.g. Vestergaard (1985).

Instead elimination methods can be applied, but only if the equations are linear. Gauss elimination (Kreyzig, 1979) is a possible way to solve the system, but for large systems of equations the method may not be very attractive. Instead two special variations of the Gauss elimination, using some further information of the system to be solved, can be applied.

The first one is perhaps the most widely used elimination algorithm in numerical modelling, namely the Double Sweep algorithm, which is a solution technique for tridiagonal systems, as e.g. the set of equations from the Crank

& Nicholson scheme, sec. 2.5. The method is easily applied and solutions are obtained very quickly. A description can be found in e.g. Cunge et al. (1980).

As mentioned above the Double Sweep algorithm are widely used in numerical modelling, and later on in this work several applications of the method can be found.

$$\begin{array}{c}
 = \\
 \left[ \begin{array}{ccccc} x & x & & & \\ x & x & x & & \\ x & x & x & & \\ x & x & x & x & \\ x & x & x & x & x \end{array} \right] \cdot \left[ \begin{array}{c} c \\ c \\ c \\ c \\ c \end{array} \right] = \left[ \begin{array}{c} x \\ x \\ x \\ x \\ x \end{array} \right] \\
 = \\
 \left[ \begin{array}{cccc} & & & \\ & x & x & x \end{array} \right] \cdot \left[ \begin{array}{c} c \\ c \\ c \\ c \\ c \end{array} \right] = \left[ \begin{array}{c} x \\ x \\ x \\ x \\ x \end{array} \right]
 \end{array}$$

Fig. 2.15. Tridiagonal linear system of equations, where  $x$  denotes an element different from zero, and  $C$  are variables to be determined.

If the system is not tridiagonal, but still only a few elements in each row in the matrix are different from zero, then the EQSOLV-procedure (Gupta & Tanji, 1977) can be applied. This algorithm is created for solution of large and sparse systems of linear equations, and only elements different from zero are treated during the elimination. An example of application can be found in Vestergaard (1985).

# Chapter 3

## Hydrodynamic Models

### 3.1 Introduction

Hydrodynamic modelling has been used for several years. A lot of different mathematical and numerical models, in a large range of complexity, have been applied on a great amount of problems.

The purpose has mainly been to determine pure hydraulic results, e.g. to determine the water level during a tidal period or to simulate the runoff in a stream during rainfall. But in the latest years another purpose has been more and more present, namely water quality modelling. In this type of models the hydrodynamic modelling is no longer the main purpose, but still it is very important, since the achieved results are used for simulation of transport, spreading and decay of pollutants. So in a very coarse way hydrodynamic modelling can be divided into two:

- Pure hydrodynamic modelling, where only hydraulic features are taken into account.
- Water quality modelling, where the hydrodynamic modelling is an important part, but not the main purpose.

Depending on the purpose different hydrodynamic models may be chosen, mathematical as well as numerical. Generally there is no need for implementation of a very general and therefore complex model, if only a few physical phenomena are important, or if only a limited number of data are available for calibration and validation.

A lot of modelling, especially water quality modelling for long time events, can be performed under assumption of steady state flow, but for short time events unsteady flow phenomena may be very important. The mathematical description is normally formulated in two equations, – one equation for conservation of mass or volume, and one equation for conservation of momentum or energy. These equations will be formulated in sec. 3.2, divided into steady and unsteady flow conditions.

The same division has been made in the description of the numerical hydrodynamic models. Models for steady flow conditions can be found in sec. 3.3, and models for unsteady flow conditions in sec. 3.4.

As a result of many years development and applications of numerical hydrodynamic models, a lot of literature is accessible, and description of hundreds of models can be found. In this work only a brief description of different types of numerical models will be given, with the purpose to create a coarse view over this extensive subject. Only a few models will be described in some details. Important subjects as stability and numerical errors will only be mentioned in a very brief way, for futher studies the reader should consult the references.

## 3.2 Mathematical Models

### 3.2.1 Steady flow

#### Piecemeal uniform flow

The most simplyfied model for steady flow assumes that normal depth is present in every cross section of the stream - a piecemeal uniform flow. Under these assumptions the continuity for mass and momentum can be written as:

Mass:

$$\frac{dQ}{dx} = q \quad (3.1)$$

Momentum:

$$I = I_o \quad (3.2)$$

where  $Q$  : flow ( $m^3/sec$ )

$q$  : lateral inflow per unit length ( $m^2/sec$ )

$x$  : space-coordinate ( $m$ )

$I_o$  : bottom slope

$I$  : friction slope

For determination of the friction slope several formulas can be used. For open channel flow normally the Chezy or the Manning formula is applied.

Chezy:

$$V = \frac{Q}{A} = C \sqrt{R \cdot I} \implies I = \frac{Q^2}{C^2 \cdot R \cdot A^2} \quad (3.3)$$

Manning:

$$V = \frac{Q}{A} = M \cdot R^{2/3} \sqrt{I} \implies I = \frac{Q^2}{M^2 \cdot R^{4/3} \cdot A^2} \quad (3.4)$$

where  $V$  : average velocity ( $m/sec$ )

$A$  : cross section area ( $m^2$ )

$C$  : Chezy number ( $m^{1/2}/sec$ )

$M$  : Manning number ( $m^{1/3}/sec$ )

and where  $R$  can be either the hydraulic radius or the resistance radius:

Hydraulic radius:

$$R = \frac{A}{P} \quad (3.5)$$

Resistance radius:

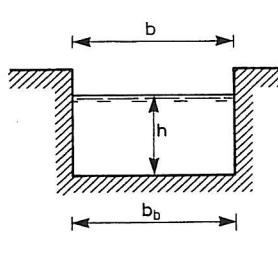
$$R = \left( \frac{1}{A} \int_0^b h^{3/2} \cdot d\beta \right)^2 \quad (3.6)$$

where  $P$  : wetted perimeter ( $m$ )

$b$  : width of cross section at the surface ( $m$ )

$h$  : local waterdepth ( $m$ )

Which one to use depends on the distribution of the bed shear stress along the wetted perimeter. If a uniform distribution can be assumed then the hydraulic radius can be applied, otherwise the resistance radius should be used. A further discussion of this choice can be found in Engelund & Pedersen (1978).



Area	$A = h \cdot b_b$
Width	$b = b_b$
Wetted perimeter	$P = 2 \cdot h + b_b$
Hydraulic radius	$R = \frac{A}{P} = \frac{h \cdot b_b}{2 \cdot h + b_b}$
Resistance radius	$R = \left( \frac{1}{A} \int_0^b h^{3/2} \cdot d\beta \right)^2 = h$

Fig. 3.1. Geometrical parameters for a rectangular cross section.

To complete this set of equations for determination of the flow  $Q$  and the depth  $h$  (or water stage  $y$ ), the cross section must be known in a way that makes it possible to determine the cross section area  $A$  and the hydraulic radius/resistance radius  $R$  as functions of the depth. Mathematical relationships can be developed if the geometry of the cross section is simple, as e.g. the rectangular cross section in Fig. 3.1. If the geometry is more complicated, as for cross sections in natural streams, a numerical cross section

analysis must be applied. How this numerical integration can be performed, can be found in Vestergaard (1985) or Vestergaard (1988).

The steady and piecemeal uniform model should only be applied if the stream is almost prismatic, which means that the variation of the cross sections is very slow, – no backwater effects due to change in cross section must be present. Furthermore, backwater effects due to constructions or fixed water levels in lakes, estuaries, etc. cannot be determined.

#### Non-uniform flow

If backwater effects are important, as in most natural streams, then the following model could be applied. Still the flow is assumed to be steady, but the flow is no longer assumed to be uniform. These conditions lead to new formulations of the two continuity equations (the development can be found in e.g. Engelund & Pedersen (1978) ):

Mass:

$$\frac{dQ}{dx} = q \quad (3.7)$$

Momentum:

$$\frac{d}{dx} \left( \alpha \frac{V^2}{2 \cdot g} + h \right) = I_o - I \quad (3.8)$$

where  $\alpha$  : velocity distribution coefficient.

The friction slope, cross section area, etc. are determined like for the uniform model mentioned above. By use of this set of equations backwater effects caused by constructions, fixed water levels or variations in cross section shape can be determined.

Often the momentum equation is exchanged with an equation describing conservation of energy. This equation is often formulated directly in a discrete manner. By using the notations in Fig. 3.2 the energy balance between the two cross-sections can be written as:

$$z_1 + h_1 + \alpha \frac{V_1^2}{2 \cdot g} = z_2 + h_2 + \alpha \frac{V_2^2}{2 \cdot g} + \Delta h \quad (3.9)$$

where  $\Delta h$  is the energy loss at the reach which, assuming that only friction loss is present, can be found from:

$$\Delta h = I \cdot \ell \quad (3.10)$$

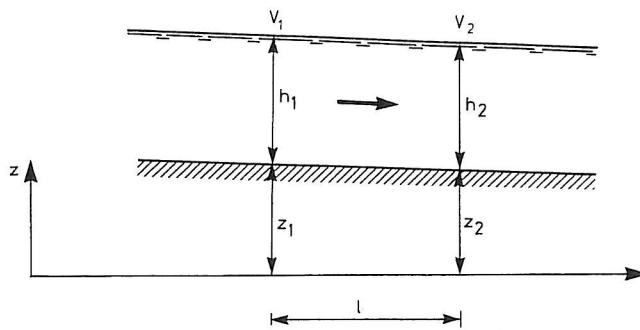


Fig. 3.2. Energy balance between two cross-sections.

An important parameter, when using the above mentioned model, is the Froude number, defined as:

$$Fr = \frac{V}{\sqrt{g \cdot D}} \quad (3.11)$$

where  $D$  is the mean depth:

$$D = \frac{A}{b} \quad (3.12)$$

For most Danish streams the Froude number will be lesser than one, which means that the flow will be subcritical, but for steep streams ( $I_o > 0.01$ ) the Froude number may be greater than one, which yields supercritical flow. For both occasions the models mentioned above may be applied, but in the area of transition, near the critical depth  $h_c$ , the basic assumption of a hydrostatic pressure field is violated, and usable results cannot be achieved.

Many efforts have been made to develop a proper mathematical description of the flow in the area of transition. An example can be found in Mandrup Andersen (1975). In Engelund & Pedersen (1978) the traditional energy formula (eq. 3.9) is extended with a term describing the curvate of the streamlines, which should make it possible to determine the water stage near critical depth. If this term is introduced, eq.(3.9) is extended to:

$$\begin{aligned} z_1 + h_1 + \alpha \frac{V_1^2}{2 \cdot g} + h_1 \frac{V_1^2}{3 \cdot g} \frac{\partial^2 h}{\partial x^2} |_1 = \\ z_2 + h_2 + \alpha \frac{V_2^2}{2 \cdot g} + h_2 \frac{V_2^2}{3 \cdot g} \frac{\partial^2 h}{\partial x^2} |_2 + \Delta h \end{aligned} \quad (3.13)$$

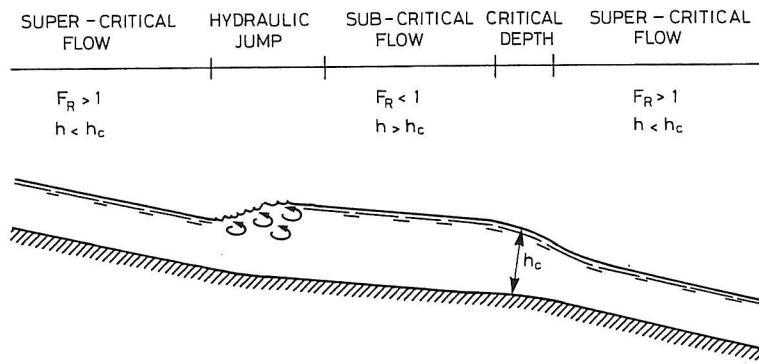


Fig. 3.3. Froude number for different flow conditions.

### 3.2.2 Unsteady flow

#### The Saint Venant equations

The most common used hydrodynamic models are based on the Saint Venant equations for unsteady flow, – one equation for continuity of mass (or volume) and one continuity equation for momentum. The equations are developed under the following assumptions:

- the water is homogeneous and incompressible
- the flow is one-dimensional
- the pressure is hydrostatic
- the friction can be determined as for steady flow
- the average bed slope is small

Often the Saint Venant equations are written as:

Mass:

$$b \frac{\partial y}{\partial t} + \frac{\partial Q}{\partial x} = q \quad (3.14)$$

### Momentum

$$\frac{\partial Q}{\partial t} + \frac{\partial}{\partial x} \left( \alpha \frac{Q^2}{A} \right) + g \cdot A \frac{\partial y}{\partial x} + g \cdot A \cdot I = q \cdot u_q \quad (3.15)$$

- where  $y$  : water level ( $m$ )  
 $Q$  : flow ( $m^3/sec$ )  
 $b$  : width ( $m$ )  
 $A$  : cross section area ( $m^2$ )  
 $I$  : energy slope  
 $\alpha$  : non-uniform velocity distribution coefficient  
 $q$  : lateral inflow ( $m^3/m \cdot sec$ )  
 $u_q$  : velocity of lateral inflow in x-direction ( $m/sec$ )  
 $g$  : gravity ( $m/sec$ )  
 $x$  : space-coordinate ( $m$ )  
 $t$  : time-coordinate ( $sec$ )

The development of the Saint Venant equations can be found in e.g. Cunge et al. (1980), Mahmood & Yevjevich (1975), or Brorsen(1988), and will not be treated any further. But it is important to remember which phenomenon the individual term in the equations is describing:

- $b \frac{\partial y}{\partial t}$  : Storage term for flow.
- $\frac{\partial Q}{\partial x}$  : Convective term for flow.
- $q$  : Source/sink term for flow.
- $\frac{\partial Q}{\partial t}$  : Local acceleration.
- $\frac{\partial}{\partial x} \left( \alpha \frac{Q^2}{A} \right)$  : Convective acceleration.
- $g \cdot A \frac{\partial y}{\partial x}$  : A double term which can be divided into two terms.  
  - $g \cdot A \frac{\partial h}{\partial x}$  : Pressure term.
  - $-g \cdot A \cdot I_o$  : Gravity term.
- $g \cdot A \cdot I$  : Friction term.
- $q \cdot u_q$  : Source/sink term.

If all these terms are included in the model, then the model will be able to describe a lot of flow events.

For some special events the model above must be extended with further terms, e.g. a term describing the shear force created by wind.

For a lot of situations a simplified model can be used with success. This reduces the complexity of the numerical model, which can be a great advantage, as well during the development of the model as when the model is used.

### Storage approximation

In a very early stage the hydrodynamic modelling was performed on basis of the storage approximation. In this model only the continuity for mass is used, – the momentum equation is totally neglected, leading to a one-equation model:

$$b \frac{\partial y}{\partial t} + \frac{\partial Q}{\partial x} = q \quad (3.16)$$

Normally the model is written directly as a continuity for a reach assuming that the lateral inflow is zero:

$$\frac{\partial W}{\partial t} = Q_i - Q_u \quad (3.17)$$

where  $W$  : volume ( $m^3$ )

$Q_i$  : inflow to the reach ( $m^3/sec$ )

$Q_u$  : outflow from the reach ( $m^3/sec$ )

Eq.(3.17) is easily obtained from eq.(3.16) by neglecting the lateral inflow and exchanging the convective term with a finite difference.

But in eq.(3.17) two unknown variables occur, namely the outflow, which is to be determined, and the storage at the reach, which must be expressed in some other way. Instead of using a physical relationship, e.g. a momentum equation, pure empirically relationships are introduced, leading to different types of storage models.

In the Muskingum model it is assumed that the volume can be expressed as a linear function of  $Q_i$  and  $Q_u$ :

$$W = K (x \cdot Q_i + (1 - x) Q_u) \quad (3.18)$$

where  $K$  and  $X$  are empirically determined constants for the reach.

Instead a more advanced non-linear expression could be introduced for the volume at the reach:

$$W = K (X \cdot Q_i + (1 - X) Q_u)^m \quad (3.19)$$

where  $m$  also is a constant.

But whether one or another expression for the storage term is applied, the model only makes it possible to determine the flow, and not the water stage (or depth). This must be determined in another way, e.g. as normal depth using a friction formula.

A further description of the storage approach can be found in e.g. Mahmood & Yevjevich (1975), but in this work it will not be treated any further.

### Kinematic wave approximation

Instead of neglecting the momentum equation, a simplified version could be introduced, and then two equations would be available for determination of flow and water stage. In the kinematic wave model it is assumed that only gravity and friction are important, leading to a simplified version of the Saint Venant equations:

Mass:

$$b \frac{\partial y}{\partial t} + \frac{\partial Q}{\partial x} = q \quad (3.20)$$

Momentum:

$$g \cdot A (I - I_o) = q \cdot u_q \quad (3.21)$$

This approximation will be good in steep streams, where only small changes in the water depth occur. Since the pressure term is neglected the model is not able to describe backwater effects.

If the lateral inflow is assumed to be zero, then it is easily seen from eq.(3.21) that the local water depth is determined as the normal depth in the cross section.

The model has mostly been used for modelling of urban runoff in sewers, where the bottom slope is quite large and where backwater effects seldom occur, but also applications for open channel flow can be found.

### Diffusive wave approximation

In the diffusive wave approximation the two initial terms in the momentum equation are neglected. Then the mathematical model can be reduced to:

Mass:

$$b \frac{\partial y}{\partial t} + \frac{\partial Q}{\partial x} = q \quad (3.22)$$

Momentum:

$$g \cdot A \frac{\partial y}{\partial x} + g \cdot A \cdot I = q \cdot u_q \quad (3.23)$$

This approximation will be good when the values of the initial terms are small compared with the other terms in the momentum equation. Normally this will be fulfilled in minor streams with a moderate bottom slope, which will be present for most of the Danish streams, except from the lower part near the mouth.

### Choice of model

Which model to choose cannot be stated in general. The choice must be based on an analysis of the specific task, – which terms are important in the momentum equation and which can be neglected.

To clarify this question several testruns have been performed (Vestergaard, 1989) using a dynamic model for determination of the relative magnitude of the terms in the momentum equation.

Only results from two testruns will be mentioned here. The exact model setup can be found in Vestergaard (1989), but it should be mentioned that the stream is a prismatic rectangular channel with a width of 5 m, bottom slope of  $5 \cdot 10^{-4}$  and a Manning number of  $30 m^{1/3}/sec$ .

In Fig. 3.4 the relative magnitude of the terms in the momentum equation, the flow, and the depth are shown at a certain station, when a flood wave is passing.

From Fig. 3.4 it can be seen that three terms are dominating, namely the gravity, the friction, and the pressure, while the two initial terms seem to be of minor importance – they even counteract each other.

Almost the same picture appears in Fig. 3.5, where the downstream water stage is changed, e.g. by tidal motion.

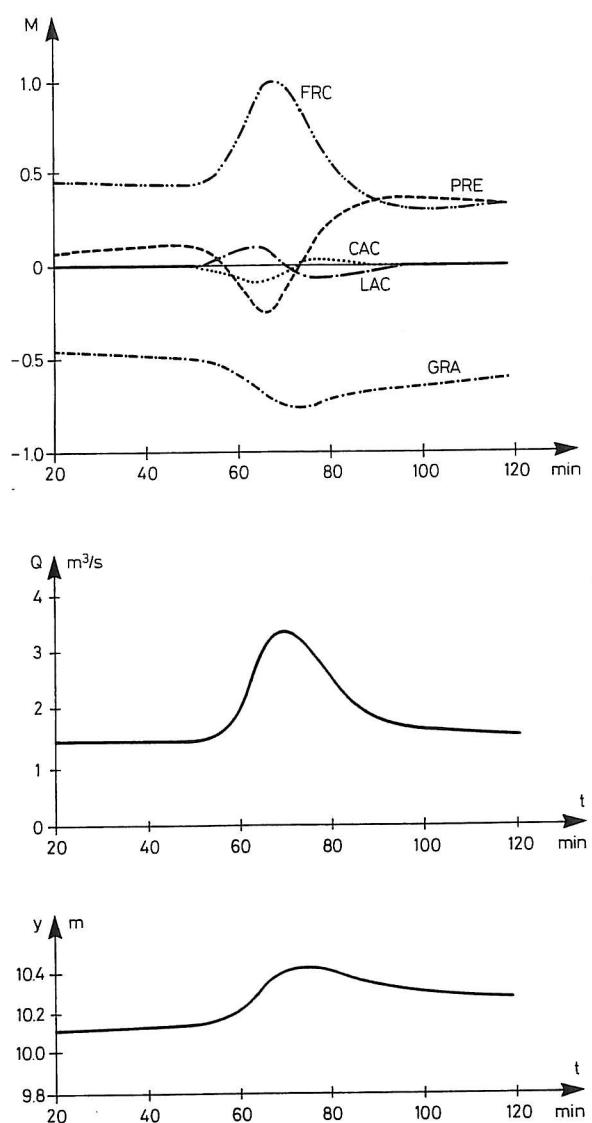


Fig. 3.4. Relative magnitude of the terms in the momentum equation, when a flood wave is passing. LAC: Local acceleration, CAC: Convective acceleration, PRE: Pressure, GRA: Gravity, FRC: Friction.

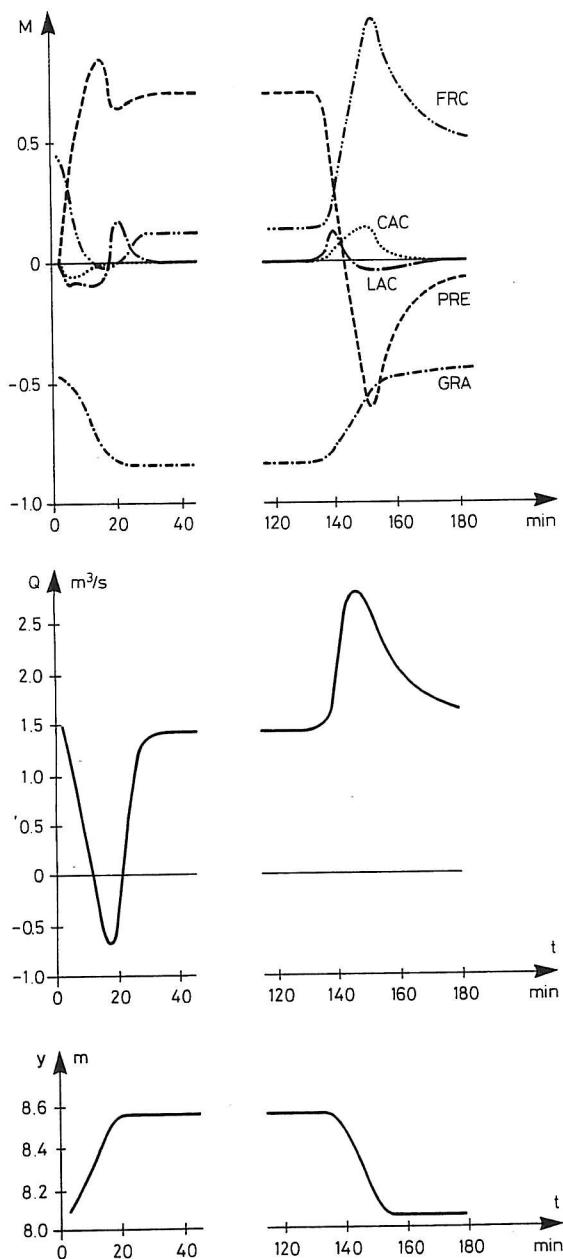


Fig. 3.5. Relative magnitude of the terms in the momentum equation, for downstream variation in the water stage. LAC: Local acceleration, CAC: Convective acceleration, PRE: Pressure, GRA: Gravity, FRC: Friction.

As mentioned, general guidelines can hardly be stated but, nevertheless, some guidelines for an initial choice of momentum equation can be seen in Fig. 3.6. The scheme is based on numerical testruns, like the two examples mentioned above, and with geometry and hydraulic phenomena characteristic for minor Danish streams. The scheme should be used with great care, and only as an initial guide for the choice of mathematical model.

		KIN	DIF	DYN
Bottomslope	large	+	+	+
	small	%	?	+
Friction	large	+	+	+
	small	?	?	+
Cross section	constant	?	?	+
	variable in space	?	?	+
Water stage at lower boundary	constant	?	+	+
	variable in time	%	?	+
Flow at upper boundary	constant	+	+	+
	variable in time	?	+	+
Lateral inflow	constant	+	+	+
	variable in time	+	+	+
Local water inlet	constant	%	+	+
	variable in time	%	?	+
Obstructions (causing backwater effects)	constant	%	+	+
	variable in time	%	?	+

Fig. 3.6. Initial guide for choice of mathematical model for determination of unsteady flow in minor Danish stream. KIN : Kinematic wave approximation, DIF : Diffusive wave approximation, DYN : Dynamic wave approximation.

### 3.3 Numerical models for steady flow

#### 3.3.1 Uniform flow

A steady and uniform flow model is easily solved by iteration. Referring to Fig. 3.7 the continuity for mass can be written as:

$$\frac{dQ}{dx} = q \sim Q_{j+1} = Q_j + \Delta x \cdot q \quad (3.24)$$

The water stage or water depth can be determined from the momentum equation by iteration. Using the Manning formula the momentum equation can be written as:

$$\begin{aligned} I = I_o &\Rightarrow V = \frac{Q}{A} = M \cdot R^{2/3} \cdot I_o^{1/2} \\ &\sim Q_{j+1} = M \cdot R_{j+1}^{2/3} \cdot I_o^{1/2} \cdot A_{j+1} \end{aligned} \quad (3.25)$$

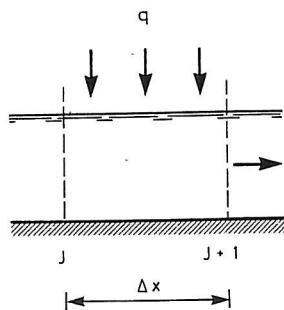


Fig 3.7. Definition sketch for a steady uniform flow model.

Since the cross section area  $A$  and the hydraulic radius  $R$  are functions of the water depth  $h$  (or stage  $y$ ), an iteration procedure must be applied for determination of  $h$ , e.g. the iteration procedure shown in Fig. 3.8.

1. Initial values for depth limits  
 $h_{min} = 0$   
 $h_{max} = h_{csmax}$  (maximum depth in the cross section)
2. Depth  $h' = \frac{1}{2} (h_{min} + h_{max})$
3. Cross section area  $A' = f(h')$   
 Hydraulic radius  $R' = f(h')$
4. Flow  $Q' = M \cdot R'^{2/3} \cdot I_o^{1/2} \cdot A'$
5. New depth limits  
 if  $Q' < Q$  then  $h_{min} = h'$   
 else  $h_{max} = h'$
6. Repeat 2 - 6 until  $|Q - Q'| < \epsilon$   
 where  $\epsilon$  is the accuracy of the iteration  
 e.g.  $\epsilon = \frac{1}{100} \cdot Q$

Fig. 3.8. Iteration procedure for determination of the normal depth.

The critical depth, determining the transition between subcritical and supercritical flow, can be determined in an equal manner. Critical depth is achieved when the Froude number is equal to one:

$$Fr = \frac{V}{\sqrt{g \cdot D}} = \frac{Q}{A \sqrt{g \cdot D}} = 1 \quad (3.26)$$

from which the critical depth can be determined by iteration, e.g. as shown in Fig. 3.9. Similar iteration procedures can be found in Vestergaard (1985) or Larsen (1988).

1. Initial values for depth limits  
 $h_{min} = 0$   
 $h_{max} = h_{csmax}$  (maximum depth in the cross section)
2. Depth  $h' = \frac{1}{2}(h_{min} + h_{max})$
3. Cross section area  $A' = f(h')$   
Average depth  $D' = f(h')$
4. Froude number  $Fr' = \frac{Q}{A' \sqrt{g \cdot D'}}$
5. New depth limits  
if  $Fr' > 1$  then  $h_{min} = h'$   
else  $h_{max} = h'$
6. Repeat 2 - 6 until  $|Fr - Fr'| < \varepsilon$   
where  $\varepsilon$  is the accuracy of iteration  
e.g.  $\varepsilon = 0.01$

Fig. 3.9. Iteration procedure for determination of critical depth.

### 3.3.2 Non-uniform flow

A steady non-uniform model is based on a continuity for mass and an equation for either momentum or energy. In this section only an example on a model based on the energy formulation will be shown.

Referring to the notation in Fig. 3.10 the governing equations can be rewritten as:

$$\frac{dQ}{dx} = q \quad \leadsto \quad Q_{j+1} = Q_j + \Delta x \cdot q \quad (3.27)$$

$$z_j + h_j + \alpha \frac{V_j^2}{2 \cdot g} = z_{j+1} + h_{j+1} + \alpha \frac{V_{j+1}^2}{2 \cdot g} + \Delta h \quad (3.28)$$

The energy loss can be determined by use of the Manning formula:

$$\Delta h = \Delta x \cdot I = \Delta x \cdot \frac{\bar{V}^2}{M^2 \cdot \bar{R}^{4/3}} \quad (3.29)$$

where

$$\bar{V} = \frac{1}{2} (V_j + V_{j+1}) \quad (3.30)$$

$$\bar{R} = \frac{1}{2} (R_j + R_{j+1}) \quad (3.31)$$

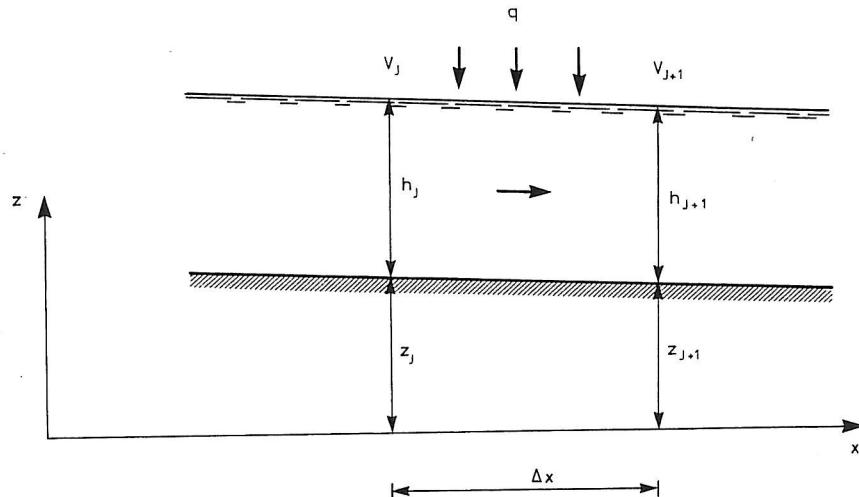


Fig. 3.10. Definition sketch for non-uniform model.

From these equations the flow (eq. 3.27) and the water depth (eq. 3.28) can be determined in a successive manner, starting at a point where the flow and the water depth is known. It is important to notice that two solutions exist for the energy formula, one for subcritical flow and one for supercritical flow. Furthermore, no usable result can be achieved in the area of transition. If these features are neglected, then the iteration in eq.(3.28) for the water depth  $h$  may not succeed.

In the Figure below a procedure is shown for a backward determination of the water depth for subcritical flow conditions. For this purpose eq.(3.28) may be written as:

$$F(h_j) = z_{j+1} + h_{j+1} + \alpha \frac{V_{j+1}^2}{2g} + \Delta h - \left( z_j + h_j + \alpha \frac{V_j^2}{2g} \right) \quad (3.32)$$

where the function  $F$  is an error function to be minimized during the iteration. A further description of this procedure can be found in Larsen (1988) or in Vestergaard (1985).

1. Initial values for depth limits  
 $h_{min} = h_c$  (critical depth)  
 $h_{max} = h_{max}$  (maximum depth in the cross section)
2. Depth  $h'_j = \frac{1}{2} (h_{min} + h_{max})$
3. Hydraulic radius  $R_j = f(h'_j)$   
Average velocity  $V_j = f(h'_j)$
4. Energy loss  $\Delta h' = f(h'_j)$
5. Error function  $F(h'_j)$
6. New depth limits  
if  $F(h'_j) > 0$  then  $h_{min} = h'_j$   
else  $h_{max} = h'_j$
7. Repeat 2 - 7 until  $F(h_j) < \varepsilon$   
where  $\varepsilon$  is the accuracy of the iteration

Fig. 3.11. Iteration procedure for determination of the water depth assuming subcritical flow.

## 3.4 Numerical models for unsteady flow

### 3.4.1 The Method of Characteristics

A way to solve the Saint Venant equations, or some simplified version, is to use the Method of Characteristics. The method was described in a very brief and general way in chapter 2 for the Transport/Dispersion model, but also when dealing with unsteady flow this method can be applied. The following description will be brief, and for further studies the reader should consult e.g. Abbott (1979), Sjöberg (1976), or Mahmood & Yevjevich (1975).

Assuming that the geometry of the channel is piecemeal uniform and the lateral inflow can be neglected, the Saint Venant equations can be written as:

$$\frac{\partial A}{\partial t} + \frac{\partial Q}{\partial x} = 0 \quad (3.33)$$

$$\frac{\partial Q}{\partial t} + \frac{\partial}{\partial x} \left( \frac{Q^2}{A} \right) + g \cdot A \frac{\partial h}{\partial x} + g \cdot A \cdot I - g \cdot A \cdot I_o = 0 \quad (3.34)$$

These equations can be transformed into the Riemann equations:

$$\frac{\partial Q}{\partial t} - \left( V - \sqrt{g \cdot D} \right) b \frac{\partial h}{\partial t} = g \cdot A (I - I_o) \quad (3.35)$$

along

$$\left( \frac{\partial x}{\partial t} \right)^+ = V + \sqrt{g \cdot D} \quad (3.36)$$

and

$$\frac{\partial Q}{\partial t} - \left( V + \sqrt{g \cdot D} \right) b \frac{\partial h}{\partial t} = g \cdot A (I - I_o) \quad (3.37)$$

along

$$\left( \frac{\partial x}{\partial t} \right)^- = V - \sqrt{g \cdot D} \quad (3.38)$$

In chapter 2 the characteristic for the Transport/Dispersion model showed up to be a straight line, which did the numerical algorithm simple and exact.

In this case it can be seen that there are two characteristics and that these are not straight lines, because as well  $V$  as  $D$  are functions of  $x$  and  $t$ . And therefore the characteristics are curved, as illustrated in Fig. 3.12.

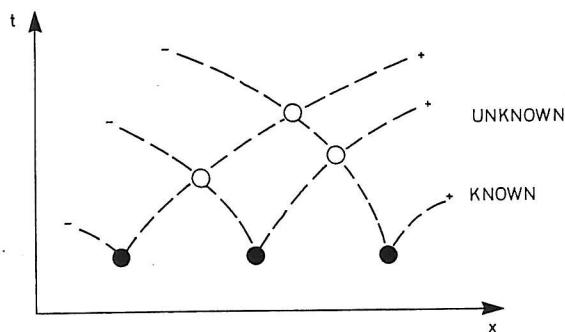


Fig. 3.12. Curved characteristics from the Riemann equations.

But still we are able to set up two equations for determination of  $h$  (or  $y$ ) and  $Q$  in every gridpoint. The only trouble is that the position of the gridpoints are no longer known, which means that a kind of double iterative procedure must be applied. But since the position of the gridpoint is dependent of the flow conditions, then the modeller is no longer able to control the numerical calculation, – he cannot decide where and when the unknown variables are determined. This fact in combination with the fact, that many iterations are needed and the method therefore is computational demanding, are the main reasons for explaining why this method seldom is used for open channel modelling.

Instead a slightly simplified method using a rectangular grid is more often used. This method is called the Hartree method, and it will be described in some details in the following. Further descriptions can be found in Mahmood & Yevjevich (1975) or Schaarup-Jensen (1984).

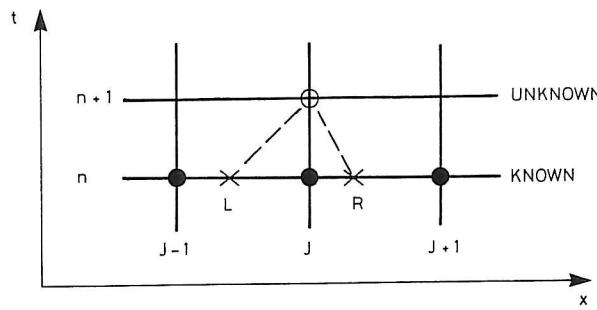


Fig. 3.13. Grid for the Hartree method

A rectangular grid is introduced, Fig. 3.13 and it is assumed that the grid is so small that the characteristics can be approximated by straight lines. Furthermore it is presumed that the characteristics intersect the time-level  $n$  between the grids  $j - 1$  and  $j + 1$ , which can be written se:

$$\left( \frac{\Delta t}{\Delta x} \right)_L = \frac{t_{n+1} - t_n}{x_j - x_{j-1}} \leq \left( \frac{dt}{dx} \right)^+ \quad (3.39)$$

$$\left( \frac{\Delta t}{\Delta x} \right)_R = \frac{t_{n+1} - t_n}{x_{j+1} - x_j} \leq \left( \frac{dt}{dx} \right)^- \quad (3.40)$$

which by introduction of the Courant number  $Cr$  can be written as:

$$Cr \leq 1 \quad \text{where} \quad Cr = \frac{\Delta t}{\Delta x} \cdot \left| V \pm \sqrt{g \cdot D} \right| \quad (3.41)$$

First the location  $x_L$  and  $x_R$  of the two points  $L$  and  $R$  must be determined. By using eq.(3.39) we get:

$$\begin{aligned} \left( \frac{dx}{dt} \right)_L &= \frac{x_j - x_L}{\Delta t} = \frac{1}{2} \left( \left( \frac{dx}{dt} \right)_{j-1}^+ + \left( \frac{dx}{dt} \right)_j^+ \right) = \\ &= \frac{1}{2} \left( (V_{j-1}^n + \sqrt{g \cdot D_{j-1}^n}) + (V_j^n + \sqrt{g \cdot D_j^n}) \right) \end{aligned} \quad (3.42)$$

from which  $x_L$  can be evaluated, and similar for  $x_R$  using eq.(3.40):

$$\left( \frac{dx}{dt} \right)_R = \frac{x_j - x_R}{\Delta t} = \frac{1}{2} \left( \left( \frac{dx}{dt} \right)_j + \left( \frac{dx}{dt} \right)_{j+1} \right) = \frac{1}{2} \left( (V_j^n - \sqrt{g \cdot D_j^n}) + (V_{j+1}^n - \sqrt{g \cdot D_{j+1}^n}) \right) \quad (3.43)$$

Secondly the values of  $h$  (or  $y$ ) and  $Q$  can be determined in point  $L$  and  $R$ . Normally this is performed by linear interpolation, but also more sofisticated methods could be introduced. A linear interpolation yields:

$$Q_L^n = \frac{x_j - x_L}{x_j - x_{j-1}} Q_{j-1}^n + \frac{x_L - x_{j-1}}{x_j - x_{j-1}} Q_j^n \quad (3.44)$$

$$Q_R^n = \frac{x_{j+1} - x_R}{x_{j+1} - x_j} Q_j^n + \frac{x_R - x_j}{x_{j+1} - x_j} Q_{j+1}^n \quad (3.45)$$

and similar for  $h$ .

Now we are ready to use the two equations, (3.35) and (3.37), for determination of  $h$  and  $Q$  at gridpoint  $(n+1, j)$ . If these two equations are integrated along the characteristics, then the following two equations appear:

$$Q_j^{n+1} - Q_L^n - (h_j^{n+1} - h_L^n) k_{1+} = k_{2+} \cdot \Delta t \quad (3.46)$$

$$Q_j^{n+1} - Q_R^n - (h_j^{n+1} - h_R^n) k_{1-} = k_{2-} \cdot \Delta t \quad (3.47)$$

where

$$k_{1+} = \frac{1}{2} \left[ (V_j^{n+1} - \sqrt{g \cdot D_j^{n+1}}) b_j^{n+1} + (V_L^n - \sqrt{g \cdot D_L^n}) b_L^n \right] \quad (3.48)$$

$$k_{1-} = \frac{1}{2} \left[ (V_j^{n+1} + \sqrt{g \cdot D_j^{n+1}}) b_j^{n+1} + (V_R^n + \sqrt{g \cdot D_R^n}) b_R^n \right] \quad (3.49)$$

$$k_{2+} = \frac{1}{2} \left( g \cdot A_j^{n+1} (I_o - I_j^{n+1}) + g \cdot A_L^n (I_o - I_L^n) \right) \quad (3.50)$$

$$k_{2-} = \frac{1}{2} \left( g \cdot A_j^{n+1} (I_o - I_j^{n+1}) + g \cdot A_R^n (I_o - I_R^n) \right) \quad (3.51)$$

where  $I$  can be found from the Manning formula.

From this set of equations  $h_j^{n+1}$  and  $Q_j^{n+1}$  can be found by use of an iterative procedure. The first step in the procedure is performed using:

$$V_j^{n+1} \simeq V_L^n, \quad D_j^{n+1} \simeq D_L^n, \quad b_j^{n+1} \simeq b_L^n, \quad I_j^{n+1} \simeq I_L^n \quad (3.52)$$

in eq.(3.48), and in eq.(3.50), and

$$V_j^{n+1} \simeq V_R^n, \quad D_j^{n+1} \simeq D_R^n, \quad b_j^{n+1} \simeq b_R^n, \quad I_j^{n+1} \simeq I_R^n \quad (3.53)$$

in eq.(3.49), and in eq.(3.51).

In case of an extremely demand of accuracy in the calculation, it is possible to correct the position of  $L$  and  $R$  using :

$$\frac{x_j - x_L}{\Delta t} = \frac{1}{2} \left[ \left( \frac{dx}{dt} \right)_L^+ + \left( \frac{dx}{dt} \right)_p^+ \right] \quad (3.54)$$

$$\frac{x_j - x_R}{\Delta t} = \frac{1}{2} \left[ \left( \frac{dx}{dt} \right)_R^- + \left( \frac{dx}{dt} \right)_p^- \right] \quad (3.55)$$

where  $p$  denotes the node  $(n+1, j)$ , and then a new determination of  $h$  and  $Q$  could be performed. The reader may have noticed that also in the Hartree method a lot of iterations must be performed and, furthermore, the grid must be relative small as the demand expressed in eq.(3.41) must be fulfilled at every location and every time during the flow event.

### 3.4.2 Finite difference schemes

Numerical solution of the Saint Venant equations, or the simplified versions, by use of finite differences, can be performed in many different ways, and during the years many different numerical schemes have been applied. It is

impossible to discuss all these methods, – instead a coarse classification will be made and only a few schemes will be described in some details.

First of all a division can be made after which mathematical model the scheme is based on. Some schemes are developed for a specific version of the Saint Venant equations, e.g. the RRL-method for Kinematic Wave approximation (Sjöberg, 1976). But many other schemes can be applied for several of the mathematical models described in sec. 3.2.

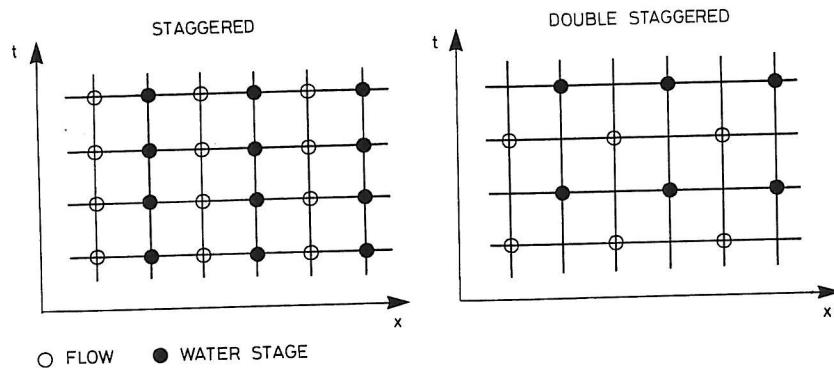


Fig. 3.14. Staggered grid

From a numerical point of view especially two concepts can be used, which will divide the schemes into four classes. At first the schemes can be divided into explicit and implicit schemes, secondly into schemes based on a staggered grid (Fig. 3.14) and schemes using the full grid, where as well the flow as the water stage are determined at each node.

At this place a lot of schemes could be mentioned, but only five well-known schemes will be considered. Perhaps it would be more correct to mention them types of schemes, since several slightly different formulations of each scheme can be found in the literature, see e.g. Mahmood & Yevjevich (1975).

In Fig. 3.15 three explicit schemes are illustrated. The RRL-scheme is an explicit scheme using four nodes on a full grid, and as mentioned above developed especially for the Kinematic Wave approximation. This scheme will be described further in sec. 3.4.3.

The Lax scheme can be applied for all versions of the Saint Venant equations and is also an explicit scheme using a full grid. During the research

some difficulties in formulation of boundary conditions has shown up for this scheme, where four boundary conditions are necessary, but it can be solved e.g. by using the Method of Characteristic for formulation of two conditions. Another solution is to apply a staggered grid, and then only two boundary conditions will be needed. The Lax scheme will not be treated any further in this work.

The third explicit scheme, the Leap Frog scheme is formulated at a staggered grid, demanding two boundary conditions. This scheme can be applied for the full Saint Venant equations, but in section 3.4.4 a modified version of the scheme will be applied for the Diffusive Wave approximation.

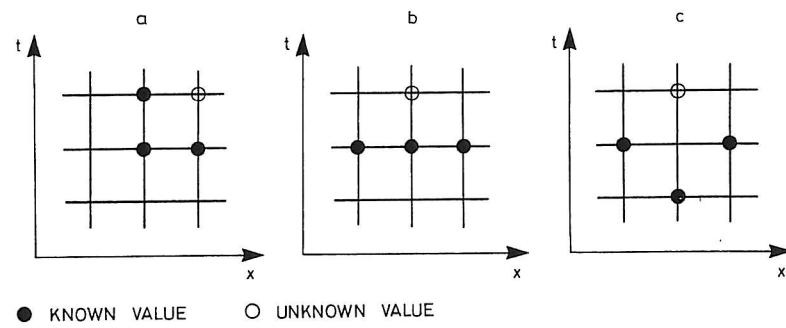


Fig. 3.15. Examples of explicit schemes, a: RRL, b: Lax, c: Leap Frog.

In Fig. 3.16 two examples of implicit schemes are shown. The first one, the Preissmann scheme, includes only four nodes on a full grid, while the Abbott scheme includes six nodes on a staggered grid. Both schemes are widely used for practical modelling, but only the Preissmann scheme will be described in the following sections.

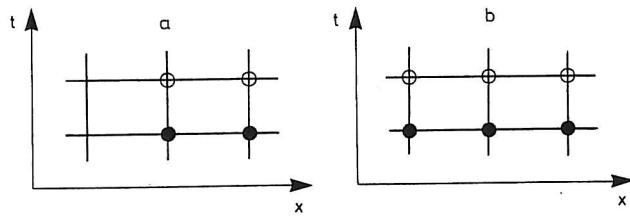


Fig. 3.16. Examples of implicit schemes, a: Preismann, b: Abbott.

As mentioned above three of these schemes, representing three different versions of the Saint Venant equations, will be considered in the following sections. The purpose is to show some different examples of how a numerical solution can be performed, and to compare the features of the three different mathematical models. The considerations in the following sections are widely based on numerical testruns. A further description of these can be found in Vestergaard (1989).

### 3.4.3 Kinematic Wave model

This numerical model, often called the RRL-model, is based on the equations for a kinematic wave, see section 3.2. Applications of this model can be found in e.g. Sjöberg (1976) or Schaarup-Jensen (1988a).

Using the Manning formula for determination of the energy slope, we get:

$$\frac{\partial A}{\partial t} + \frac{\partial Q}{\partial x} = q \quad (3.56)$$

$$I = I_o \quad \Rightarrow \quad Q = M \cdot R^{2/3} \cdot I_o^{1/2} \cdot A \quad (3.57)$$

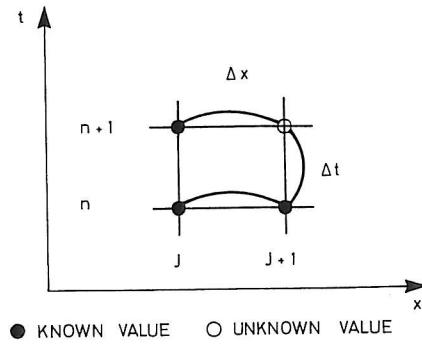


Fig. 3.17. Numerical grid for the RRL-scheme.

Referring to the numerical grid in Fig. 3.17 the following discrete terms are introduced:

$$\frac{\partial A}{\partial t} \simeq \frac{A_{j+1}^{n+1} - A_j^n}{\Delta t} \quad (3.58)$$

$$\frac{\partial Q}{\partial x} \simeq \frac{1}{2} \left( \frac{Q_{j+1}^{n+1} - Q_j^{n+1}}{\Delta x} + \frac{Q_{j+1}^n - Q_j^n}{\Delta x} \right) \quad (3.59)$$

$$Q_{j+1}^{n+1} \simeq M \cdot (R_{j+1}^{n+1})^{2/3} \cdot I_o^{1/2} \cdot A_{j+1}^{n+1} \quad (3.60)$$

Inserting these approximations in eq.(3.56) and (3.57) leads to:

$$\frac{1}{2 \cdot \Delta x} (Q_{j+1}^{n+1} - Q_j^{n+1} + Q_{j+1}^n - Q_j^n) + \frac{1}{\Delta t} (A_{j+1}^{n+1} - A_j^n) = q \quad (3.61)$$

$$Q_{j+1}^{n+1} = M \cdot (R_{j+1}^{n+1})^{2/3} \cdot I_o^{1/2} \cdot A_{j+1}^{n+1} \quad (3.62)$$

from which the unknown flow and depth in gridpoint  $(n+1, j+1)$  can be determined by applying some iterative procedure, having in mind that as well  $A$  as  $R$  are functions of  $h$ .

A possible procedure is to combine eq.(3.61) and eq.(3.62) :

$$M \left( R_{j+1}^{n+1} \right)^{2/3} I_o^{1/2} \cdot A_{j+1}^{n+1} - Q_j^{n+1} + Q_{j+1}^n - Q_j^n + \frac{2 \cdot \Delta x}{\Delta t} (A_{j+1}^{n+1} - A_{j+1}^n) - 2 \cdot \Delta x \cdot q = 0 \quad (3.63)$$

From this equation the unknown depth at  $(n+1, j+1)$  can be found by iteration. The iteration can be started by assuming that:

$$h_{j+1}^{n+1} \simeq h_{j+1}^n \quad \text{and therefore} \quad R_{j+1}^{n+1} \simeq R_{j+1}^n \quad \text{and} \quad A_{j+1}^{n+1} \simeq A_{n+1}^n \quad (3.64)$$

When the depth is known the flow is easily found from eq.(3.62), and the next gridpoint can be treated.

To start the numerical calculation some initial conditions must be known. For this model as well  $Q$  as  $h$  must be known at each node at the initial time level.

From Fig. 3.17 it is easily seen that no lower boundary condition is needed. At the upper boundary the flow or the depth must be known at each time level.

The choice of  $\Delta x$  is essential for this model. If the numerical model was a perfect approximation to the Kinematic Wave model, it could hardly be used for any practical purpose, since the true kinematic wave is not damped (Schaarup-Jensen, 1984). But it can be proved that the finite difference scheme above is encumbered with numerical errors in such a way that a special choice of  $\Delta x$  will result in a model approximating the diffusive kinematic wave, which is more sufficient for practical purpose. This is achieved if  $\Delta x$  is chosen as:

$$\Delta x = \frac{Q_o}{b \cdot I_o \cdot C_k} \quad (3.65)$$

where  $C_k$  is the kinematic wave celerity, which can be approximated by

$$C_k = \frac{\partial Q}{\partial A} \simeq \beta \cdot V \quad (3.66)$$

The coefficient  $\beta$  is dependent of the cross section shape. Referring to Schaarup-Jensen (1984) a proper choice would stay between 1.2 and 1.7.

### 3.4.4 Diffusiv Wave model

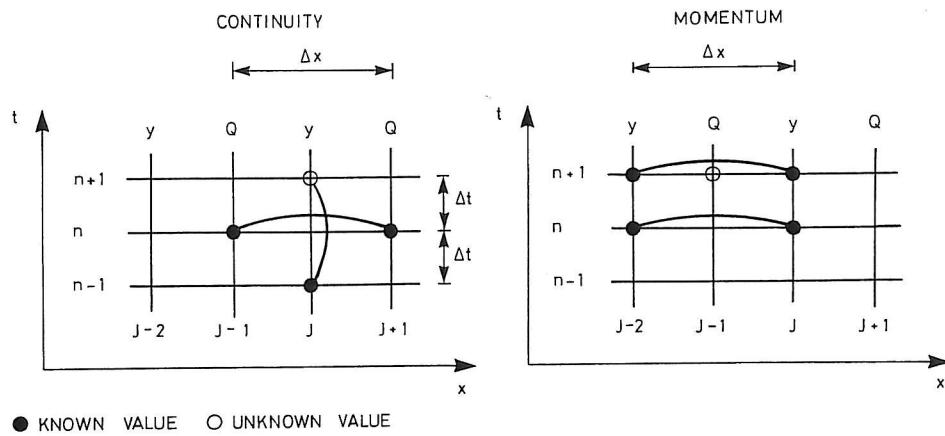


Fig. 3.18. Numerical grid for the modified Leap Frog scheme.

The mathematical model is the Diffusive Wave approximation, which was described in sec. 3.2:

$$b \frac{\partial y}{\partial t} + \frac{\partial Q}{\partial x} = q \quad (3.67)$$

$$\frac{\partial y}{\partial x} + I = 0 \quad \Rightarrow \quad \frac{\partial y}{\partial x} + \frac{Q^2}{M^2 \cdot R^{2/3} \cdot A^2} = 0 \quad (3.68)$$

where the Manning formula is introduced for determination of the energy slope and the lateral inflow is assumed to be perpendicular to the mean flow direction.

The original Leap Frog scheme is based on a double staggered grid, while the modified version only applies a grid staggered in space, see Fig. 3.15 and Fig. 3.18.

Referring to the notation in Fig. 3.18 the following discretization can be performed:

$$b \frac{\partial y}{\partial t} \simeq b_j^n \frac{y_j^{n+1} - y_j^{n-1}}{2 \cdot \Delta t} \quad (3.69)$$

$$\frac{\partial Q}{\partial x} \simeq \frac{Q_{j+1}^n - Q_{j-1}^n}{\Delta x} \quad (3.70)$$

$$\begin{aligned}\frac{\partial y}{\partial x} &\simeq \frac{1}{2} \frac{y_j^{n+1} - y_{j-2}^{n+1}}{\Delta x} + \frac{1}{2} \frac{y_j^n - y_{j-2}^n}{\Delta x} \\ &= \frac{y_j^{n+1} - y_{j-2}^{n+1} + y_j^n - y_{j-2}^n}{2 \cdot \Delta x}\end{aligned}\quad (3.71)$$

This means that eq.(3.67) can be written as:

$$\begin{aligned}\Downarrow \quad b_j^n \frac{y_j^{n+1} - y_j^{n-1}}{2 \cdot \Delta t} + \frac{Q_{j+1}^n - Q_{j-1}^n}{\Delta x} &= q \\ y_j^{n+1} &= y_j^{n-1} + \frac{2 \cdot \Delta t \cdot q}{b_j^n} - \frac{2 \cdot \Delta t (Q_{j+1}^n - Q_{j-1}^n)}{\Delta x \cdot b_j^n}\end{aligned}\quad (3.72)$$

from which the water stage at  $(n+1, j)$  can be determined. When the water stage is known the unknown flow at  $(n+1, j+1)$  can be determined of eq.(3.68) , which by use from eq.(3.71) can be written as:

$$\begin{aligned}\Downarrow \quad \frac{y_j^{n+1} - y_{j-2}^{n+1} + y_j^n - y_{j-2}^n}{2 \cdot \Delta x} + \frac{(Q_{j-1}^{n+1})^2}{M^2 \cdot \bar{R}^{4/3} \cdot \bar{A}^2} &= 0 \\ Q_{j-1}^{n+1} &= -M \cdot \bar{R}^{2/3} \cdot \bar{A} \frac{1}{\sqrt{2 \cdot \Delta x}} (y_j^{n+1} - y_{j-2}^{n+1} + y_j^n - y_{j-2}^n) \cdot \\ &\quad |y_j^{n+1} - y_{j-2}^{n+1} + y_j^n - y_{j-2}^n|^{-1/2}\end{aligned}\quad (3.73)$$

where the average cross section parameters are determined as:

$$\bar{R} = \frac{1}{4} (R_j^{n+1} + R_{j-2}^{n+1} + R_j^n + R_{j-2}^n) \quad (3.74)$$

$$\bar{A} = \frac{1}{4} (A_j^{n+1} + A_{j-2}^{n+1} + A_j^n + A_{j-2}^n) \quad (3.75)$$

Two boundary conditions must be introduced. At the upper boundary the flow must be known at every time level, and at the lower boundary the water stage must be known. Often the water stage at the lower boundary is assumed to be equal to the normal depth, and then the water stage can be determined by iteration from:

$$Q_{jm-1}^n = M (R_{jm}^{n+1})^{2/3} (A_{jm}^{n+1}) \cdot I_o \quad (3.76)$$

As initial conditions the flow and water stage must be known at two time levels. Often the simulation can be started from a situation, where the flow is steady, and then the water stage can be determined by use of a steady non-uniform model, see sec. 3.3.

During testruns this explicit model has shown good features (Hummelhøj & Nielsen, 1988) (Vestergaard, 1989). In Fig. 3.19 the result from a testrun is shown. A triangular hydrograf with a peak value of  $3 m^3/sec$  is introduced into a minor stream at  $x = 4000 m$ . The cross section of the stream is rectangular with a width of  $5 m$ , a bottom slope of  $5 \cdot 10^{-4}$  and a Manning number of  $40 m^{1/3}/sec$ .

The greatest disadvantage for this explicit model is the restrictions for the choice of  $\Delta t$  and  $\Delta x$ . The stability condition for the explicit Leap Frog scheme can be stated as (Falconer, 1986):

$$Cr = \frac{\Delta t}{\Delta x} \sqrt{g \cdot D} \leq 1 \quad (3.77)$$

But for some flow events, like the one shown in Fig. 3.19, even more restrictive demands seem to be valid, which may lead to insufficient small  $\Delta t$ .

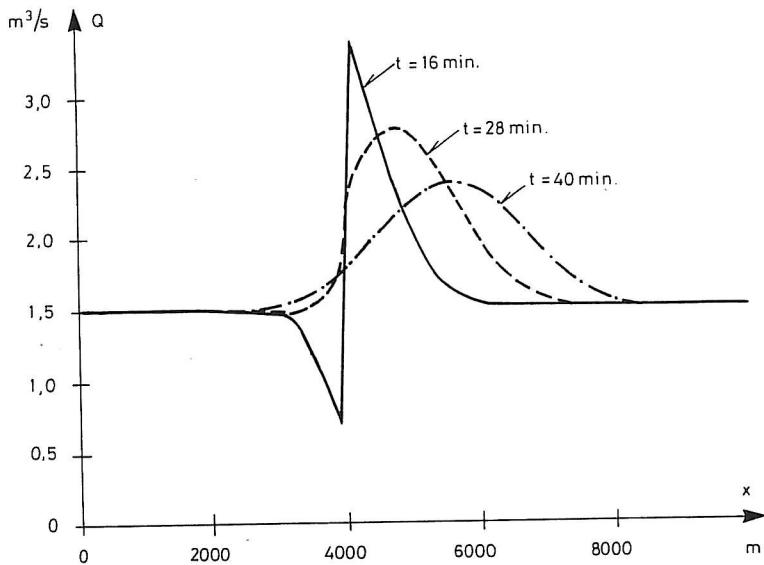


Fig. 3.19. Testrun with the modified Leap Frog model,  $\Delta x = 100 \text{ m}$ ,  $\Delta t = 5 \text{ sec}$  (Hummelshøj & Nielsen, 1988).

### 3.4.5 Dynamic Wave model

The Dynamic Wave model includes the full Saint Venant equations:

$$b \frac{\partial y}{\partial t} + \frac{\partial Q}{\partial x} = q \quad (3.78)$$

$$\frac{\partial Q}{\partial t} + \frac{\partial}{\partial x} \left( \frac{Q^2}{A} \right) + g \cdot A \frac{\partial y}{\partial x} + g \cdot A \cdot I = q \cdot u_q \quad (3.79)$$

where again the Manning formula is introduced for determination of the energy slope.

The Preissmann scheme can be formulated and implemented in many different ways. The following version is very like the version described by Verwey (Cunge et al., 1980). The scheme is a four node scheme, where as well the flow as the water stage are determined at each node.

The scheme is based on the following form of discretization:

$$\frac{\partial f}{\partial x} \simeq \Theta \frac{f_{j+1}^{n+1} - f_j^{n+1}}{\Delta x} + (1 - \Theta) \frac{f_{j+1}^n - f_j^n}{\Delta x} \quad (3.80)$$

$$\frac{\partial f}{\partial t} \simeq \frac{1}{2} \frac{f_{j+1}^{n+1} - f_{j+1}^n}{\Delta t} + \frac{1}{2} \frac{f_j^{n+1} - f_j^n}{\Delta t} \quad (3.81)$$

where  $\Theta$  is a coefficient for centering in time ( $0 \leq \Theta \leq 1$ ).

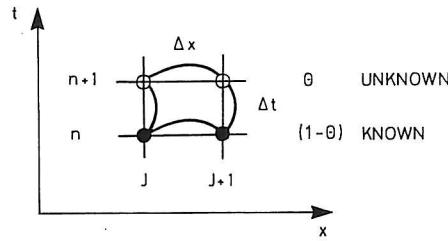


Fig. 3.20. Numerical grid for the Preissmann scheme.

Referring to Fig. 3.20 the Preissmann scheme can be written as:

Continuity:

$$\bar{b} \cdot \left( \frac{1}{2} \frac{y_{j+1}^{n+1} - y_{j+1}^n}{\Delta t} + \frac{1}{2} \frac{y_j^{n+1} - y_j^n}{\Delta t} \right) + \Theta \frac{Q_{j+1}^{n+1} - Q_j^{n+1}}{\Delta x} + (1 - \Theta) \frac{Q_{j+1}^n - Q_j^n}{\Delta x} = q \quad (3.82)$$

Momentum:

$$\begin{aligned} & \frac{1}{2} \frac{Q_{j+1}^{n+1} - Q_{j+1}^n}{\Delta t} + \frac{1}{2} \frac{Q_j^{n+1} - Q_j^n}{\Delta t} + \\ & \frac{1}{\Delta x} \left( \frac{Q_{j+1}^n \cdot Q_{j+1}^{n+1}}{A_{j+1}^{n+1/2}} - \frac{Q_j^n \cdot Q_j^{n+1}}{A_j^{n+1/2}} \right) + \\ & g \cdot \bar{A} \left( \Theta \frac{y_{j+1}^{n+1} - y_j^{n+1}}{\Delta x} + (1 - \Theta) \frac{y_{j+1}^n - y_j^n}{\Delta x} \right) + \end{aligned}$$

$$g \cdot \bar{A} \left( \frac{1}{2} \frac{|Q_j^n| Q_j^{n+1}}{\left( M \left( R_j^{n+1/2} \right)^{2/3} A_j^{n+1/2} \right)^2} + \frac{1}{2} \frac{|Q_{j+1}^n| Q_{j+1}^{n+1}}{\left( M \left( R_{j+1}^{n+1/2} \right)^{2/3} A_{j+1}^{n+1/2} \right)^2} \right) = q \cdot u_q \quad (3.83)$$

where

$$A_j^{n+1/2} = \frac{A_j^n + A_j^{n+1}}{2} \quad (3.84)$$

$$A_{j+1}^{n+1/2} = \frac{A_{j+1}^n + A_{j+1}^{n+1}}{2} \quad (3.85)$$

$$\bar{A} = \frac{A_j^{n+1/2} + A_{j+1}^{n+1/2}}{2} \quad (3.86)$$

and similar for  $b$  and  $R$ .

If  $jm$  space levels are present it is possible to set up  $2 \cdot jm - 2$  equations at each time level. If two boundary conditions are added, then the system can be solved for the unknown flow and water stage at time level ( $n + 1$ ). Since the equations are non-linear,  $-b$ ,  $A$  and  $R$  are functions of the water stage, an iterative solution technique must be implemented.

In the first step in the iteration,  $b$ ,  $R$  and  $A$  (eq. 3.83 - 3.86) are determined at the known time level  $n$ .

Eq.(3.82) as well as eq.(3.83) can be rearranged introducing the coefficients  $a_i$ , leading to equations of the form:

$$a_1 \cdot y_j^{n+1} + a_2 \cdot Q_j^{n+1} + a_3 \cdot y_{j+1}^{n+1} + a_4 \cdot Q_{j+1}^{n+1} = a_5 \quad (3.87)$$

If the continuity equation and the momentum equation are applied in a successive manner a linear system of equations can be obtained:

$$\left[ \begin{array}{cccc|c} x & x & & & y_1 \\ x & x & x & x & Q_1 \\ x & x & x & x & y_2 \\ & x & x & x & Q_2 \\ & x & x & x & y_3 \\ \hline & & & & - \\ & & & & - \\ & & & & - \\ x & x & x & x & Q_{jm-1} \\ x & x & x & x & y_{jm} \\ x & x & & & Q_{jm} \end{array} \right] = \left[ \begin{array}{c} x \\ x \\ x \\ x \\ x \\ x \\ x \end{array} \right]$$

which either can be solved directly by using Gauss elimination, e.g. the EQSOLV algorithm, or the quicker Double Sweep algorithm after a local elimination, which must lead to a system of the form:

$$\left[ \begin{array}{cccc|c} x & x & & & y_1 \\ x & x & x & & Q_1 \\ x & x & x & & y_2 \\ x & x & x & & Q_2 \\ x & x & x & & y_3 \\ \hline & & & & - \\ & & & & - \\ & & & & - \\ x & x & x & & Q_{jm-1} \\ x & x & x & & y_{jm} \\ x & x & & & Q_{jm} \end{array} \right] = \left[ \begin{array}{c} x \\ x \\ x \\ x \\ x \\ x \\ x \end{array} \right]$$

When the new water stages at time level  $(n+1)$  are determined,  $b$ ,  $A$  and  $R$  are updated using eq.(3.84) – (3.86), and a new set of equations can be obtained and solved, and so on, until the wanted accuracy is achieved. Often only very few steps are needed in this iteration.

As initial conditions the flow and water stage must be known at each node at the lowest time level. Two boundary conditions are needed, and every combination of  $Q$  and  $y$  would allow the system to be solved, but some of these combinations can lead to bad results. An often used combination,

without any problems, is known flow at the upper boundary and normal depth at the lower boundary, determined from the Manning formula using the known values at time level  $n$ .

The Preissmann scheme has been tested through a large number of testruns (Vestergaard, 1989) (Brorsen, 1988). The result from one of these is shown in Fig. 3.21. The model setup is identical to the setup described in sec. 3.4.4, – a triangular hydrograf is introduced in a stream at  $x = 4000 \text{ m}$ .

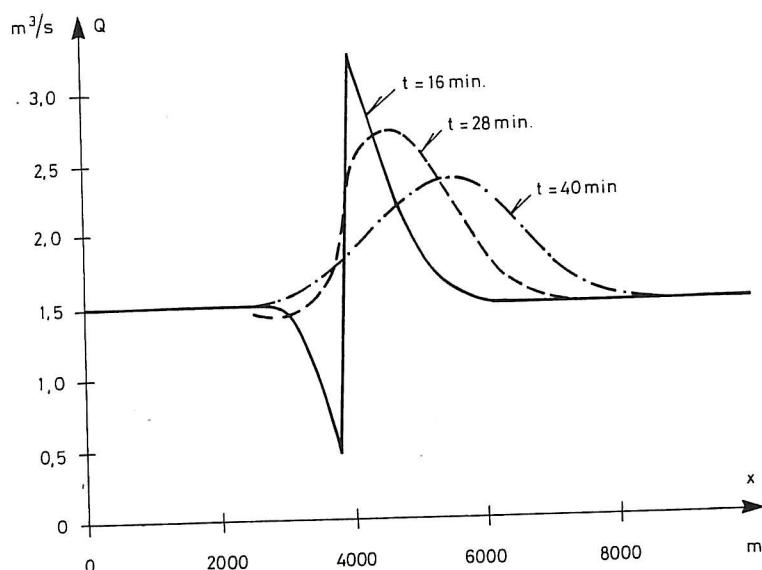


Fig. 3.21. Testrun with the Preissmann scheme,  $\Delta x = 200 \text{ m}$ ,  $\Delta t = 120 \text{ sec}$  (Brorsen, 1988).

If the results achieved with the Preissmann model (Fig. 3.21) are compared with the results achieved from the modified Leap Frog model (Fig. 3.19), no important deviations can be observed. But since this flow event can be modelled with the Preissmann model by use of a time step more than 20 times greater the time step used in the explicit model, it follows that the implicit scheme is much more usable for modelling of large water systems and flow events of rather long duration. Some applications of the scheme can be found in Vestergaard & Larsen (1987) and Schaaruup-Jensen (1988b).

### 3.5 Discussion

The use of numerical models for open channel flow has already been extensive for some years, and there is no doubt that the application will be even more extensive in the future, including modelling of hydraulic phenomena in Danish streams.

Which model to choose for a specific task can hardly be stated in general, since more than one model may lead to sufficient results. For some years ago it was very important to be aware of, and to minimize the demand for computer speed and store, but the almost explosive development in hardware capacity during the latest years, has made this demand lesser restrictive.

But still there is no need for implementation of large and complex models, if only a limited number of data are available, or if only some coarse results are needed. Therefore the choice of model should be based on a careful analysis of the specific task, with the purpose to fulfill the stated aims using a minimum of resources.

For this analysis it could be valuable to draw up some general properties for hydrodynamic models, in an attempt to create a coarse view over advantages and disadvantages for the different mathematical models and numerical schemes.

There is no doubt that a lot of modelling, especially water quality modelling, can be based on steady flow, or at least quasi-steady flow. For natural streams it will normally be necessary to apply a non-uniform model. The steady non-uniform model is easily solved numerically by use of iteration procedures.

It is important to notice that the transition between subcritical and supercritical flow is difficult to describe in an accurate manner, and numerical solutions are very difficult to obtain. Another weakness in the model is the description of the energy loss, especially if seaweed is present, like in many minor Danish streams. For these occasions a further development of the models is needed.

Unsteady flow models are normally based on a version of the Saint Venant equations. The storage approximation seems to be of minor interest, since a lot of empirical parameters must be determined through calibration. There is no valid argument for not using a version of the momentum equation. Which one to use depends on which hydraulic phenomenon to be modelled. An attempt to create a guide for this choice was made in sec. 3.4, but generally

it seems as if the Diffusive Wave approximation would be sufficient for most of the hydraulic events in Danish streams. An exception is tidal motion in large, flat streams, where the Dynamic Wave model may be necessary.

A large amount of numerical schemes can be chosen. The first decision to make is whether the scheme should be explicit or implicit. An explicit scheme is normally far lesser complicated than an implicit scheme, and therefore much quicker to develop. But the price is restrictive demands for the choice of  $\Delta x$  and  $\Delta t$ , as explicit schemes generally are conditionally stable.

Generally implicit schemes are unconditionally stable, and therefore much larger values of  $\Delta x$  and  $\Delta t$  may be chosen, resulting in lesser need for computer speed. But since large systems of equations must be handled and solved, the implicit model may demand more computer storage than the explicit. If the hydraulic phenomenon is of a very short duration, it might be necessary to choose small values for  $\Delta t$  anyway, and for such events the explicit model may be faster than the implicit one.

Boundary conditions are often difficult to describe and many errors are introduced through a poor description of the boundary conditions. For some schemes four boundary conditions are needed, which can be very difficult to describe in an accurate manner. Therefore, schemes with only two boundary conditions are preferable. This feature is normally obtained when a staggered grid is used, but also schemes on non-staggered grid can have this feature, if only two nodes at each time level are used in the discretization.

In large commercial model systems, such as MOUSE and MIKE 11 from the Danish Hydraulic Institute, an implicit hydrodynamic model is applied, – in these models the Abbott scheme. This is necessary and preferable since these modelsystems are very general and can be applied on a large amount of hydraulic events. But if the model has been built directly for a specific task, the choice between explicit, implicit, staggered, and non-staggered is very open and further recommendations cannot be stated, – the final choice belongs to the person who has to develop and use the model.



# **Chapter 4**

## **Models for Transport and Spreading of Pollutants**

### **4.1 Introduction**

Water quality modelling has become a more and more commonly used engineering tool during the latest years. In streams normally one-dimensional models are applied, and these can be divided into three steps:

- Hydrodynamic modelling as described in chapter 3. In the following considerations the flow will be assumed to be steady and uniform.
- Modelling of transport and spreading caused by "mechanical" processes, such as convective transport by the mean flow and spreading caused by dispersion. The pollutant is perceived as a non-reactive or conservative matter and therefore the mass will be conserved. Modelling of these processes will be the main subject in this chapter.
- Modelling of decay and growth caused by biological or chemical processes/reactions. This extensive subject will not be treated in this work, but an example of a numerical oxygen model for streams can be found in Schaarup-Jensen (1988b).

Transport and spreading of pollutants in streams can be described in several ways. The most simple model is to assume that only transport caused

by convection is important. This can be a good approximation in steep, nearly uniform channels, but often the spreading cannot be neglected.

The most commonly used model is the one-dimensional Transport/Dispersion model, where the spreading is described as a Fickian diffusion process. The weakness of this model is that only symmetrical distributions can be described, and often measurements show that distributions are skew, – a long tail is present.

This phenomenon can be described by use of a Dead Zone model, where the Transport/Dispersion equation is expanded with a term, describing the exchange of matter between the flowing area and some totally mixed non-flowing area, the dead zone. These three models will be considered in the following sections.

For some occasions an analytical solution can be found to the models. Often these analytical solutions are based on so restrictive assumptions that the solution cannot be used in practice. But the analytical solutions can tell a lot about the behaviour of the model, and it can be used for testing of a numerical model. Therefore, some of the relevant analytical solutions will be mentioned in the next sections.

A wide range of numerical methods can be applied, but in this chapter mainly finite difference methods will be treated. An attempt to classify these methods is made, and a number of schemes, including the most commonly used, are described in some details.

Numerical properties, such as stability conditions and magnitude of numerical errors, are very important features in transport/dispersion modelling. The first numerical schemes were encumbered with serious numerical errors, providing erroneously results, and since then a lot of efforts have been spent in developing more accurate schemes. A large amount of papers can be studied, but often the obtained results are not comparable. With the purpose to review this subject and to obtain some general information, the numerical properties for a number of schemes have been examined and compared, using analytical as well as numerical methods.

## 4.2 Mathematical models for transport & spreading

### 4.2.1 Continuity for a conservative matter

The following three models are all based on a continuity a conservative pollutant. The continuity is developed for a small element of the stream (length  $dx$ ) and for a small amount of time ( $dt$ ).

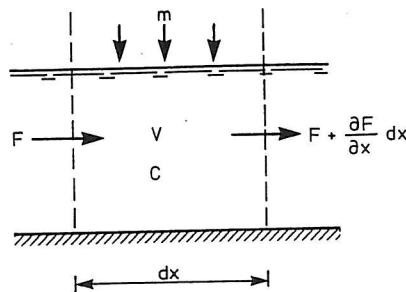


Fig. 4.1. Continuity for a small element of a stream (For explanation of symbols - look below).

$$\text{Amount of matter in the element at time } t : V \cdot C \quad (4.1)$$

$$\text{Amount of matter in the element at time } t + dt : V \cdot C + \frac{\partial(V \cdot C)}{\partial t} dt \quad (4.2)$$

$$\text{Transport into the element : } F \cdot dt \quad (4.3)$$

$$\text{Transport out of the element : } \left( F + \frac{\partial F}{\partial x} dx \right) dt \quad (4.4)$$

$$\text{Source term : } m \cdot dx \cdot dt \quad (4.5)$$

where  $dx$  : length of the element ( $m$ )  
 $dt$  : a small amount of time ( $sec$ )  
 $C$  : concentration of a conservative pollutant ( $gr/m^3$ )  
 $V$  : volume of the element ( $m^3$ )  
 $F$  : flux of matter through a surface ( $gr/sec$ )  
 $m$  : source input per unit length ( $gr/m \cdot sec$ )

Then a general continuity equation can be written, using that

$$\text{storage} = \text{inflow} - \text{outflow} + \text{source}$$

$$\left( V \cdot C + \frac{\partial(V \cdot C)}{\partial t} \right) - V \cdot C = F \cdot dt - \left( F + \frac{\partial F}{\partial x} \right) dt + m \cdot dx \cdot dt$$

↓

$$\frac{\partial(A \cdot C)}{\partial t} = -\frac{\partial F}{\partial x} + m \quad (4.6)$$

This is the basic continuity equation for all of the following models. They only differ from each other by the expressions of the transport flux  $F$  and the source term  $m$ .

#### 4.2.2 The Transport model

This model is based on the assumption that transport of a pollutant in a stream is caused by convection only. This means that a distribution of matter will be convected downstream with a celerity equal to the average flow velocity, and without any change in shape.

The transport can be expressed as:

$$F = Q \cdot C \quad (4.7)$$

where  $Q$  ( $m^3/sec$ ) is the flow.

Combining this with eq.(4.6) leads to:

$$\frac{\partial(A \cdot C)}{\partial t} + \frac{\partial(Q \cdot C)}{\partial x} = m \quad (4.8)$$

where  $A$  ( $m^2$ ) is the cross section area.

This equation is the general one-dimensional Transport equation for unsteady, non-uniform flow.

Assuming steady flow, and neglecting the source term, the equation can be reduced to:

$$\frac{\partial C}{\partial t} + u \frac{\partial C}{\partial x} = 0 \quad (4.9)$$

where  $u$  ( $m/sec$ ) is the average flow velocity.

If the flow is assumed to be steady an analytical solution can be obtained. Since  $C$  is a function of  $t$  and  $x$  we get:

$$dC = \frac{\partial C}{\partial t} dt + \frac{\partial C}{\partial x} dx$$

↓

$$\frac{dC}{dt} = \frac{\partial C}{\partial t} + \frac{\partial C}{\partial x} \frac{dx}{dt} \quad (4.10)$$

A combination of eq.(4.9) and eq.(4.10) leads to:

$$\frac{dC}{dt} = 0 \quad \text{for} \quad u = \frac{dx}{dt} \quad (4.11)$$

which also can be found from eq.(4.9) by changing the coordinate system to a system moving with a celerity of  $u$ .

We now assume that the concentration  $C(x_0, t)$  at the upper end of the stream (called  $x_0$ ) is known as a function of time. By moving this known profile downstream with the celerity  $u$ , the concentration at a certain place and time can be found. The travel time  $tt$  from  $x_0$  to  $x$  can be found from:

$$tt = \int_{x_0}^x \frac{1}{u} dx \quad (4.12)$$

and the solution can then be expressed as:

$$C(x, t) = C \left( x_0, t - \int_{x_0}^x \frac{1}{u} dx \right) \quad (4.13)$$

If the flowfield is uniform, the solution can be reduced to:

$$C(x, t) = C \left( x_o, t - \frac{1}{u}(x - x_o) \right) \quad (4.14)$$

The Transport model is a very plain and usable model, especially when the flow velocity is constant. The model should only be used when longitudinal dispersion can be neglected, which often can be performed in sewer networks and open channels with a uniform velocity distribution in the cross section.

In natural streams dispersion seldom can be neglected, and therefore the Transport model should be used by care and only for providing initial results.

#### 4.2.3 The Transport/Dispersion model

This model is based on the assumption that the transport (the flux  $F$ ) through a surface can be described by convection, and a Fickian diffusion. Then a distribution of matter will be convected downstream with the average flow velocity and the shape will be changed by the diffusion term.

The flux through a surface is now expressed as:

$$F = Q \cdot C - K_x \cdot A \frac{\partial C}{\partial x} \quad (4.15)$$

where  $K_x$  ( $m^2/sec$ ) is the longitudinal dispersion coefficient.

Combining this with eq.(4.6) yields:

$$\begin{aligned} \frac{\partial(A \cdot C)}{\partial t} &= - \frac{\partial(Q \cdot C - K_x \cdot A \frac{\partial C}{\partial x})}{\partial x} + m \\ \Downarrow \\ \frac{\partial(A \cdot C)}{\partial t} + \frac{\partial(Q \cdot C)}{\partial x} &= \frac{\partial}{\partial x} \left( K_x \cdot A \frac{\partial C}{\partial x} \right) + m \end{aligned} \quad (4.16)$$

This equation is the most common used to describe transport and spreading of pollutants in streams and is called the one-dimensional Transport/Dispersion model for unsteady non-uniform flow.

Assuming a steady uniform flow, a constant dispersion coefficient, and a source term of zero eq.(4.16) leads to:

$$\frac{\partial C}{\partial t} + u \frac{\partial C}{\partial x} = K_x \frac{\partial^2 C}{\partial x^2} \quad (4.17)$$

An analytical solution can be obtained for one very important case, under assumption of a steady and uniform flow, eq.(4.17).

Eq.(4.17) can be solved if the upper boundary (located at  $x_0$ ) is specified in a certain manner:

$$x_0 = 0$$

$$C(x_0) = \infty \quad \text{for } \tau = 0 \quad \text{else} \quad C(x_0) = 0$$

$$\int_{-\infty}^{\infty} C(x_0) d\tau \neq 0 \quad (4.18)$$

describing the concentration profile at the upper boundary as a delta function, which is a good approximation to a pulse injection of tracer.

For these conditions the solution is found to:

$$C(x, \tau) = \frac{\frac{m}{A}}{\sqrt{4 \cdot \pi \cdot K_x \cdot \tau}} \exp\left(\frac{-(x' - u \cdot \tau)^2}{4 \cdot K \cdot \tau}\right) \quad (4.19)$$

where  $m$  : injected mass (gr)  
 $A$  : cross section area ( $m^2$ )  
 $K_x$  : dispersion coefficient ( $m^2/sec$ )  
 $\tau$  : time since injection (sec)  
 $x'$  : distance from injection point (m)

Introducing

$$x' = x - x_0 \quad \text{and} \quad \tau = t - t_0 \quad (4.20)$$

where  $x_0$  : space for injection (m)  
 $t_0$  : time for injection (sec)

the general solution for a pulse injection at station  $x_0$  and time  $t_0$  can be expressed as:

$$C(x, t) = \frac{\frac{m}{A}}{\sqrt{4 \cdot \pi \cdot K_x(t - t_0)}} \exp\left(\frac{-((x - x_0) - u(t - t_0))^2}{4 \cdot K_x(t - t_0)}\right) \quad (4.21)$$

This expression can be expanded to a semi-analytical solution for an arbitrary concentration profile at station  $x_0$ , using that eq.(4.17) is linear, which means that a solution can be found as a sum of independent solutions (superposition).

An arbitrary concentration profile at  $x_0$  can be approximated with a number ( $k_x$ ) of delta functions, Fig. 4.2.

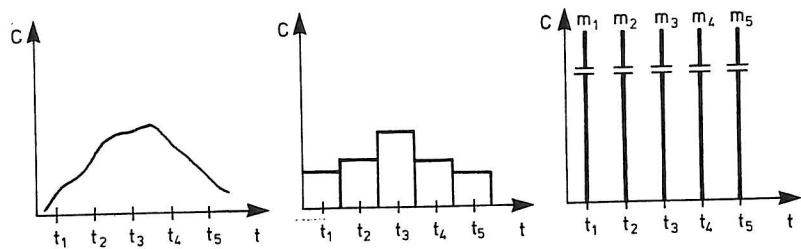


Fig. 4.2. Approximation of concentration profile with delta functions.

For each delta function the injected mass  $m_k$  and the time for injection  $t_k$  has to be specified. The final solution can be expressed as a sum:

$$C(x, t) = \sum_{k=1}^{k_m} \frac{\frac{m_k}{A}}{\sqrt{4 \cdot \pi \cdot K_x(t - t_k)}} \exp\left(\frac{-((x - x_0) - u(t - t_k))^2}{4 \cdot K_x(t - t_k)}\right) \quad (4.22)$$

where index  $k$  refers to injection no.  $k$ . By increasing  $k$  eq.(4.22) will converge against the true solution (found by convolution of eq.(4.21)).

It is very important to notice that the Transport/Dispersion model tends against solutions, which are Gaussian distributions in the x-domain, symmetrical around the mean position (equal to the peak position). The Transport/Dispersion model will be a sufficient model for many natural streams, as long as the variation of the geometry and especially the velocity distribution in the cross sections are moderate. Large almost non-flowing areas will provide a skew distribution, and if such phenomena are important, then the Transport/Dispersion model should be replaced with the following model.

#### 4.2.4 The Transport/Dispersion/Dead Zone model

This model is based on the assumption that the cross section is divided into two sub-areas, – a flowing area and a non-flowing area, also called the dead zone (Pedersen, 1977).

In the flowing zone the flux through a surface is described by convection and Fickian diffusion, like the traditional Transport/Dispersion model.

$$F = Q \cdot C - K_x \cdot A \frac{\partial C}{\partial x} \quad (4.23)$$

Between the flowing zone and the dead zone, which is assumed to be totally mixed, the transport of matter is caused by an exchange of water. In the model this is expressed as a special source term:

$$m_* = q_d \cdot C_d - q_d \cdot C = q_d (C_d - C) \quad (4.24)$$

where  $q_d$  is the exchange of water per unit length ( $m^3/m \cdot sec$ )  
 $C_d$  is the concentration in the dead zone ( $gr/m^3$ ).

These expressions can be combined with eq.(4.6) leading to:

$$\frac{\partial(A \cdot C)}{\partial t} = -\frac{\partial(Q \cdot C)}{\partial x} + \frac{\partial}{\partial x} \left( K_x \cdot A \frac{\partial C}{\partial x} \right) + q_d (C_d - C) + m \quad (4.25)$$

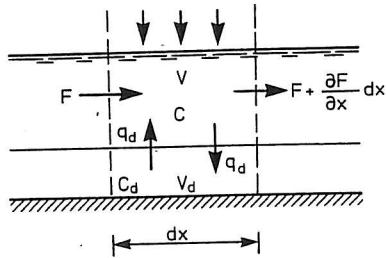


Fig. 4.3. Dead Zone model.

Introducing the cross section area of the dead zone:

$$A_d = \frac{V_d}{dx} \quad (4.26)$$

where  $V_d$  denotes the dead zone volume, a continuity consideration for the dead zone yields:

Quantity of matter at time  $t$ :

$$A_d \cdot C_d \cdot dx \quad (4.27)$$

Quantity of matter at time  $t + dt$ :

$$A_d \cdot C_d \cdot dx + \frac{\partial(A_d \cdot C_d \cdot dx)}{\partial t} dt \quad (4.28)$$

Transport into the dead zone:

$$q_d \cdot C \cdot dx \cdot dt \quad (4.29)$$

Transport out of the dead zone:

$$q_d \cdot C_d \cdot dx \cdot dt \quad (4.30)$$

From which we get:

$$\left( A_d \cdot C_d \cdot dx + \frac{\partial(A_d \cdot C_d \cdot dx)}{\partial t} dt \right) - (A_d \cdot C_d \cdot dx) =$$

$$q_d \cdot C \cdot dx \cdot dt - q_d \cdot C_d \cdot dx \cdot dt$$

↓

$$\frac{\partial(A_d \cdot C_d)}{\partial t} = q_d(C - C_d) \quad (4.31)$$

This equation in combination with eq.(4.25) is the Transport/Dispersion/Dead zone model for unsteady, non-uniform flow.

Assuming that the flow is steady and uniform, and the dispersion coefficient and the cross section area of the dead zone are constants, the model can be reduced to:

$$\frac{\partial C}{\partial t} + u \frac{\partial C}{\partial x} = K_x \frac{\partial^2 C}{\partial x^2} + \frac{\varepsilon}{T_d} (C_d - C) + \frac{1}{A} m \quad (4.32)$$

$$\frac{\partial C_d}{\partial t} = \frac{1}{T_d} (C - C_d) \quad (4.33)$$

where the volume fraction dead zone

$$\varepsilon = \frac{V_d}{V} = \frac{A_d}{A} \quad (4.34)$$

and the residence time for the dead zone

$$T_d = \frac{A_d}{q_d} \quad (4.35)$$

have been introduced.

Eq.(4.32) and eq.(4.33) can be transformed to a higher order differential equation:

$$T_d \frac{\partial}{\partial t} \left( \frac{\partial C}{\partial t} + u \frac{\partial C}{\partial x} - K_x \frac{\partial^2 C}{\partial x^2} \right) + \\ (1 + \varepsilon) \left( \frac{\partial C}{\partial t} + \frac{u}{1 + \varepsilon} \frac{\partial C}{\partial x} - \frac{K_x}{1 + \varepsilon} \frac{\partial^2 C}{\partial x^2} \right) = 0 \quad (4.36)$$

The model above will be able to simulate skew concentration distributions, which often can be observed in natural streams. A further description of the features of the model and how the dead zone parameters  $T_d$  and  $\varepsilon$  can be determined, can be found in Pedersen (1977) and in Bjerrekjær, Mark and Tornbjerg (1988).

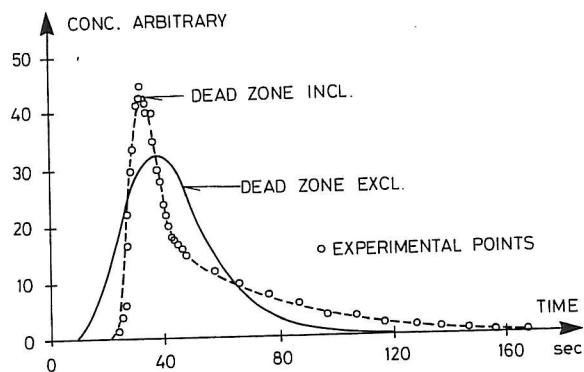


Fig. 4.4. Fit of two models to experimental data (Pedersen, 1977).

## 4.3 Numerical solution of the Transport model

### 4.3.1 Method of Characteristics

The most obvious choice, with section 4.2 in mind, would be to use the Method of Characteristics for a numerical solution of the Transport model. In sec. 4.2.2 the Transport equation was rewritten as:

$$\frac{dC}{dt} = 0 \quad \text{for} \quad u = \frac{dx}{dt} \quad (4.37)$$

This means that if the grid is chosen in a way that

$$u = \frac{\Delta x}{\Delta t} \quad \text{or} \quad u \frac{\Delta x}{\Delta t} = 1 \quad (4.38)$$

then the numerical scheme becomes very simple, namely

$$C_j^{n+1} = C_j^n \quad (4.39)$$

referring to Fig. 4.5 where the characteristic determined by eq.(4.38) is shown.

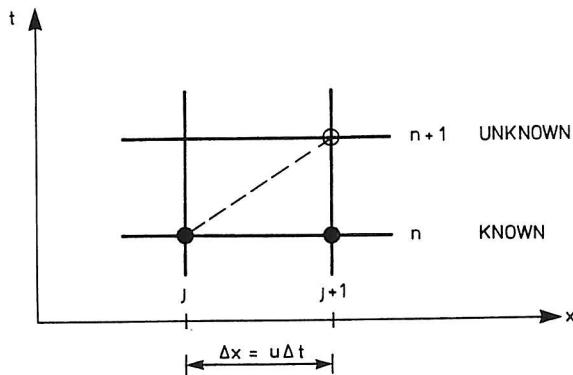


Fig. 4.5. The Method of Characteristics.

But this means that strong restrictions are put on the choice of grid, which can be most inconvenient, but accurate results are achieved, – no numerical errors are present.

Instead a more convenient grid, which do not fulfil eq.(4.38), could be chosen. This situation is illustrated in Fig. 4.6, where the characteristic is shown, but in this case it intersects the lower time level between two nodes.

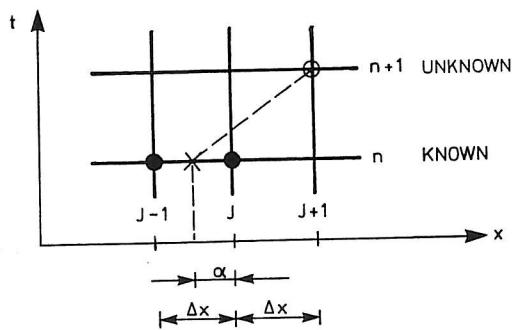


Fig. 4.6. Modified Method of Characteristics.

Eq.(4.37) is still valid along the characteristic, but the problem is that the value of the concentration at the point of intersection is not known. This value can be found by interpolation between the known values at the nodes ( $j$ ) and ( $j - 1$ ).

If this is done by linear interpolation we get the Bella Dobbins scheme, and using the notation in Fig. 4.6 this scheme can be written as (Cunge et al., 1980):

$$C_{j+1}^{n+1} = \frac{(\Delta x - \alpha) C_j^n + \alpha \cdot C_{j-1}^n}{\Delta x} \quad (4.40)$$

$$\alpha = \Delta x - u \cdot \Delta t$$

If this scheme is examined for numerical errors by use of Taylor analysis, see sec. 4.5.2, then we get:

$$\frac{\partial C}{\partial t} + u \frac{\partial C}{\partial x} = \frac{\Delta x^2}{2 \cdot \Delta t} \left( 1 - u \frac{\Delta t}{\Delta x} \right) \left( u \frac{\Delta t}{\Delta x} - 2 \right) \frac{\partial^2 C}{\partial x^2} \quad (4.41)$$

which shows that some numerical errors have been introduced as a result of the applied interpolation technique. But it can be seen from eq.(4.41) that the error will be eliminated if a special combination of  $\Delta x$  and  $\Delta t$  is chosen, in accordance with eq.(4.38) and Fig. 4.5.

A lot of work has been done in trying to apply a better interpolation technique. The most obvious way is to use a higher order interpolation, where more than two nodes are used in the interpolation. Another way of creating a better interpolation is to include the derivative of the dependent variable. This performance has been used of Cunge et al. (1980) in the scheme called "Two Point Fourth Order". In this scheme a cubic interpolation is performed:

$$C_{j+1}^{n+1} = a_1 \cdot C_{j-1}^n + a_2 \cdot C_j^n + a_3 \left( \frac{\partial C}{\partial x} \right)_{j-1}^n + a_4 \left( \frac{\partial C}{\partial x} \right)_j^n \quad (4.42)$$

The coefficients  $a_i$  can be found in Cunge et al. (1980).

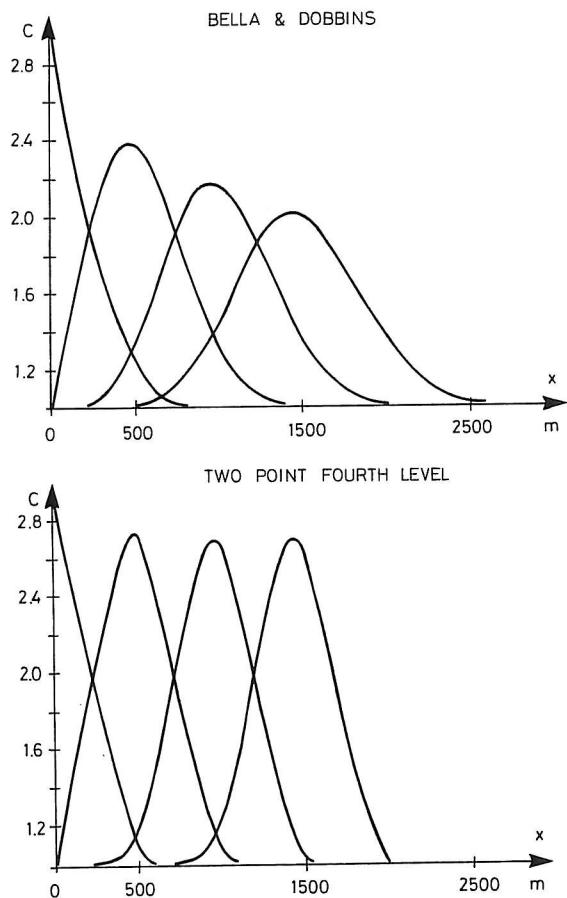


Fig. 4.7. Testrun with the Bella Dobbins scheme, and the Two Point Fourth Order scheme applied for the Transport model.

This scheme shows very good features in comparison with the traditional linear interpolation as performed in the Bella Dobbins scheme, which is illustrated in Fig. 4.7, where results from a testrun are shown. A narrow triangel (with a peak value of 3) is convected in a uniform flowfield.

Both schemes are able to simulate a correct transport celerity of the mean value. But as seen in Fig. 4.7 the Bella Dobbins model provides a large unexpected spreading of the triangel, while the Two Point Fourth Order scheme shows much better results. Only a slightly smoothing of the triangel, leading to a smaller peak value, can be observed.

Fig. 4.7 is an excellent example of the phenomenon "numerical dispersion", which will be described further in section 4.5.

### 4.3.2 Control Volume approach

A similar problem of interpolation can be recognized in the Control Volume (CV) approach. Referring to Fig. 4.8, the continuity for the CV can be written in an explicit manner as:

$$V_j (C_j^{n+1} - C_j^n) = F_{j-\frac{1}{2}} \cdot \Delta t - F_{j+\frac{1}{2}} \cdot \Delta t \quad (4.43)$$

where  $F = Q \cdot C^*$ .

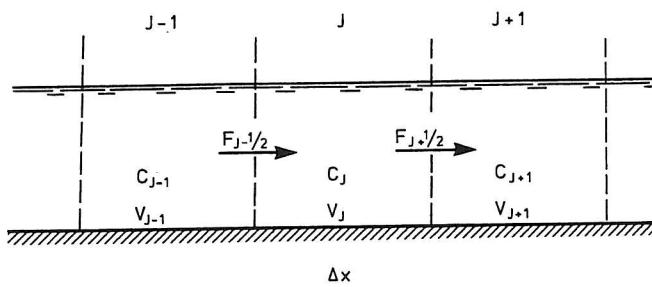


Fig. 4.8. Control Volume approach.

Now the problem is to determine which concentration  $C^*$  to use in the flux into and out of the CV. We can choose to use the concentration from the upper CV and then we get the upwind scheme, which can be written as:

$$C_j^{n+1} = u \frac{\Delta t}{\Delta x} (C_{j-1}^n - C_j^n) + C_j^n \quad (4.44)$$

or instead a linear interpolation between the concentrations in the two CV can be used, leading to:

$$C_j^{n+1} = C_j^n + u \frac{\Delta t}{2 \cdot \Delta x} (C_{j-1}^n - C_{j+1}^n) \quad (4.45)$$

In a similar way as above different types of higher order interpolation could be introduced. The features of the two CV models will be treated further in sec. 4.4, where two finite difference schemes, almost identical to eq.(4.44) and eq.(4.45) will be considered.

Further descriptions of Control Volume models can be found e.g. in Patanka (1980).

## 4.4 Numerical solution of the Transport/ Dispersion model

### 4.4.1 Finite difference schemes

The most commonly used model for description of transport and spreading of pollutants in streams is the Transport/Dispersion model, which in a general form can be written as:

$$\frac{\partial(A \cdot C)}{\partial t} + \frac{\partial(Q \cdot C)}{\partial x} = \frac{\partial}{\partial x} \left( K_x \cdot A \frac{\partial C}{\partial x} \right) + m \quad (4.46)$$

where  $C$  : concentration of matter ( $gr/m^3$ )  
 $A$  : cross section area ( $m^2$ )  
 $Q$  : flow ( $m^3/sec$ )  
 $K_x$  : longitudinal dispersion coefficient ( $m^2/sec$ )  
 $m$  : source/sink ( $gr/m \cdot sec$ )  
 $x$  : space coordinate ( $m$ )  
 $t$  : time coordinate ( $sec$ )

Assuming that there are no sinks or sources, that the longitudinal dispersion coefficient is constant, and that the flow is steady, then eq.(4.46) can be reduced to:

$$\frac{\partial C}{\partial t} + u \frac{\partial C}{\partial x} = K_x \frac{\partial^2 C}{\partial x^2} \quad (4.47)$$

where  $u$ : average flow velocity ( $m/sec$ ).

In this section all considerations will be related to the simplified eq.(4.47), because this simplified version makes it possible to determine stability conditions (see sec. 4.6) and error terms (see sec. 4.5) in an analytical way. Furthermore, an analytical solution exists for some specific conditions, as described in sec. 4.2.3, which can be used for comparison with the numerical solution. But on the other hand this means that the achieved results cannot be used directly for unsteady flow, further considerations might be necessary.

In the past mostly finite difference schemes have been used for numerical solution of the Transport/Dispersion model, whether these have been implemented directly in the differential equation, or indirectly through a Control

Volume model. In the following section all schemes are not represented, of course, but instead the schemes have been divided into four classes, from which some characteristic schemes will be described. The four classes to be mentioned are:

- Two Level schemes. Two time levels and up to three nodes at each time level are used in the discretization. Explicit as well as implicit schemes are included.
- Three Level schemes. Three time levels and up to three nodes at each time level are used.
- Quick schemes. A class of schemes inspired from the Quick scheme (Leonard, 1979), where two time levels and up to four nodes at each are used.
- Other schemes. This class includes the rest, e.g. schemes using more than four nodes at each time level, etc.

A number of schemes, belonging to the three classes shown in Fig. 4.9, will be treated further in sec. 4.5 and sec. 4.6, where some comparison will be made by mean of numerical error properties and stability conditions.

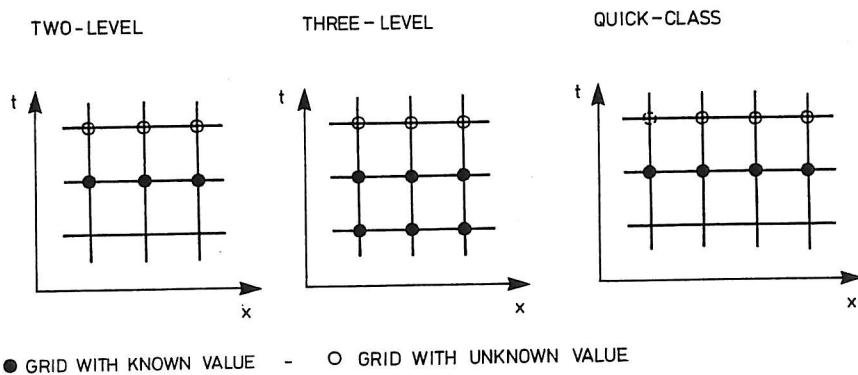


Fig. 4.9. Three classes of finite difference schemes.

#### 4.4.2 Two Level schemes

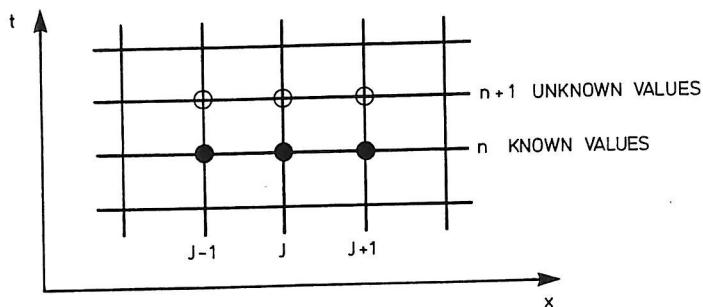


Fig. 4.10. Class of Two Level schemes.

This type of schemes includes the most commonly used numerical schemes for the Transport/Dispersion model. In the discretization two time levels and up to three nodes at each time level are used, as illustrated in Fig. 4.10.

#### Explicit schemes

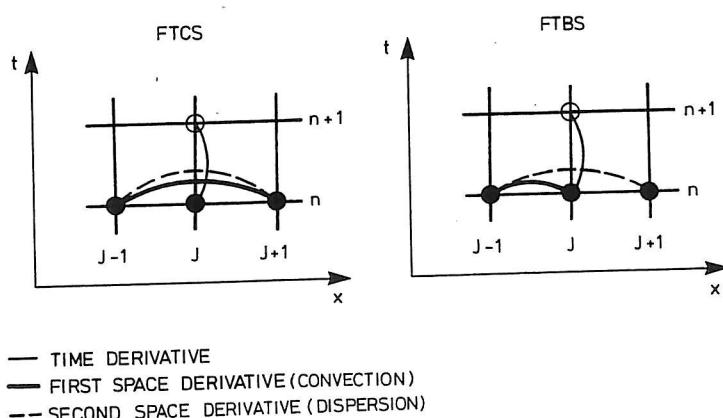


Fig. 4.11. Discretization of the FTCS scheme and the FTBS scheme.

Two often mentioned explicit schemes are included in this class. The first one is the Forward Time Central Space scheme (FTCS) and the second one is the Forward Time Backward Space (or upwind) scheme (FTBS). The

discretization of time derivative and the second space derivative are similar in the two schemes, the only difference is the discretization of the convective term, – the first space derivative. In the FTCS scheme a central difference is used, while a backward difference is used in the FTBS scheme, which is illustrated in Fig. 4.11.

FTCS:

$$C_j^{n+1} = C_j^n - u \frac{\Delta t}{2 \cdot \Delta x} (C_{j+1}^n - C_{j-1}^n) + K_x \frac{\Delta t}{\Delta x^2} (C_{j+1}^n - 2 \cdot C_j^n + C_{j-1}^n) \quad (4.48)$$

FTBS:

$$C_j^{n+1} = C_j^n - u \frac{\Delta t}{\Delta x} (C_j^n - C_{j-1}^n) + K_x \frac{\Delta t}{\Delta x^2} (C_{j+1}^n - 2 \cdot C_j^n + C_{j-1}^n) \quad (4.49)$$

Even though the difference between these two schemes seems to be small, the properties are quite different. If the dispersion terms are removed, then the two schemes above are identical to the two schemes obtained in sec. 4.3.2 by use of the Control Volume approach.

### Implicit schemes.

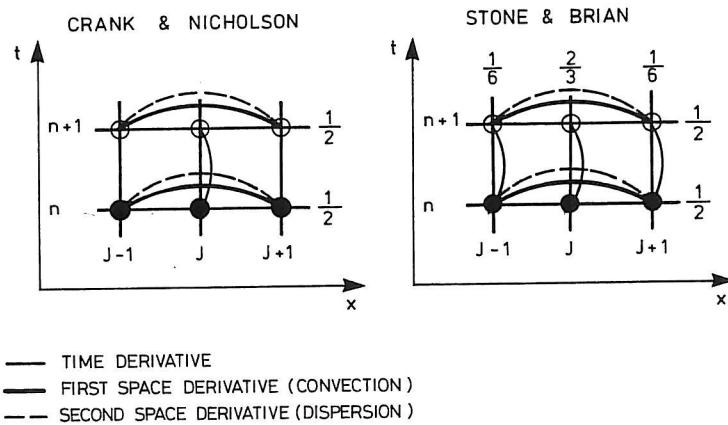


Fig. 4.12. The Crank & Nicholson scheme and the Stone & Brian scheme.

A lot of implicit schemes can be mentioned, but only two will be considered. The first one will be called Crank & Nicholson, because the well-known Crank Nicholson formula is used in combination with a central difference for the convective term.

The second one is the Stone & Brian scheme (Fischer, 1979), which is identical to the Crank & Nicholson except from a speciel formulation of the time derivative. This is formed as a weighted sum of differences, where the central grid  $j$  has a weight of  $2/3$  and each of the outer grid a weight of  $1/6$ .

The two difference equations can be written as:

Crank & Nicholson:

$$\begin{aligned}
 & \frac{1}{2} \left( -u \frac{\Delta t}{2 \cdot \Delta x} - K_x \frac{\Delta t}{\Delta x^2} \right) C_{j-1}^{n+1} + \\
 & \left( K_x \frac{\Delta t}{\Delta x^2} \right) C_j^{n+1} + \\
 & \frac{1}{2} \left( u \frac{\Delta t}{2 \cdot \Delta x} - K \frac{\Delta t}{\Delta x^2} \right) C_{j+1}^{n+1} = \\
 & \frac{1}{2} \left( u \frac{\Delta t}{2 \cdot \Delta x} + K_x \frac{\Delta t}{\Delta x^2} \right) C_{j-1}^n + \\
 & \left( -K_x \frac{\Delta t}{\Delta x^2} \right) C_j^n + \\
 & \frac{1}{2} \left( -u \frac{\Delta t}{2 \cdot \Delta x} + K_x \frac{\Delta t}{\Delta x^2} \right) C_{j+1}^n
 \end{aligned} \tag{4.50}$$

Stone & Brian:

$$\begin{aligned}
 & \left( \frac{1}{6} + \frac{1}{2} \left( -u \frac{\Delta t}{2 \cdot \Delta x} - K_x \frac{\Delta t}{\Delta x^2} \right) \right) C_{j-1}^{n+1} + \\
 & \left( \frac{2}{3} + K_x \frac{\Delta t}{\Delta x^2} \right) C_j^{n+1} + \\
 & \left( \frac{1}{6} + \frac{1}{2} \left( u \frac{\Delta t}{2 \cdot \Delta x} - K_x \frac{\Delta t}{\Delta x^2} \right) \right) C_{j+1}^{n+1} = \\
 & \left( \frac{1}{6} + \frac{1}{2} \left( u \frac{\Delta t}{2 \cdot \Delta x} + K_x \frac{\Delta t}{\Delta x^2} \right) \right) C_{j-1}^n +
 \end{aligned}$$

$$\begin{aligned} & \left( \frac{2}{3} - K_x \frac{\Delta t}{\Delta x^2} \right) C_j^n + \\ & \left( \frac{1}{6} + \frac{1}{2} \left( -u \frac{\Delta t}{2 \cdot \Delta x} + K_x \frac{\Delta t}{\Delta x^2} \right) \right) C_{j+1}^n \end{aligned} \quad (4.51)$$

These schemes lead to a system of linear equations, which can be solved by use of one of the methods mentioned in sec 2.6. The most commonly used method is the Double Sweep algorithm.

### The Two Level Multischeme

The Two Level Multischeme is a scheme developed for use in test of the behaviour of the Two Level schemes. The scheme contains three coefficients, which can be varied, and thus provide different schemes. These coefficients are:

- $\Theta$ : A coefficient used in the space derivatives for centering in time. If  $\Theta$  is zero then pure explicit schemes are obtained. If  $\Theta = 0.5$  then the scheme is fully centered in time, as e.g. the Crank & Nicholson scheme.
- $\alpha$ : A coefficient used in the time derivative. If  $\alpha$  is zero then the time derivative is approximated by a difference only at the central nodes, as in the FTCS scheme and the Crank and Nicholson scheme. If  $\alpha$  is  $1/6$  then the Stone & Brian formulation is achieved.
- $\beta$ : A coefficient used in the first space derivative, – the convective term. If  $\beta$  is zero then a backward difference is used as in the FTBS scheme, and if  $\beta$  is  $1/2$  then a central difference is used (FTCS).

The derivation is shown in Appendix and leads to an expression of the form:

Two Level Multischeme:

$$\begin{aligned} & a_1 \cdot C_{j-1}^{n+1} + a_2 \cdot C_j^{n+1} + a_3 \cdot C_{j+1}^{n+1} = \\ & b - 1 \cdot C_{j-1}^n + b - 2 \cdot C_j^n + b - 3 \cdot C_{j+1}^n \end{aligned} \quad (4.52)$$

where the coefficients  $a_i$  and  $b_i$  can be found in Appendix.

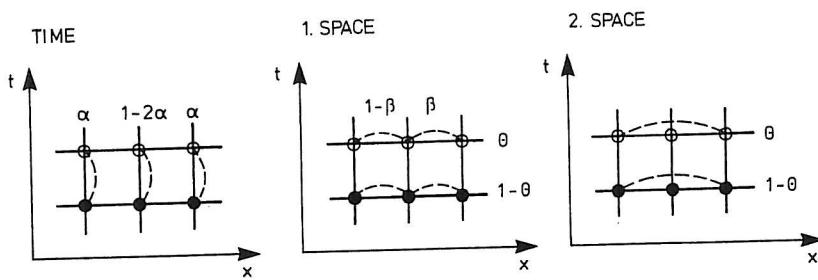


Fig. 4.13. Coefficients in the Two Level Multischeme.

For a certain choice of the coefficients  $\Theta$ ,  $\alpha$ , and  $\beta$  all the four schemes mentioned above can be obtained. The choice of the coefficients is shown in Table 4.1.

Furthermore, the coefficients for two other implicit Two Level schemes are shown in Table 4.1. The first one is the Backward Time Central Space (BTCS) and the second one the Backward Time Backward Space scheme (BTBS). In these schemes only values at time level  $n+1$  are used in the discretization of the space derivatives. Later on in section 4.5 all these schemes will be compared by means of numerical error properties.

Table 4.1. Choice of coefficients in the Two Level Multischeme.

	$\Theta$	$\alpha$	$\beta$
FTCS	0	0	$\frac{1}{2}$
FTBS	0	0	0
Crank & Nich.	$\frac{1}{2}$	0	$\frac{1}{2}$
Stone & Brian	$\frac{1}{2}$	$\frac{1}{6}$	$\frac{1}{2}$
BTCS	1	0	$\frac{1}{2}$
BTBS	1	0	0

#### 4.4.3 Three Level schemes

This type of scheme is not used so often for Transport/Dispersion modelling. As the name indicates, this group of schemes includes three time levels in the discretization, and up to three nodes at each time level.

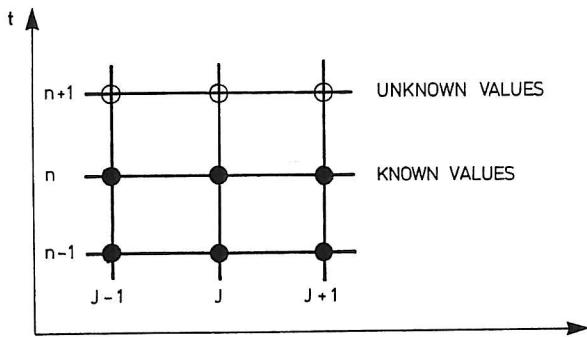


Fig. 4.14. Class of Three Level schemes.

#### Explicit schemes

Two explicit schemes will be mentioned. The first one is a fully centered scheme, which will be called Leap Frog, because the basic scheme is identical to the original Leap Frog scheme, well known from the hydrodynamic modelling (sec. 3.4.2). The discretization is very straightforward and is illustrated in Fig. 4.15.

The second scheme is almost identical, except from a slightly different discretization of the dispersion term, – the second space derivative. The value at the central grid ( $j, n$ ) is exchanged with the mean of the values at  $(j, n + 1)$  and  $(j, n - 1)$ . This has some positive effect on the stability properties. The scheme is called the Du Fort & Frankel scheme, and it should be mentioned that this scheme is conditionally consistent, while all the other schemes mentioned up to now were unconditionally consistent.

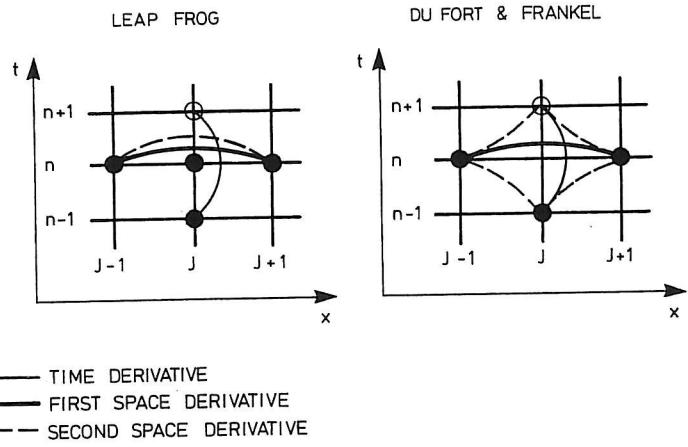


Fig. 4.15. The Leap Frog scheme and the Du Fort & Frankel scheme.

Leap Frog:

$$\begin{aligned}
 C_j^{n+1} = & C_j^{n-1} - u \frac{\Delta t}{2 \cdot \Delta x} (C_{j+1}^n - C_{j-1}^n) + \\
 & K_x \frac{2 \cdot \Delta t}{\Delta x^2} (C_{j+1}^n - 2 \cdot C_j^n + C_{j-1}^n)
 \end{aligned} \tag{4.53}$$

Du Fort & Frankel:

$$\begin{aligned}
 C_j^{n+1} = & \frac{1}{\left(1 + K_x \frac{2 \cdot \Delta t}{\Delta x^2}\right)} \cdot \\
 & \left( C_j^{n-1} - u \frac{\Delta t}{\Delta x} (C_{j+1}^n - C_{j-1}^n) + \right. \\
 & \left. K_x \frac{2 \cdot \Delta t}{\Delta x^2} (C_{j+1}^n - C_j^n + C_{j-1}^n) \right)
 \end{aligned} \tag{4.54}$$

### The Blockscheme.

Implicit Three Level schemes have not been used so widely in modelling of transport and dispersion, but for Diffusion models some schemes can be found in Richtmyer & Morton (1967). No specific scheme will be described here. Instead a more general scheme, like the Two Level Multischeme, has been developed and used in the investigations.

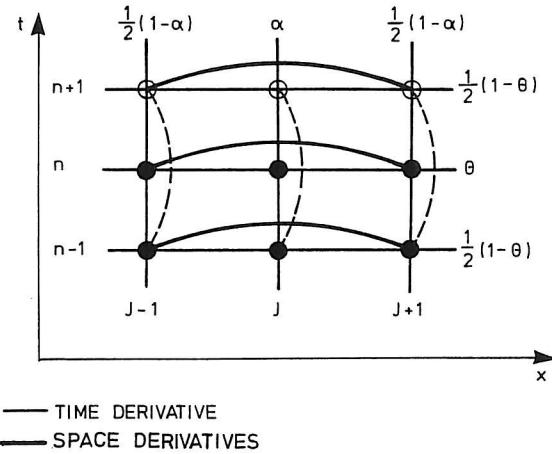


Fig. 4.16. Coefficients in the Blockscheme.

Many possible coefficients can be introduced in a scheme where up to nine nodes can be used in the discretization. In this scheme, called the Blockscheme (the scheme is symmetrical around the centernode), only two coefficients are introduced:

- $\Theta$ : A coefficient used in the discretization of the space derivatives. If  $\Theta$  is equal to one, then the space derivatives are expressed by use of values from time level  $n$  only, for all other values all three time levels are used in the discretization.
- $\alpha$ : A coefficient used in the discretization of the time derivative. If  $\alpha$  is equal to one, then only the nodes at  $j$  are used.

This leads to the difference equation:

$$a_1 \cdot C_{j+1}^{n+1} + a_2 \cdot C_j^{n+1} + a_3 \cdot C_{j-1}^{n+1} = b \quad (4.55)$$

where the coefficients  $a_i$  are functions of  $(u, K_x, \Delta t, \Delta x, \Theta, \alpha)$  and the right hand side  $b$  is a function of  $(u, K_x, \Delta t, \Delta x, \Theta, \alpha)$  and the known values at time level  $n$  and  $n - 1$ . The coefficients can be found in Appendix.

If  $\Theta$  and  $\alpha$  are equal to one, then this expression can be reduced to the explicit Leap Frog scheme. For all other values of  $\Theta$  and  $\alpha$  the scheme becomes implicit, and some method for solving systems of equations must be introduced.

#### 4.4.4 Quick schemes

This group of schemes have been developed in an attempt to create a scheme without wiggles, – a phenomenon which will be treated further in sec. 4.5. It is widely known that the discretization of the convective term is very sensitive. If a backward difference is used, then the scheme suffers from large numerical errors, but if a central difference is used, then wiggles can become a problem. A further description of this phenomenon can also be found in Leonard (1979).

Instead another way of treating the convective term was introduced by Leonard (1979), who developed the Quick scheme for steady conditions, where an equilibrium between convection and dispersion is present. Instead of using linear interpolation in the expression for the convection, a Quadratic Upstream Interpolation for Convective Kinematics (QUICK) was used.

Using this approach for Transport/Dispersion modelling the following three schemes have been obtained. The three schemes will only be described very briefly. For further information the reader should consult the references.

##### Quickest

This explicit scheme using four nodes at time level  $n$ , Fig. 4.17, was developed by Leonard (1979).

$$C_j^{n+1} = b_1 \cdot C_{j+1}^n + b_2 \cdot C_j^n + b_3 \cdot C_{j-1}^n + b_4 \cdot C_{j-2}^n \quad (4.56)$$

where the coefficients  $b_i$  are functions of  $(u, K_x, \Delta x, \Delta t)$  (see Appendix). It can be shown (Basco, 1984) that the Quickest scheme also can be obtained,

if the numerical errors in the FTCS scheme are removed by introducing some correction terms.

### Quickist

This scheme was developed by Basco (Basco, 1984), with the purpose to create a scheme, with the same good properties as the Quickest, but with a greater stability area, see sec. 4.6. The Quickist scheme is a semi-implicit scheme (not all terms are expressed implicit) using three nodes at time level  $n + 1$  and four nodes at time level  $n$ , Fig. 4.17. But the stability was not improved as much as expected. The coefficients can be found in Appendix.

$$\begin{aligned} a_1 \cdot C_{j+1}^{n+1} + a_2 \cdot C_j^{n+1} + a_3 \cdot C_{j-1}^{n+1} = \\ b_1 \cdot C_{j+1}^n + b_2 \cdot C_j^n + b_3 \cdot C_{j-1}^n + b_4 \cdot C_{j-2}^n \end{aligned} \quad (4.57)$$

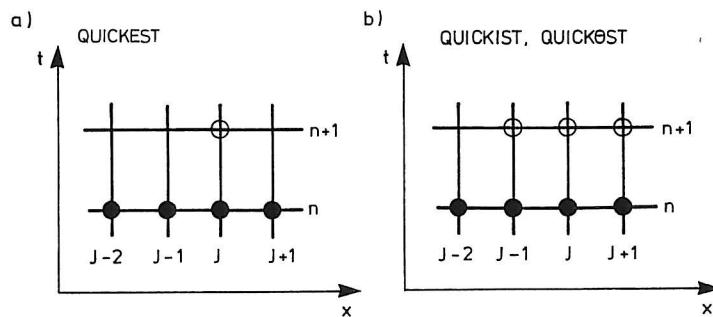


Fig. 4.17. Schematic discretization of Quickest , Quickist and Quickθst.

### Quickθst

Instead the Quickθst was developed, also by Basco (1984). The centering of the Quickist scheme was improved, and the Quickθst showed up with better stability properties.

$$\begin{aligned} a_1 \cdot C_{j+1}^{n+1} + a_2 \cdot C_j^{n+1} + a_3 \cdot C_{j-1}^{n+1} = \\ b_1 \cdot C_{j+1}^n + b_2 \cdot C_j^n + b_3 \cdot C_{j-1}^n + b_4 \cdot C_{j-2}^n \end{aligned} \quad (4.58)$$

Also these coefficients can be found in Appendix.

## 4.5 Numerical errors in Transport/ Dispersion models

### 4.5.1 Description of numerical errors

One of the most important properties of a numerical method or model is the accuracy of the numerical solution, having in mind that a numerical solution only is an approximation to the real solution.

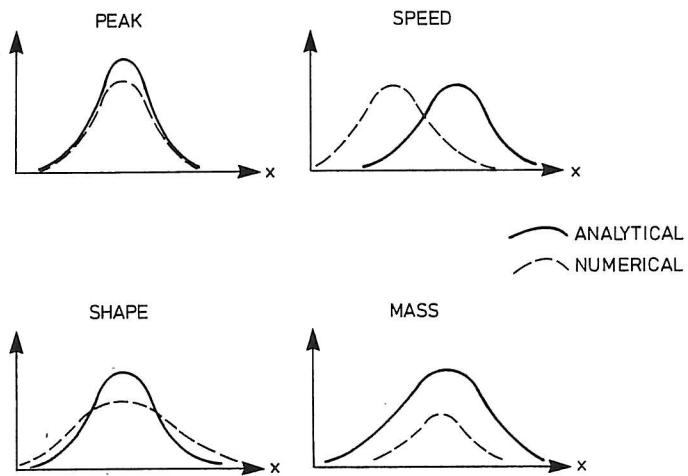


Fig. 4.18. Illustration of four types of numerical errors.

As mentioned in chapter 2 the numerical error can be divided into two classes:

- round off errors caused by the computer, which only works with a limited number of digits. In transport/dispersion modelling this type of error is often of minor importance, and therefore no further considerations on this type of error will be made in this work.
- truncation errors provided by the numerical scheme. A description of this type of error will be the main subject in the following section. The description will be limited to Transport/Dispersion models.

If an analytical and a numerical solution are compared visually, four types of errors can be discovered. These are illustrated in Fig. 4.18.

The first error is a deviation in the peak value. Normally this is caused by numerical or artificial dispersion, – an unwanted spreading of the pollutant is present.

The second error is a deviation in the location of the distribution (of the solution), caused by an error in travel speed. This error is often called a phase error.

The third error is more complex and is connected to the form or shape of the distribution. This error is caused by more than one numerical phenomenon, but numerical dispersion and skewness can be mentioned as important quantities. These phenomena will be treated in details in the following sections.

The last type of error is more difficult to discover visually, but is perhaps the most important. A model must be able to preserve mass, and often this can be expressed as the area limited by the distribution.

The classification above is very rough and the numerical error will often be a sum of several types of errors, and therefore it can be very difficult to describe the properties and magnitudes of the numerical errors, but in general a numerical error can be observed as a deviation in some of the parameters describing the phenomenon transport and dispersion of a pollutant, namely:

- Conservation of mass.
- Average transport velocity.
- Longitudinal spreading.

The finite difference schemes mentioned in section 4.4 are all able to provide conservation of mass, and a correct transport velocity, so these types of errors will not be treated any further. But some of the schemes suffer from numerical or artificial dispersion, leading to an error in the spreading of the pollutant, and some of the schemes lead to skew concentration profiles in the x-domain, where a symmetric profile should be expected as shown in section 4.2.3. And it is mainly these two types of errors, which will be the subject for further study in this work.

Description of error properties in numerical schemes can be found in many references, but often the results cannot be compared, since different methods

of description of the errors have been applied. The main intention with this work is to obtain comparable results for a number of schemes, and in this way be able to extract some general properties, – a knowledge which could lead to methods to reduce/minimize the numerical errors in the present schemes, or even to new more efficient schemes.

In this work three different methods for determination of numerical errors will be described and applied for a number of numerical schemes, providing comparable results. The three methods are:

- Taylor analysis, – a mathematical method based on Taylor expansions of the difference schemes, leading to an analytical expression for each of the numerical error terms.
- The Method of Moments, – a computer-based numerical method, leading to the magnitude of each numerical error term, obtained by comparison of the numerical solution and the corresponding analytical solution.
- The Root Mean Square method, – a computer-based numerical method, leading to the magnitude of the total numerical error, obtained by comparison of the numerical and analytical solutions.

Based on the obtained comparable results some general properties will be extracted and some methods for reducing the numerical errors will be stated.

#### 4.5.2 Taylor Analysis

##### Taylor expansions

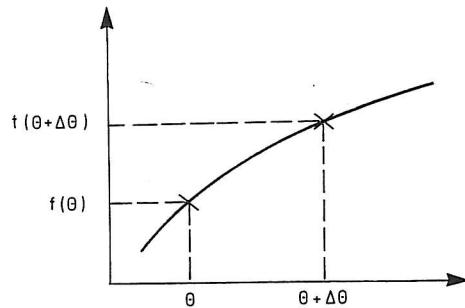


Fig. 4.19. Definition sketch for Taylor Analysis.

If  $f$  is a function where the value and the derivatives of the function are known at point  $\Theta$ , then the value at point  $\Theta + \Delta\Theta$  can be approximated by use of a Taylor expansion:

$$f(\Theta + \Delta\Theta) = f(\Theta) + \frac{\Delta\Theta}{1!} \frac{\partial f}{\partial\Theta} + \frac{\Delta\Theta^2}{2!} \frac{\partial^2 f}{\partial\Theta^2} + \frac{\Delta\Theta^3}{3!} \frac{\partial^3 f}{\partial\Theta^3} + HOT \quad (4.59)$$

where HOT denotes Higher Order Terms. The accuracy of the expansion only depends on the number of terms.

### The Forward Time Central Space scheme (FTCS)

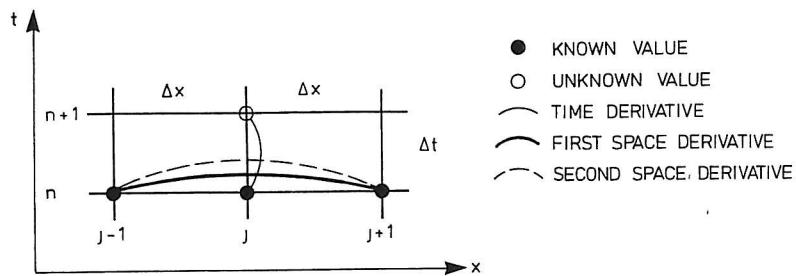


Fig. 4.20. The Forward Time Central Space scheme (FTCS) applied for the Transport/Dispersion model.

The method will be illustrated for the explicit FTCS scheme (sec. 4.4.2.). Referring to the notation in Fig. 4.20 the scheme can be written as:

$$\frac{C_j^{n+1} - C_j^n}{\Delta t} + u \frac{C_{j+1}^n - C_{j-1}^n}{2 \cdot \Delta x} = K_x \frac{C_{j+1}^n - 2 \cdot C_j^n + C_{j-1}^n}{\Delta x^2} \quad (4.60)$$

A Taylor expansion at gridpoint  $(j, n)$  can be developed for all dependent variables in the scheme. If terms of fourth and higher order are neglected, then the four values in the scheme can be approximated with:

$$C_j^n = C_j^n$$

$$C_j^{n+1} \simeq C_j^n + \Delta t \frac{\partial C}{\partial t} + \frac{\Delta t^2}{2} \frac{\partial^2 C}{\partial t^2} + \frac{\Delta t^3}{6} \frac{\partial^3 C}{\partial t^3}$$

$$C_{j+1}^n \simeq C_j^n + \Delta x \frac{\partial C}{\partial x} + \frac{\Delta x^2}{2} \frac{\partial^2 C}{\partial x^2} + \frac{\Delta x^3}{6} \frac{\partial^3 C}{\partial x^3}$$

$$C_{j-1}^n \simeq C_j^n - \Delta x \frac{\partial C}{\partial x} + \frac{\Delta x^2}{2} \frac{\partial^2 C}{\partial x^2} - \frac{\Delta x^3}{6} \frac{\partial^3 C}{\partial x^3} \quad (4.61)$$

Inserting these expressions in eq. (4.60) yields:

$$\frac{\partial C}{\partial t} + u \frac{\partial C}{\partial x} = K_x \frac{\partial^2 C}{\partial x^2} - \frac{\Delta t}{2} \frac{\partial^2 C}{\partial t^2} - \frac{\Delta t^2}{6} \frac{\partial^3 C}{\partial t^3} - u \frac{\Delta x^2}{6} \frac{\partial^3 C}{\partial x^3}$$

↓

$$\begin{aligned} \frac{\partial C}{\partial t} + u \frac{\partial C}{\partial x} &= \left( K_x - u^2 \frac{\Delta t}{2} \right) \frac{\partial^2 C}{\partial x^2} + \\ &\quad \left( u^3 \frac{\Delta t^2}{6} - u \frac{\Delta x^2}{6} + u K_x \Delta t \right) \frac{\partial^3 C}{\partial x^3} \end{aligned} \quad (4.62)$$

If this expression is compared with the original equation:

$$\frac{\partial C}{\partial t} + u \frac{\partial C}{\partial x} = K_x \frac{\partial^2 C}{\partial x^2} \quad (4.63)$$

then the error terms can be identified directly as a second order term and a third order term:

$$-u^2 \frac{\Delta t}{2} \frac{\partial^2 C}{\partial x^2} + \left( u^3 \frac{\Delta t^2}{6} - u \frac{\Delta x^2}{6} + u K_x \Delta t \right) \frac{\partial^3 C}{\partial x^3} \quad (4.64)$$

from which the numerical dispersion coefficient  $K_2$  can be determined to:

$$K_2 = -u^2 \frac{\Delta t}{2} \quad (4.65)$$

and the numerical skewness coefficient  $K_3$  to:

$$K_3 = u^3 \frac{\Delta t^2}{6} - u \frac{\Delta x^2}{6} + u K_x \Delta t \quad (4.66)$$

The order of the truncation error can be identified from eq.(4.64), and for the FTCS scheme it is normally written as  $O(\Delta t, \Delta x^2)$ . Furthermore, the consistency of the scheme can be controlled from eq.(4.62). If  $\Delta x$  and  $\Delta t$  tend to zero then eq.(4.62) will tend to the original differential equation, eq.(4.63). This means that the FTCS scheme is consistent.

Taylor expansions can also be developed for implicit schemes, but the development becomes more complicated as mixed derivatives will be present, e.g. a term like:

$$\frac{\partial^3 C}{\partial x^2 \cdot \partial t} \quad (4.67)$$

### Centering in space

It is wellknown that the discretization of the convective transport term is very important for the magnitude of the numerical error. The choice is between a backward difference (an upwind discretization) or a central difference, since a forward discretization of the convective term leads to an unstable scheme. In Table 4.2 the error terms for the FTBS scheme (Forward Time Backward Space) and the FTCS scheme can be seen.

*Table 4.2. Space centering*

Scheme	2. order term	3. order term
FTBS	$u \frac{\Delta x}{2} - u^2 \frac{\Delta t}{2}$	$u^3 \frac{\Delta t^2}{6} - u \frac{\Delta x^2}{6} + u K_x \Delta t$
FTCS	$-u^2 \frac{\Delta t}{2}$	$u^3 \frac{\Delta t^2}{6} - u \frac{\Delta x^2}{6} + u K_x \Delta t$

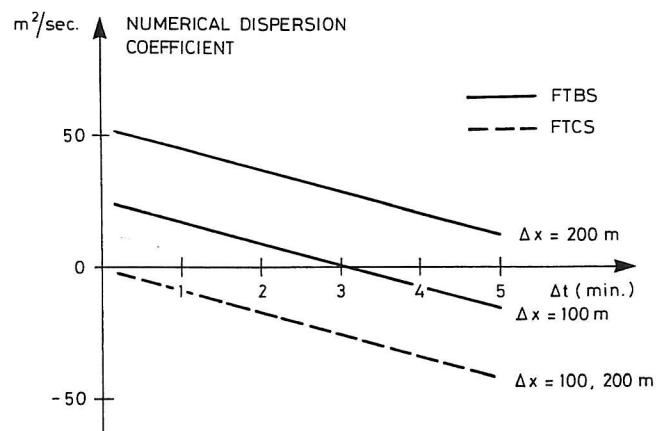


Fig. 4.21. Magnitude of the numerical dispersion coefficient in the FTCS scheme, and the FTBS schemes for an average velocity  $u = 0.53 \text{ m/sec.}$

The third order term is independent of the discretization of the convective term, while the second order term, – the numerical dispersion, depends on the choice of discretization. It can be seen that the numerical dispersion in the FTCS scheme always will be negative and only depends of the magnitude of  $\Delta t$ , while the numerical dispersion in the FTBS scheme is dependent of as well  $\Delta t$  as  $\Delta x$ . This is illustrated in Fig. 4.21, where the magnitude of the numerical dispersion coefficient is shown for different values of  $\Delta t$  and  $\Delta x$ .

### Choice of $\Delta x$ and $\Delta t$

It can be seen from Fig. 4.21 that a specific choice of  $\Delta t$  and  $\Delta x$  will remove the numerical dispersion in the FTBS scheme:

$$u \frac{\Delta x}{2} - u^2 \frac{\Delta t}{2} = 0 \quad \Rightarrow \quad \Delta x = u \cdot \Delta t \quad (4.68)$$

Furthermore, this choice will reduce the third order term to  $u \cdot K_x \cdot \Delta t$ .

This performance cannot be applied for the FTCS scheme as only a choice of  $\Delta t = 0$  will remove the numerical dispersion.

### Centering in time

Instead of using a forward time differences, a central time difference (Crank & Nicholson) or even a backward time difference (BTCS) could be applied, leading to implicit finite difference schemes. The two schemes mentioned above and a general scheme where  $\Theta$  denotes a coefficient for centering in time (FTCS:  $\Theta = 0$ , Crank & Nicholson:  $\Theta = 0.5$ , BTCS:  $\Theta = 1$ ) are compared with the FTCS scheme in Table 4.3.

*Table 4.3. Time centering*

<u>Scheme</u>	<u>2. order term</u>	<u>3. order term</u>
FTCS	$-u^2 \frac{\Delta t}{2}$	$u^3 \frac{\Delta t^2}{6} - u \frac{\Delta x^2}{6} + u K_x \Delta t$
Crank & Nicholson	0	$-u^3 \frac{\Delta t^2}{12} - u \frac{\Delta x^2}{6}$
BTCS	$u^2 \frac{\Delta t}{2}$	$-u^3 \frac{\Delta t^2}{3} - u \frac{\Delta x^2}{6} - u K_x \Delta t$
General scheme	$u^2 \frac{\Delta t}{2} (1 - 2\Theta)$	$u^3 \frac{\Delta t^2}{6} (1 - 3\Theta) - u \frac{\Delta x^2}{6} + u K_x \Delta t (1 - 2\Theta)$

From this Table it can be seen that the numerical dispersion coefficient is negative for  $\Theta < 0.5$ , zero for  $\Theta = 0.5$  and positive for  $\Theta > 0.5$ , which means that a fully time centered scheme is free of numerical dispersion. Also the numerical skewness is affected of the choice of  $\Theta$ , but general properties can hardly be extracted.

### Explicit time centered schemes

The explicit Leap Frog scheme is also a fully time centered scheme, and it can be shown by Taylor analysis that also this scheme is free of numerical dispersion, but unfortunately the scheme is unstable (sec. 4.6). Instead the conditionally stable Du Fort & Frankel scheme can be applied, but in this scheme numerical dispersion will be present. The error terms can be found in Table 4.6.

### Reduction of third order term

The time centered Crank & Nicholson scheme is free of numerical dispersion, but still numerical skewness is present. The magnitude of the third order term (or numerical skewness coefficient) can be reduced by applying a slightly different finite difference in time. If all six nodes are used for discretization of the time derivative, as e.g. in the Stone & Brian scheme (sec. 4.4.2), then the third order term will be reduced, but it cannot be removed.

*Table 4.4. Reduction of third order term*

Scheme	<u>3. order term</u>
Crank & Nicholson	$-u^3 \frac{\Delta t^2}{12} - u \frac{\Delta x^2}{6}$
Stone & Brian	$-u^3 \frac{\Delta t^2}{12}$

### Non-uniform grid

All the schemes considered above have been applied on a uniform grid, where  $\Delta x$  and  $\Delta t$  are constants. Often it will be necessary to apply a scheme on a grid with varying  $\Delta x$ , and then numerical errors are introduced. In Table 4.5 the results from a Taylor analysis of the Crank & Nicholson scheme on a uniform grid, and on a non-uniform grid are shown, respectively. It can

be seen that a non-uniform grid will introduce numerical dispersion in the scheme and some change in the numerical skewness will occur.

*Table 4.5. Non-uniform grid for the Crank & Nicholson scheme, where  $\Delta x_1 = x_j - x_{j-1}$  and  $\Delta x_2 = x_{j+1} - x_j$ , referring to the notation in Fig. 4.12.*

<u>Scheme</u>	<u>2. order term</u>	<u>3. order term</u>
Constant $\Delta x$	0	$-u^3 \frac{\Delta t^2}{12} - u \frac{\Delta x^2}{6}$
Variabel $\Delta x$	$-u \frac{\Delta x_2 - \Delta x_1}{4}$	$-u^3 \frac{\Delta t^2}{12} - u \frac{\Delta x_1^2 + \Delta x_2^2}{12}$ $+u^2 \frac{\Delta t(\Delta x_2 - \Delta x_1)}{8} + \frac{1}{3} K_x \left( \frac{\Delta x_2^2 - \Delta x_1^2}{\Delta x_1 + \Delta x_2} \right)$

### Removing the truncation error

A way to remove the numerical dispersion in the FTCS scheme is to introduce a correction to the dispersion coefficient. If the dispersion coefficient is replaced by:

$$K_* = K_x + u^2 \frac{\Delta t}{2} \quad (4.69)$$

then a correct simulation of the dispersion will be obtained. The same approach for removing the numerical dispersion can be applied for the other schemes, but at first sight the third order error cannot be removed in this manner, as no third order term is present in the difference equations.

But if an artificial third order term is introduced, then also the third order error can be removed. This is in fact what happens in the Quickest scheme, where neither second order nor third order errors are present. Originally the scheme was developed by use of a quadratic interpolation technique (Leonard, 1979), but Basco (1984) showed that the Quickest scheme also could be obtained from the FTCS scheme, using a correction to the dispersion coefficient combined with an introduction of an artificial third order term.

### General properties

The results from above and results from several other Taylor analyses are shown in Table 4.6. It is important to remember that all these results are valid only for steady flow conditions.

Table 4.6. Truncation errors determined by Taylor analysis, where  $\Delta x_1 = x_j - x_{j-1}$  and  $\Delta x_2 = x_{j+1} - x_j$ .

<u>Scheme</u>	<u>2. order term</u>	<u>3. order term</u>
<b>FTBS</b>		
$\Delta x = \text{const.}$	$u \frac{\Delta x}{2} - u^2 \frac{\Delta t}{2}$	$u^3 \frac{\Delta t^2}{6} - u \frac{\Delta x^2}{6} + u K_x \Delta t$
$\Delta x \neq \text{const.}$	$u \frac{\Delta x_1}{2} - u^2 \frac{\Delta t}{2}$	$u^3 \frac{\Delta t^2}{6} - u \frac{\Delta x_1^2}{6} + u K_x \Delta t$ $+ \frac{1}{3} K_x \left( \frac{\Delta x_2^2 - \Delta x_1^2}{\Delta x_1 + \Delta x_2} \right)$
<b>FTCS</b>		
$\Delta x = \text{const.}$	$-u^2 \frac{\Delta t}{2}$	$u^3 \frac{\Delta t^2}{6} - u \frac{\Delta x^2}{6} + u K_x \Delta t$
$\Delta x \neq \text{const.}$	$-u^2 \frac{\Delta t}{2} - u \frac{\Delta x_2 - \Delta x_1}{4}$	$u^3 \frac{\Delta t^2}{6} - u \frac{\Delta x_1^2 + \Delta x_2^2}{12} + u K_x \Delta t$ $+ \frac{1}{3} K_x \left( \frac{\Delta x_2^2 - \Delta x_1^2}{\Delta x_1 + \Delta x_2} \right)$
<b>BTBS</b>		
$\Delta x = \text{const.}$	$u \frac{\Delta x}{2} + u^2 \frac{\Delta t}{2}$	$-u^3 \frac{\Delta t^2}{3} - u \frac{\Delta x^2}{6} - u K_x \Delta t$
$\Delta x \neq \text{const.}$	$u \frac{\Delta x_1}{2} + u^2 \frac{\Delta t}{2}$	$-u^3 \frac{\Delta t^2}{3} - u \frac{\Delta x_1^2}{6} - u K_x \Delta t$ $- u^2 \frac{\Delta x_1 \cdot \Delta t}{2} + \frac{1}{3} K_x \left( \frac{\Delta x_2^2 - \Delta x_1^2}{\Delta x_1 + \Delta x_2} \right)$
<b>BTCS</b>		
$\Delta x = \text{const.}$	$u^2 \frac{\Delta t}{2}$	$-u^3 \frac{\Delta t^2}{3} - u \frac{\Delta x^2}{6} - u K_x \Delta t$
$\Delta x \neq \text{const.}$	$u^2 \frac{\Delta t}{2} - u \frac{\Delta x_2 - \Delta x_1}{4}$	$-u^3 \frac{\Delta t^2}{3} - u \frac{\Delta x_1^2 + \Delta x_2^2}{12} - u K_x \Delta t$ $+ u^2 \frac{\Delta t (\Delta x_2 - \Delta x_1)}{4} + \frac{1}{3} K_x \left( \frac{\Delta x_2^2 - \Delta x_1^2}{\Delta x_1 + \Delta x_2} \right)$
<b>Crank &amp; Nicholson</b>		
$\Delta x = \text{const.}$	0	$-\frac{1}{6} u \Delta x^2 - u^3 \frac{\Delta t^2}{12}$
$\Delta x \neq \text{const.}$	$-u \frac{\Delta x_2 - \Delta x_1}{4}$	$-u \frac{\Delta x_1^2 + \Delta x_2^2}{12} - u^3 \frac{\Delta t^2}{12}$ $+ u^2 \frac{\Delta t (\Delta x_2 - \Delta x_1)}{8} + \frac{1}{3} K_x \left( \frac{\Delta x_2^2 - \Delta x_1^2}{\Delta x_1 + \Delta x_2} \right)$

Stone & Brian

$$\begin{array}{lll} \Delta x = \text{const.} & 0 & -u^3 \frac{\Delta t^2}{12} \\ \Delta x \neq \text{const.} & -u \frac{\Delta x_2 - \Delta x_1}{12} & -u^3 \frac{\Delta t^2}{12} + u^2 \frac{5 \Delta t}{24(\Delta x_2 - \Delta x_1)} \\ & & -K_x \frac{\Delta x_2 - \Delta x_1}{6} + \frac{1}{3} K_x \left( \frac{\Delta x_2^2 - \Delta x_1^2}{\Delta x_1 + \Delta x_2} \right) \end{array}$$

General Two Level scheme

$$\begin{array}{lll} \Delta x = \text{const.} & -u^2 \frac{\Delta t}{2} (1 - 2 \Theta) & u^3 \frac{\Delta t^2}{6} (1 - 3 \Theta) - u \frac{\Delta x^2}{6} \\ & + u K_x \Delta t (1 - 2 \Theta) & \\ \Delta x \neq \text{const.} & -u^2 \frac{\Delta t}{2} (1 - 2 \Theta) & u^3 \frac{\Delta t^2}{6} (1 - 3 \Theta) - u \frac{\Delta x^2}{6} \\ & - u \frac{\Delta x_2 - \Delta x_1}{4} & + u K_x \Delta t (1 - 2 \Theta) \\ & & + u^2 \Theta \frac{\Delta t (\Delta x_2 - \Delta x_1)}{4} + \frac{1}{3} K_x \left( \frac{\Delta x_2^2 - \Delta x_1^2}{\Delta x_1 + \Delta x_2} \right) \end{array}$$

Leap Frog

$$\Delta x = \text{const.} \quad 0 \quad u^3 \frac{\Delta t^2}{6} - u \frac{\Delta x^2}{6}$$

Du Fort & Frankel

$$\Delta x = \text{const.} \quad -K_x u^2 \frac{\Delta t^2}{\Delta x^2} \quad u^3 \frac{\Delta t^2}{6} - u \frac{\Delta x^2}{6} + 2 u K_x^2 \frac{\Delta t^2}{\Delta x^2}$$

Quickest

$$\Delta x = \text{const.} \quad 0 \quad 0$$

From the Taylor analyses some general properties can be extracted:

- A fully centered scheme is free of numerical dispersion.
- From the General Two Level scheme it is seen that the numerical dispersion will be negative for  $\Theta < \frac{1}{2}$  (like for the FTCS scheme), zero for  $\Theta = \frac{1}{2}$  (like for the Crank & Nicholson scheme), and positive for  $\Theta > \frac{1}{2}$  (like for the BTCS scheme).
- The numerical dispersion can be related to the discretization of the convective term, except in the Du Fort & Frankel scheme.

- The third order error, – the numerical skewness, can be reduced by choosing a slightly different discretization of the time derivative (like in the Stone & Brian), but it cannot be removed.
- By introducing a correction term to the dispersion coefficient and an artificial third order term it is possible to remove the numerical errors, as e.g. performed in the Quickest scheme for a constant  $\Delta x$ .
- A non-uniform grid will introduce numerical dispersion and some change in the numerical skewness can be expected.

### **Summary**

The method applied above is a very straightforward method, and it is easy to apply on simple schemes, as e.g. the FTCS scheme. For more complicated schemes, e.g. the Stone & Brian scheme, the method becomes more and more complicated (many terms), and for the implicit versions of the Quickest scheme the method cannot be recommended. This statement is also valid for unsteady flow conditions, where a Taylor analysis generally cannot lead to any valuable results. For these schemes and/or for unsteady flow conditions other methods must be applied.

But the results from the Taylor analysis can be very valuable, as the error terms are expressed analytically in terms of  $\Delta x$  and  $\Delta t$ , which makes it possible to extract some general properties, and this could lead to some guidelines for the choice of  $\Delta x$  and  $\Delta t$ , or to some methods for removing/reducing the numerical errors in the schemes.

### **4.5.3 The Method of Moments**

Where Taylor analysis is a mathematical method the Method of Moments is a computer-based method. It is a condition to know the analytical solution, because the magnitude of each numerical error is obtained by comparison of the numerical solution and the corresponding analytical solution.

The advantage of the Method of Moments is the possibility to perform a numerical determination of the error terms. As seen in the previous section it is often without any problems to determine the numerical error analytical for simple explicit schemes, such as e.g. the FTCS scheme. But it takes a greater effort to analyse more complicated schemes like the implicit schemes,

and for these schemes the Method of Moments is a usable alternative, since the application of the method is independent of complexity of the actual numerical scheme.

The following examination of finite difference schemes is based on a comparison of moments of a numerical solution in the  $x$ -domain and moments of the corresponding analytical solution for a pulse injection.

### Determination of the error coefficients

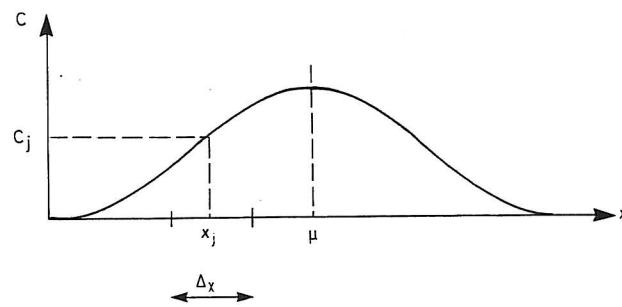


Fig. 4.22. Definition sketch.

The mass can be expressed through the area of the distribution or the zero order moment:

$$M_0 = \int_0^\infty C_j \cdot dx \sim \sum_j C_j \cdot \Delta \chi_j \quad (4.70)$$

where  $\Delta \chi_j$  is a finite length used in the numerical determination of the moment.

The position of the distribution, – the mean value  $\mu$ , which leads to the transport velocity, can be found from the first moment around  $x = 0$ :

$$M_1 = \int_0^\infty x_j \cdot C_j \cdot dx \sim \sum_j x_j \cdot C_j \cdot \Delta \chi_j \quad (4.71)$$

The mean value  $\mu$  can then be found as:

$$\mu = \frac{M_1}{M_0} \quad (4.72)$$

The shape of the distribution can be expressed through central moments of second and higher order, which in a general form can be written as:

$$M_k = \int_0^\infty (x_j - \mu)^k \cdot C_j \cdot dx \sim \sum_j (x_j - \mu)^k C_j \cdot \Delta \chi_j \quad (4.73)$$

where  $k$  denotes the order of the moment. Using these moments a comparison of mass, center of gravity, variance, skewness, flatness etc. can be performed. As mentioned in the introduction all examined schemes are able to provide conservation of mass and a correct centering of gravity (correct transport velocity), so these types of errors will not be treated any further.

The moment of second order leads to the variance of the distribution, which can be written as:

$$\sigma^2 = \frac{M_2}{M_0} = \frac{\sum_j (x_j - \mu)^2 C_j \cdot \Delta \chi_j}{\sum_j C_j \cdot \Delta \chi_j} \quad (4.74)$$

For comparison it is important to know the analytical variance, which can be found from

$$\sigma_a^2 = 2 \cdot K_x \cdot tt + \sigma_i^2 \quad (4.75)$$

where  $tt$  denotes the travel time and  $\sigma_i^2$  the initial variance of the distribution, which for a pulse injection will be zero. Then the second order error can be expressed as:

$$\sigma^2 - \sigma_a^2 \quad (4.76)$$

and the numerical dispersion coefficient determined as:

$$K_2 = \frac{1}{2 \cdot tt} (\sigma^2 - \sigma_a^2) \quad (4.77)$$

The third order error term can be determined in an almost similar way. The third order moment can be found as:

$$M_3 = \sum_j (x_j - \mu)^3 C_j \cdot \Delta \chi_j \quad (4.78)$$

Since the third order moment of the analytical solution is equal to zero, – a normal distribution contains no skewness, the numerical skewness coefficient

can be determined directly from the third order moment of the numerical solution:

$$K_3 = \frac{1}{6 \cdot tt} \frac{M_3}{M_0} \quad (4.79)$$

Since the determination of the numerical dispersion coefficient and the numerical skewness coefficient is based on a comparison of an analytical and a numerical solution the results obtained will be dependent on the choice of four parameters:

- $u$ , the mean flow velocity.
- $K_x$ , the dispersion coefficient.
- $\Delta x$ , the step in space.
- $\Delta t$ , the step in time.

The following analysis is based on a specific choice of mean flow velocity and dispersion coefficient, while the step in time and the step in space have been varied, providing a large number of results. These results have been plotted into a coordinate system and through linear interpolation iso-curves for the magnitude of the numerical dispersion coefficient, and the numerical skewness coefficient have been obtained.

The applied coordinate system is the Courant coordinate system, where the abscissa is formed by the dispersive Courant number, defined as:

$$Cr_d = K_x \frac{\Delta t}{\Delta x^2} \quad (4.80)$$

while the ordinate is formed by the convective Courant number:

$$Cr_c = u \frac{\Delta t}{\Delta x} \quad (4.81)$$

The value of the flow velocity and the dispersion coefficient have been choosen as:

$$u = 0.53 \text{ m/sec} \quad \text{and} \quad K_x = 5 \text{ m}^2/\text{sec}$$

and the comparison of the moments has been performed after 50 time steps.

This means that the following results must be treated with care, as the magnitude of the numerical error coefficients are dependent of this specific choice, but since all results in this paper are based on the same data, the Figures may be compared.

The Method of Moments has been applied for a number of numerical schemes. The presentation and the discussion of the results will be divided into two sections, where the class of Two Level Schemes will be treated first. Secondly the results for the class of Quick Schemes will be treated, and finally, some general properties will be outlined.

### Two Level Schemes

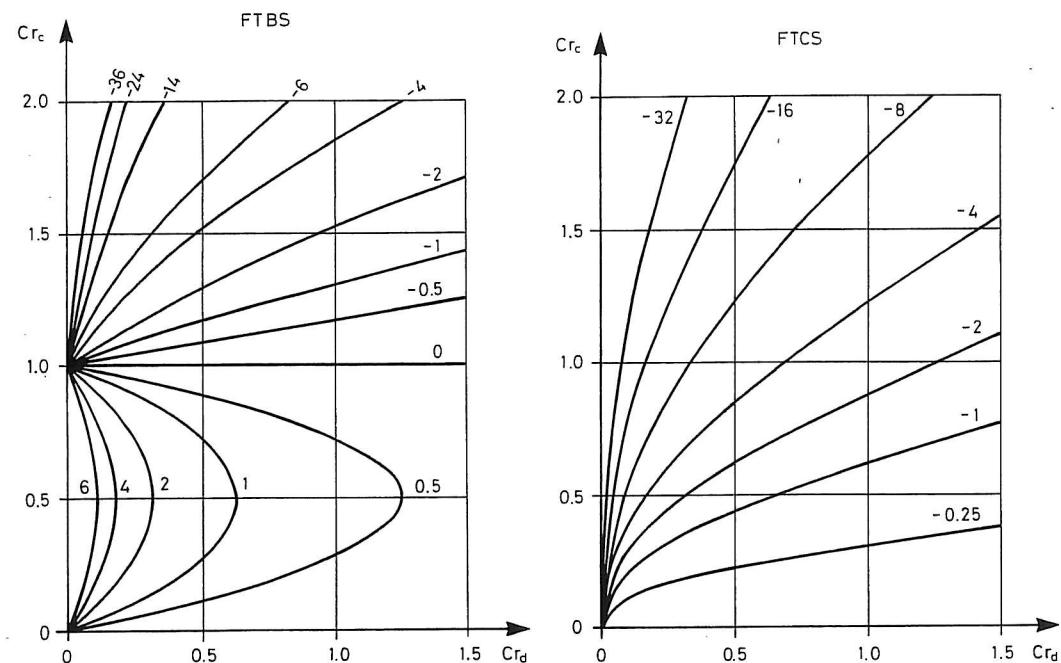


Fig. 4.23. Iso-curves for the numerical dispersion coefficient  $K_2 [m^2/sec]$  for the Forward Time Backward Space scheme (FTBS), and the Forward Time Central Space scheme (FTCS),  $u = 0.53 m/sec$ ,  $K_x = 5 m^2/sec$ .

In numerical modelling it is normally preferable to use large steps as well in time as in space. In the Courant coordinate system the time and space step

will increase for increasing convective Courant number and decreasing dispersive Courant number. This means that it would be preferable to perform the numerical modelling in the "upper left corner" in the Courant coordinate system.

In Fig. 4.23 iso-curves for the magnitude of the numerical dispersion coefficient in the FTBS scheme and in the FTCS scheme are shown. In accordance with the results from the Taylor analysis the numerical dispersion can be eliminated in the FTBS scheme by choosing a convective Courant number of one. For larger Courant numbers the numerical dispersion will be negative and for Courant number lesser than one the numerical dispersion will be positive.

In the FTCS scheme the numerical dispersion is always negative and it can only be minimized by choosing Courant numbers in the "lower part" of the Courant coordinate system, which will lead to small time steps.

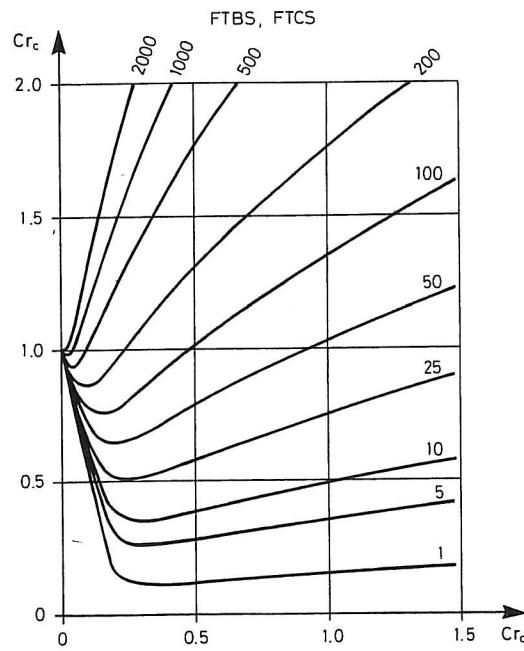


Fig. 4.24. Iso-curves for the numerical skewness coefficient  $K_3 [m^3/sec]$  for the Forward Time Backward Space scheme (FTBS) , and for the Forward Time Central Space scheme (FTCS),  $u = 0.53 m/sec$  ,  $K_x = 5 m^2/sec$ .

The numerical skewness coefficient is identical for the FTBS scheme and the FTCS scheme, and the iso-curves are shown in Fig. 4.24. The picture is almost the same as for the numerical dispersion coefficient, – the numerical error is increasing for increasing convective Courant number.

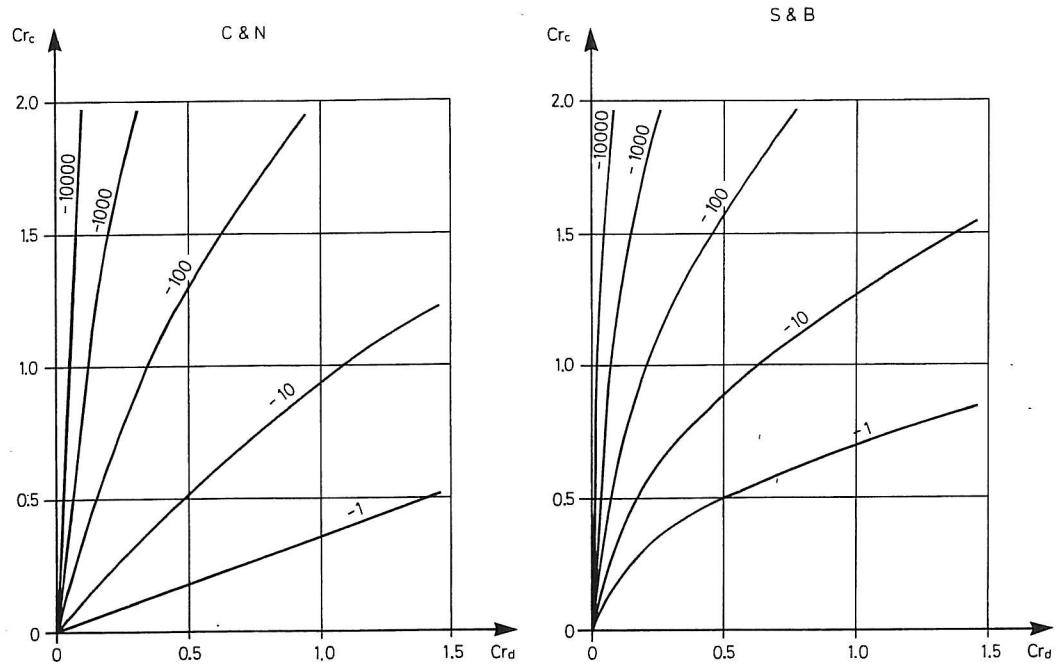


Fig. 4.25. Iso-curves for the numerical skewness coefficient  $K_3 [m^3/sec]$  for the Crank & Nicholson scheme (C & N), and for the Stone & Brian scheme (S & B),  $u = 0.53 m/sec$ ,  $K_x = 5 m^2/sec$ .

The same picture appears in Fig. 4.25 for the two implicit schemes, Crank & Nicholson and Stone & Brian, but a comparison will show that the magnitude of the numerical skewness coefficient is significantly lesser in the Stone & Brian scheme than in the FTCS scheme. This is also illustrated in Tabel 4.7 where the magnitude of the numerical skewness coefficient is determined for some combinations of the two Courant numbers.

Table 4.7. Magnitude of the numerical skewness coefficient for some combinations of Courant numbers

<u><math>Cr_c</math></u>	<u><math>Cr_d</math></u>	<u>FTCS</u>	<u>C &amp; N</u>	<u>S &amp; B</u>
1.5	0.5	300	-150	-79
0.5	1.0	10	-2.3	-0.25

### Quick schemes

As mentioned above the Taylor analysis can hardly be applied for the implicit Quick schemes, but instead the Method of Moments can be applied leading to the same results as shown for the Two Level schemes.

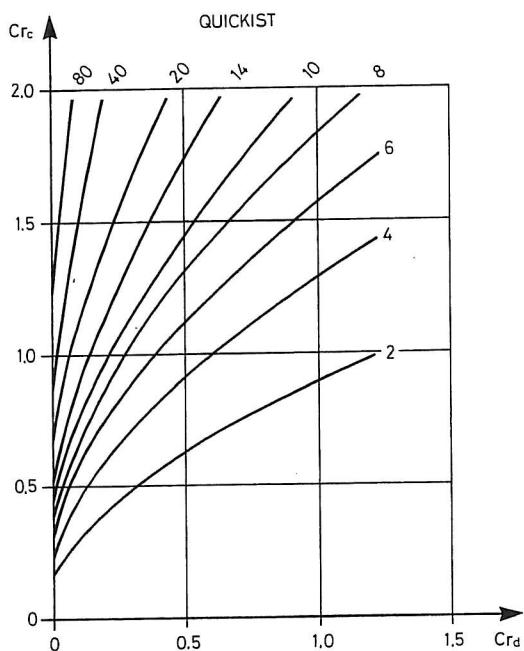


Fig. 4.26. Iso-curves for the numerical dispersion coefficient  $K_2$  [ $m^2/sec$ ] for the Quickist scheme,  $u = 0.53 m/sec$ ,  $K_x = 5 m^2/sec$ .

Only one of the three Quick schemes contains numerical dispersion, – the Quickist scheme, and iso-curves for the numerical dispersion coefficient are

shown in Fig. 4.26. The magnitude of the numerical dispersion coefficient is approximately the same as for the FTCS scheme (Fig. 4.23), but the sign is opposite.

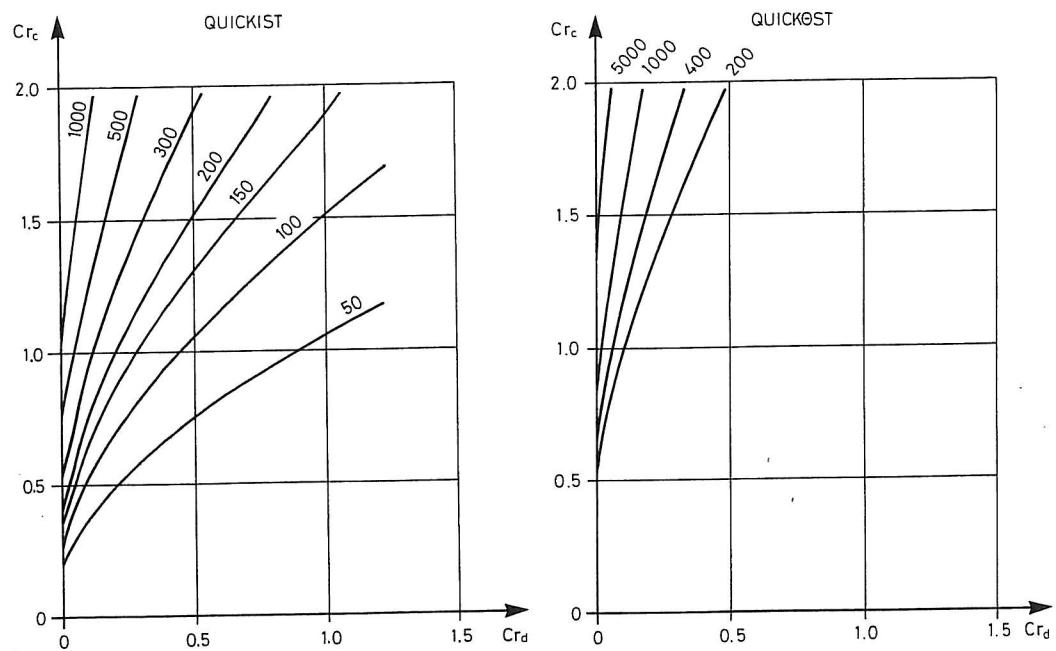


Fig. 4.27. Iso-curves for the numerical skewness coefficient  $K_3 [m^3/sec]$  for the Quickist scheme, and for the QuickOst scheme,  $u = 0.53 m/sec$ ,  $K_x = 5 m^2/sec$ .

The Quickest scheme and the QuickOst scheme are free of numerical dispersion, but only the Quickest scheme is free of numerical skewness. In Fig. 4.27 the numerical skewness coefficients for the Quickist scheme and the QuickOst scheme are shown. In the "upper left corner" the magnitude of the coefficient is quite equal, but it seems as if the skewness coefficient in the QuickOst scheme decreases more rapidly for decreasing  $Cr_d$  than in the Quickist scheme. There is no significant difference in the magnitude of the skewness coefficients if the QuickOst scheme and the Stone & Brian scheme (Fig. 4.25) are compared.

### Summary

The Method of Moments seems to be an easy and reliable method for comparison of numerical schemes with each other. The advantages of the method is primarily that the error can be divided into different error terms, and that very complicated numerical schemes can be analysed. The disadvantages are that the magnitude of the error terms is dependent of the chosen example, and that the method demands a knowledge of the corresponding analytical solution, which limits the application to a few simplified events, such as a sudden release of a tracer assuming steady flow conditions.

The achieved results indicate that for Two Level schemes the Stone & Brian scheme seems to be superior, while the explicit Quickest scheme and the semi-implicit Quick $\theta$ st scheme show the best error properties of the Quick schemes.

#### 4.5.4 The Root Mean Square Method (RMS)

The RMS method is very like the Method of Moments, but instead of determination of each error coefficient the RMS method provides the value of the total numerical error, - all orders of error are included in one value. This value is obtained by determination of the root mean square between the numerical solution and the corresponding analytical solution.

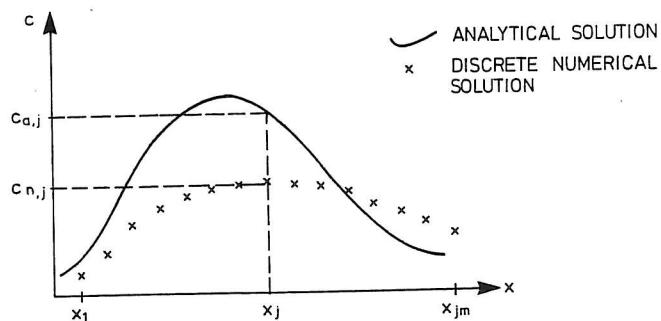


Fig. 4.28. Definition sketch for determination of the root mean square value.

Referring to the notation in Fig. 4.28 the root mean square value can be determined as:

$$RMS = \sqrt{\frac{1}{jm} \sum_{j=1}^{jm} (C_{a,j} - C_{n,j})^2} \quad (4.82)$$

The RMS value is determined for a large number of combinations of the Courant numbers  $Cr_d$  and  $Cr_c$ , and then iso-curves for the RMS value can be drawn in the Courant coordinate system.

As for the Method of Moments the magnitude of the RMS value is dependent of the choice of data, and furthermore, the RMS value will be dependent of the number of time steps performed by the numerical model before analysis. Finally, the choice of event, i.e. the shape of the initial concentration profile, will have some influence on the result. In the following all RMS values are based on:

- $u = 0.53 \text{ m/sec.}$
- $K_x = 5 \text{ m}^2/\text{sec.}$
- Determination of the RMS value after one timestep
- The initial concentration profile is a triangel.

Having this in mind the following Figures may be compared with each other, but they should be treated with great care if used in other connections.

#### **The results from the RMS analysis**

The RMS analysis has been performed for four numerical schemes, the two level Stone & Brian scheme and the three Quick schemes. The results are shown in Fig. 4.29 and 4.30.

The RMS value acts in a different way for the schemes. The RMS value is increasing against "the upper left corner" for the Stone & Brian scheme and the Quick $\varnothing$ st scheme, while the RMS value for the Quickest scheme is increasing against "the upper right corner". The Quickist scheme seems to provide the largest RMS values, while no significant difference can be observed in the three other schemes, although Quickest seems to provide slightly lesser values.

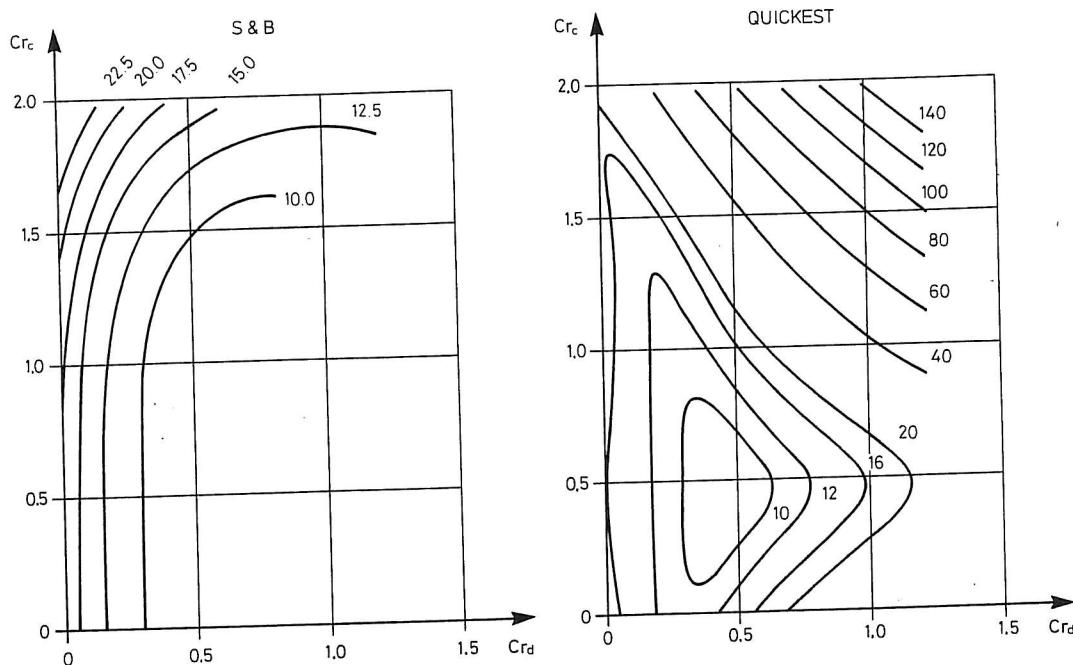


Fig. 4.29 Iso-curves for the RMS value for the Stone & Brian scheme (S&B), and for the Quickest scheme, determined after one time step for a triangel as the initial concentration profile,  $u = 0.53 \text{ m/sec}$  and  $K_x = 5 \text{ m/sec}$ .

### Summary

The RMS Method is a computer-based method, which is easily applied for a wide range of numerical schemes. The method provides a single value including all orders of numerical errors, which makes a comparison between different schemes simple. But it is important to notice that the method is encumbered with a number of disadvantages, which limits the application of the method.

The achieved results seem to support that the Stone & Brian scheme provides the best result for the class of Two Level schemes, while the Quick $\Theta$ st and the Quickest schemes are superior in the class of Quick schemes.

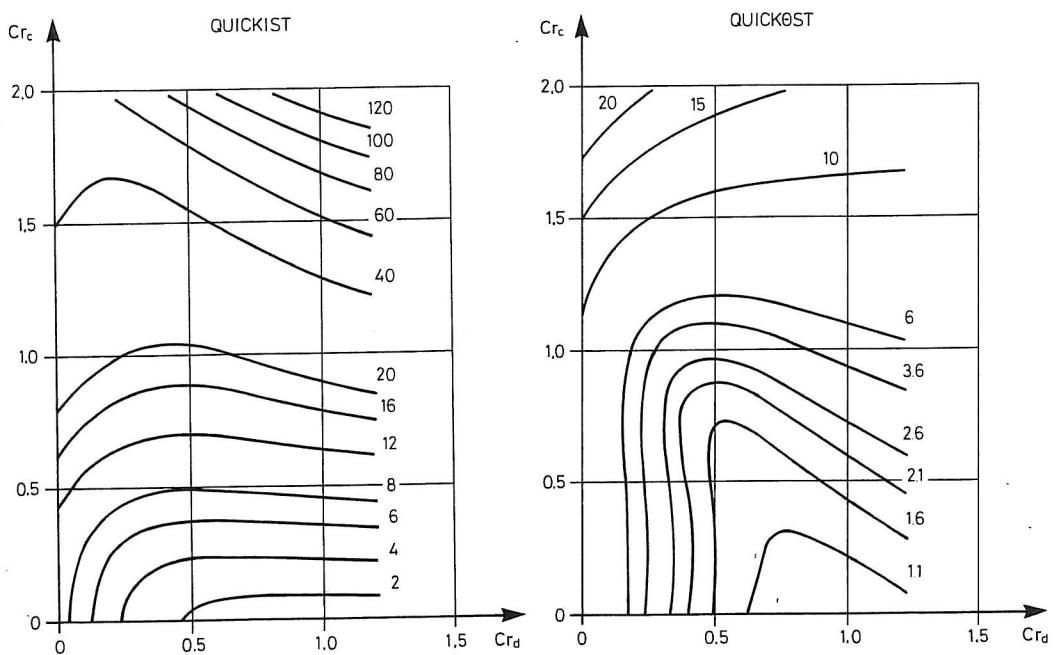


Fig. 4.30. Iso-curves for the RMS value for the Quickist scheme, and for the Quick $\theta$ st scheme, determined after one time step for a triangulation as the initial concentration profile,  $u = 0.53 \text{ m/sec}$  and  $K_x = 5 \text{ m/sec}$ .

#### 4.5.5 Wiggles

Wiggles is a phenomenon which can be observed when central differences are used for discretization of the convective term. The phenomenon is treated in details in Leonard (1979), in which wiggles are defined as: "... spatially decaying or growing oscillations of movelength  $2 \cdot \Delta x$  ...".

If the FTCS scheme is applied for simulation of transport and spreading of a concentration-impulse, then wiggles can be observed at the upstream end of the concentration-profile at the initial time steps, but as the simulation proceeds, the wiggles seem to develop to some oscillations with a movelength larger than  $2 \cdot \Delta x$ , as shown in Fig. 4.31.

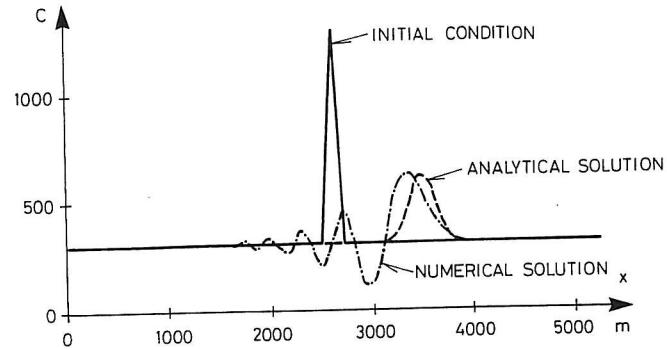


Fig. 4.31. Example of the development of wiggles in the FTCS scheme after 49 time steps for  $Cr_c = 0.17$ ,  $Cr_d = 0.015$  and  $Pe = 11.3$ , after Hummelshøj & Nielsen (1988).

#### Comparison of some schemes

It has been shown (Leonard, 1979) that the presence of wiggles is dependent of the Peclet number, defined as:

$$Pe = \frac{Cr_c}{Cr_d} \quad (4.83)$$

and the condition for a wiggle-free solution, using the FTCS scheme, can be expressed as:

$$Pe \leq 2 \quad (4.84)$$

This demand is also valid for implicit schemes using central differences, such as the Crank & Nicholson scheme and the Stone & Brian scheme, but a comparison of results from the two schemes will show that the magnitude of the wiggles is significantly reduced in the Stone & Brian scheme, see Fig. 4.32.

If a backward difference is used, like in the FTBS scheme, then wiggles will not be present, but instead the numerical dispersion will increase. In the Quick schemes the wiggles are eliminated by use of an upstream interpolation technique, as described in Leonard (1979) and Basco (1984). In Fig. 4.33 the result from a testrun with the Quickst scheme and the Quickθst scheme

is shown. The wiggles are almost eliminated, but it can be seen that the price is an increased numerical dispersion in the Quickist scheme, while the Quick $\theta$ st scheme seem to be able to provide accurate wiggle-free results even for a large Peclet number.

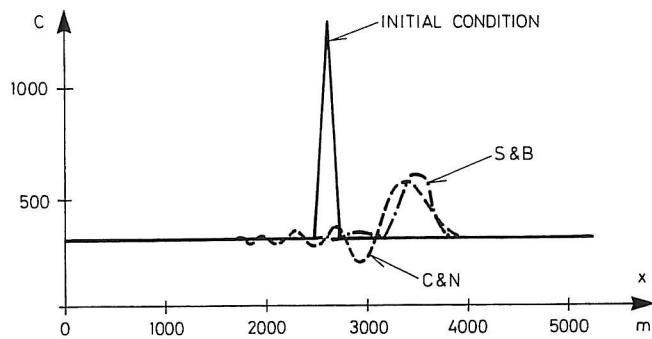


Fig. 4.32. Comparison of the development of wiggles in the Crank & Nicholson scheme (C&N), and in the Stone & Brian scheme (S&B) after 49 time steps for  $Cr_c = 0.17$ ,  $Cr_d = 0.015$  and  $Pe = 11.3$ , after Hummelshøj & Nielsen (1988).

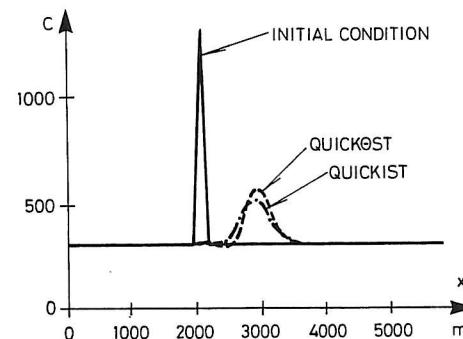


Fig. 4.33. Comparison of the development of wiggles in the Quickist scheme, and in the Quick $\theta$ st scheme after 49 time steps for  $Cr_c = 0.17$ ,  $Cr_d = 0.015$  and  $Pe = 11.3$ .

### **Summary**

The presence of wiggles can be related to the discretization of the convective transport term. If a central difference is applied the condition for a wiggle-free scheme will be a Peclet number minor than two, but it is possible to obtain usable result for quite large Peclet numbers, if the Stone & Brian is applied.

An upwind discretization of the convective term will eliminate the phenomenon wiggles, but in general the price will be an increased numerical dispersion, e.g. as shown for the Quickist scheme in Fig. 4.33. But in the Quickest scheme and the Quick $\theta$ st scheme neither numerical dispersion nor wiggles are present, and therefore these two schemes seem to be a good choice. The disadvantages for these schemes, - a limited stability area, will be treated in the next section.

## 4.6 Stability conditions for Transport/ Dispersion models

### 4.6.1 Determination of the stability condition

In almost every numerical calculation some numerical errors will be present. If these errors tend to accumulate during the simulation then the numerical scheme is unstable. This is normally recognized as quickly growing oscillations, often resulting in an interruption of the computer program.

Several parameters are important when the stability conditions for a specific numerical scheme shall be predicted, including which physical phenomenon to simulate. For the Transport/Dispersion equation the stability conditions are normally expressed through three parameters:

- The convective Courant number:

$$C_{rc} = u \frac{\Delta t}{\Delta x}$$

which is the proportion between the convective speed  $u$  and the "speed" of the numerical scheme.

- The dispersive Courant number or the diffusion number:

$$C_{rd} = K_x \frac{\Delta t}{\Delta x^2}$$

which can be perceived as the proportion between the dispersive speed and the "speed" of the scheme.

- The Peclet number:

$$Pe = \frac{C_{rc}}{C_{rd}} = \frac{u}{K_x} \Delta x$$

which is the proportion between the two Courant numbers above, or between the speeds of the two involved physical phenomena, convection and dispersion.

Furthermore, a fourth parameter can be mentioned, namely the description of a phenomenon in discrete terms, e.g. a sudden change in the concentration at the upper boundary. If the description is too coarse (the time step is too large), important numerical errors can be introduced, which may affect the stability conditions.

#### Methods for determination of the stability condition

The stability conditions for a specific scheme can be predicted in several ways. At this place only three different methods shall be mentioned. A more complete description can be found in e.g. Roache (1976).

The first and perhaps the most obvious method is the method of trial and error. Knowing that an unstable scheme normally will provide results, which cannot be misunderstood, the method could seem usable. But as seen above the stability depends on some parameters, which may change during the calculation. This means that the scheme may be unstable for some few steps, where errors are accumulated and perhaps reinforced, providing an erroneously final result, though it looks stable.

Another and more informative method is the "Discrete Perturbation Stability Analysis", e.g. described in Roache (1976). A discrete perturbation is introduced in the scheme and the numerical calculation is performed step by step. If the scheme is stable then the perturbation must die out. This is illustrated in Fig. 4.34, where results after one respectively five time steps are shown for three different combinations of convective and dispersive Courant numbers.

The method can be applied in a pure numerical and systematical manner, The Impulse Method, as described in Hummelhøj & Nielsen (1988), leading to general stability conditions equal to conditions obtained by use of the last method to be mentioned here.

The von Neumann stability analysis is perhaps the most commonly used. The method is based on a rewriting of the scheme in finite Fourier components, leading to a determination of the amplification factor. If the scheme is stable the amplification factor must be lesser than one for each Fourier component, leading to the stability conditions. For e.g. the FTCS scheme these conditions can be expressed in terms of the convective and dispersive Courant number. The stability conditions are forming the limits for the stability area, which is normally shown in the Courant coordinate system, see Fig. 4.35.

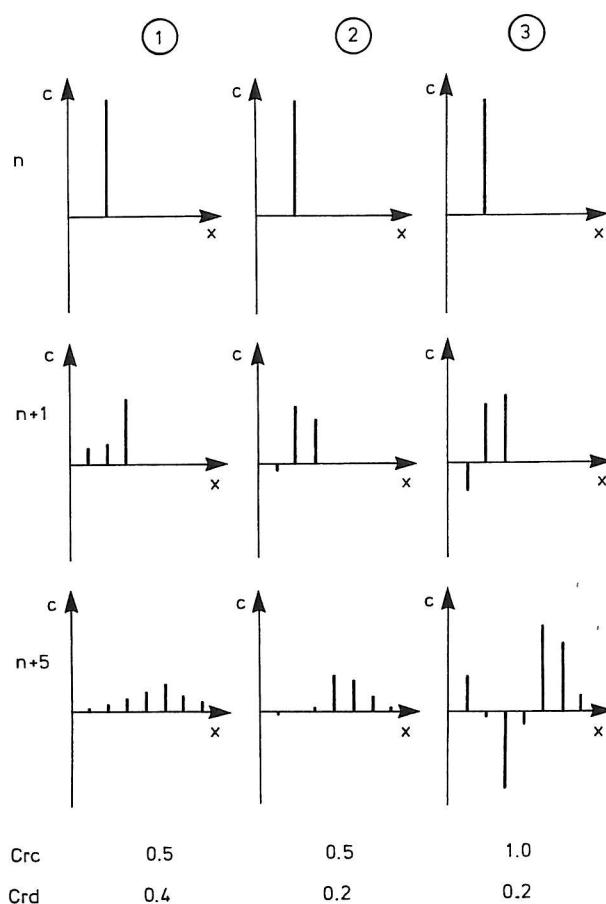


Fig. 4.34. Discrete Perturbation Analysis for the FTCS scheme for three different combinations of convective and dispersive Courant number, where no. 1 & 2 provide stable results, while no. 3 provides unstable results.

Which method to choose among the three mentioned above cannot be specified in a general way. The von Neumann analysis is a purely mathematical method, which should provide the best results, but for more complicated schemes it might be impossible to extract usable stability conditions. For these occasions the Discrete Perturbation Analysis may be easier, especially the numerical version. As mentioned previous the Impulse Method and the

von Neumann analysis provide identical results for simple schemes, such as the FTCS scheme, but it has not been proved that the Impulse Method can be applied in general.

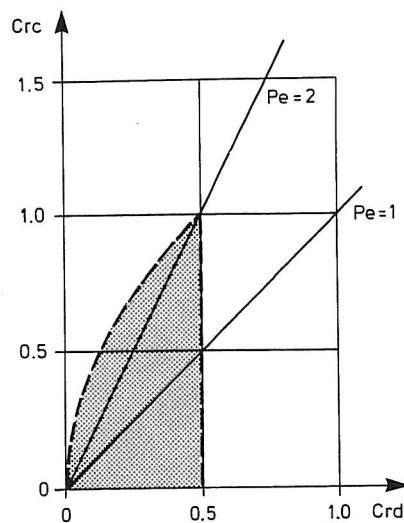


Fig. 4.35. Stability area for the FTCS scheme applied at the Transport/Dispersion equation.

#### 4.6.2 Stability conditions

In the following some of the previous mentioned schemes for the Transport/Dispersion model will be considered, and the stability conditions will be shown in the Courant coordinate system. The results have been found in several references, but most of them have also been found by use of The Impulse Method (Hummelshøj & Nielsen, 1988).

But before the stability conditions for Transport/Dispersion models are examined further, it might be valuable to consider the stability properties for two sub-models, the Transport model and the Diffusion model.

##### **The Transport model**

For this model only the two explicit models, obtained in sec. 4.3.2, will be considered. If a Discrete Perturbation Analysis is performed, it is easily

seen that the model using linear interpolation (FTCS) always will provide unstable results, while the stability condition for the upwind scheme (FTBS) can be expressed as:

$$Cr_c \leq 1 \quad (4.85)$$

### The Diffusion model

Table 4.8. Stability conditions for FD-schemes for the diffusion equation (or heat flow equation) (Richtmyer & Morton, 1967).

	<p>1. <math>\frac{u_j^{n+1} - u_j^n}{\Delta t} = \sigma \frac{(\delta^2 u)_j^n}{(\Delta x)^2}</math></p> <p><math>e = 0[(\Delta t)] + 0[(\Delta x)^2]</math></p> <p>explicit, stable if <math>\sigma \cdot \Delta t / (\Delta x)^2 = \text{const.} \leq 1/2</math> as <math>\Delta t, \Delta x \rightarrow 0</math>.</p>
	<p>2. <math>\frac{u_j^{n+1} - u_j^n}{\Delta t} = \sigma \frac{(\delta^2 u)_j^n + (\delta^2 u)_j^{n+1}}{2(\Delta x)^2}</math></p> <p>Crank and Nicholson (1947)</p> <p><math>e = 0[(\Delta t)^2] = 0[(\Delta x)^2]</math></p> <p>implicit, always stable.</p>
	<p>3. <math>\frac{u_j^{n+1} - u_j^{n-1}}{2 \cdot \Delta t} = \sigma \frac{(\delta^2 u)_j^n}{\Delta x^2}</math></p> <p>always unstable.</p>
	<p>4. <math>\frac{u_j^{n+1} - u_j^{n-1}}{2 \cdot \Delta t} = \sigma \frac{u_{j+1}^n - u_j^{n+1} - u_j^{n-1} + u_{j-1}^n}{(\Delta x)^2}</math></p> <p>where <math>\Delta t / \Delta x \rightarrow 0</math> as <math>\Delta t, \Delta x \rightarrow 0</math></p> <p><math>e = 0[(\Delta t)^2] + 0[(\Delta x)^2] + 0 \left[ \left( \frac{\Delta t}{\Delta x} \right)^2 \right]</math></p> <p>Du Fort and Frankel (1953)</p> <p>explicit, always stable.</p>

A wide range of numerical schemes has been applied for the Diffusion model (or the Heat Flow model), and the stability conditions for a large number of these schemes have been examined by Richtmyer & Morton (1967). Some of these results are shown in Table 4.8, where  $\sigma$  denotes the diffusion coefficient.

### The Transport/Dispersion model

In the Transport/Dispersion model the two sub-models above are combined and then the determination of the stability properties becomes more complicated.

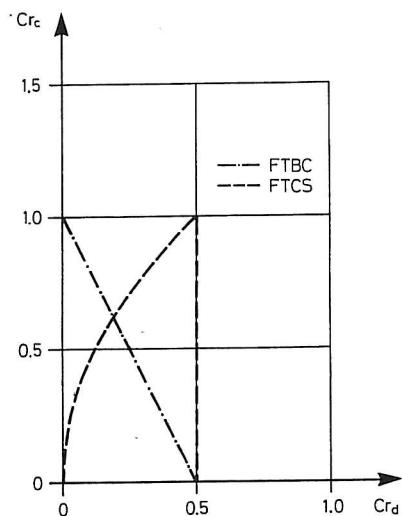


Fig. 4.36. Stability conditions for the FTCS scheme, and for the FTBS scheme (Leonard, 1979).

The Two Level Multischeme has been examined for different values of the coefficients, using a numerical Discrete Perturbation Analysis (Hummelshøj & Nielsen, 1988) as well as an analytical linear stability analysis (Basco, 1984). The examinations have shown that the time centering is essential and that the Two Level Multischeme always will provide stable results if:

$$\Theta \geq \frac{1}{2} \quad (4.86)$$

This means that fully centered schemes like the Crank & Nicholson scheme

and the Stone & Brian scheme always will provide stable solutions, in accordance with the Diffusion model (Table 4.8, no. 2). Explicit models as the FTCS scheme and the FTBS scheme are conditionally stable as shown in Fig. 4.36, and the stability conditions mentioned for the Transport model ( $Cr_c = 0$ ) and the Diffusion model ( $Cr_d = 0$ , Table 4.8, no 1) can easily be recognized.

Since Two Level schemes centered in time are unconditionally stable, it might be expected that also time centered three level schemes would show good stability properties. But this expectation is not fulfilled. Testruns have shown that the Leap Frog scheme (sec. 4.4.3) always will be unstable, while the Du Fort & Frankel scheme seems to be able to provide stable solutions if the convective term is of minor magnitude. These results are in agreement with the results obtained for the Diffusion model (Table 4.8, no. 3 & 4).

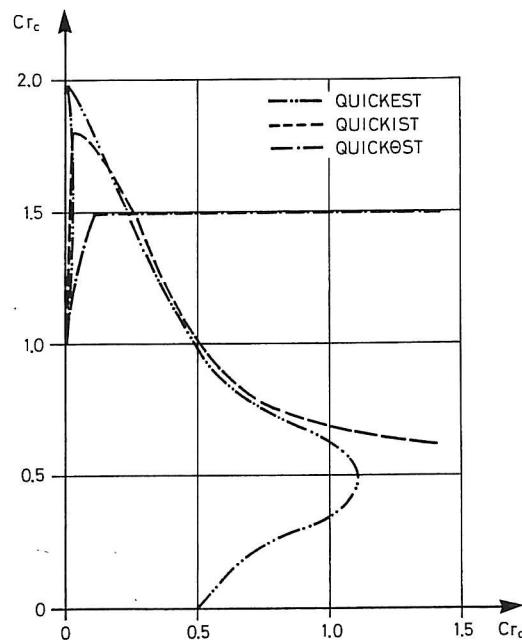


Fig. 4.37. Stability conditions for the Quickest scheme, the Quickist scheme, and the QuickØst scheme (Basco, 1984).

The Blockscheme (sec. 4.4.3) has not been examined for stability properties, but since the scheme is identical to the Leap Frog scheme for  $\alpha = 1$  and  $\Theta = 1$  (unstable), and identical to the Crank & Nicholson scheme for  $\alpha = 0$  and  $\Theta = 0$  (unconditional stable), then it must be expected that the scheme will be conditionally stable for all other combinations of  $\alpha$  and  $\Theta$ . Testruns seem to support this.

The explicit Quickest scheme developed by Leonard (1979) was found to be conditionally stable, but with a better stability area than the FTCS scheme, see Fig. 4.36 and Fig. 4.37. The main purpose with the development of the two implicit schemes, - Quickist and Quick $\Theta$ st (Basco, 1984), was to improve the stability properties, but it can be seen from Fig. 4.37 that the stability properties for the Quickist scheme is only slightly improved, and though the stability properties for the Quick $\Theta$ st is quite better, yet a further improvement could be desirable.

### Summary

In general explicit and semi-implicit finite difference schemes for the Transport/Dispersion model are conditionally stable. This limits the possibility for the choice of desirable values of  $\Delta x$  and  $\Delta t$  in opposition to the fully implicit schemes, which seem to be unconditionally stable, leading to an unlimited choice of  $\Delta x$  and  $\Delta t$ .

## 4.7 Numerical Solution of the Dead Zone model

### 4.7.1 Finite difference models

If the flow is steady and uniform, the dispersion coefficient is constant, the lateral inflow is equal to zero, and the distribution of the dead zones are uniform, then the Dead Zone model can be written as (sec. 4.2.4):

Main stream:

$$\frac{\partial C}{\partial t} + u \frac{\partial C}{\partial x} = K_x \frac{\partial^2 C}{\partial x^2} + \frac{\varepsilon}{T_d} (C_d - C) \quad (4.87)$$

Dead zone:

$$\frac{\partial C_d}{\partial t} = \frac{1}{T_d} (C - C_d) \quad (4.88)$$

where  $C$  : concentration in the main stream ( $gr/m^3$ )

$C_d$  : concentration in the dead zone ( $gr/m^3$ )

$u$  : average flow velocity ( $m/sec$ )

$K_x$  : longitudinal dispersion coefficient ( $m^2/sec$ )

$\varepsilon$  : volume fraction dead zone

$T_d$  : residence time in dead zone ( $sec$ )

$x$  : space-coordinate ( $m$ )

$t$  : time-coordinate ( $sec$ )

Numerical solution of the Dead Zone model is only slightly different from numerical solution of the ordinary Transport/Dispersion model (sec. 4.4), and almost identical finite difference schemes can be applied for solution of the equation for the main stream, eq.(4.87), when the exchange term with the dead zone is perceived as a source/sink term.

But the model is extended with a continuity equation for the dead zone. Several numerical methods can be applied for eq.(4.88), e.g. the Runge-Kutta method (Kreysig, 1979), and even semi-analytical methods (based on superposition of analytical solutions) can be applied for a number of events.

But it is very important being aware that eq.(4.88) describes an exchange of the pollutant between the dead zone and the main stream, and therefore,

the description (discretization) of the exchange term as well in eq.(4.88) as in eq.(4.87) must be identical, if conservation of mass shall be secured. Therefore, it might be necessary to choose a more simple finite difference scheme for the Dead Zone equation, because this scheme can be implemented in e.g. the Two Level Multischeme for solution of eq.(4.87). Some applications of the Dead Zone model can be found in Bjerrekær, Mark & Tornbjerg (1988).

### Numerical solution of the Dead Zone equation

Introducing a coefficient  $\Theta$  for centering in time, the discretization of eq.(4.88) can be performed as:

$$\frac{C_d - C_d^n}{\Delta t} = \frac{1}{T_d} (\Theta(C^{n+1} - C_d^{n+1}) + (1 - \Theta)(C^n - C_d^n)) \quad (4.89)$$

when the index for space is neglected. If  $\Theta = 0$  the well-known Euler algorithm appears.

This finite difference scheme is encumbered with numerical errors and before implementation in the model it would be suitable to examine the behaviour of these errors.

Eq.(4.88) can be solved analytically if the concentration in the main stream is assumed to be constant and equal to  $C_0$ , and the initial concentration in the dead zone is zero. For these conditions the analytical solution can be written as:

$$C_d(t) = C_0 - C_0 \cdot e^{-\frac{t}{T_d}} \quad (4.90)$$

From a Taylor analysis it can be seen that the scheme, eq.(4.89) is of order  $O(\Delta t)$  and the only way to remove the truncation errors is to minimize  $\Delta t$ . The behaviour of the scheme for different values of  $\Theta$  is illustrated in Fig. 4.38 and Fig. 4.39 ( $C_0 = 1 \text{ gr/m}^3$ ), and it can be seen that the model is able to perform accurate results for  $\Theta = \frac{1}{2}$  even for large values of  $\Delta t$  compared with the residence time  $T_d$ , but  $\Delta t$  should not be chosen greater than  $T_d$ .

Furthermore, it can be seen that a choice of  $\Theta > \frac{1}{2}$  will tend to damp the solution.

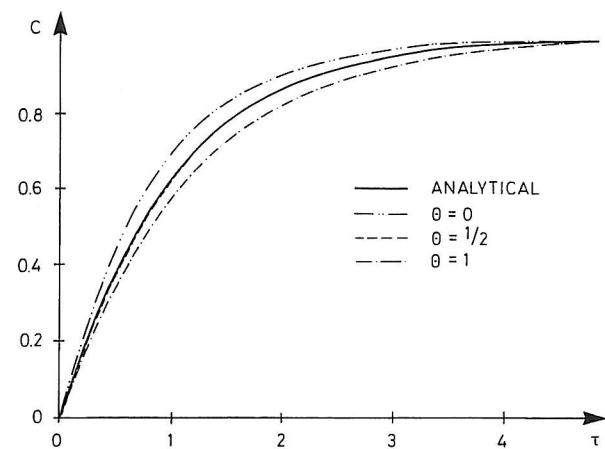


Fig. 4.38. Numerical solution of the Dead Zone model for  $\Delta t = 0.3 \cdot T_d$ .

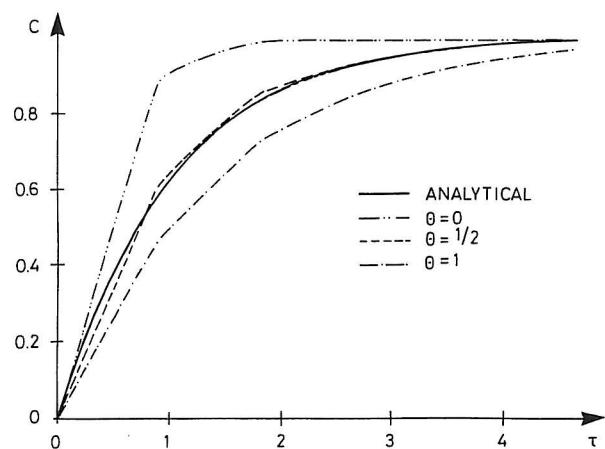


Fig. 4.39. Numerical solution of the Dead Zone model for  $\Delta t = 0.9 \cdot T_d$ .

### An explicit model

A combination of eq.(4.89) and the explicit FTCS scheme (sec. 4.4.2) and a choice of  $\Theta = 0$  lead to:

Main stream:

$$\frac{C_j^{n+1} - C_j^n}{\Delta t} + u \frac{C_{j+1}^n - C_{j-1}^n}{2 \cdot \Delta x} = \\ K_x \frac{C_{j-1}^n - 2 \cdot C_j^n + C_{j+1}^n}{\Delta x^2} + \frac{\epsilon}{T_d} (C_{d,j}^n - C_j^n)$$

↓

$$C_j^{n+1} = C_j^n - \frac{1}{2} Cr_c (C_{j+1}^n - C_{j-1}^n) + \\ Cr_d (C_{j-1}^n - 2 \cdot C_j^n + C_{j+1}^n) + h \cdot \epsilon (C_{d,j}^n - C_j^n) \quad (4.91)$$

where

$$Cr_c = u \frac{\Delta t}{\Delta x}, \quad Cr_d = K_x \frac{\Delta t}{\Delta x^2}, \quad h = \frac{\Delta t}{T_d}$$

Dead zone:

$$\frac{C_{d,j}^{n+1} - C_j^n}{\Delta t} = \frac{1}{T_d} (C_j^n - C_{d,j}^n)$$

↓

$$C_{d,j}^{n+1} = C_j^n + h (C_j^n - C_{d,j}^n) \quad (4.92)$$

Adding boundary conditions like for the original FTCS scheme and initial conditions extended to include initial values for the concentration in the dead zones, the explicit model above is easily solved. Like the FTCS scheme the model above is only conditional stable (sec. 4.6), and important numerical errors may occur, though the exchange term with the dead zone will tend to damp the errors.

### An implicit model

Instead an implicit formulation could be chosen. A combination of eq.(4.89) and the Two Level Multischeme (sec 4.4.2) leads to:

Main stream:

$$\begin{aligned}
 & a_1 \cdot C_{j-1}^{n+1} + a_2 \cdot C_j^{n+1} + a_3 \cdot C_{j+1}^{n+1} = \\
 & b_1 \cdot C_{j-1}^n + b_2 \cdot C_j^n + b_3 \cdot C_{j+1}^n + \\
 & \Delta t \cdot \Theta \frac{\varepsilon}{T_d} (C_{d,j}^{n+1} - C_j^{n+1}) + \Delta t (1 - \Theta) \frac{\varepsilon}{T_d} (C_{d,j}^n - C_j^n) \\
 & \Downarrow \\
 & a_1 \cdot C_{j-1}^{n+1} + (a_2 + \Theta \cdot \varepsilon \cdot h) C_j^{n+1} - \\
 & \Theta \cdot \varepsilon \cdot h \cdot C_{d,j}^{n+1} + a_3 \cdot C_{j+1}^{n+1} = \\
 & b_1 \cdot C_{j-1}^n + (b_2 - (1 - \Theta) \varepsilon \cdot h) C_j^n + \\
 & (1 - \Theta) \varepsilon \cdot h \cdot C_{d,j}^n + b_3 \cdot C_{j+1}^n
 \end{aligned} \tag{4.93}$$

Dead zone:

$$\begin{aligned}
 \frac{C_{d,j}^{n+1} - C_{d,j}^n}{\Delta t} &= \frac{1}{T_d} \left( \Theta (C_j^{n+1} - C_{d,j}^{n+1}) + (1 - \Theta) (C_j^n - C_{d,j}^n) \right) \\
 & \Downarrow \\
 & (1 + h \cdot \Theta) C_n + 1_{d,j} - h \cdot \Theta \cdot C_j^{n+1} = \\
 & (1 - (1 - \Theta) h) C_{d,j}^n + (1 - \Theta) h \cdot C_j^n
 \end{aligned} \tag{4.94}$$

Adding boundary conditions like for the Two Level Multischeme, a system of linear equations can be developed for determination of the concentrations in the main stream as well as in the dead zone. Depending on the arrangement of the equations the system may look as:

$$\begin{bmatrix} x & x & x \\ x & x & \\ x & x & x & x \\ x & x & \\ x & x & x & x \\ x & x & \\ x & x & x & x \\ x & x & \\ - & - & - \\ - & - & \end{bmatrix} \cdot \begin{bmatrix} C_1 \\ C_{d,1} \\ C_2 \\ C_{d,2} \\ C_3 \\ C_{d,3} \\ C_4 \\ C_{d,4} \\ - \\ - \end{bmatrix} = \begin{bmatrix} x \\ - \\ - \end{bmatrix}$$

where  $x$  denotes a coefficient different from zero. This system can be solved by Gauss elimination, e.g. by use of the EQSOLV algorithm (Gupta & Tanji, 1977).

Also the quicker Double Sweep algorithm can be applied after rewriting the equations. From eq.(4.94) the unknown concentration in the dead zone  $C_{d,j}^{n+1}$  can be found. Inserting this in eq.(4.93) yields:

$$a_1 \cdot C_{j-1}^{n+1} + \left( a_2 + \frac{\Theta \cdot \varepsilon \cdot h}{1 + \Theta \cdot h} \right) C_j^{n+1} + a_3 \cdot C_{j+1}^{n+1} = \\ b_1 \cdot C_{j-1}^n + \left( b_2 - \frac{(1 - \Theta) \varepsilon \cdot h}{1 + \Theta \cdot h} \right) C_j^n + b_3 \cdot C_{j+1}^n + \frac{\varepsilon \cdot h}{1 + \Theta \cdot h} C_{d,j}^n \quad (4.95)$$

By use of this expression a tridiagonal system of equations can be obtained and solved by using the Double Sweep algorithm, leading to new values for the main stream concentration. Afterwards the concentration in the dead zones can be found from eq.(4.94).

This implicit model is much more sufficient than the explicit model mentioned above, since no stability conditions are present and numerical errors are of minor importance when  $\Theta = \frac{1}{2}$ . To avoid wiggles the Peclet number should not exceed a value of 2 (sec. 4.5.5).

### Solution of higher order equation

The last model to be mentioned is a finite difference model for the higher order equation (sec. 4.2.4):

$$T_d \frac{\partial}{\partial t} \left( \frac{\partial C}{\partial t} + u \frac{\partial C}{\partial x} - K_x \frac{\partial^2 C}{\partial x^2} \right) + \\ (1 + \varepsilon) \left( \frac{\partial C}{\partial t} + \frac{u}{1 + \varepsilon} \frac{\partial C}{\partial x} - \frac{K_x}{1 + \varepsilon} \frac{\partial^2 C}{\partial x^2} \right) = 0 \quad (4.96)$$

No specific numerical scheme will be mentioned, but a discretization of eq.(4.96) can only be performed if at least three space levels and three time levels are included, since a second derivative is present in  $x$  as well as in  $t$ . The discretization could lead to a tridiagonal system of linear equations, from which the concentrations in the main stream could be determined.

## 4.8 Discussion

In this chapter three mathematical models for transport and spreading of pollutants have been treated, namely, the Transport model, the Transport/Dispersion model, and the Transport/Dispersion/Dead Zone model. Which one to choose depends on the features of the stream, the event and for which purpose the modelling is performed.

If the variation in geometry and bottom slope is very small, and the velocity distribution in the cross section is nearly uniform, then the Transport model might lead to sufficient results, since the longitudinal dispersion might be expected to be of minor importance. Furthermore, if only small variations in the concentrations (small gradients) are expected, then the Transport model could be a proper choice. But if large and rapid variations in the concentration of the pollutant are expected, e.g. caused by storm sewer overflow, then the longitudinal dispersion should not be ignored, and then the Transport/Dispersion model would be a better choice. The variation in the geometry should not be too strong, and if large almost non-flowing areas are present, then the Transport/Dispersion model should not be applied for events, where rapidly varying concentrations are expected.

Instead the Dead Zone model should be applied, since this model is able to describe the influence (long tails) from these non-flowing areas on rapidly varying concentrations. If only moderate gradients of the concentration are present, then there is no need for implementation of the Dead Zone model, since the influence from the dead zones will act like a Fickian dispersion (Pedersen, 1977). For practical modelling the Dead Zone model is difficult to apply, since three parameters must be known or found through a calibration, namely the longitudinal dispersion coefficient  $K_x$ , the dead zone volume fraction  $\varepsilon$ , and the residence time for the dead zone  $T_d$ . Furthermore, some variation in space (and perhaps in time) of these parameters might be expected. An attempt to develop mathematical expressions for these parameters can be found in Pedersen (1977), while an attempt to determine the parameters through calibration can be found in Bjerrekær et al. (1988).

A number of different numerical models have been examined, primarily by mean of stability conditions and numerical error properties. If the purpose was to identify the best scheme the examinations have not succeeded, but a number of general properties have been identified. Having these properties in mind, the choice of a numerical model and the application for a specific

task should be easier and the risk for serious mistakes reduced.

The Method of Characteristics or the movable coordinate system seem to be superior for the Transport model and the Transport/Dispersion model, as long as the flow is steady, but for unsteady flow other methods are preferable. The modified Method of Characteristics cannot be recommended, since this model suffers from serious numerical dispersion.

The Control Volume approach can be recommended for new modellers, since the method is very straightforward and the physical relationships easy to understand, especially for formulation of boundary conditions, but basically the method will provide schemes identical to finite difference schemes.

The main part of the models treated in chapter 4 are based on finite differences. The advantage by using this approach is a more stringent mathematical formulation, but often the formulation of boundary conditions must be based on the Control Volume approach.

Generally implicit schemes seem to be preferable, since the stability properties are much better here than for the explicit schemes. Furthermore, the stability properties for three level schemes seem to be poor and these schemes cannot be recommended for Transport/Dispersion models.

The Two Level Multischeme includes a lot of schemes, e.g. the Stone & Brian scheme, which seems to be a good choice for a lot of events. The scheme is unconditional stable, free of numerical dispersion, but wiggles will be present unless very small space steps are chosen. This phenomenon can be avoided by using a backward difference instead of a central difference for the convective term, but this performance introduce numerical dispersion, and therefore it cannot be recommended.

An attempt to develop schemes without any numerical dispersion and without wiggles has been performed by Leonard (1979) and Basco (1984). The explicit Quickest scheme has shown up very good properties, - no numerical dispersion or wiggles are present, but the scheme is only conditional stable. The stability area has been extended in the semi-implicit Quick $\Theta$ st scheme, but further improvement could be desirable. Nevertheless, the Quick $\Theta$ st scheme seems to be a very good choice, but whether it would be a better choice than the Stone & Brian cannot be stated in general.

It is important to have in mind that all the considerations in this chapter have been performed under assumption of steady flow, and therefore further examinations should be performed for unsteady flow conditions, e.g. a number of testruns for some characteristic events in Danish streams.

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## APPENDIX

### Two Level Multischeme

Differential equation:

$$\frac{\partial c}{\partial t} + u \frac{\partial c}{\partial x} = K_x \frac{\partial^2 c}{\partial x^2}$$

Discretization :

$$\begin{aligned}\frac{\partial c}{\partial t} &\simeq \alpha \frac{C_{j-1}^{n+1} - C_{j-1}^n}{\Delta t} + (1 - 2 \cdot \alpha) \frac{C_j^{n+1} - C_j^n}{\Delta t} + \alpha \frac{C_{j+1}^{n+1} - C_{j+1}^n}{\Delta t} \\ \frac{\partial c}{\partial x} &\simeq \Theta \left( \beta \frac{C_{j+1}^{n+1} - C_j^{n+1}}{x_{j+1} - x_j} + (1 - \beta) \frac{C_j^{n+1} - C_{j-1}^{n+1}}{x_j - x_{j-1}} \right) + \\ &\quad (1 - \Theta) \left( \beta \frac{C_{j+1}^n - C_j^n}{x_{j+1} - x_j} + (1 - \beta) \frac{C_j^n - C_{j-1}^n}{x_j - x_{j-1}} \right) \\ \frac{\partial^2 c}{\partial x^2} &\simeq \Theta \frac{\frac{C_{j+1}^{n+1} - C_j^{n+1}}{x_{j+1} - x_j} - \frac{C_j^{n+1} - C_{j-1}^{n+1}}{x_j - x_{j-1}}}{\frac{1}{2}(x_{j+1} - x_{j-1})} + (1 - \Theta) \frac{\frac{C_{j+1}^n - C_j^n}{x_{j+1} - x_j} - \frac{C_j^n - C_{j-1}^n}{x_j - x_{j-1}}}{\frac{1}{2}(x_{j+1} - x_{j-1})}\end{aligned}$$

Difference equation ( $\Delta x = const.$ ):

$$\begin{aligned}&\left[ \alpha + \Theta \left( -(1 - \beta) u \frac{\Delta t}{\Delta x} - K_x \frac{\Delta t}{\Delta x^2} \right) \right] C_{j-1}^{n+1} + \\ &\left[ (1 - 2 \cdot \alpha) + \Theta \left( (1 - 2 \cdot \beta) u \frac{\Delta t}{\Delta x} + 2 \cdot K_x \frac{\Delta t}{\Delta x^2} \right) \right] C_j^{n+1} + \\ &\left[ \alpha + \Theta \left( \beta \cdot u \frac{\Delta t}{\Delta x} - K_x \frac{\Delta t}{\Delta x^2} \right) \right] C_{j+1}^{n+1} = \\ &\left[ \alpha + (1 - \Theta) \left( (1 - \beta) u \frac{\Delta t}{\Delta x} + K_x \frac{\Delta t}{\Delta x^2} \right) \right] C_{j-1}^n + \\ &\left[ (1 - 2 \cdot \alpha) + (1 - \Theta) \left( -(1 - 2 \cdot \beta) u \frac{\Delta t}{\Delta x} - 2 \cdot K_x \frac{\Delta t}{\Delta x^2} \right) \right] C_j^n + \\ &\left[ \alpha + (1 - \Theta) \left( -\beta \cdot u \frac{\Delta t}{\Delta x} + K_x \frac{\Delta t}{\Delta x^2} \right) \right] C_{j+1}^n\end{aligned}$$

## Du Fort & Frankel scheme

Differential equation:

$$\frac{\partial c}{\partial t} + u \frac{\partial c}{\partial x} = K_x \frac{\partial^2 c}{\partial x^2}$$

Discretization :

$$\frac{\partial c}{\partial t} \simeq \frac{C_j^{n+1} - C_j^{n-1}}{2 \cdot \Delta t}$$

$$\frac{\partial c}{\partial x} \simeq \frac{C_{j+1}^n - C_{j-1}^n}{x_{j+1} - x_{j-1}}$$

$$\frac{\partial^2 c}{\partial x^2} \simeq \frac{\frac{C_{j+1}^n - \frac{1}{2}(C_j^{n+1} + C_j^{n-1})}{x_{j+1} - x_j} - \frac{\frac{1}{2}(C_j^{n+1} + C_j^{n-1}) - C_{j-1}^n}{x_j - x_{j-1}}}{\frac{1}{2}(x_{j+1} - x_{j-1})}$$

Difference equation ( $\Delta x = \text{const.}$ ):

$$\frac{C_j^{n+1} - C_j^{n-1}}{2 \cdot \Delta t} + u \frac{C_{j+1}^n - C_{j-1}^n}{2 \cdot \Delta x} = K_x \frac{C_{j+1}^n - C_j^{n+1} - C_j^{n-1} + C_{j-1}^n}{\Delta x^2}$$

## The Blokcscheme

Differential equation:

$$\frac{\partial c}{\partial t} + u \frac{\partial c}{\partial x} = K_x \frac{\partial^2 c}{\partial x^2}$$

Discretization ( $\Delta x = \text{const.}$ ):

$$\begin{aligned} \frac{\partial c}{\partial t} &\simeq \frac{1-\alpha}{2} \left( \frac{C_{j-1}^{n+1} - C_{j-1}^{n-1}}{2 \cdot \Delta t} \right) + \\ &\quad \frac{1-\alpha}{2} \left( \frac{C_{j+1}^{n+1} - C_{j+1}^{n-1}}{2 \cdot \Delta t} \right) \end{aligned}$$

$$\begin{aligned}
\frac{\partial c}{\partial x} &\simeq \frac{1-\Theta}{2} \left( \frac{C_{j+1}^{n+1} - C_{j-1}^{n+1}}{2 \cdot \Delta x} \right) + \Theta \left( \frac{C_{j+1}^n - C_{j-1}^n}{2 \cdot \Delta x} \right) + \\
&\quad \frac{1-\Theta}{2} \left( \frac{C_{j+1}^{n-1} - C_{j-1}^{n-1}}{2 \cdot \Delta x} \right) \\
\frac{\partial^2 c}{\partial x^2} &\simeq \frac{1-\Theta}{2} \left( \frac{C_{j+1}^{n+1} - 2 \cdot C_j^{n+1} + C_{j-1}^{n+1}}{\Delta x^2} \right) + \\
&\quad \Theta \left( \frac{C_{j+1}^n - 2 \cdot C_j^n + C_{j-1}^n}{\Delta x^2} \right) + \\
&\quad \frac{1-\Theta}{2} \left( \frac{C_{j+1}^{n-1} - 2 \cdot C_j^{n-1} + C_{j-1}^{n-1}}{\Delta x^2} \right)
\end{aligned}$$

Difference equation:

$$\begin{aligned}
&\left( \frac{1-\alpha}{4 \cdot \Delta t} - u \frac{1-\Theta}{4 \cdot \Delta x} - K_x \frac{1-\Theta}{2 \cdot \Delta x^2} \right) C_{j-1}^{n+1} + \\
&\left( \frac{\alpha}{2 \cdot \Delta t} + K_x \frac{1-\Theta}{\Delta x^2} \right) C_j^{n+1} + \\
&\left( \frac{1-\alpha}{4 \cdot \Delta t} + u \frac{1-\Theta}{4 \cdot \Delta x} - K_x \frac{(1-\Theta)}{2 \cdot \Delta x^2} \right) C_{j+1}^{n+1} = \\
&\left( u \frac{\Theta}{2 \cdot \Delta x} + K_x \frac{\Theta}{\Delta x^2} \right) C_{j-1}^n + \\
&\left( -K_x \frac{2 \cdot \Theta}{\Delta x^2} \right) C_j^n + \\
&\left( -u \frac{\Theta}{2 \cdot \Delta x} + K_x \frac{\Theta}{\Delta x^2} \right) C_{j+1}^n + \\
&\left( \frac{1-\alpha}{4 \cdot \Delta t} + u \frac{1-\Theta}{4 \cdot \Delta x} + K_x \frac{1-\Theta}{2 \cdot \Delta x^2} \right) C_{j-1}^{n-1} + \\
&\left( \frac{\alpha}{2 \cdot \Delta t} - K_x \frac{1-\Theta}{\Delta x^2} \right) C_j^{n-1} + \\
&\left( \frac{1-\alpha}{4 \cdot \Delta t} - u \frac{1-\Theta}{4 \cdot \Delta x} + K_x \frac{1-\Theta}{2 \cdot \Delta x^2} \right) C_{j+1}^{n-1}
\end{aligned}$$

Coefficients in the Quick schemes (Basco, 1984)

Quickest:

$$b_1 = -\frac{1}{2} Cr_c + Cr_d + \frac{1}{2} Cr_c^2 + \frac{1}{6} Cr_c (1 - Cr_c^2 - 6 \cdot Cr_d)$$

$$b_2 = 1 - 2 \cdot Cr_d - Cr_c^2 - \frac{1}{2} Cr_c (1 - Cr_c^2 - 6 \cdot Cr_d)$$

$$b_3 = \frac{1}{2} Cr_c + Cr_d + \frac{1}{2} Cr_c^2 + \frac{1}{2} Cr_c (1 - Cr_c^2 - 6 \cdot Cr_d)$$

$$b_4 = -\frac{1}{6} Cr_c (1 - Cr_c^2 - 6 \cdot Cr_d)$$

Quickist:

$$a_1 = \frac{1}{2} \Theta \cdot Cr_c - \Theta \cdot Cr_d$$

$$a_2 = 1 + 2 \cdot \Theta \cdot Cr_d$$

$$a_3 = -\frac{1}{2} \Theta \cdot Cr_c - \Theta \cdot Cr_d$$

$$b_1 = (1 - \Theta) (-\frac{1}{2} Cr_c + Cr_d) + \frac{1}{2} Cr_c^2 + \frac{1}{6} Cr_c (1 - Cr_c^2 - 6 \cdot Cr_d)$$

$$b_2 = 1 - 2(1 - \Theta) Cr_d - Cr_c^2 - \frac{1}{2} Cr_c (1 - Cr_c^2 - 6 \cdot Cr_d)$$

$$b_3 = (1 - \Theta) (\frac{1}{2} Cr_c + Cr_d) + \frac{1}{2} Cr_c^2 + \frac{1}{2} Cr_c (1 - Cr_c^2 - 6 \cdot Cr_d)$$

$$b_4 = -\frac{1}{6} Cr_c (1 - Cr_c^2 - 6 \cdot Cr_d)$$

Quick $\Theta$ st:

$$a_1 = \Theta \left( \frac{1}{2} Cr_c - Cr_d \right)$$

$$a_2 = 1 + 2 \cdot \Theta \cdot Cr_d$$

$$a_3 = \Theta \left( -\frac{1}{2} Cr_c - Cr_d \right)$$

$$b_1 = (1 - \Theta) \left( -\frac{1}{2} Cr_c + Cr_d \right) +$$

$$(1 - 2 \cdot \Theta) \left( \frac{1}{4} Cr_c^2 - \frac{5}{12} Cr_c \cdot Cr_d \right) + \frac{1}{6} Cr_c$$

$$b_2 = 1 - 2 \cdot (1 - \Theta) Cr_d +$$

$$(1 - 2 \cdot \Theta) \left( -\frac{1}{2} Cr_c^2 + \frac{15}{12} Cr_c \cdot Cr_d \right) - \frac{1}{2} Cr_c$$

$$b_3 = (1 - \Theta) \left( \frac{1}{2} Cr_c + Cr_d \right) +$$

$$(1 - 2 \cdot \Theta) \left( \frac{1}{4} Cr_c^2 - \frac{15}{12} Cr_c \cdot Cr_d \right) + \frac{1}{2} Cr_c$$

$$b_4 = -\frac{1}{6} Cr_c + (1 - 2 \cdot \Theta) \frac{5}{12} Cr_c \cdot Cr_d$$

where  $Cr_c = u \frac{\Delta t}{\Delta x}$  and  $Cr_d = K_x \frac{\Delta t}{\Delta x^2}$



## DANSK RESUME

I de seneste år er der sket en kraftig stigning i anvendelsen af numeriske vandkvalitetsmodeller. Numerisk vandkvalitetsmodellering kan opdeles i tre trin:

- Hydrodynamisk modellering til bestemmelse af vandføring og vandstand.
- Modellering af transport og spredning af en opløst konservativt stof
- Modellering af kemiske og biologiske omsætningsprocesser

I denne rapport er kun de to førstnævnte typer modeller behandlet direkte, men indirekte er mange andre typer modeller, f.eks. sedimenttransportmodeller, også behandlet, idet en lang række aspekter er fælles i numerisk modellering. En del af disse fælles træk er behandlet i kapitel 2.

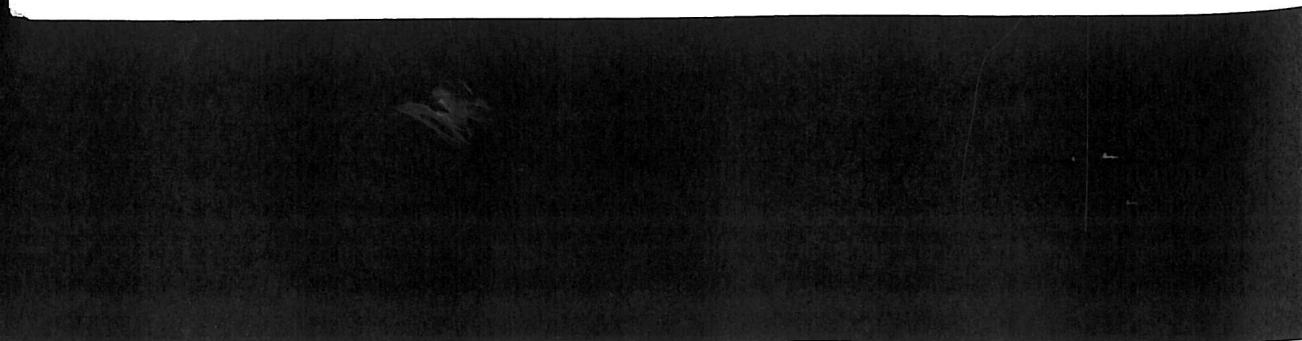
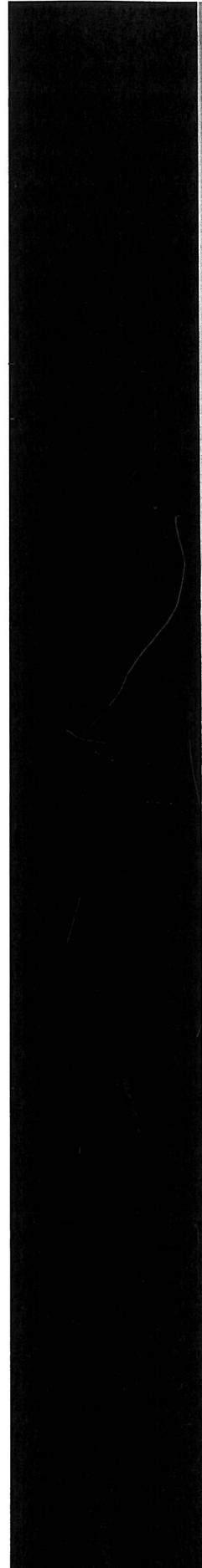
I kapitel 3 behandles den hydrodynamiske modellering. En række matematiske modeller opstilles, såvel for stationært som ikke-stationært flow, og en række forenklede udgaver af de Saint Venants ligninger behandles. Eksempler på numeriske modeller angives, idet hovedvægten er lagt på finite differens modeller.

Kapitel 4 er rapportens hovedkapitel, hvori modellering af transport og spredning af opløst konservativt stof behandles. Der opstilles tre matematiske modeller:

- Transport model, hvor kun konvektiv transport medtages, – det vil sige at spredning af stof ikke kan simuleres.
- Transport/Dispersions model, hvor stofspreddningen antages at følge Fick's diffusions love, hvilket indebærer en symmetrisk spredning af stoffet.
- Transport/Dispersion/Død Zone model, hvor den usymmetriske stofspreddning (lange haler på koncentrationsforløbene) simuleres ved at medtage en stofudveksling mellem den strømmende zone og død zonen, som opfattes som et fuldt op blandet, men stillestående vandvolumen.

Forskellige numeriske løsningsmetoder for de tre modeller behandles, idet hovedvægten lægges på finite differens skemaer for Transport/Dispersions modellen.

En række af de behandlede numeriske skemaer undersøges med hensyn til numeriske egenskaber, – stabilitet og numeriske fejl. Ved beskrivelse af de numeriske fejl skelnes mellem forskellige typer af fejl, såsom numerisk dispersion, numerisk skævhed og fænomenet "wiggles". Der anvendes både matematiske og numeriske analysemetoder, såvel til at uddrage en række generelle egenskaber som til en indbyrdes sammenligning imellem de undersøgte skemaer.



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