3 MATHEMATICAL MODEL

The AQUASEA model consists of the following two models:

Hydrodynamic flow model

Transport-dispersion model

The flow model can simulate water level variations and flows in response to various forcing functions in lakes, estuaries, bays and coastal areas. The water levels and flows are approximated in a numerical finite element grid and calculated on the basis of information on the bathymetry, bed resistance coefficients, wind field and boundary conditions.

The transport-dispersion model simulates the spreading of a substance in the environment under the influence of the fluid flow and the existing dispersion processes. The substance may be a pollutant of any kind, conservative or non-conservative, inorganic or organic: salt, heat, suspended sediments, dissolved oxygen, inorganic phosphorus, nitrogen and other water quality parameters.

3.1 Flow models

In surface water flows, which can be considered shallow in the sense that the depth of flow is small compared with the horizontal lengths involved, a depth averaged flow model is a good approximation to real flow situations. In this case we only have two dimensional flow equations which are solved by AQUASEA.

3.1.1 The equation of continuity

The equation of continuity is given by:

$$\frac{\partial}{\partial x}(uH) + \frac{\partial}{\partial y}(vH) + \frac{\partial h}{\partial t} = Q$$

where

$$H = h + h$$

Explanation:

h	is mean water depth, m
η	is change in water level, m
H	is total water depth, m

u	is velocity component in x-direction, m/s
v	is velocity component in y-direction, m/s
t	is time, s
Q	is injected water, m^3/s.

As the continuity equation includes three unknown variables u,v, and h, we need two more equations to complete the solution of the problem. These are given by the momentum equations in two directions and are introduced in the following section.

3.1.2 The momentum equations

We assume hydrostatic pressure variations across all verticals. The momentum equations in the x and y directions are then given by:

$$\frac{\partial u}{\partial t} + u\frac{\partial u}{\partial x} + v\frac{\partial u}{\partial y} = -g\frac{\partial \eta}{\partial x} + fv - \frac{g}{HC^2}(u^2 + v^2)^{1/2}u + \frac{k}{H}W_x|W| - \frac{Q}{H}(u - u_o)$$

$$\frac{\partial v}{\partial t} + u\frac{\partial v}{\partial x} + v\frac{\partial v}{\partial y} = -g\frac{\partial \eta}{\partial y} - fu - \frac{g}{HC^2}(u^2 + v^2)^{1/2}v + \frac{k}{H}W_y|W| - \frac{Q}{H}(v - v_o)$$

The Coriolis parameter, f, is defined as:

$$f = 2\omega \sin \varphi$$

where φ is the latitude and ω is the Earth's rate of rotation equal to $7.2722\times10^{-5}\ s^{-1}$.

The wind shear stress parameter, k, is defined as:

$$k = \frac{\rho_a C_D}{\rho}$$

Explanation:

η	Change in water level, m
H	Total water depth, m
u	Velocity in x-direction, m/s
v	Velocity in y-direction, m/s
t	Time, s

g	Acceleration of gravity, m/s^2
ω	The Earth's rate of rotation, s^{-1}
φ	Latitude, deg
C	Chézy bottom friction coefficient, m$^{1/2}$/s
ρ_a	Density of air, kg/m^3
C_D	Wind drag coefficient
ρ	Fluid density, kg/m^3
W_x	Wind velocity in x-direction, m/s
W_y	Wind velocity in y-direction, m/s
$\|W\|$	Wind speed, m/s
u_o	Velocity of injected water in x-direction, m/s
v_o	Velocity of injected water in y-direction, m/s

The momentum equations together with the equation of continuity complete the specification of the shallow water flow problem. While these equations also form the basis of the finite element approximations the final integration procedure is such that it is more akin to integrating the momentum equations along with a wave equation rather than the continuity equation of section 4.4.

3.1.3 Boundary conditions

The following boundary conditions are allowed.

1) Specified time variation of water level.

2) No-flow boundary condition.

Specified flow at a boundary can be modeled by defining source nodes at the no flow boundary nodes.

In AQUASEA the time variation of the water level is specified by an external file or by the following sinusoidal variation: η=c+a sin w(t+α) where c,a,w,α are given constants.

3.2 Transport model

AQUASEA is designed to solve the equations of mass- and heat-transport. By proper selection of the parameters transport of faecal coliforms, suspended sediments and heat can be solved.

3.2.1 The transport equation

AQUASEA solves the equation for transport of mass or heat. The transport equation is given by:

$$\frac{\partial}{\partial x}(HD_x\frac{\partial c}{\partial x}) + \frac{\partial}{\partial y}(HD_y\frac{\partial c}{\partial y}) - \frac{\partial}{\partial x}(Hcu) = \frac{\partial}{\partial t}(Hc) + S - Qc_o$$

or alternatively, if we substitute in from the continuity equation:

$$\frac{\partial}{\partial x}(HD_x\frac{\partial c}{\partial x}) + \frac{\partial}{\partial y}(HD_y\frac{\partial c}{\partial y}) - Hu\frac{\partial c}{\partial x} = H\frac{\partial c}{\partial t} + S - Q(c_o - c)$$

AQUASEA solves the transport equations in this latter form. The above equations apply to a local coordinate system having the x-axis along the flow direction, so that v=0. In the finite element approximation such a local system can be introduced within each element at any given time.

Explanation:

c	is Concentration, excess suspended sediment or excess temperature.
u	is Velocity within each element taken from the solution of the flow problem, m/s
D_x	is Longitudinal dispersion coefficient, m^2/s
D_y	is Transversal dispersion coefficient, m^2/s
H	is Total water depth, m
S	is the mass flux term in kg/m^3
Q	is Injected water, m^3/s
c_o	is Concentration, excess sediment concentration/ temperature of the injected water.

3.2.2 Boundary conditions

The following two kinds of boundary conditions are allowed.

1) Specified concentration or temperature at the boundary.

2) Zero concentration or temperature gradient, indicating just convective transport of mass or heat through the boundary.

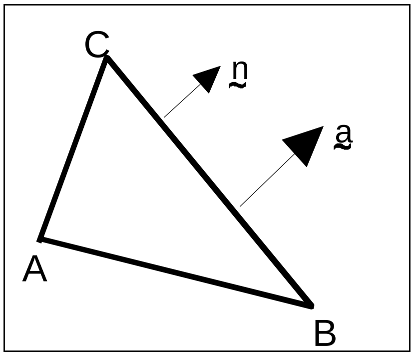
4. NUMERICAL MODEL

In AQUASEA all model equations are approximated using a Galerkin finite element method on triangular elements. Continuous approximations are used for water elevation (η and H) and concentration or temperature or suspended sediments (c), linear within elements, but piecewise constant approximations for the velocities (u and v). Such a choice has been shown to lead to a spatially stable approximation.

4.1 Finite element notation

The approximation is most readily described in terms of a general triangular element ABC (see figure below). We introduce the following notation:

Δ	the triangular element
$\partial\Delta$	the boundary of Δ
$\partial\Delta_a$	the boundary edge BC opposite A
$\|\Delta\|$	the area of Δ
$\mathbf{n}$	a general outward unit normal vector on $\partial\Delta$
$\mathbf{a}=(a_x,a_y)$	the outward normal vector on $\partial\Delta_a$, whose length is that of the edge, i.e. if (x_B, y_B) and (x_C,y_C) denote the coordinates of B and C respectively. $\mathbf{a} = (y_C-y_B, x_B-x_C)$ **b** and **c** are defined similarly
$\mathbf{k}$	Unit vector in the z-direction (vertically upwards)



We also define the following element matrices:

The element divergence matrix:

$$N = 1/2 \begin{vmatrix} a_x & a_y \\ b_x & b_y \\ c_x & c_y \end{vmatrix}$$

The element mass matrix:

$$M = \frac{|\Delta|}{12} \begin{vmatrix} 2 & 1 & 1 \\ 1 & 2 & 1 \\ 1 & 1 & 2 \end{vmatrix}$$

The lumped element mass matrix:

$$M_1 = \frac{|\Delta|}{3} \begin{vmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{vmatrix}$$

The element x-stiffness matrix:

$$K_x = \frac{1}{4|\Delta|} \begin{bmatrix} a_x^2 & a_x b_x & a_x c_x \\ a_x b_x & b_x^2 & b_x c_x \\ a_x c_x & b_x c_x & c_x^2 \end{bmatrix}$$

K_y is defined similarly

The element stiffness matrix:

$$K = K_x + K_y = \frac{1}{|\Delta|} N N^T$$

The element x-derivative matrix:

The approximation of the continuity equation in chapter 3.1.1 is based on the followir reformulation of that equation:

L_y is defined similarly.

We further retain the notation introduced in the previous chapters with following additions:

Approximate velocity within the element: $\mathbf{V} = (u,v)$

Approximate velocity within the adjacent element that **a** points into: $\mathbf{V}_a = (u_a,v_a)$

Velocity of injected water: $\mathbf{V}_o = (u_o,v_o)$

Approximate water level at nodes A,B and C: $\boldsymbol{\eta} = (\eta_A,\eta_B,\eta_C)$

Average water level within the element: $\eta_m = 1/3(\eta_A+\eta_B+\eta_C)$

$\mathbf{H}$, H_m, $\mathbf{h}$ and h_m are defined similarly

Approximate concentration or temperature at nodes A,B and C: $\mathbf{c} = (c_A,c_B,c_C)$

Wind stress vector: $\mathbf{S} = (S_x,S_y)$

Decay vector $s = (s_a,s_b,s_c)$

$$L_X = -\frac{1}{6}\begin{bmatrix} a_X & b_X & c_X \\ a_X & b_X & c_X \\ a_X & b_X & c_X \end{bmatrix}$$

4.2 Finite element continuity equation and calculation of flow

$$\int_{\partial\Delta} H\mathbf{V}\cdot\mathbf{n}\psi\, ds - \iint_{\Delta} H\mathbf{V}\cdot\nabla\psi\, dxdy + \iint_{\Delta}\frac{\partial\eta}{\partial t}\psi\, dxdy = \iint_{\Delta} Q\psi\, dxdy$$

for appropriate test (weight) functions ψ. In AQUASEA the test functions are ψ_i, i = A,B,C, where ψ_i is a linear function taking the value 1 at node i and the value 0 on the opposite edge. The resulting finite element approximation becomes:

$$\mathbf{q} + H_m N\mathbf{V} + M\frac{d}{dt}\eta = \mathbf{Q}$$

where all vectors in the formula are to be viewed as column vectors and:

$$Q = (Q_A, Q_B, Q_C) \qquad Q_i = \iint_{\Delta} Q y_i \, dxdy$$

$$q = (q_A, q_B, q_C) \qquad q_i = \int_{\partial\Delta} q y_i \, ds \quad i = A, B, C$$

Here Q is injected water whereas q denotes the boundary normal outflow H**V** · **n**. However, only q-values at an outer boundary where we have a no-flow boundary condition (cf. section 3.1.4) will enter into the global assembled system and are there set to zero. On inner boundaries between elements the q-values cancel out, thus indirectly ensuring that continuity of flow is preserved in spite of the jumps in the constant velocity approximations between elements. In AQUASEA the continuity equation above is not integrated directly but it forms the basis of the approximate wave equation as shown in section 4.4. Further when flow across outer boundaries with specified water level or across inner boundaries is calculated in AQUASEA these calculations are based on the dependence of **q** on **V**,η and **Q** as given by the finite element continuity equation which in turn ensures continuity of mass. For the sake of simplicity M is, however, replaced by its lumped counterpart, M_l.

4.3 Finite element momentum equations

In order to simplify the presentation we assume below that at the given time $\partial\Delta_a$ is the only upstream edge in the sense that $(\mathbf{V}+\mathbf{V}_a) \cdot \mathbf{a} < 0$. When there is another upstream edge the contribution from it will be analogous to that described for $\partial\Delta_a$.

The approximations of the momentum equations in chapter 3.1.2 are based on the following weak reformulation of those equations:

$$\iint_{\Delta} \left[\frac{\partial u}{\partial t} + u\frac{\partial u}{\partial x} + v\frac{\partial u}{\partial y}\right]\psi dxdy + \int_{\partial\Delta_a} \left[\frac{1}{2}(\mathbf{V} + \mathbf{V}_a) \cdot \mathbf{a}\right](u_a - u)\psi ds$$
$$= \iint_{\Delta} \left[-g\frac{\partial \eta}{\partial x} - \beta u + fv + \frac{1}{H}S_x - \frac{Q}{H}(u - u_o)\right]\psi dxdy$$

$$\iint_{\Delta} \left[\frac{\partial v}{\partial t} + u\frac{\partial v}{\partial x} + v\frac{\partial v}{\partial y}\right]\psi dxdy + \int_{\partial\Delta_a} \left[\frac{1}{2}(\mathbf{V} + \mathbf{V}_a) \cdot \mathbf{a}\right](v_a - v)\psi ds$$
$$= \iint_{\Delta} \left[-g\frac{\partial \eta}{\partial y} - \beta v - fu + \frac{1}{H}S_y - \frac{Q}{H}(v - v_o)\right]\psi dxdy$$

for appropriate test (weight) functions ψ. In AQUASEA the test functions are constant functions over the element. The resulting finite element approximation becomes in vector notation:

$$|\Delta|\frac{d}{dt}\mathbf{V}+[\frac{1}{2}(\mathbf{V}+\mathbf{V}_a)\cdot\mathbf{a}](\mathbf{V}_a-\mathbf{V})=gN^T\boldsymbol{ç}-|\Delta|[\beta\mathbf{V}+f\,kx\mathbf{V}-\frac{1}{H}S+\frac{Q}{H}(\mathbf{V}-\mathbf{V}_o)]$$

When $\partial\Delta_a$ is part of the outer boundary $\mathbf{V}_a$-$\mathbf{V}$ replaced by **O.** Possible inflow at such a boundary is entered in AQUASEA through $\mathbf{V}_o$ which effectively amounts to setting $\mathbf{V}_a=\mathbf{V}_o$ and $Q=-(\mathbf{V}_o\cdot\mathbf{a})H/|\Delta|$. The use of upstream approximations for the velocity derivatives is consistent with the specification of velocity on outer inflow boundaries, has a stabilizing effect on the spatial approximation, and makes it possible to integrate the momentum equations locally, even if we use an implicit method, as described in section 4.4.

4.4 Time integration and the approximate wave equation

In AQUASEA the global counterpart of the continuity and momentum equations are integrated in time by a first order backward difference fully implicit method. This amounts to approximating the time derivatives.

$$\frac{d}{dt}\boldsymbol{\eta} \quad \text{and} \quad \frac{d}{dt}\mathbf{V}$$

by

$$\frac{1}{\Delta t}(\boldsymbol{\eta}-\boldsymbol{\eta}^P) \quad \text{and} \quad \frac{1}{\Delta t}(\mathbf{V}-\mathbf{V}^P)$$

where $\boldsymbol{\eta}^P$ and $\mathbf{V}^P$ denote approximations to $\boldsymbol{\eta}$ and $\mathbf{V}$ resp. at the previous time step t-Δt. However, rather then advancing the mass equation as it stands, we eliminate $\mathbf{V}$ from the momentum equation and substitute it into the continuity equation obtaining the equation:

$$\left[\frac{1}{\Delta t}M+\Delta tgH_m(gK+dG)\right]h$$

$$=\Delta tNF\left[\frac{H_m}{|\Delta|}(\frac{1}{2}(\mathbf{V}-\mathbf{V}_a)\cdot\mathbf{a})(\mathbf{V}-\mathbf{V}_a)-\mathbf{S}+Q(\mathbf{V}-\mathbf{V}_o)-\frac{H_m}{\Delta t}\mathbf{V}^P\right]+(\mathbf{Q}-\mathbf{q})+\frac{1}{\Delta t}M\eta^P$$

where

$$F=\begin{bmatrix}\gamma & \delta\\ -\delta & \gamma\end{bmatrix}=\left[I+\Delta t\begin{bmatrix}\beta & -f\\ f & \beta\end{bmatrix}\right]^{-1}$$

and

$$\begin{bmatrix} 0 & 1 & -1 \end{bmatrix}$$

While this is a one-step procedure it is analogous to the integration of the solaced second order wave equation. It does, however, entail a further decoupling between elevation and velocity and the fact that, unlike the wave equation, it does not involve the continuity equation in differentiated form is of consequence in retaining mass conservation over long time intervals. Finally all boundary conditions may be unincorporated in a natural way within the framework of the primary continuity and momentum equations.

The solution to the global counterpart of the equation above is obtained by iteration where we retain on left-hand side the global counterpart of the matrix

$$\left[\frac{1}{\Delta t}M + \Delta t \cdot gh_m K\right]$$

a symmetric positive definite matrix which remains constant while the timestep, Δt, is constant, and thus only has to be refactored when the timestep is changed. The linear system is solved by a band Choleski factorization, the bandwidth of the matrix having been minimized by ordering the nodes using the Gibbs-Stockmeyer-Poole algorithm. For simplicity M is replaced by M_l in AQUASEA. In general convergence is obtained within five iterations, but when this fails the time-step is halved, since it can be shown that $\gamma K+\delta G-K$ is 0 (Δt).

AQUASEA then advances **V** by integrating the finite element momentum equation using again a fully implicit method. This integration can, however, be carried out locally within elements, due to the upstream approximations of the velocity derivatives, by proceeding through the elements in downstream fashion. In AQUASEA the elements are ordered in such a way at the beginning of each timestep if that is possible. In cases when such an ordering does not exist due to circulation in the flow AQUASEA proceeds iteratively, starting the calculations again at the element where the downstream ordering first broke down.

In the solution of each local system a quadratic equation in u and v has to be solved in the presence of convective terms. These equations are solved fully by a Newton type iterative method. Convergence problems may arise if the timestep, Δt, has been chosen too large. When this happens AQUASEA halves the timestep automatically.

Finally AQUASEA repeats the two integrations before proceeding to the next timestep, using updated velocity approximations when advancing η and updated elevation approximations and values for β when advancing u and v.

In the absence of convective terms the local time integrations of the momentum equation can be carried out in any order, so that element ordering is not required. Furthermore only a linear system in u and v has to be solved for each element. This reduces the total solution time considerably.

4.5 Finite element transport equation

The approximation of the transport equation (chapter 3.2.1) is based on the following weak reformulation of that equation:

$$\int_{\partial\Delta} H(D_x \frac{\partial c}{\partial x}, D_y \frac{\partial c}{\partial y}) \cdot \mathbf{n}\psi ds - \iint_{\Delta} H(D_x \frac{\partial c}{\partial x}\frac{\partial \psi}{\partial x} + D_y \frac{\partial c}{\partial y}\frac{\partial \psi}{\partial y})dxdy - \iint_{\Delta} Hu\frac{\partial c}{\partial x}\psi dxdy$$

$$= \iint_{\Delta} [H\frac{\partial c}{\partial t} + s - Q(c_o - c)]\psi dxdy$$

for appropriate test (weight)functions ψ. In AQUASEA the test functions are the same as for the continuity equation (see section 4.2) resulting in the finite element approximation:

$$-\mathbf{P}^d - H_m(D_x K_x + D_y K_y)c - H_m u L_x c = H_m M\frac{d}{dt}c + M\mathbf{s} - QM(c_o - c)$$

where as before all vectors are to be viewed as column vectors and

$$\mathbf{P}^d = (p^d{}_A, p^d{}_B, p^d{}_C) \quad p^d{}_i = \int_{\partial\Delta} p^d \psi_i ds, \quad i = A, B, C$$

and p^d denotes the boundary normal mass outflow

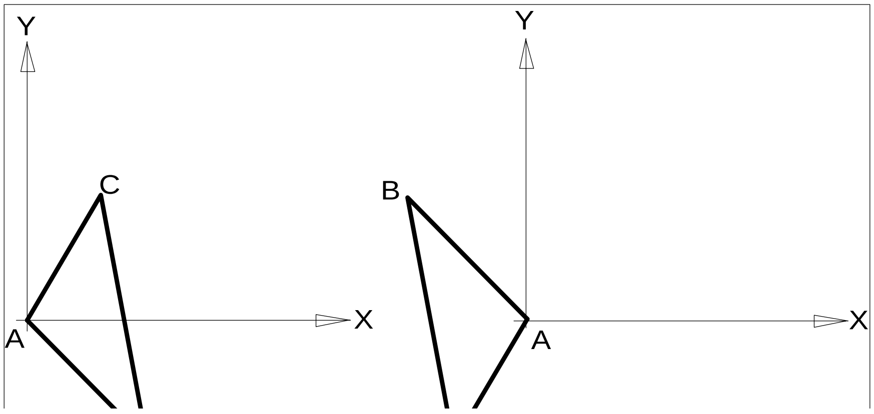
$$-H(D_x \frac{\partial c}{\partial x}, D_y \frac{\partial c}{\partial y}) \cdot \mathbf{n}$$

due to dispersion. These p^d values do in fact not enter into the global system since they cancel out on inner boundaries and are set to zero on no-flow outer boundaries. For the sake of simplicity M is again replaced by M_l.

4.6 Upstream modifications

Optionally, in AQUASEA the spatial approximation can be stabilized by modifying the test functions within the element as:

$$y_i + m\frac{2}{3}\frac{|\Delta|}{|a_x|}\frac{\partial y}{\partial x} \ , \ 0 \leq m \leq 1 \ , \ i = A, B, C$$



where the coordinates within the element have been chosen so that the velocity **V** = (u,0) is in the positive x-direction and Δ is supposed to have one of the two configurations shown in figure 4.2 and μ is a free parameter. Such a modification will in general damp out spurious oscillations that may arise in the case of large Peclet numbers (typically 5). For the configurations in figure above the Peclet number may be defined as (cf. section 4.9):

$$Pe = 2\frac{|\Delta|}{|a_x|}\frac{u}{D_x}$$

The modification amounts to a so called Streamline Upstream Petrov Galerkin method or Localized Adjoint Method, the modified test functions in the extreme case when μ = 1 being local solutions to the "adjoint" equation, in the limit as u/D→ ∞:

$$\frac{\partial}{\partial x}(D\frac{\partial c}{\partial x})+\frac{\partial}{\partial y}(D\frac{\partial c}{\partial y})+u\frac{\partial c}{\partial x}=0$$

The resulting modification to the finite element transport equation is that:

$$L_x \; is \; replaced \;\; by \; L_x + m\frac{2}{3}\frac{|\Delta|}{|a_x|}K_x$$

$$M_l \; is \; replaced \;\; by \; M_l - m\frac{|\Delta|}{3|a_x|}\begin{vmatrix} a_x & 0 & 0 \\ 0 & b_x & 0 \\ 0 & 0 & c_x \end{vmatrix}$$

The first modification amounts to adding the dispersive term

$$m\frac{2}{3}\frac{|\Delta|}{|a_x|}Hu\frac{\partial^2 c}{\partial x^2}$$

to the transport equation ie. replacing D_x by D_x (1+ μ/3 Pe) where Pe is the Peclet number defined above. The modifications of the remaining terms ensure, however, that the resulting approximations remains consistent with the original transport equation. In AQUASEA the value of μ is chosen by the user and only one global value can be chosen.

4.7 Time integration of transport equation

In AQUASEA the global counterpart of equation 4.4 is integrated using a fully implicit method based on a first order backward difference approximation to the time derivative. The resulting linear system involves a matrix which is the global counterpart of:

$$(\frac{Hm}{\Delta t} + Q)M_l + H_m(D_x K_x + D_y K_y + uL_x)$$

Due to the presence of L_x the matrix will not be symmetric so that this linear system is solved by LU-factorization using the same ordering of nodes as in the solution of the wave equation. In this case we may get numerical instability unless pivoting is introduced. Resulting row exchanges in the global matrix will on the other hand increase the bandwidth of the matrix and thus add to the solution time and memory requirements. In AQUASEA the approach is taken not to introduce row-exchanges but to print a warning if the size of a multiplier during the factorization exceeds 10. This may happen in the case of large Peclet numbers when no modification of the test function is introduced, but such a modification will in general remedy the situation.

In AQUASEA the matrix is updated and factored again at each timepoint that corresponds to a specified velocity output.

4.8 Calculation of mass or heat flow

The approximation of the transport equation is based on the following weak reformulation before the equation of continuity is inserted into the transport equation (refer chapter 3.2.1).

$$\int_{\partial\Delta} H(D_x \frac{\partial c}{\partial x} - uc, D_y \frac{\partial c}{\partial y}) \cdot n\psi ds - \iint_{\Delta} H(D_x \frac{\partial c}{\partial x}\frac{\partial \psi}{\partial x} + D_y \frac{\partial c}{\partial y}\frac{\partial \psi}{\partial y})dxdy$$

$$+ \iint_{\Delta} Huc\frac{\partial \psi}{\partial x}dxdy = \iint_{\Delta} [\frac{\partial}{\partial t}(Hc) + s - Q\,c_o)]\psi dxdy$$

using the same test functions as before, results in the finite element approximation:

$$- P^t - H_m(D_x K_x + D_y K_y)c + H_m u\, L_x{}^T c = M\frac{d}{dt}(Hc) + M\mathbf{s} - QM\,c_o$$

Here $\mathbf{p}^t$ corresponds to $\mathbf{p}^d$ in equation 4.4 except that $\mathbf{p}^t$ now denotes the total boundary normal mass or heat outflow

$$- H(\, D_x \frac{\partial c}{\partial x} - uc,\; D_y \frac{\partial c}{\partial y}) \cdot \mathbf{n}$$

due to dispersion and advection. When mass or heat outflow across outer or inner boundaries are calculated in AQUASEA these calculations are based on the dependence on $\mathbf{p}^t$ of $\mathbf{c}$ as given in equation 4.5 which in turn ensures continuity of mass or heat . As before M is replaced by M_l.

4.9 Grid size and time step requirements

It is well known that the advective-dispersive transport equation is more difficult to solve numerically. The problems are particularly severe when advection dominates over dispersion. In this situation, the Galerkin finite element solution usually exhibits numerical spatial oscillations - overshoot and undershoot - near the concentration (temperature) front. Overshoot describes the erroneously high values of concentration encountered upstream of the moving front. The analogous behavior on the downstream side is called undershoot. These numerical oscillations tend to be more severe as advection becomes more dominant. General experience indicates that in a case where the dispersion coefficient, D, is greater than zero, numerical oscillations in the Galerkin finite element solution using linear basis functions can be virtually eliminated if the element size is selected so that its local Peclet number does not exceed 2. The Peclet number is defined as:

$$Pe = \frac{V\Delta l}{D}$$

where $\Delta 1$ is a characteristic length of the finite element grid and D is the dispersion coefficient. In most cases involving nonuniform flow, acceptable numerical solutions with very mild oscillations are achieved even when the local Peclet number is as high as 10. A simple guideline for selecting the finite element mesh and time step size can be given:

$$\text{The Peclet number} < 10$$

$$\text{The Courant number} = \frac{\mathrm{V}\Delta \mathrm{t}}{\Delta \mathrm{l}} < 1$$

The characteristic grid size is then given by:

$$\Delta \mathrm{l} \leq \frac{10\mathrm{D}}{\mathrm{V}}$$

The characteristic time step size is given by:

$$\Delta \mathrm{t} \leq \frac{\Delta \mathrm{l}}{\mathrm{V}}$$

It should be born in mind that in most cases it is acceptable to keep the grid size small locally around contamination or heat sources where the numerical results are of importance, but ignoring the numerical oscillations in the far field, and instead being able to have large grid sizes far away from the sources.

It should also be noted that for low Peclet numbers (<2) a better solution may be obtained without the upstream correction mentioned in section 4.6.

For flow calculations we recommend that the Courant number based on the flow velocities should not exceed one.