MOUSE TRAP

Technical Reference
Advection-Dispersion Module

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Contents

1 INTRODUCTION

Driven by ever-increasing legal requirements and public interest, emissions of pollution from urban sewer and drainage systems into the receiving waters become, both in quantitative and qualitative terms, a focus of particular interest in many evaluations of the system's performance. The knowledge of temporal and spatial distribution of water discharges at outlets and at combined sewer overflows (CSOs), generated by hydrodynamic model simulations, provides useful information about the system operation under given conditions. However, this information is insufficient for the evaluation of e.g. dynamics of the pollution loads at the wastewater treatment plant or the real scale of the problem associated with CSOs. In order to fulfil the articulated demand, the simulation tools must include the description of the pollution transport process.

Transport of pollutants in sewer networks is an extremely complex process and cannot be described with a single transport mechanism. This complexity is due to the nature of the transported pollutants. These occur both as dissolved matter and as pollutant particles. The particulate phase of sewage-borne pollution includes a wide range of particle sizes, which implies various transport mechanisms. E.g. extremely fine suspended pollutant particles (so called "wash-load") behave practically as dissolved. On the other hand, pollutants are attached to the sediments of various grain sizes, which can either be transported as suspended or as bed load, depending on the actual grain size and hydraulic conditions.

The variety of pollutants and their forms in sewage include further complication to the understanding of pollution transport in sewers. Certain types of pollutants occur exclusively in dissolved form, while some other appear only as particles. Organic pollution (e.g. expressed as BOD) is present both in dissolved and particulate phase, with the possibility to move between the suspended and bed load.

Hence, a comprehensive description of the pollution transport process, appropriate for practical numerical modelling applications, must essentially be constituted of several fundamentally different formulations. Transport of dissolved pollutants can successfully be described by the Advection-Dispersion (AD) formulation. This formulation, implemented in MOUSE TRAP AD, is based on mass continuity and advection-dispersion equations, where phenomena like mass conservation, advective transport, molecular and turbulent diffusion and the diffusive effect from the non-uniform velocity distribution are included.

Experience shows that the AD formulation can also be used for the simulation of suspended (fine) fraction of particulate pollutants and sediments. Hence, MOUSE TRAP AD is essential for the simulation of sediment transport processes (suspended sediment fractions), with or without interaction of sediments and pollutants.

Thus, MOUSE TRAP AD is a cornerstone of the MOUSE TRAP suite, essential for the analysis of temporal and spatial distribution of pollution emissions, WWTP loading patterns, morphological studies, etc.

This Technical Reference manual provides an insight into the theoretical aspects of the numerical solution implemented in MOUSE TRAP AD. In association with MOUSE TRAP User guide, this manual should be sufficient for a sensible and effective use of the AD module.

2 SOURCES OF DISSOLVED SUBSTANCES IN SEWER SYSTEMS

Dissolved substances in sewers originate from several sources. These are:

- surface runoff,
- build up in gully pots during dry weather,
- infiltration,
- waste water.

The sources are described in more detail below.

2.1 Dissolved Substances in Surface Runoff

Dissolved substances in surface runoff consist of two components:

- dissolved substances in the precipitation,
- wash-off from the surface.

Precipitation is far from clean. As it passes though the atmosphere, there is an uptake of substances such as nutrients, organic material, solids, metals and pesticides. American researchers have found higher levels of ammonia in precipitation than in runoff from the residential areas and they found that nitrate in the precipitation in some urban areas accounted for 20-90 % of the nitrate in the storm water runoff. The remaining part of the dissolved substances in the surface runoff comes from the erosion of mass on the surface by surface runoff.

2.2 Build up of Dissolved Substances in Gully Pots

The purpose of a gully pot is to trap particles and to prevent them from entering the pipe system. Also, gully pots prevent the release of odour from the pipe system. During dry weather, the amount of dissolved pollutants (e.g. ammonia) builds up in the gully pot liquid. The rate of build up is dependent on the type of pollutant, the biological/chemical conditions in the gully pot and the temperature. During rain storms, the gully pot liquid mixes with the incoming rain water and the polluted water is released. Under some circumstances this phenomena contributes significantly to the First Foul Flush.

2.3 Infiltration Into the Sewer System

Few data are available describing the concentrations in infiltration water. It is often assumed to be clean due to its origin in the soil layers. Infiltration originates from three sources:

- antecedent precipitation,
- frozen residual moisture,
- ground water.

If the quality of the ground water is known or an infiltration study has been carried out, the concentrations of the infiltration can be estimated from these.

2.4 Wastewater

Wastewater originates from residential, commercial and industrial sources. The concentrations of the dissolved substances in the wastewater strongly depend on the local conditions e.g. land use type, number of inhabitants in the catchment and type of industry. Typically, concentrations in wastewater vary on an hourly and daily basis.

3 TRANSPORT OF DISSOLVED SUBSTANCES IN SEWER SYSTEMS

The transport of dissolved substances is traditionally described by the advection-dispersion equations. These equations describe the one-dimensional mass-conservative transport of dissolved material.

The advection-dispersion equation needs inputs from a hydrodynamic model in terms of water levels and discharges. The hydrodynamic basis of the MOUSE TRAP advection-dispersion model is the hydrodynamic model in MOUSE. This model solves the full St. Venant equations for looped systems with free surface flow or pressurized flow. The hydrodynamic model is described in the "MOUSE User's Guide & Technical Reference".

The main assumptions of the one dimensional advection-dispersion equation are:

- the considered substance is completely mixed over the water column. This implies that a source/sink term is considered to mix instantaneously,
- the substance is considered to be conservative or subject to a first order decay,
- Fick's diffusion law can be applied, i.e. the dispersive transport is proportional to the gradient of the concentration.

If the flow passes rapidly through the sewer system, the decay will seldom be important. In general, the dissolved substances/pollutants can be modelled as conservative or with a first order decay. The decay can be used e.g. for the description of the de-oxygenation of BOD.

3.1 The Continuity Equation for the Transport of Dissolved Substances

The one-dimensional, vertically-integrated equation for the conservation of mass of a substance in solution is given as:

$$\frac{\partial (AC)}{\partial t} + \frac{\partial T}{\partial x} = - A \cdot K \cdot C + C_S \cdot q \qquad (1)$$

where:

C is the concentration (arbitrary unit),
A is the area of the cross-section (m^2),
T is the transport,
K is the linear decay coefficient (s^{-1}),
C_s is the source/sink concentration,
q is the lateral inflow (m^2/s),
x is the space co-ordinate (m),
t is the time co-ordinate (s).

3.2 The Advection-Dispersion Equation

The advection-dispersion equation reflects two transport mechanisms:

- the advective transport of the dissolved substances with the mean flow velocity,
- the dispersive transport due to concentration gradients of the dissolved substance in the water.

The dispersion again reflects several phenomena, i.e. molecular diffusion, turbulent diffusion and the effect from the non-uniform velocity distribution over the cross-section.

The two first mentioned diffusion processes are rather insignificant compared the effect from the non-uniform velocity distribution. The dispersion coefficient for the turbulent flow in a full running pipe was found through theoretical analysis by **Taylor in 1954** to be:

$$k_x = \frac{D}{u_f \cdot R} = 20.2 \tag{2}$$

where:

k_x is the dimensionless dispersion coefficient,
D is the dispersion coefficient (m^2/s),
u_f is the friction velocity (m/s),
R is the hydraulic radius (m).

The theoretical analysis by Taylor was verified against experimental data. For a 1-meter pipe with a slope of 1.0E-2 the dispersion coefficient D is:

$$D = 20.2 \cdot \sqrt{gRI} \cdot R =$$

$$20.2 \sqrt{9.81 \cdot 0.25 \cdot 1.0E-2} \cdot 0.25 = 0.8\, m^2/s \tag{3}$$

The effect of the dispersion term is probably small for sewer systems with high flow velocities, but it may become important in systems with small gradients and backwater effects. The one-dimensional vertically integrated equation for the conservation of mass of a substance in solution, i.e. the one dimensional advection-dispersion equation reads:

$$\frac{\partial(AC)}{\partial t} + \frac{\partial(QC)}{\partial x} - \frac{\partial}{\partial x}\left(AD\frac{\partial C}{\partial x}\right) = -A \cdot K \cdot C + C_c \cdot q \tag{4}$$

In the present numerical model, a more general description of the dispersion coefficient has been implemented. The dispersion coefficient is determined as a function of the mean flow velocity:

$$D = a \cdot |u|^b \tag{5}$$

where:

u is the mean velocity (m/s),
a,b are user specified constants.

Equation (5) can be turned into Equation (2) by selecting:

$$a = 20.0 \frac{\sqrt{g}}{M} R^{5/6} \quad and \quad b = 1 \tag{6}$$

3.3 Boundary Conditions for the Advection-Dispersion Equation

The advection-dispersion model needs boundary conditions at all external boundaries. At external boundaries several different boundary conditions can be applied:

- outflow from an the open boundary,
- flow into an open boundary,
- closed boundary.

3.3.1 Outflow From an Open Boundary

When outflow occur, the concentration is only dependent on the concentration in the model area. The open boundary outflow condition is:

$$\frac{\partial^2 C}{\partial x^2} = 0 \tag{7}$$

This specifies that the gradient of the concentration with respect to the distance is constant at the outflow boundary and that the transport across the boundary is pure advection.

3.3.2 Flow Into an Open Boundary

At an open inflow boundary the concentration must be specified as function of time. If the flow direction changes an outflow boundary becomes an inflow boundary and vice versa. This scenario will typically happen when the receiving water is tidal influenced. The boundary condition then changes between the concentration in the sewer system and the concentration in the receiving water according to:

$$C = C_r + \left(C_s - C_r\right) \; e^{\frac{-t_{mix}}{K_{mix}}} \tag{8}$$

where:

c_r is the concentration in the receiving water,
c_s is the concentration in the sewer system immediately before the flow direction changed,
K_{mix} is a time scale (hrs^{-1}),
t_{mix} is the elapsed time since the flow direction changed (hrs).

Equation (8) reflects that the first water, which enters the sewer system has the concentration of the water which last has left the sewer before the flow reversal occurred. By selecting a small value of K_{mix}, the inflow concentration changes almost immediately to the concentration in the receiving water. On the contrary, by selecting a large k_{mix}, the inflow concentration changes very slowly from the concentration in the sewer system to the concentration in the recipient.

3.3.3 Closed Boundaries

No mass is transported across a closed boundary, hence it is characterized by q = 0.0 and

$$\frac{\partial C}{\partial x} = 0 \tag{9}$$

3.4 Solution of the Advection-Dispersion Equation at Structures and Manholes

The solution of the advection-dispersion equation has to be modified at hydraulic structures in sewer systems. The general way to describe the transport at a nodal point is to set up a local continuity equation. Further, special cases exist where the local continuity equation has to be modified, e.g. when free flow into a manhole is present. The modification to the advection-dispersion equation is described below.

3.4.1 Manholes and Structures - General Solution

At manholes a local continuity equation is applied. It is assumed that the substance in the nodal point is fully mixed over the volume. This assumption might not always be fulfilled, e.g. when flooding occurs. The continuity equation for a manhole reads:

$$\frac{\partial(V_N C_N)}{\partial t} + \sum_{i=1}^{i=kk} T = -V_N \cdot C_N \cdot K_N \tag{10}$$

where:

V_N is the volume of the structure (m^3/s),
C_N is the concentration in the node,
T is the transport into the node (kg/s),
K_N is the decay constant for the node,
kk is the number of connecting pipes.

The continuity equation for the water flow to and from a node can be written as:

$$\frac{\partial V_N}{\partial t} + \sum_{i=1}^{i=kk} Q = 0 \tag{11}$$

where Q (m^3/s) is the discharge in the connecting branches.

The continuity equation for a nodal point, Equation (10), can be re-arranged by use of the continuity equation for water, Equation (11):

$$V_n \frac{\partial C_N}{\partial t} - C_N \sum_{i=1}^{i=kk} Q + \sum_{i=1}^{i=kk} T = - V_N \cdot C_N \cdot K_N \qquad (12)$$

3.4.2 Free Flow Into a Manhole

When free flow into a structure occurs, i.e. the water level in the structure is lower than the water level in the inlet pipe, the concentration in the pipe is independent of the concentration at the structure. Hence, the dispersion term in the formulation of the transport is neglected, i.e. the transport is pure advection, see Figure 1. The transport at a structure is now formulated as:

$$T = Q \cdot C \qquad (13)$$

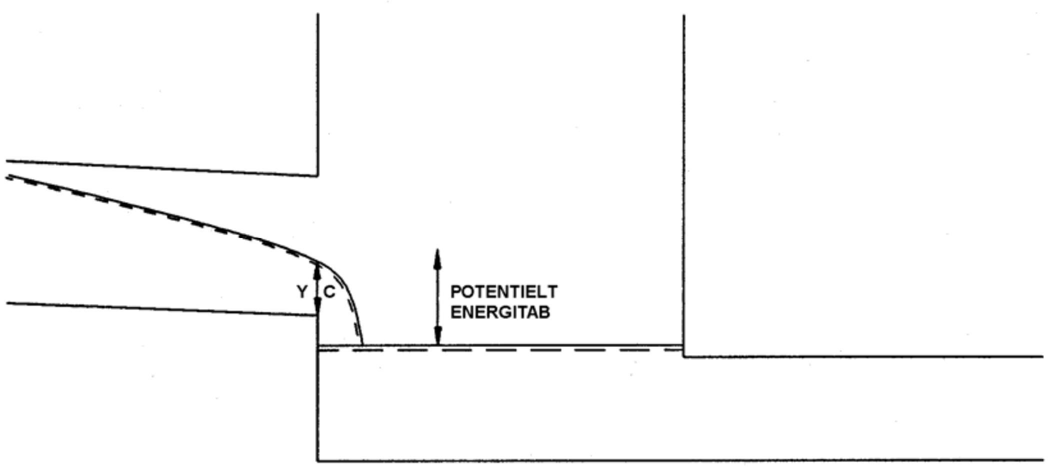

Figure 1 Free inflow to a manhole.

3.4.3 No Outflow From a Structure To a Pipe

This condition occurs when the water level at the structure is lower than the bottom invert of the outlet pipe, see Figure 2. When such a situation arises, a local continuity equation is applied. The transport into the outlet pipe is described by:

$$T = Q_{pipe} \cdot C_N \qquad (14)$$

where Q_{pipe} (m^3/s) is the discharge at the first grid point in the outlet pipe.

In reality the discharge in the outlet pipe ought to be zero. However, due to the stability of the numerical scheme in the hydrodynamic model a minimum water depth of 0.5% of the pipe diameter (maximum 0.5 cm) will always be present in the pipes. Hence, a small discharge will be present.

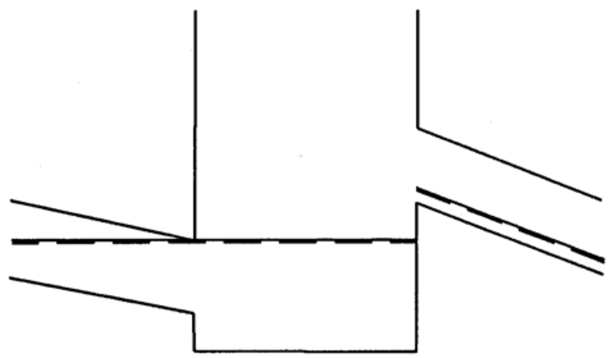

Figure 2 No flow from the manhole to the outlet pipe.

3.5 Formulation of the Transport of Dissolved Substances Through Pumps

In general, the formulation of the transport of a dissolved substance is based on the hydrodynamic solutions of the MOUSE model. In the hydrodynamic model of MOUSE, pumps are normally described as functions between two nodes, i.e. without explicit definition of rising mains. This simplification implies instantaneous water transport and consequently, the impossibility to apply the advection-dispersion equations in such cases. The only information available is the distance between the pump and the tail node (approx. the length of the rising main) and the discharge of the pump. Hence, dissolved matter is routed through such a system with no time lag between the pump and the end of the conduit. This results in significant errors in the transport time for dissolved substances in the pipe, if the retention time of water in the conduit is much larger than the time step of the simulation. The pumped mass $q_s{\cdot}c_s$ is added to in the source term of the continuity equation at the tail node.

3.6 Formulation of the Transport of Dissolved Substances Over Weirs

Transport over a weir is formulated as routing between the weir node and the destination node. The transport rate is determined on the basis of the concentration in the weir node and the weir flow. The mass flowing over the weir $q_s{\cdot}c_s$ is added to the source term of the continuity equation at the destination node.

4 THE NUMERICAL SOLUTION FOR THE ADVECTION-DISPERSION MODEL

4.1 Numerical Scheme

The advection-dispersion equation is solved using an implicit finite-difference scheme, which is centred in time and space in order to avoid the numerical dispersion. The concentrations are defined in each grid point, i.e. the grid is a non-staggered grid. A third-order correction term has been included in order to eliminate the third-order truncation error. A sketch of the numerical scheme is shown in Figure 3.

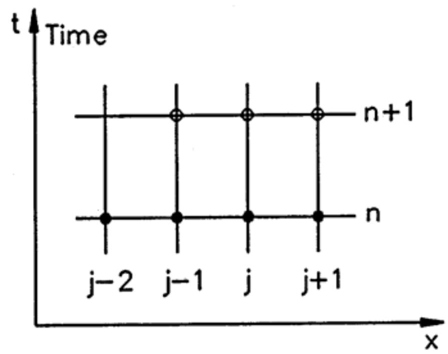

Figure 3 The numerical scheme for the advection-dispersion.

The two equations considered are the continuity equation and the advection-dispersion equation. The continuity equation is given in Equation (1). A sketch of the transport of dissolved substances through a small element of water is shown in Figure 4.

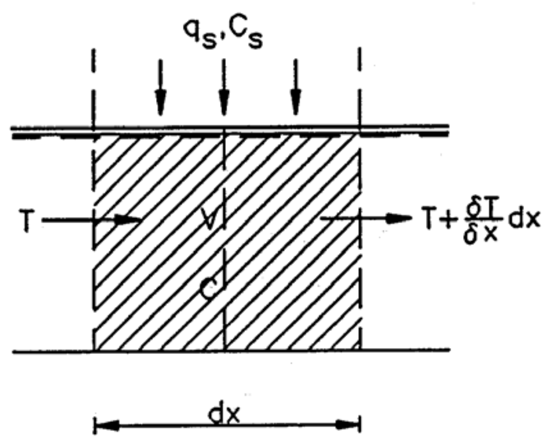

Figure 4 Sketch of the transport of dissolved substances through a small element of water

The continuity equation can be written in discrete form as given below:

$$\frac{(V_j C_j)^{n+1} - (V_j C_j)^n}{\Delta t} + T_{j+½}^{n+½} - T_{j-½}^{n+½} = Q_s^{n+½} C_s^{n+½} - K C_j^{n+½} V_j^{n+½} \quad (15)$$

where:

T is the transport through the box walls,
j is the grid point number,
n is the time level.

The advection-dispersion equation is given below in discrete form:

$$T_{j+½}^{n+½} = Q_{j+½}^{n+½} C_{j+½}^{*} - A_{j+½}^{n+½} D_{j+½}^{n+½} \frac{C_{j+1}^{n+½} - C_j^{n+½}}{\Delta x} \quad (16)$$

where:

$Q_{j+½}^{n+½}$ is the discharge at the right wall of the box (m^3/s),

$A_{j+½}^{n+½}$ is the cross sectional area of the right wall (m^2),

$D_{j+½}^{n+½}$ is the dispersion coefficient (m^2/s) given by Equation (17),

$C_{j+½}{}^{*}$ is an upstream interpolated concentration given by Equation s (66) and (67).

The dispersion coefficient is calculated as:

$$D_{j+½}^{n+½} = a \cdot \left| \frac{Q_{j+½}^{n+½}}{A_{j+½}^{n+½}} \right|^b \quad (17)$$

where *a* and *b* are constants.

4.2 Discretization of the Boundary Conditions

4.2.1 Outflow From an Open Boundary

The open outflow boundary condition is given by Equation (7). The discrete form of Equation (7) is:

$$\frac{(V_N C_N)^{n+1} - (V_N C_N)^n}{\Delta t} + (\Delta T)^{n+½} = Q_s^{n+½} C_s^{n+½} - K_N C_N^{n+½} V_N^{n+½} \tag{18}$$

where $\Delta T^{n+½}$ is the transport given as:

$$\Delta T^{n+½} = Q_{j-½}^{n+½} C_{j-½}^{*} - Q_N^{n+½} C_N^{n+½} \tag{19}$$

4.2.2 Flow Into an Open Boundary

The discrete form of the inflow boundary condition is:

$$C_N^{n+½} = C_B^{n+½} \tag{20}$$

where C_B is the concentration at the boundary. If a flow reversal occurs at the boundary the outflow boundary changes to an inflow boundary and the boundary condition is given as in Equation (8). The discrete form of Equation (8) is:

$$C_N^{n+½} = C_r^{n+½} + (C_s^{n+½} - C_r^{n+½})\, e^{\frac{-t_{mix}}{K_{mix}}} \tag{21}$$

4.2.3 Closed Boundaries

The closed boundary condition is given in Equation (9). The discrete form for the closed boundary is equivalent to the discrete form of the continuity equation for a manhole, which is given in the next section.

4.3 Discretization at Manholes and Structures

The continuity equation around manholes and structures, Equation (10), is given in the discrete form below:

$$V_N^{n+½} \frac{C_N^{n+1} - C_N^n}{\Delta t} + ½ (C_N^{n+1} + C_N^n) \frac{\partial V_N}{\partial t} + \sum_{k=1}^{k=kk} T \quad =$$

$$Q_s C_s \; - \; ½ \, K \, V_N^{n+½} (C_N^n + C_N^{n+1}) \tag{22}$$

The transport T to and from the node is given as:

$$T \; = \; 1/4 \, Q_{j+½}^{n+½} (C_N^{n+1} + C_N^n + C_{N-1}^{n+1} + C_{N-1}^n) \; +$$

$$A_{N-½}^{n+½} D_{N-½}^{n+½} \left[\frac{1/2(C_N^{n+1} + C_N^n) - 1/2(C_{N-1}^{n+1} + C_{N-1}^n)}{1/2 \, \Delta x} \right] \tag{23}$$

where $N\text{-}1$ is the grid point in pipe k at a distance Δx from the node.

4.3.1 Free Flow Into a Manhole

When free inflow to the node occurs the dispersion term in the formulation of the transport is neglected. The discrete form of the transport then yields:

$$T_j^{n+½} \; = \; 1/2 \, Q_j^{n+½} (C_j^{n+1} + C_j^n) \tag{24}$$

4.3.2 No Outflow From a Structure to a Pipe

When the water level in the structure is lower than the invert of the outlet pipe, a local continuity equation is applied. The discrete form of the transport into the outlet pipe is:

$$T_j^{n+½} \; = \; Q_j^{n+½} \cdot 1/2(C_N^{n+1} + C_N^n) \tag{25}$$

4.4 Solution of the Finite Difference Equations

Substitution and re-arrangement of the above equations give a general implicit finite difference equation which relates the concentration in three neighbouring grid points to each other at any time level as follows:

$$\alpha_j C_{j-1}^{n+1} + \beta_j C_j^{n+1} + \gamma_j C_{j+1}^{n+1} = \delta^n \qquad (26)$$

where α, β and γ are constants.

Equation (26) gives a tri-diagonal matrix, i.e. a system of linear equations which is solved by the "double sweep" algorithm, as described in the MOUSE HD Technical Reference Manual.

4.5 The Accuracy of the Numerical Scheme

The third order Taylor series expansion is used to ensure that the scheme has a third order accuracy. Elimination of the third order truncation error makes it possible to simulate concentration profiles with steep fronts. In general, the third order terms are associated with phase errors and wiggles in the scheme while the second order terms lead to numerical diffusion. The Taylor expansions yields:

$$C_j^{n+1} = C_j^n + \Delta t \frac{\partial C_j^n}{\partial t} + \frac{\Delta t^2}{2} \frac{\partial^2 C_j^n}{\partial t^2} + \frac{\Delta t^3}{6} \frac{\partial^3 C_j^n}{\partial t^3} \qquad (27)$$

$$C_{j-1}^n = C_j^n - \Delta x \frac{\partial C_j^n}{\partial x} + \frac{\Delta x^2}{2} \frac{\partial^2 C_j^n}{\partial x^2} - \frac{\Delta x^3}{6} \frac{\partial^3 C_j^n}{\partial x^3} \qquad (28)$$

$$C_{j+1}^n = C_j^n + \Delta x \frac{\partial C_j^n}{\partial x} + \frac{\Delta x^2}{2} \frac{\partial^2 C_j^n}{\partial x^2} + \frac{\Delta x^3}{6} \frac{\partial^3 C_j^n}{\partial x^3} \qquad (29)$$

$$C_{j-2}^n = C_j^n - 2\Delta x \frac{\partial C_j^n}{\partial x} + \frac{(2\Delta x)^2}{2} \frac{\partial^2 C_j^n}{\partial x^2} - \frac{(2\Delta x)^3}{6} \frac{\partial^3 C_j^n}{\partial x^3} \qquad (30)$$

$$C^{n+1}_{j+1} = C^n_j + \Delta t \frac{\partial C^n_j}{\partial t} + \Delta x \frac{\partial C^n_j}{\partial x} + \frac{\Delta t^2}{2}\frac{\partial^2 C^n_j}{\partial t^2} +$$

$$\frac{\partial x^2}{2}\frac{\partial^2 C^n_j}{\partial x^2} + \frac{2\Delta x \Delta t}{2}\frac{\partial^2 C^n_j}{\partial x \partial t} + \frac{\Delta t^3}{6}\frac{\partial^3 C^n_j}{\partial t^3} +$$

$$\frac{\Delta x^3}{6}\frac{\partial^3 C^n_j}{\partial x^3} + \frac{3\Delta x^2 \Delta t}{6}\frac{\partial^3 C^n_j}{\partial x^2 \partial t} + \tag{31}$$

$$\frac{3\Delta x \Delta t^2}{6}\frac{\partial^3 C^n_j}{\partial x \partial t^2}$$

$$C^{n+1}_{j-1} = C^n_j + \Delta t \frac{\partial C^n_j}{\partial t} - \Delta x \frac{\partial C^n_j}{\partial x} +$$

$$1/2 \left\{ \Delta t^2 \frac{\partial^2 C^n_j}{\partial t^2} + \Delta x^2 \frac{\partial^2 C^n_j}{\partial x^2} - 2\Delta x \Delta t \frac{\partial^2 C^n_j}{\partial x \partial t} \right\} + \tag{32}$$

$$1/6 \left\{ \Delta t^3 \frac{\partial^3 C^n_j}{\partial t^3} - \Delta x^3 \frac{\partial^3 C^n_j}{\partial x^3} + 3\Delta x^2 \Delta t \frac{\partial^3 C^n_j}{\partial x^2 \partial t} \right.$$

$$\left. - 3\Delta x \Delta t^2 \frac{\partial^3 C^n_j}{\partial x \partial t^2} \right\}$$

By assuming that the velocity is constant locally, the second and third order derivatives in Equations (27) to

(32) can be transformed to a more convenient form. The transformations used are:

$$\frac{\partial C}{\partial t} = - u \frac{\partial C}{\partial x} \tag{33}$$

$$\frac{\partial^2 C}{\partial x \partial t} = -u \frac{\partial^2 C}{\partial x^2} \tag{34}$$

$$\frac{1}{u^2}\frac{\partial^3 C}{\partial x \partial t^2} = \frac{\partial^3 c}{\partial x^3} \tag{35}$$

$$\frac{\partial^3 C}{\partial x^2 \partial t} = -\frac{1}{u}\frac{\partial^3 C}{\partial x \partial t^2} \tag{36}$$

$$\frac{\partial^3 C}{\partial t^3} = -u \frac{\partial^3 C}{\partial x \partial t^2} \tag{37}$$

Equation (33) can be turned into the general formulation:

$$\frac{\partial^n C}{\partial t^n} = (-u)^n \frac{\partial^n C}{\partial x^n} \tag{38}$$

The results of the Taylor expansions are inserted in the advection dispersion equation, e.g. Equation (27) is rewritten as:

$$C_j^{n+1} = C_j^n + \Delta t \frac{\partial C_j^n}{\partial t} + \frac{\Delta t^2}{2} u^2 \frac{\partial^2 C_j^n}{\partial x^2} - \frac{\Delta t^3}{6} u^3 \frac{\partial^3 C_j^n}{\partial x^3} \tag{39}$$

The explicit third order correction term can be found from the solution to four equations with four variables. The solution to the equations is:

$$-1/6\,(1 + \frac{\delta^2}{2})(c_{j-2}^n - 3c_{j-1}^n + 3c_j^n - c_{j+1}^n) = 0 \tag{40}$$

where δ is the convective Courant number defined in Equation (68).

4.6 The Stability of the Numerical Scheme

4.6.1 Linear Stability Analysis of the Numerical Scheme

The stability of the advection equation is evaluated by applying the von Neumann condition for stability. The stability criteria is only evaluated for the advection and not for the advection-dispersion equation, since the case with pure advection sets the strongest stability criteria. The advection equation is given below:

$$\frac{\partial c}{\partial t} + u\frac{\partial c}{\partial x} = 0 \qquad (41)$$

The analytical solution to Equation (41) is:

$$c(x,t) = c_0 \cos(k\,(x - ut),0) = \sum_{j=1}^{\infty} c_j \cos\{\, k_j (x - ut)\} \qquad (42)$$

The harmonic solution to Equation (41) is:

$$c(x,t) = c_0 \cos\{k\,(x - ut)\} = Re[\, c_0\, e^{i\,k\,(x-ut)}\,] \qquad (43)$$

where:

$x \quad = j{\cdot}\Delta x,$
$t \quad = n{\cdot}\Delta t.$

The numerical harmonic solution to Equation (41) can be written as:

$$c(x = j\,\Delta x, t = n\,\Delta t) = c_0\, \rho^n\, e^{i\,k\,j\,\Delta x} \qquad (44)$$

If the analytical equation is equal to the numerical solution the following equation has to be fulfilled:

$$\rho = e^{-i\,k\,u\,\Delta t} \qquad (45)$$

The concentration in grid point j at time level n can now be written as:

$$c_j^n = c_0\, \rho^n\, e^{i\,j\,\xi} \qquad (46)$$

with:

$$\xi = \Delta x \cdot k = 2\pi \frac{\Delta x}{L} \qquad (47)$$

The von Neumann stability condition is based on a linear stability analysis in which it is assumed that the solution to the finite difference scheme can be written as a Fourier series in complex, exponential form for any time level, n, in the form:

$$c_j^n = \sum_{k=1}^{k=kk} \rho_k^n \, e^{ik\alpha_j} \qquad k = 1,2,3,...,kk \tag{48}$$

where:

α is the dimensionless wave number,
k is a finite index.

The linear stability analysis determines how the Fourier coefficients behave in time for a fixed wave number. The concentration at grid point j at time n for the wave number k = 1, can be written as:

$$c_j^n = c_0 \, \rho^n \, e^{i\,j\,\xi} \tag{49}$$

In a similar way, the concentration at grid point j at time level $n+1$ and the concentration at grid point $j+1$ at time level n can be written as:

$$c_j^{n+1} = \rho^{n+1} e^{i\alpha j} \tag{50}$$

and

$$c_{j+1}^n = \rho^n \, e^{i\alpha(j+1)} \tag{51}$$

4.6.2 The Stability of the Advection Equation

The one-dimensional advection equation is given by:

$$\frac{\partial c}{\partial t} = u \frac{\partial c}{\partial x} \tag{52}$$

The discretization of the one-dimensional advection equation, accurate to the third order, is given by:

$$\frac{c_j^n + 1 - c_j^n}{\Delta t} = u \frac{c_{j+½}^{n+½} + (\, c_{j+1}^n - 2\, c_j^n + c_{j-1}^n \,) - c_{j-½}^{n+½} - (\, c_j - 2\, c_{j-}}{\Delta x} \tag{53}$$

Equation (53) is transformed to complex numbers by using the following substitutions:

$$c_j^{n+½} = 1/2(\, c_j^{n+1} + c_j^n \,) = \frac{\rho + 1}{2} c_j^n \tag{54}$$

$$\frac{c_{j+1}^n - c_{j-1}^n}{2} \cdot \frac{1}{c_j^n} = \frac{e^{i\xi} - e^{-i\xi}}{2} = i \sin\xi \tag{55}$$

$$c_{j+½}^{n+½} - c_{j-½}^{n+½} = c_j^n \frac{1+\rho}{2}\left(e^{\frac{i\xi}{2}} - e^{\frac{-i\xi}{2}} \right) = c_j^n \frac{1+\rho}{2} \cdot 2i \sin(\frac{\xi}{2}) \tag{56}$$

$$c_{j+1}^n - 2\, c_j^n + c_{j-1}^n = \rho^n e^{i\xi} - 2\,\rho^n + \rho^n e^{-i\xi} = \rho^n \left(-2 + 2\cos\xi \right) \tag{57}$$

$$c_j^n - 2\, c_{j-1}^n + c_{j-2}^n = \rho^n - 2\,\rho^n e^{-i\xi} + \rho^n e^{-2i\xi} = e^{-i\xi} \rho^n \left(-2 + 2\cos\xi \right) \tag{58}$$

Using the Equations (54) to (58), the equation (53) can be written as:

$$\rho^{n+1} - \rho^n = \sigma \left[\rho^n \text{‰} (1+\rho)\, i \sin\xi - \rho^n \left(-2 + 2\cos\xi \right) \cdot \left(1 - \cos\xi + i \sin\xi \right) \right] \tag{59}$$

where σ is the Courant number ($u{\cdot}\Delta t/\Delta x$).

Short waves:

For the shortest resolvable wave (the Nyquist frequency) the wave length, L, is given as:

$$L = 2\pi \;\; => \;\; \xi = \pi, \quad \text{i.e.} \quad \sin\xi = 0 \qquad \cos\xi = -1 \tag{60}$$

Equation (59) now gives:

$$\rho^{n+1} = \beta\, \rho^n (1 - 8\,\sigma) \tag{61}$$

where ($1 - 8\sigma$) is the amplification factor E.

The stability criterion is:

$$\left| E \right| \leq 1 \tag{62}$$

The solution to Equation (62) is:

$$\beta = \frac{1}{4\sigma} \tag{63}$$

Long waves:

For the longest the wave length, L, is given as:

$$L = 2\pi \;\; => \;\; \xi \_ 0, \quad i.e. \quad \sin\xi = \xi \quad \cos\xi = 1 - \frac{\xi^2}{2} \tag{64}$$

Equation now gives:

$$\rho^{n+1} - \rho^n = \sigma\left[\rho^n \frac{1+\rho}{2} i\,\xi - \rho^n \left(-2 + 2(1 - \frac{\xi^2}{2})\right)\cdot\left(1 - (1 - \frac{\xi^2}{2}) + i\,\xi\right)\right] \tag{65}$$

The approximation to the upstream-interpolated concentration can now be given as:

If $\sigma < 1$ then:

$$C^*_{j+½} = \frac{1}{4}\left(C^{n+1}_{j+1} + C^{n+1}_j + C^n_{j+1} + C^n_j\right) - \frac{1}{6}\left(1 + \frac{\sigma^2}{2}\right)\cdot\left(C^n_{j+1} - 2\,C^n_j + C^n_{j-1}\right) \tag{66}$$

If $\sigma \geq 1$ then

$$C^*_{j+½} = \frac{1}{4}\left(C^{n+1}_{j+1} + C^{n+1}_j + C^n_{j+1} + C^n_j\right) \tag{67}$$

The phase and the amplitude portraits of the numerical scheme are shown in Figure 5 and Figure 6.

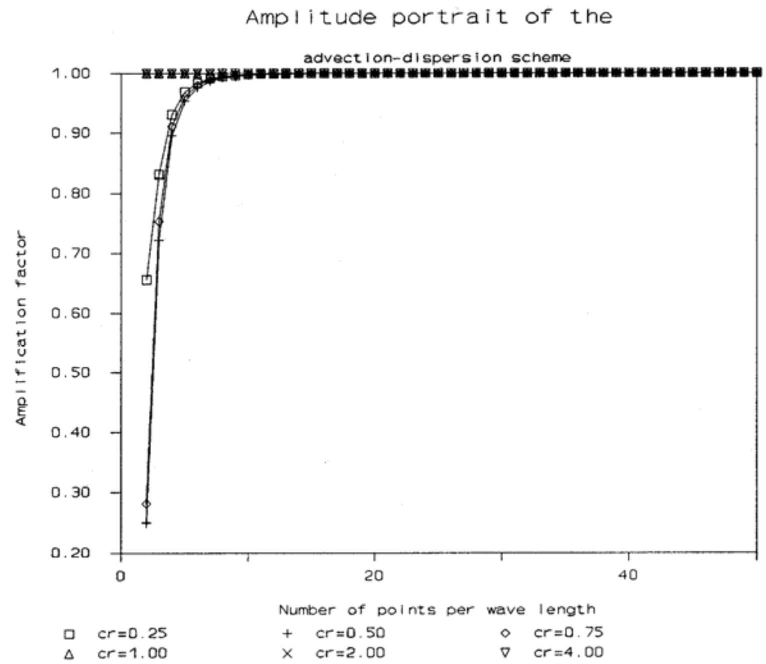

Figure 5 The amplitude portrait of the advection-dispersion schemes.

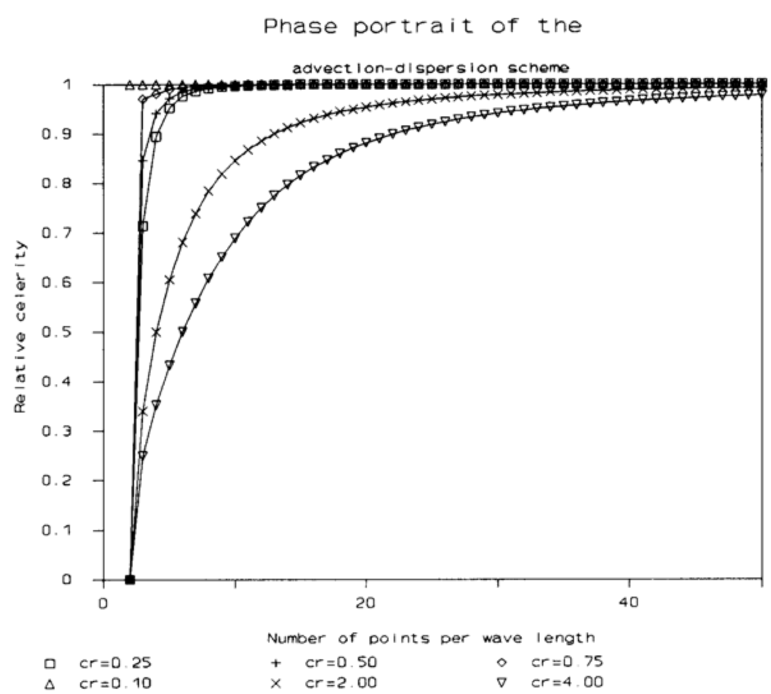

Figure 6 The phase portrait of the advection-dispersion scheme.

Even if the scheme is stable there are some restrictions on the selection of the time step, Δt, and the grid size, Δx. The stability criterion is expressed in terms of the convective Courant number, defined as:

$$\delta = \frac{|u| \cdot \Delta t}{\Delta x} \tag{68}$$

The stability criterion is:

$$C_c = \frac{|u| \cdot \Delta t}{\Delta x} < 1 \tag{69}$$

Another dimensionless number used to describe the numerical scheme is the Peclet number. This is defined as:

$$Pe = \frac{|u| \cdot \Delta x}{D} \tag{70}$$

The numerical scheme is stable even for large Peclet numbers, i.e. $Pe > 2$. However, the Peclet number is associated with numerical oscillations, wiggles, which grow or decay spatially with a wave length of $2\Delta x$. In a diffusion-free scheme which is stable in the von Neumann, wiggles are likely to occur when large gradients in the concentration are present. The criterion for the absence of wiggles is:

$$Pe \le 2 \tag{71}$$

The wiggles can be eliminated from the numerical scheme by an upstream centring of the numerical scheme, which introduces numerical diffusion into the scheme or by use of the *n-1* time step in the computations.

5 NOMENCLATURE

A	cross-sectional area (m^2),
a	constant in Equation (17),
b	constant in Equation (17),
c	concentration (arbitrary unit),
c_r	boundary concentrations,
c_N	concentration in the node,
c_q	concentration of lateral inflow source,
c_s	is the concentration at the boundary immediately before the flow direction changed,
c_s	source/sink concentration,
D	dispersion coefficient (m^2/s),
E	amplification factor,
j	grid point number,
K	linear decay coefficient (s^{-1}),
K_{mix}	a time scale ($hours^{-1}$),
K_N	decay constant for the node (s^{-1}),
kk	the number of connecting pipes,
k_x	dimensionless dispersion coefficient,
n	time level,
Pe	the Peclet number,
Q	discharge (m^3/s),
Q_{pipe}	discharge at the first grid point in the outlet pipe, (m^3/s),
q	discharge per unit width (m^2/s),
R	hydraulic radius (m),
T	transport through box walls,
t	time coordinate (s),
t_{mix}	is the time passed since the flow direction changed (s),
u	mean velocity (m/s),
u_f	friction velocity (m/s),
V	volume (m^3/s),
V_N	is the volume of the structure (m^3/s),
x	space coordinate (m),
α	constant in Equation (26),
β	constant in Equation (26),
γ	constant in Equation (26),
δ	convective Courant number.

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