

APPENDIX A THEORETICAL BACKGROUND OF C-DIVAST AND STM

1.1 Governing Hydrodynamic Processes

Numerical modelling of fluid flow is based on the principles of continuity of mass and conservation of momentum within the body of fluid to be modelled. In many cases, the flow is defined by the Reynolds equations, which describe the three-dimensional turbulent motion of an incompressible fluid. For flows which show little variation in the vertical direction, it is appropriate to integrate these equations over the depth of water, resulting in simplified two-dimensional shallow water equations (Falconer 1977). To obtain the solution on a boundary-fitted curvilinear grid, the two-dimensional shallow water equations are transformed and expressed as (Lin and Chandler-Wilde 1996):

Conservation of mass:

$$\frac{\partial \zeta}{\partial t} + \frac{1}{J} \frac{\partial (h_s p)}{\partial \xi} + \frac{1}{J} \frac{\partial (h_1 q)}{\partial \eta} = q_m$$

Conservation of momentum:

$$\begin{aligned} & \frac{\partial p}{\partial t} + \beta \left[\frac{1}{J} \left(\frac{\partial (h_2 p U)}{\partial \xi} + \frac{\partial (h_1 q U)}{\partial \eta} \right) + \frac{V}{J} \left(p \frac{\partial h_1}{\partial \eta} - q \frac{\partial h_2}{\partial \xi} \right) \right] \\ &= f q - \frac{gH}{h_1} \frac{\partial \zeta}{\partial \xi} + \frac{\rho_a}{\rho} C_w W_\xi \sqrt{W_\xi^2 + W_\eta^2} - \frac{g p \sqrt{p^2 + q^2}}{H^2 C^2} \\ &+ \varepsilon \left[\frac{1}{h_1} \frac{\partial}{\partial \xi} \left(\frac{1}{J} \frac{\partial}{\partial \xi} (h_2 p) \right) + \frac{1}{h_2} \frac{\partial}{\partial \eta} \left(\frac{1}{J} \frac{\partial}{\partial \eta} (h_1 p) \right) - \frac{1}{h_1} \frac{\partial}{\partial \xi} \left(\frac{1}{J} \frac{\partial}{\partial \eta} (h_1 q) \right) \right. \\ &\quad \left. - \frac{1}{h_2} \frac{\partial}{\partial \eta} \left(\frac{1}{J} \frac{\partial}{\partial \xi} (h_2 q) \right) \right] \end{aligned}$$

$$\begin{aligned} & \frac{\partial q}{\partial t} + \beta \left[\frac{1}{J} \left(\frac{\partial (h_2 p V)}{\partial \xi} + \frac{\partial (h_1 q V)}{\partial \eta} \right) + \frac{U}{J} \left(q \frac{\partial h_2}{\partial \xi} - p \frac{\partial h_1}{\partial \eta} \right) \right] \\ &= -f p - \frac{gH}{h_2} \frac{\partial \zeta}{\partial \eta} + \frac{\rho_a}{\rho} C_w W_\eta \sqrt{W_\xi^2 + W_\eta^2} - \frac{g p \sqrt{p^2 + q^2}}{H^2 C^2} \\ &+ \varepsilon \left[\frac{1}{h_1} \frac{\partial}{\partial \xi} \left(\frac{1}{J} \frac{\partial}{\partial \xi} (h_2 q) \right) + \frac{1}{h_2} \frac{\partial}{\partial \eta} \left(\frac{1}{J} \frac{\partial}{\partial \eta} (h_1 q) \right) - \frac{1}{h_2} \frac{\partial}{\partial \xi} \left(\frac{1}{J} \frac{\partial}{\partial \eta} (h_2 p) \right) \right. \\ &\quad \left. - \frac{1}{h_1} \frac{\partial}{\partial \eta} \left(\frac{1}{J} \frac{\partial}{\partial \xi} (h_1 p) \right) \right] \end{aligned}$$

where:

$p(=UH)$, $q(=VH)$	discharges per unit width in the ξ and η directions respectively ($m^3/s/m$);
q_m	source discharge per unit horizontal area ($m^3/s/m^2$);
U, V	depth average velocity components in the ξ and η directions respectively (m/s);
β	momentum correction factor for a non-uniform vertical velocity profile;
f	Coriolis parameter due to the Earth's rotation ($=2\omega \sin\phi$, with ω = angular rotation speed of the Earth and ϕ = geographical angle of latitude; $\omega = 2\pi/(24 \times 3600) = 7.27 \times 10^{-5}$ radians/s);
g	gravitational acceleration ($= 9.806 m/s^2$);
H	total water depth $= \eta + h$;
ζ	water surface elevation above datum;
h	water depth below datum;
ρ_a	density of air ($\approx 1.292 kg/m^3$);
ρ	density of fluid (kg/m^3);
C	Chezy roughness coefficient ($m^{1/2}/s$);
C_w	air/fluid resistance coefficient (assumed to be 2.6×10^{-3} [5]);
ε	depth averaged turbulent eddy viscosity (m^2/s);
C_d	vegetation drag coefficient
m	vegetation density
D	vegetation diameter
ξ, η	co-ordinates in a curvilinear system
h_1, h_2	the transformation scale factors in ξ and η directions
J	$J=h_1 \cdot h_2$

Time derivative

Denotes the local change of the quantities water elevation and momentum with time. In C-DIVAST, this is due to tidal action at the boundaries.

Advective terms

Describes the change of momentum in the direction of flow. The non-cross term $u\partial u/\partial \xi$ contains information on the velocity gradient in the same direction as the flow, while the cross term $v\partial u/\partial \xi$ contains information on the velocity gradient in the other co-ordinate direction. These terms are important to describe the flow field in curved channels, around objects, etc. and in generating vorticity. Due to their non-linearity, they may cause computational instability and may be neglected under low Reynolds conditions for the sake of stability.

The momentum correction factor

For an assumed logarithmic vertical velocity profile, the momentum correction factors may be calculated from:

$$\beta = 1 + \frac{g}{C^2 \kappa^2}$$

where κ = von Karman's constant = 0.4. For an assumed seventh power law velocity profile the value of β is 1.016 and 1.20 for an assumed quadratic velocity profile (Falconer and Chen 1991).

Coriolis term

The Coriolis term describes the effect of the earth's rotation on the flow. It is dependent on the latitude and the flow velocity and acts at right angles to the flow. It deflects currents in a channel and can indirectly influence river alignment and sediment transport. On the coast it affects tidal currents and amplitude, causing the flow to rotate around points of zero amplitude. In estuaries, the Coriolis influence is usually very small compared with other effects, unless the modelling domain is very large.

Surface slope term

This term represents the action of gravity and takes into account both the topography and the water elevation. In C-DIVAST, the term contains both the mean depth + water elevation and the derivative of the water elevation, making the term non-linear.

The effect of wind

Wind exerts a drag force as it blows over the water surface. The shear stress at the air-water interface is calculated by assuming that it is proportional to the square of the wind speed at a particular height above the water surface. Various empirical formulae have been proposed to calculate an air-water resistance coefficient similar to the drag coefficient in turbulent flow field. In C-DIVAST, Wilson's (Weiyan, 1992) value is used, which refers to the resistance height $z = 10$ m above the water surface.

In water bodies with strong currents such as estuaries and rivers, wind stress is often small when compared to bottom shear stress. It plays predominantly a role in open sea and in lakes.

Bottom friction

Bottom friction has a non-linear, retarding effect on the flow. The Chezy coefficient is a semi-empirical bottom friction coefficient, which was originally developed to describe uniform flow in open channels. Under rough turbulent flow, i.e. Reynolds number $Re \gg 1000$ and an assumed logarithmic velocity-depth profile, the Chezy bottom friction coefficient is assumed to be independent of the flow and varies only with the relative roughness of the bed:

$$C = -18.0 * \text{Log}_{10} \left(\frac{k}{H * 12.0} \right)$$

Under transitional flow conditions, i.e. if Re 2000 - 4000, the Chezy coefficient varies with the flow conditions. The user can decide to switch to a different mode of calculating the Chezy coefficient by setting the corresponding flag in the data file. Under transitional conditions, the Chezy coefficient is calculated by iteration from:

$$C = -18.0 * \text{Log}_{10} \left(\frac{k}{H} + \frac{5}{\text{Re} * 18.0} * C \right)$$

where

- k = roughness length (data file)
 Re = Reynolds number
 Re_{min} = minimum Reynolds number for calculation of Chezy coefficient under transitional conditions (data file)

Within C-DIVAST, the Chezy coefficient is recalculated in time steps, the length of which is specified by the user in the data file. The coefficient may vary between 20-70 in floodplains and rivers (Weiyan, 1992).

Turbulence

The turbulent shear stress refers to the flow resistance associated with the random fluctuation of water in space and time. The momentum exchange brought about by turbulence causes the velocity-depth distribution to be more uniform than under laminar conditions. C-DIVAST only considers turbulent shear stress near the bed. The turbulence model in C-DIVAST relates to Boussinesq's approximation for the mean shear stress τ_e in turbulent flow:

$$\tau_e = \varepsilon \frac{dv}{dy}$$

where ε is the eddy viscosity, which is dependent on the turbulence characteristics of the flow and may be thousands of times larger than the molecular viscosity. If the turbulent shear stress is dominated by bottom friction, a relationship between the Chezy coefficient and the eddy viscosity exists. In C-DIVAST, the depth-integrated eddy viscosity is calculated (after Fischer, 1979) from:

$$\varepsilon = C_e \frac{H}{C} \sqrt{g(U^2 + V^2)}$$

where

C_e = eddy viscosity coefficient (data file)

Fischer's (1979) suggestion of $C_e =$ eddy viscosity coefficient ≈ 0.15 is based upon laboratory data. For actual tidal flows in estuaries and coastal areas, the value of C_e is frequently much larger and $C_e \approx 1.0$ is used in the current version of the model.

The turbulence model as specified in C-DIVAST gives an indication of the impact of bed generated turbulent momentum exchange on the overall time-averaged flow profile. This approach assumes that the turbulent shear stress is dominated by turbulence near the bottom and that it is equal in ξ - and η -direction. It cannot describe the turbulent fluctuation of the velocity, or specific flow features such as turbulent wakes behind objects etc. Its effect is to smooth velocity gradients and to enhance the stability of the numerical solution. It also contributes to the generation of vorticity. Because C-DIVAST uses a depth-integrated turbulence model, turbulent features that are 3-dimensional in nature, such as transport of horizontal eddies cannot be modelled. Nadaoka & Yagi (1997) discuss an approach to model horizontal turbulence with length scales larger than the water depth.

Stratification

C-DIVAST is a two-dimensional model, in which the vertical component is neglected. Such models are valid when the flow is predominantly horizontal with good vertical mixing or if the vertical variations are insignificant. This is mostly the case in shallow, tidal bays and estuaries with moderate freshwater inflow, but not in fjords and lakes at medium latitude. Whether the effects of stratification may be neglected does not only depend on the physical properties of the water body of interest, but also on the scale of the modelling. Most estuaries show some degree of salinity stratification during some time. Stratification increases when the freshwater flux increases relative to the tidal flux and is therefore likely to be stronger during low tide.

1.2 Governing Solute Transport Processes

In the conformal boundary-fitted coordinate system, the depth-integrated form of the advective-diffusion equation for suspended sediment transport (Falconer and Owens 1990) was expressed in the following form:

$$\frac{\partial(SH)}{\partial t} + \frac{1}{h_1 h_2} \left(\frac{\partial(h_2 p S)}{\partial \xi} + \frac{\partial(h_1 q S)}{\partial \eta} \right) - \frac{1}{h_1 h_2} \left(\frac{\partial}{\partial \xi} (HD_{11} \frac{\partial S}{\partial \xi} +) + \frac{\partial}{\partial \xi} (HD_{12} \frac{h_1}{h_2} \frac{\partial S}{\partial \eta} +) \right) - \frac{1}{h_1 h_2} \left(\frac{\partial}{\partial \eta} (HD_{21} \frac{h_2}{h_1} \frac{\partial S}{\partial \xi} +) + \frac{\partial}{\partial \eta} (HD_{22} \frac{\partial S}{\partial \eta} +) \right) = E$$

where:

S	the depth-mean solute concentration (kg/s);
E	net rate of erosion or deposition per unit area of bed (see Section 1.3);
$D_{11}, D_{12}, D_{21}, D_{22}$	depth mean dispersion coefficients;

When a cloud of dissolved or suspended material is released into the receiving water, the cloud will propagate, dilute and spread as it moves with the flow due to the effects of advective, diffusive and dispersive transport processes. The advection refers to the transport of the material by an imposed current system, such as that due to a tide in estuarine and coastal waters. Diffusion includes the scattering of particles by molecular and turbulent motion. The dispersion, as distinct from diffusion, is the dilution process associated with the stretching out and distortion of a cloud of solute in a non-uniform flow by the effect of velocity shear and consequential averaging of the flow distribution over the depth for two-dimensional models (Smith, 1992).

Time derivative and advective terms

The first three terms of the solute transport equation describe the local change with time of a solute and its advective flux. In C-DIVAST, the discharge from outfalls and the solute

concentrations at the boundary are constant, so that the change of the solute concentration with time is brought about by tidal changes in the water depth.

The dispersion-diffusion terms

The dispersion-diffusion terms summarise all non-advective transport processes, such as molecular diffusion, turbulent diffusion and dispersion due to shear flow. Molecular diffusion is usually negligible in turbulence flow.

1.3 Governing Sediment Transport Processes

The net erosion or deposition rate E in the above equation can be expressed in the form (Lin and Falconer 1995):

$$E = W_s \frac{S_{ae}}{S_e} (S_e - S)$$

where S_{ae} is the equilibrium sediment concentration at the reference level "a"; S_e is the depth mean equilibrium sediment concentration; W_s is the particle falling velocity. S_e can be calculated from the ratio of the depth integrated equilibrium suspended sediment flux q_s and the depth integrated fluid flux q , giving:

$$S_e = a \frac{q_s}{q}$$

The expression for S_{ae} was given by van Rijn (1984) and can be written as:

$$S_{ae} = 0.015 \frac{D_{50} T^{1.5}}{a D_*^{0.3}}$$

To obtain values for q_s , vertical solution was required for the following equation:

$$q_s = \frac{u_* S_{ae}}{\kappa} \left[\frac{a}{d-a} \right]^{Z'} \left[\int_a^{0.5d} \left[\frac{d-z}{z} \right]^{Z'} \ln \left(\frac{z}{z_0} \right) + \int_{0.5d}^d [e]^{-4Z'(z/d-0.5)} \ln \left(\frac{z}{z_0} \right) dz \right]$$

where u_* is the bed shear velocity; z is the vertical coordinate; z_0 is the zero velocity level; d is the water depth; Z' is the suspension number; and κ the von Karman constant.

1.4 Finite Difference Schemes

The finite difference method has been used to solve the governing differential equations previously given for the hydrodynamic and solute transport processes. The curvilinear grid is transformed to a regular computational mesh. In order to make this transformation, the curvilinear grid must be conformal coordinate grid, a special type of orthogonal grid. It is not easy to generate a conformal coordinate grid, which is not further discussed in the report. The

Techniques to generate conformal coordinate grids were discussed by Lin and Chandler-Wilde (1996).

The partial differential equations are replaced by finite difference equations on the computational mesh based upon the Taylor's series approximation. Solutions of the finite difference equations will introduce numerical errors, mainly due to computer round-off errors. For a given partial differential equation, there are a number of different ways in which its finite difference representations can be equivalently expressed. These include numerical schemes which progressively solve forward, backward or centrally in space; time-marching explicit solutions, where the unknown value can be calculated directly from known values without solving a matrix; and implicit solutions, where the unknown value is represented in terms of other neighbouring unknowns.

Generally speaking, explicit schemes have more restrictive time step constraints than implicit schemes. In order to obtain correct computational predictions, it is necessary to analyse the numerical properties associated with the finite difference scheme representation, including: consistency, stability, convergence and accuracy.

The finite difference equation must be consistent with the partial differential equation so that both equations describe the same physical phenomena. The finite difference scheme must be stable so that the cumulative effects of all the round-off errors of a computer at any stage of the computation are negligible, and that the computed solutions only differ insignificantly from the exact solutions of the finite difference equation. The convergence condition relates the computed solution of the finite difference equation to the exact solution of the partial differential equation. The accuracy criterion defines the permissible magnitudes of the truncation error for a finite difference scheme. A good finite difference scheme should satisfy the first three conditions and maintain a high order of accuracy.

The particular type of finite difference scheme used in this model is based upon the Alternating Direction Implicit, or ADI, technique which involves the sub-division of each time step into two half time steps. Thus a two-dimensional implicit scheme can be applied but considering only one dimension implicitly for each half time step, without the solution of a full two-dimensional matrix. On the first half time step the water elevation, the U velocity component (or the unit width discharge p) and the solute concentration are solved implicitly in the x-direction, whilst the other variables are represented explicitly. Similarly, for the second half time step, the water elevation, the V velocity component (or the unit width discharge q) and the solute concentration are solved for implicitly in the y-direction, with other variables being represented explicitly. With the boundary conditions included, the resulting finite difference equations for each half time step are solved using the method of Gauss elimination and back substitution (see e.g. Gerald & Wheatly, 1994 for details)

A space staggered grid system is used, with the variables ζ (elevation) and S (concentration) being located at the grid centre and with U and V at the centre of the grid sides as shown in Figure 1. The use of a staggered grid system prevents the appearance of oscillatory solutions which tend to occur in a non-staggered grid for space centred differences (Fletcher, 1991).

The depths are specified directly at the centre of the grid sides so that twice as much bathymetric detail can be included as in the traditional way, which gives depths at corners. This method also allows bed topography to be represented more accurately, particularly for non-linear bed variations and complicated bed elevations. However, in practice, specification of bed topography is often restricted by the data available.

For solutions to the solute transport equation, C-DIVAST provides three solvers, ADI-TOASOD, ADI-QUICK and second order central difference schemes respectively, where TOASOD stands for Third Order Advection and Second Order Diffusion, and QUICK stands for Quadratic Upwind Interpolation for Convective Kinematics. Although the ADI-TOASOD and ADI-QUICK schemes are similar in formulation, the former has a third order accuracy in space whereas the latter only has a second order accuracy. Therefore the current version of the C-DIVAST model uses the ADI-TOASOD scheme in view of its higher order accuracy.

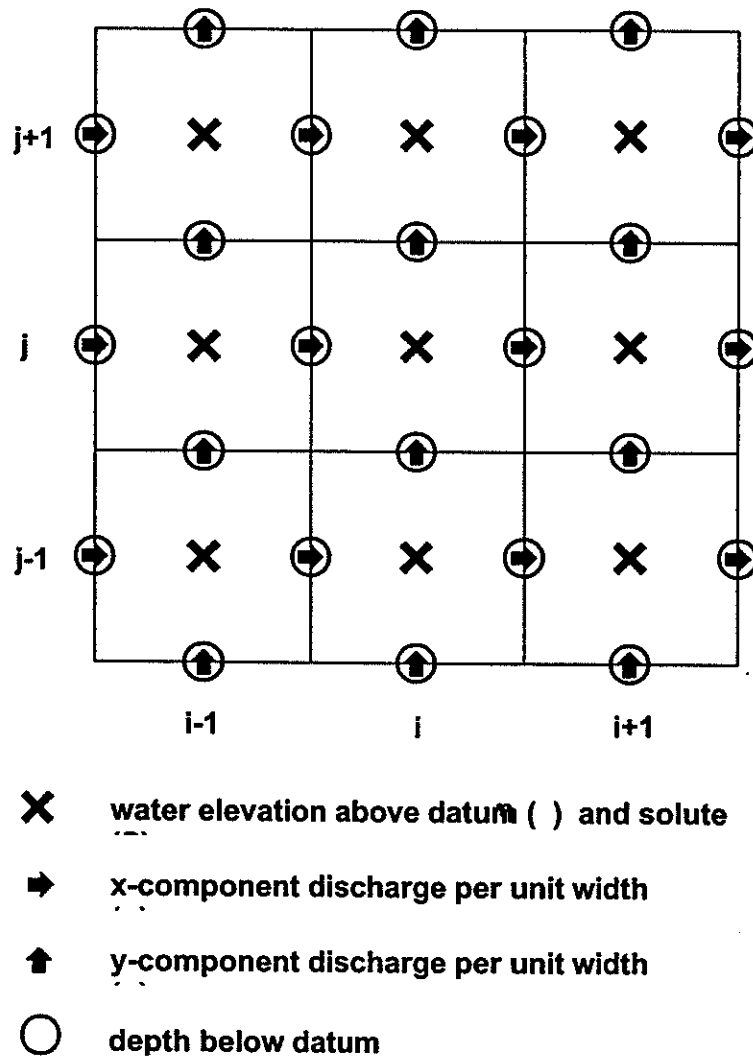


Figure 1: Computational Space Staggered Grid System

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