NUMERICAL MODELLING OF ADVECTION–DISPERSION EQUATION IN A STRETCHED CURVILINEAR GRID USING THE QUICKEST SCHEME

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SUMMARY

A stretched version of the QUICKEST scheme for solutions of the advection–dispersion equation is presented. The scheme is accurate for large degrees of stretching, so that it can be used where large gradients are present, e.g. for the calculation of sediment in suspension close to the bed. The scheme is tested for various cases of sediment advection and dispersion in one and two dimensions. © 1998 John Wiley & Sons, Ltd.

KEY WORDS: QUICKEST; curvilinear grid; advection–dispersion; stretched grid; suspended sediment

1. INTRODUCTION

In many hydrodynamic problems, the flow close to solid boundaries has a large influence on the entire flow field. Close to the solid boundaries, large gradients in the physical parameters, such as the velocities and the turbulent intensities, are present, making the numerical modeling a challenging task in these areas.

In this work, the advection–dispersion (AD) modelling close to a solid boundary is studied. An important engineering application for such modelling is within the sediment transport field, where an accurate prediction of suspended sediment near the bed is of major importance for predicting the sediment transport and scour development. For such problems, the vertical length scale close to the bed is determined by the sediment grain size, and will typically be in the order of 0.1–1 mm. A numerical model aiming to resolve the near-bed processes and still cover the whole fluid domain will, as a natural choice, have a stretched grid [1].

For flow cases where turbulent dispersion of the sediment is the major transport mechanism, the requirements to the AD scheme are not crucial for the results. For flow cases where advection dominates the transport, the requirements to the scheme increase. The main problems with low-order finite difference advection schemes are numerical dispersion and volume falsification. An alternative to finite difference schemes could be Lagrangean models [2]. Another alternative is higher-order finite difference schemes, where such problems are minimized. The QUICKEST scheme introduced in [3], is an explicit higher-order scheme for unsteady flow, where the above mentioned problems are avoided. The scheme was extended to

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two and three dimensions in References [4,5], and the results of test cases presented in these papers are very convincing for the properties of this model. In addition, the model is very easily implemented because of the explicit control volume formulation.

When using a higher-order scheme on a stretched grid, one must be very careful not to loose the high-order accuracy due to the grid derivatives. If, however, this is done carefully, very high degrees of stretching are possible without loosing any accuracy, as will be shown in this paper. The scheme is tested on three one-dimensional and two two-dimensional cases; testing pure advection of fronts and diffusion of an initially sharp front.

2. ADVECTION–DISPERSION EQUATION

The examples presented in this paper all deal with sediment in suspension. The outlined expressions can, however, be used for other AD cases (e.g. the vorticity transport equation and the heat exchange equation), where a detailed discretization is required close to the boundaries.

Following Reference [1], the suspended sediment can be described with a usual AD equation, modified in the vertical direction by the settling velocity of the sediment. In two dimensions, the equation reads as

$$
\frac{\partial c}{\partial t} = -u \frac{\partial c}{\partial x} - (w - w_s) \frac{\partial c}{\partial z} + \frac{\partial}{\partial x} \left(\epsilon_s \frac{\partial c}{\partial x} \right) - \frac{\partial}{\partial z} \left(\epsilon_s \frac{\partial c}{\partial z} \right),\tag{1}
$$

where c is the concentration of suspended sediment; u and w are the horizontal and vertical water velocities, respectively; w_s is the fall velocity of the sediment; ϵ_s is the turbulent diffusion coefficient; z is the vertical co-ordinate and x is the horizontal co-ordinate.

By applying the continuity equation for the fluid, Equation (1) can be written in terms of transports as

$$
\frac{\partial c}{\partial t} = -\frac{\partial}{\partial x} \left(uc - \epsilon_s \frac{\partial c}{\partial x} \right) - \frac{\partial}{\partial z} \left((w - w_s)c - \epsilon_s \frac{\partial c}{\partial z} \right).
$$
\n(2)

The boundary condition at the bed may be either the vertical transport of sediment at the bed or the bed concentration, c_b , see Reference [1].

At the water surface, the vertical transport of sediment is zero. At the vertical boundaries, the boundary conditions may either be a specification of transports, concentrations or periodic conditions. In the case of an impermeable wall, the relevant boundary condition at the wall is zero transport.

The numerical solution of Equations (1) or (2) can be time consuming because it has to be solved in two spatial dimensions and time, and because the gradients of the concentrations, velocities and diffusion coefficients are large inside the bottom boundary layer. Therefore, the choice of solution method is crucial for achieving acceptable solutions within a reasonable calculation time.

Here, QUICKEST formulated in a stretched grid has been chosen. The next section will be a presentation of QUICKEST in two dimensions in a regular grid. In the following sections, this model will be extended to a stretched curvilinear grid.

2.1. *Regular grid*

In the 2D version of QUICKEST, the AD equation is discretized in a staggered grid and stepped forward in time using operator splitting as follows:

$$
c_{j,k}^{n+1/2} = c_{j,k}^{n} - (T_{x,j,k}^{n} - T_{x,j-1,k}^{n}),
$$

\n
$$
c_{j,k}^{n+1} = c_{j,k}^{n+1/2} - (T_{z,j,k}^{n+1/2} - T_{z,j,k-1}^{n+1/2}),
$$
\n(3)

where *n* indicates the time step, and j and k indicate the horizontal and vertical grid point, respectively. T_x and T_z are, respectively, the horizontal and vertical transports of sediment given as

$$
T_x = \left(uc - \epsilon_s \frac{\partial c}{\partial x} \right) \frac{\Delta t}{\Delta x},\tag{5}
$$

and

 $T_{x,j,k}$ and $T_{z,j,k}$ are the third-order interpolations of these transports through the control surfaces

$$
T_z = \left(\left(w - w_s \right) c - \epsilon_s \frac{\partial c}{\partial z} \right) \frac{\Delta t}{\Delta z} \tag{6}
$$

shown in Figure 1(a). These transports are outlined in Appendix B.

In order to achieve a second-order-accurate scheme with the operator splitting technique, the velocity field has to be modified [6]. However, no corrections are necessary for the examples presented below.

The scheme is stable for $\sigma_x + \sigma_z \leq 1/2$ and $\alpha < 1/2$, where σ_x and σ_z are the Courant numbers in the horizontal and vertical direction, respectively, while α is the non-dimensional diffusion coefficient [4].

2.2. *Stretched grid*

Introducing a stretching function, $r(z)$, Equation (2) yields

$$
\frac{\partial c}{\partial t} + \frac{\partial c}{\partial x} \left(uc - \epsilon_s \frac{\partial c}{\partial x} \right) - \frac{\partial}{\partial r} \left[(w - w_s)c - \epsilon_s \frac{\partial c}{\partial r} r' \right] r',\tag{7}
$$

where *r'* is the derivative of $r(z)$. After division with *r'* this equation can be written as

$$
\frac{\partial}{\partial t} \left(c \frac{dz}{dr} \right) + \frac{\partial}{\partial x} \left[u \left(c \frac{dz}{dr} \right) - \epsilon_s \frac{\partial}{\partial x} \left(c \frac{dz}{dr} \right) \right]
$$
\n
$$
= -\frac{\partial}{\partial r} \left[(w - w_s) r' \left(c \frac{dz}{dr} \right) - \epsilon_s r'^2 \left(\frac{\partial}{\partial r} \left(c \frac{dz}{dr} \right) - c \frac{d^2 z}{dr^2} \right) \right],
$$
\n(8)

i.e.

$$
\frac{\partial C}{\partial t} + \frac{\partial}{\partial x} \left(uC - \epsilon_s \frac{\partial C}{\partial x} \right) = -\frac{\partial}{\partial r} \left[\left((w - w_s)r' + r'^3 \frac{d^2 z}{dr^2} \epsilon_s \right) C - \epsilon_s r'^2 \frac{dC}{dr} \right]
$$

$$
= -\frac{\partial}{\partial r} \left(W C - E_s \frac{dC}{dr} \right), \tag{9}
$$

where

$$
C = c \cdot \frac{\mathrm{d}z}{\mathrm{d}r};\tag{10}
$$

$$
W = (w - w_s) \cdot \frac{dr}{dz} + \epsilon_s \cdot \left(\frac{dr}{dz}\right)^3 \cdot \frac{d^2z}{dr^2};
$$
\n(11)

$$
E_{\rm s} = \epsilon_{\rm s} \cdot \left(\frac{\mathrm{d}r}{\mathrm{d}z}\right)^2. \tag{12}
$$

An example of the stretched grid is shown in Figure 1(b). *C* is a measure for the sand volume rather than the concentration. The second term in W is a diffusion correction because

Figure 1. Grid used in the 'original' QUICKEST scheme (a), grid used in the stretched version of the QUICKEST scheme (b), and grid used in the stretched curvilinear version of the QUICKEST scheme (c).

the diffusion is due to concentration gradients rather than volume gradients. If care is taken to discretize these terms correctly, the scheme will maintain its accuracy after stretching. This is not the case with the variable grid method presented in Appendix of Leonard (1979), where the diffusion correction is not included. Equation (9) can be solved with respect to $C(x, r, t)$ using the original QUICKEST scheme, with the modified vertical velocity, *W*, and with the modified diffusion coefficient, E_s .

The stability of this scheme is determined by using the vertical Courant number, $\sigma_z = W \Delta t / T$ Δr , and the vertical non-dimensional diffusion coefficient, $\alpha_z = E_s \cdot \Delta t / \Delta r^2$, but since $W \approx w \cdot dr /$ dz and $E_s = \epsilon_s (dr/dz)^2$, it is still the smallest grid size Δz_{min} that determines the stability of the scheme.

2.3. *Varying bed*

In case of a varying bed, the AD equation is written in an orthogonal curvilinear co-ordinate system (α, β) , see Figure 1(c). In this system, the stretch function is introduced in the β -direction.

By further restricting the orthogonal curvilinear co-ordinate system to be a conformal mapping, one can introduce the Jacobian:

Figure 2. Examples of stretched co-ordinate systems with $d_{50} = 0.5$ mm, $h = 10$ m, and: (a) $s = 0.1$, $nk = 20$; (b) $s = 0.5$, $nk = 20$; (c) $s = 0.1$, $nk = 30$.

The AD equation is first written in terms of (α, β) co-ordinates:

$$
\frac{1}{J^2}\frac{\partial c}{\partial t} = -\frac{\partial}{\partial \alpha} \left[\frac{1}{J} \left(\left(u_x - w_s \frac{1}{J} \frac{\partial \alpha}{\partial z} \right) c - \epsilon_s \frac{\partial c}{\partial \alpha} J \right) \right] - \frac{\partial}{\partial \beta} \left[\frac{1}{J} \left(\left(u_\beta - w_s \frac{1}{J} \frac{\partial \beta}{\partial z} \right) c - \epsilon_s \frac{\partial c}{\partial \beta} J \right) \right],
$$
\n(14)

where u_{α} and u_{β} are the velocity components in the α - and the β -directions, respectively. This can be written as

$$
\frac{\partial}{\partial t} \left(\frac{c}{J^2} \right) = -\frac{\partial}{\partial \alpha} \left[\left(u_\alpha J - w_s \frac{\partial \alpha}{\partial z} \right) \left(\frac{c}{J^2} \right) - \epsilon_s \left(J^2 \frac{\partial}{\partial \alpha} \left(\frac{c}{J^2} \right) + \frac{\partial J^2}{\partial \alpha} \left(\frac{c}{J^2} \right) \right) \right] \n- \frac{\partial}{\partial \beta} \left[\left(u_\beta J - w_s \frac{\partial \beta}{\partial z} \right) \left(\frac{c}{J^2} \right) - \epsilon_s \left(J^2 \frac{\partial}{\partial \beta} \left(\frac{c}{J^2} \right) + \frac{\partial J^2}{\partial \beta} \left(\frac{c}{J^2} \right) \right) \right] \n= -\frac{\partial}{\partial \alpha} \left[\left(u_\alpha J - w_s \frac{\partial \alpha}{\partial z} - \epsilon_s \frac{\partial J^2}{\partial z} \right) \left(\frac{c}{J^2} \right) - \epsilon_s J^2 \frac{\partial}{\partial \alpha} \left(\frac{c}{J^2} \right) \right] \n- \frac{\partial}{\partial \beta} \left[\left(u_\beta J - w_s \frac{\partial \beta}{\partial z} - \epsilon_s J^2 \frac{\partial J^2}{\partial \beta} \right) \left(\frac{c}{J^2} \right) - \epsilon_s J^2 \frac{\partial}{\partial \beta} \left(\frac{c}{J^2} \right) \right].
$$
\n(15)

Stretching is introduced in the β -direction by introducing the function of β , $r(\beta)$, giving the equation

$$
\frac{\partial C'}{\partial t} = -\frac{\partial}{\partial \alpha} \left(U'C' - \epsilon'_s \frac{\partial C'}{\partial \alpha} \right) - \frac{\partial}{\partial r} \left[W'C' - E'_s \frac{\partial C'}{\partial r} \right],\tag{16}
$$

where

$$
C' = c \cdot J^{-2} \frac{\mathrm{d}\beta}{\mathrm{d}r};\tag{17}
$$

$$
U' = \left(u_{\alpha} J - w_{\alpha} \frac{\partial \alpha}{\partial z} - \epsilon_{\alpha} \frac{\partial J^2}{\partial \alpha}\right);
$$
\n(18)

$$
W' = \left(\left(u_{\beta} J - w_{s} \frac{\partial \alpha}{\partial z} - \epsilon_{s} \frac{\partial J^{2}}{\partial \beta} \right) \frac{dr}{d\beta} + \epsilon_{s} J^{2} \left(\frac{dr}{d\beta} \right)^{3} \frac{d^{2} \beta}{dr^{2}} \right);
$$
\n(19)

$$
\epsilon'_{s} = \epsilon_{s} J^{2};\tag{20}
$$

$$
E'_{s} = \epsilon_{s} J^{2} \left(\frac{\mathrm{d}r}{\mathrm{d}\beta}\right)^{2}.
$$
 (21)

Also, Equation (16) is an equation that can be solved with the original QUICKEST scheme.

3. ANALYTICAL STRETCHING

In order to avoid uncertainties in the determination of the first- and second-derivatives of the stretching function, analytical stretching functions are recommended. In the following examples, the stretching function has the form

$$
z(r) = -h + 2d_{50}(s * r + 1)^R,
$$
\n(22)

where $r = 0$ at the bottom, $z = -h + 2d_{50}$ corresponding to a reference concentration two grain diameters above the bed, $r = nr$ at the surface $z(nr) = 0$. The two parameters *s* and *R* are stretching parameters, where *R* is linked to *s* by

Figure 3. Grid with $d_{50} = 0.5$ mm, $h = 10$ m, $nk = 100$, and $s = 0.1$; (a) entire system, (b) close up near-bed grid lines.

Figure 4. Concentration profile as function of time for pure diffusion. Each 500 s is shown. Grain diameter $d_{50}=0.5$ mm, water depth $h=10$ m, friction velocity $u_f=0.05$ m s⁻¹. The co-ordinate system is shown in Figure 3. The time step is equal to 0.01 s.

$$
R = \frac{\log\left(\frac{h}{2d_{50}}\right)}{\log(s \cdot nr + 1)}.
$$
\n(23)

Examples of grids with $s = 0.1$ and $s = 0.5$ for $d_{50} = 0.5$ mm and $h = 10$ m are presented in Figure 2. The first- and second-derivatives are found from Equation (22),

$$
\frac{dz(r)}{dr} = 2d_{50}sR(s*r + 1)^{R-1},
$$
\n(24)

$$
\frac{d^2z(r)}{dr^2} = 2d_{50}s^2R(R-1)(s*r+1)^{R-2}.
$$
\n(25)

Using a staggered grid, the derivatives have to be determined in the grid points as well as in between the grid points. The concentration (C) , Equations (10) or (17), uses the derivatives at the grid points, while the fluxes (T_z) , the vertical velocities (W) , Equations (11) or (19), and vertical diffusion (E_s) , Equations (12) or (21), use the derivatives between the grid points.

4. ONE-DIMENSIONAL TEST EXAMPLES

Three one-dimensional tests have been set up: (1) pure dispersion, (2) pure advection, and (3) combined dispersion–advection.

4.1. *Pure dispersion*

At time equal 0, the bed concentration is increased from zero to 1 in a 10-m deep channel. A parabolic diffusion coefficient (eddy viscosity), corresponding to a fully developed logarithmic velocity profile, is assumed in the channel:

$$
\epsilon(z) = \kappa u_f(z+h) \frac{(-z)}{h},\tag{26}
$$

where $\kappa = 0.4$ is von Karman's number, the friction factor is taken to be $u_f = 0.05$ m s⁻¹, the simulation is carried out with $nk = 100$ grid points in the vertical direction. A stretching parameter, $s = 0.1$, is used; the grid is shown in Figure 3. The sand diameter is $d_{50} = 0.5$ mm.

The simulation was performed with a time step of 0.01 s, corresponding to a maximum non-dimensional diffusion coefficient $\alpha=0.65$ and a Courant number due to the diffusion correction, $\sigma = 0.35$. At the upper boundary, the flux is zero. The results of the simulation are presented in Figure 4, the concentration profile is shown for every 500 s.

4.2. Pure advection

In the next test, the scheme's ability to maintain a sharp front is tested. At time equal 0, the concentration at the bed is increased from zero to 1 in the same grid as used in the previous example. A constant vertical velocity $w = 0.01$ m s^{−1} is imposed and no diffusion is present. At the upper boundary, the gradient in the concentration is taken to be zero. A time step of 0.01 s was used, corresponding to a maximum Courant number $\sigma = 0.23$. The results of the simulation are presented in Figure 5, where the concentration profile is shown for every 50 s (corresponding to a 0.5 m movement of the front). The classical 'over' and 'under' shoots are seen to have a constant value, and the slope of the front is seen to increase with the increased grid spacing, as could be expected, so that the front stays intact in the stretched co-ordinate system.

Figure 5. Concentration profile as function of time for pure advection. Each 50 s is shown. Grain diameter $d_{50}=0.5$ mm, water depth *h* = 10 m, constant vertical velocity *w* = 0.01 m s^{−1}. The co-ordinate system is shown in Figure 3. The time step is equal to 0.01 s.

Figure 6. Concentration profile as function of time for combined advection–dispersion. Every other second is shown in the interval between 0 and 20 s. Every tenth s is shown in the interval between 20 and 100 s and finally $t=1000$ s. The full line corresponds to the Vanoni profile (Equation (28)). Grain diameter $d_{50}=0.5$ mm, water depth $h=10$ m, constant vertical velocity $w = 0.0005$ m s⁻¹, friction factor $u_f = 0.025$ m s⁻¹ The co-ordinate system is shown in Figure 3. The time step is equal to 0.01 s.

4.3. *Combined ad*6*ection*–*dispersion*

In the third example, see Figure 6, the magnitude of diffusion is given by Equation (26), with friction velocity $u_f = 0.025$ m s^{−1}. The settling velocity is $w_s = 0.0005$ m s^{−1}. The ratio between the settling velocity w_s and the diffusion can be characterized by the Rouse number,

$$
Ro = \frac{w_s}{\kappa u_f},\tag{27}
$$

which in this example is $Ro = 0.4$. The profile converges towards the Vanoni profile, which is shown as the thick line. The Vanoni profile is the solution to the steady state diffusion equation (1) and is given analytically by

$$
c = c_0 \bigg(\frac{-z \cdot 2d_{50}}{(h+z) \cdot (h-2d_{50})} \bigg). \tag{28}
$$

The same grid and time step as the previous examples are used, corresponding to a maximum Courant number and non-dimensional diffusion: $\sigma = 0.62$, $\alpha = 0.05$.

Figure 7. Concentration development for pure advection with constant velocities, $(u, w) = (0.005, 0.01)$ m s^{−1} at time equal 250 s (a), 500 s (b), and 1250 s (c). Bed concentration is equal to 1 for $x < -5$ m and equal 0 for $x > -5$ m, periodic flow conditions, time step d*t*=0.01 s. The vertical discretization of the co-ordinate system is shown in Figure 3.

Figure 7 (*Continued*)

5. TWO-DIMENSIONAL TEST EXAMPLES

5.1. *Pure ad*6*ection in stretched grid*

In an area 10×10 m², there is a constant horizontal velocity of 0.005 m s⁻¹ and constant vertical velocity of 0.01 m s⁻¹. The area is described with 40 grid points in the horizontal direction and 100 grid points in the vertical direction, using the stretching shown in Figure 3. The bed concentration is constant, equal 1 for $-10 < x < -5$ m, and equal 0 for $-5 < x < 0$ m. Periodic flow conditions are used in the horizontal direction. A constant time step, $dt = 0.01$ s, is used, corresponding to $\sigma_{\text{max}}=0.24$. The calculated concentrations are shown in Figure 7 after 250, 500 and 1250 s. The scheme is seen to capture the correct movement of the front.

5.2. Pure advection in a curvilinear stretched grid

Flow in the area shown in Figure 8 described by 40×100 grid points is considered. The area is 50 m long and the water depth is between 7.5 and 11 m. The grid is stretched in the β -direction with a stretching factor, $s=0.1$, and grain diameter $d_{50}=0.5$ mm. The boundary condition at the bed is zero concentration along the bed except for $-27.2 < x < -22.2$ m, where the concentration is 1. The neutrally buoyant sand ($w_s = 0$) is advected by an oscillating velocity field given as

$$
(u_{\alpha}, u_{\beta}) = J \cos \frac{\pi t}{T} (0.01, 0.05), \tag{29}
$$

where J is the grid Jacobian, and T is the (half) period of the oscillation here taken as $T = 100$ s. A velocity field given by $(u_{\alpha}, u_{\beta}) = (J, 0)$ corresponds to a potential flow along the *x*-axis, while a velocity field given by $(u_a, u_\beta) = (0, J)$ corresponds to a potential flow along the β -axis. The time step is 0.01 s, corresponding to a maximum courant number of 0.42.

The concentration and velocity results are shown for $t = 0.02T$ (Figure 9), $t = 0.24T$ (Figure 10), $t = 0.48T$ (Figure 11), $t = 0.76$ (Figure 12), and $t = 0.98$ (Figure 13). In theory, Figure 9 should be identical to Figure 13, and Figure 10 should be identical to Figure 12. The errors are of the same magnitude as the ones present in a similar test in a rectangular grid.

6. CONCLUSION

An accurate solver for near-bed advection–dispersion processes has been developed for two-dimensional cases. The explicit finite difference scheme, QUICKEST, has been used in a stretched curvilinear grid, where care has been taken to keep the second-order derivatives of the

Figure 8. Curvilinear co-ordinate system with 40×100 grid points, $s = 0.1$ and $d_{50} = 0.5$ mm, (a) entire system, (b) close up near-bed grid lines.

Figure 9. Concentrations at $t = 0.02T$ for pure advection. The co-ordinate system is shown in Figure 8. Bed concentration equal 0 for the entire bed except for $-27.2 < x < -22.2$. The time varying velocity field is given by

Figure 10. Concentrations at $t = 0.24T$ for pure advection. The co-ordinate system is shown in Figure 8. Bed concentration equal 0 for the entire bed except for $-27.2 < x < -22.2$ m. The time varying velocity field is given

Figure 11. Concentrations at $t = 0.48T$ for pure advection. The co-ordinate system is shown in Figure 8. Bed concentration equal 0 for the entire bed except for $-27.2 < x < -22.2$ m. The time varying velocity field is given

Figure 12. Concentrations at $t = 0.76T$ for pure advection. The co-ordinate system is shown in Figure 8. Bed concentration equal 0 for the entire bed except for $-27.2 < x < -22.2$ m. The time varying velocity field is given

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Figure 13. Concentrations at $t = 0.98T$ for pure advection. The co-ordinate system is shown iffin Figure 8. Bed concentration equal 0 for the entire bed except for $-27.2 < x < -22.2$ m. The time varying velocity field is giv

stretched grid, so that no errors are introduced due to stretching. In the present formulation, the second-order grid derivatives enter as diffusion corrections to the advection velocities. The examples show an ability to keep fronts relatively sharp, even for very high degrees of grid stretching. The explicit control volume formulation makes the method easily implemented, and it is therefore a good choice, e.g. for sediment transport and scour modelling. The extension to three dimensions is straightforward with the work done in Reference [5], although the curvilinear version becomes more complicated.

APPENDIX A. NOMENCLATURE

APPENDIX B. DISCRETIZATION OF TRANSPORTS IN QUICKEST

This case is for a positive velocity *uj*:

$$
T_j = \sigma_x \left[c_{j-1} \left(\frac{1}{6} \sigma_x^2 - \frac{1}{6} + \sigma_x \right) + c_j \left(-\frac{1}{3} \sigma_x^2 + \frac{1}{2} \sigma_x + \frac{5}{6} - 2\alpha_x \right) \right] + \left[c_{j+1} \left(\frac{1}{6} \sigma_x^2 - \frac{1}{2} + \sigma_x + \frac{1}{3} + \alpha_x \right) \right] - \alpha_x (c_j - c_{j-1}).
$$

Figure A1. Discretization of differential equation.

The location of the concentrations and transport is shown in Figure A1, where

 $\sigma_x = u_i \cdot \Delta t / \Delta x$, $\alpha_x = \epsilon_j \cdot \Delta t / \Delta x^2$.

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