

HEC-RAS Water Quality Technical Reference

HEC-RAS Water Quality User's Manual

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1 The Advection-Diffusion Equation

The mass balance equation describes a change in mass (or energy) within a control volume as flux into and out of a control volume (mass transport) and external gains or losses (sources and sinks).

$$\left(\begin{array}{c} \text{Net rate of} \\ \text{change} \\ \text{mass / energy} \end{array} \right) = \left(\begin{array}{c} \text{Flux in} \\ \text{by advection} \\ \text{or dispersion} \end{array} \right) - \left(\begin{array}{c} \text{Flux out} \\ \text{by advection} \\ \text{or dispersion} \end{array} \right) + / - \left(\begin{array}{c} \text{Sources} \\ \text{and/or sinks} \end{array} \right)$$

1.1 State Variables

The state variable for advection-diffusion are concentration of mass or concentration of heat,

Generally, the water quality state variable is concentration of mass,

$$\phi = \frac{M}{V}$$

Symbol	Definition	Units
ϕ	Concentration of constituent	g/m^3
M	Mass of constituent	g
V	Volume of the water quality cell	m^3

For temperature modeling, the concentration of heat, θ is,

$$\theta = \frac{E}{V}$$

Symbol	Definition	Units
θ	Concentration	J/m^3
E	Heat energy	J

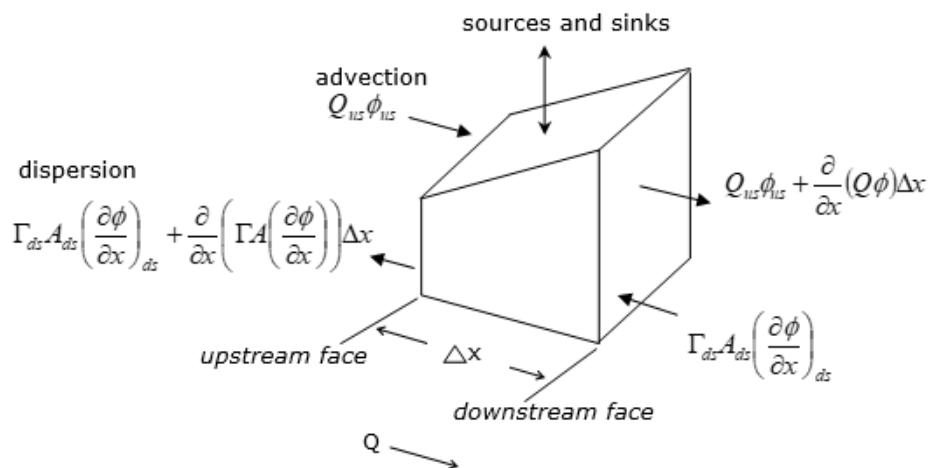
A change in heat content is reported (and measured) as a change in temperature,

$$T = \frac{\theta}{\rho C_p}$$

Symbol	Definition	Units
ρ	Density of water (function of temperature)	kg/m ³
C_p	Specific heat of water at constant pressure (weak function of temperature)	J/kg/K

1.2 Advection

Advection is the organized movement of contaminants, dissolved or suspended, in fluid.



The flux of mass transport due to advection is

$$\frac{\partial M}{\partial t} \text{ advection} = Q \phi$$

Symbol	Definition	Units
M	Mass of constituent	g
ϕ	Concentration of constituent	g/m ³
Q	Bulk flow	m ³ /s
t	Time	s

1.3 Mixing Processes - Diffusion and Dispersion

Three diffusion processes are of interest: molecular diffusion; turbulent diffusion; and shear flow dispersion. All three minimize concentration gradients by moving mass from regions of high to low concentration.

Diffusion processes are most commonly modeled using Fick's Law. Although Fick's Law applies to molecular diffusion, it is also used to simulate other gradient-driven mixing processes, including turbulent mixing, and shear flow dispersion. All three of these processes act to soften a steep front. In a one-dimensional model, particularly a gravity driven fluid problem, shear flow dispersion is of primary concern.

1.3.1 Molecular Diffusion

Molecular diffusion is a specific term for diffusion resulting from random motion of particles. Fick's law states that the mass of contaminant crossing a unit area (per unit time) is proportional to the gradient of contaminant concentration in that direction.

The negative sign indicates that the transport is from high to low concentration. Molecular diffusion coefficients are properties of the solute and the solvent, are nearly constant, and are on order of $10^{-9} m^2 s^{-1}$.

$$\frac{\partial M}{\partial t}_{diffusion} = -\Gamma A \frac{\partial \phi}{\partial x}$$

Symbol	Definition	Units
M	Mass of constituent	g
Γ	Diffusion coefficient	m^2/s
ϕ	Concentration of constituent	g/m^3
A	Cross sectional area perpendicular to flow direction	m^2
x	Streamwise direction	m

1.3.2 Turbulent Diffusion

Fick's law is applicable to turbulent diffusion under conditions of stationary homogenous turbulence. Fick's law is generally satisfactory for modeling purposes provided that sufficient time has passed since introduction of the contaminant. Turbulent diffusion coefficients are properties of the flow, are not constant, and are on order of $10^{-3} m^2 s^{-1}$.

1.3.3 Shear Flow Dispersion

Differences in velocity between the center of the channel, its bed, and its banks smear the leading edge of a steep face of constituent as it moves downstream. Including shear flow dispersion in a one-dimensional model compensates somewhat for the loss of representation that occurs when a three-dimensional system is reduced to one. Shear flow dispersion provides a mechanism to describe lateral variations in stream velocity.

Unlike molecular and turbulent diffusion, shear flow dispersion is not a fundamental physical process. However, Fick's laws is often used to simulate shear flow dispersion under particular conditions. The primary requirement is that enough (travel) time has elapsed in order to ensure that the contaminant has mixed fully in both the lateral and vertical directions.

Shear flow dispersion coefficients vary with properties of the flow, including the shape of the channel. Shear flow is greater in magnitude than both turbulent and molecular diffusion. Shear flow dispersion coefficients are on order of 1 to $10^3 m^2 s^{-1}$.

1.3.4 Shear Flow Dispersion Coefficients for One-Dimensional Modeling

The one-dimensional water quality model allows specification of dispersion coefficients globally, or at individual water quality cell faces. Dispersion coefficients may also be computed based on hydraulic characteristics such as cell width, face velocity, average depth and shear velocity. This latter option is especially useful for situations where abrupt discontinuities in hydraulic parameters are encountered.

1.3.4.1 Generic Equation for Shear Flow Dispersion

1.3.4.2 Fischer's Equation for Shear Flow Dispersion

An approximation for the dispersion coefficient in real streams was given by Fischer (1979).

$$\Gamma = 0.011 \lambda \frac{u^2 W^2}{Du^*}$$

Symbol	Definition	Units
Γ	Shear flow dispersion coefficient	m^2/s
λ	User specified multiplier (default is 1.0)	unitless
u	Face velocity	m^2/s

Symbol	Definition	Units
W	Face top width	m
D	Hydraulic depth	m

Shear flow velocity is computed as

$$u^* = \sqrt{g D S_f}$$

Symbol	Definition	Units
u^*	Shear flow velocity	m/s
S_f	Friction slope	unitless
g	Gravitational constant	m/s ²

1.3.4.3 Experimental Measurements of Shear Flow Dispersion

The dispersion coefficient is often used as a calibration parameter. Measured values are somewhat difficult to obtain. Below are from Fischer (1979).

Channel	Depth (m)	Width (m)	Mean Velocity (m/s)	Shear Velocity (m/s)	Observed Dispersion Coefficient (m ² /s)
Comite	0.43	16	0.37	0.050	14
Powell River, Tennessee	0.85	34	0.15	0.055	9.5
Sacramento	4.00	n/a	0.53	0.051	15
South Platte	0.46	n/a	0.66	0.069	16.2
Missouri	2.70	200	1.55	0.074	1500
Sabine	2.04	104	0.58	0.050	315

Channel	Depth (m)	Width (m)	Mean Velocity (m/s)	Shear Velocity (m/s)	Observed Dispersion Coefficient (m ² /s)
Yadkin	2.35	70	0.43	0.100	110
John Day	0.58	25	1.01	0.140	14

Shear velocity is computed as $u^* = \sqrt{gdS}$ where g = gravitational constant; d = average channel depth and S= channel slope

2 Numerical Scheme

HEC-RAS solves the advection-dispersion equation using the QUICKEST scheme for the state variable concentrations, reporting results at the centers of fully mixed cells. This section explains the water quality model numerical scheme. It also describes details regarding interfacing hydrodynamic results with the water quality model.

2.1 The Advection-Dispersion Equation

Any change in mass over time is equal to net mass transported by advection and diffusion, and sources and sinks. Written in different form, the equation is

$$\frac{\partial M}{\partial t} = Q_{us}\phi_{us} - \left[Q_{us}\phi_{us} + \frac{\partial}{\partial x}(Q\phi)\Delta x \right] - \Gamma_{ds}A_{ds}\left(\frac{\partial\phi}{\partial x}\right)_{ds} + \left[\Gamma_{ds}A_{ds}\left(\frac{\partial\phi}{\partial x}\right)_{ds} + \frac{\partial}{\partial x}\left(\Gamma A\frac{\partial\phi}{\partial x}\right)\Delta x \right] \pm S$$

Substituting $M = V\phi$ and $V = A\Delta x$, dividing through by Δx and canceling terms yields the conservation form of the advection-diffusion equation

$$\frac{\partial}{\partial t}(A\phi) = -\frac{\partial}{\partial x}(Q\phi) + \frac{\partial}{\partial x}\left(\Gamma A\frac{\partial\phi}{\partial x}\right) \pm \frac{S}{\Delta x}$$

2.2 Water Quality Cells

The QUICKEST numerical scheme is a control volume approach. When first initialed, the water quality model automatically constructs control volumes (cells), between each pair of HEC-RAS cross-sections. Although this is the default configuration, it is easily changed by the user.

HEC-RAS hydraulic cross sections are sometimes intentionally closely spaced. One example is hydraulic structures, where closely spaced cross sections are necessary to fully characterize the geometry for hydrodynamics computations. In areas such as this, very small water quality cells might automatically be created. These water quality cells will be short in length and relatively small in volume.

Small water quality cells are problematic, because in order to satisfy the stability condition imposed by the (QUICKEST) computational scheme, finely spaced water quality cells require correspondingly small time steps. In order to maximize the computational time step (and Minimize run times), it may become necessary to merge adjoining small water quality cells to form a larger cell. Merged cells must be contiguous and they must begin and end on existing cross sections.

2.3 Quickest Implementation

Symbol	Description	Units
A	Cell face area	m^2
\bar{V}	Time averaged volume of water quality cell	m^3
ϕ_f^*	QUICKEST estimated time averaged concentration at any face	kg m^{-3}
ϕ_{us}^*	QUICKEST estimated time averaged concentration at upstream face	kg m^{-3}
ϕ_{ds}^*	QUICKEST estimated time averaged concentration at downstream face	kg m^{-3}
ϕ_C	QUICKEST Computed Concentration (Center Cell)	kg m^{-3}
ϕ_{UP}	QUICKEST Computed Concentration (Upstream Cell)	kg m^{-3}
ϕ_{FUP}	QUICKEST Computed Concentration (Far Upstream Cell)	kg m^{-3}
ϕ_{DN}	QUICKEST Computed Concentration (Downstream Cell)	kg m^{-3}
Δx_{UP}	Distance between faces (upstream cell)	m
Δx_{FUP}	Distance between faces (far upstream cell)	m
Δx_{DN}	Distance between faces (downstream cell)	m
Δx_{us}	Distance between faces (center cell and upstream cell)	m
Δx_{fus}	Distance between faces (upstream and far upstream cell)	m

Symbol	Description	Units
Δx_{ds}	Distance between faces (center and downstream cell)	m
\bar{Q}	Time averaged flow at any face	$\text{m}^3 \text{s}^{-1}$
Q_{us}	Flow across (upstream) face	$\text{m}^3 \text{s}^{-1}$
Q_{ds}	Flow across (downstream) face	$\text{m}^3 \text{s}^{-1}$
u_{us}	Velocity across (upstream) face	ms^{-1}
u_{ds}	Velocity across (downstream) face	ms^{-1}

3 QUICKEST Implementation

The QUICKEST solution scheme estimates the fully mixed concentration at the center of each cell, as a function of computed fluxes across each cell face. Face fluxes are computed based on (previously computed) cell concentrations at cells located upstream and downstream of each cell face.

3.1 Variables

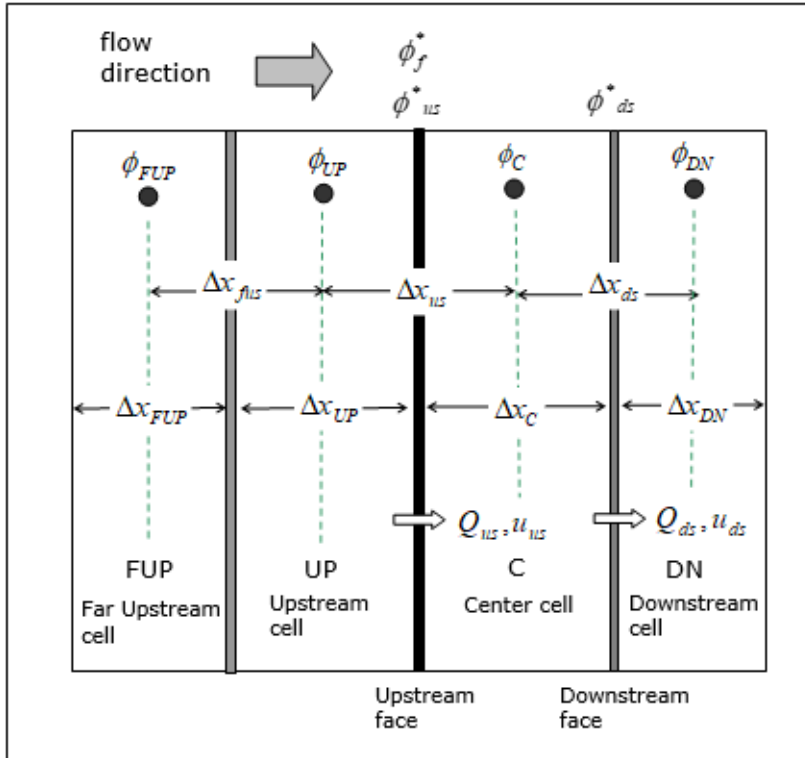
HEC-RAS naming conventions are referenced to an active (center) cell. Variables that describe cell faces are indicated with lower case subscripts; variables that describe cell centers are indicated with upper case subscripts.

Although this naming convention differs slightly from that presented in the QUICKEST scheme developed by Leonard (reference), computations are identical.

Symbol	Description	Units
A	Cell face area	m^2
\bar{V}	Time averaged volume of water quality cell	m^3
ϕ_f^*	QUICKEST estimated time averaged concentration at any face	kg m^{-3}
ϕ_{us}^*	QUICKEST estimated time averaged concentration at upstream face	kg m^{-3}
ϕ_{ds}^*	QUICKEST estimated time averaged concentration at downstream face	kg m^{-3}
ϕ_C	QUICKEST Computed Concentration (Center Cell)	kg m^{-3}
ϕ_{UP}	QUICKEST Computed Concentration (Upstream Cell)	kg m^{-3}
ϕ_{FUP}	QUICKEST Computed Concentration (Far Upstream Cell)	kg m^{-3}
ϕ_{DN}	QUICKEST Computed Concentration (Downstream Cell)	kg m^{-3}

Symbol	Description	Units
Δx_{UP}	Distance between faces (upstream cell)	m
Δx_{FUP}	Distance between faces (far upstream cell)	m
Δx_{DN}	Distance between faces (downstream cell)	m
Δx_{us}	Distance between faces (center cell and upstream cell)	m
Δx_{fus}	Distance between faces (upstream and far upstream cell)	m
Δx_{ds}	Distance between faces (center and downstream cell)	m
\bar{Q}	Time averaged flow at any face	$\text{m}^3 \text{s}^{-1}$
Q_{us}	Flow across (upstream) face	$\text{m}^3 \text{s}^{-1}$
Q_{ds}	Flow across (downstream) face	$\text{m}^3 \text{s}^{-1}$
u_{us}	Velocity across (upstream) face	ms^{-1}
u_{ds}	Velocity across (downstream) face	ms^{-1}

3.2 Computational Points



Computational points are placed between pairs of cross-sections (cell faces) so that the following relationships always hold,

$$\Delta_{ds} = \frac{1}{2}(\Delta_C + \Delta_{DN})$$

$$\Delta_{us} = \frac{1}{2}(\Delta_{UP} + \Delta_C)$$

3.3 Computing GRAD and CURV

GRAD and CURV are shorthand notation for his expressions of the first and second spatial derivatives.

The gradient, or GRAD, is the finite difference expression for the first derivative

$$GRAD \approx \frac{\partial \phi}{\partial x}$$

$$GRAD_{fus} = \frac{1}{\Delta_{fus}}(\phi_{UP} - \phi_{FUP})$$

$$GRAD_{us} = \frac{1}{\Delta_{us}}(\phi_C - \phi_{UP})$$

$$GRAD_{ds} = \frac{1}{\Delta_{ds}}(\phi_{DN} - \phi_C)$$

Curvature, or CURV, is an approximation for the second derivative

$$CURV \approx \frac{\partial^2 \phi}{\partial x^2}$$

CURV approaches zero when a function is nearly flat. In this context, CURV is upwind biased. Its definition is adjusted for the direction of flow across the face.

Written across the upstream and downstream face, CURVs are

$$CURV_{us} = \begin{cases} CURV_{UP} & \text{if } Q_{us} \geq 0 \\ CURV_C & \text{if } Q_{us} < 0 \end{cases}$$

$$CURV_{ds} = \begin{cases} CURV_C & \text{if } Q_{ds} \geq 0 \\ CURV_{DN} & \text{if } Q_{ds} < 0 \end{cases}$$

$$\begin{aligned} CURV_{UP} &= \frac{1}{\Delta x_{UP}} (GRAD_{us} - GRAD_{fus}) \\ &= \frac{1}{\Delta x_{UP}} \left(\frac{1}{\Delta x_{us}} (\phi_C - \phi_{UP}) - \frac{1}{\Delta x_{fus}} (\phi_{UP} - \phi_{FUP}) \right) \end{aligned}$$

$$\begin{aligned} CURV_C &= \frac{1}{\Delta x_C} (GRAD_{ds} - GRAD_{us}) \\ &= \frac{1}{\Delta x_C} \left(\frac{1}{\Delta x_{ds}} (\phi_{DN} - \phi_C) - \frac{1}{\Delta x_{us}} (\phi_C - \phi_{UP}) \right) \end{aligned}$$

$$\begin{aligned} CURV_{DN} &= \frac{1}{\Delta x_{DN}} (GRAD_{fds} - GRAD_{ds}) \\ &= \frac{1}{\Delta x_{DN}} \left(\frac{1}{\Delta x_{fds}} (\phi_{FDN} - \phi_{DN}) - \frac{1}{\Delta x_{ds}} (\phi_{DN} - \phi_C) \right) \end{aligned}$$

3.4 Difference Form of Advection-Dispersion Equation

The equation originally solved by Leonard is

$$\frac{\partial \phi}{\partial t} = -\frac{\partial(u\phi)}{\partial x} + \Gamma \frac{\partial^2 \phi}{\partial x^2}$$

HEC-RAS incorporates time varying and non-uniform area, as well as non-uniform into the equation so that it becomes

$$\frac{\partial(A\phi)}{\partial t} = -\frac{\partial(Q\phi)}{\partial x} + \frac{\partial}{\partial x} \left(\Gamma A \frac{\partial \phi}{\partial x} \right)$$

Writing the equation in finite difference form,

$$\frac{A_i^{n+1} \phi_i^{n+1} - A_i^n \phi_i^n}{\Delta t} = -\frac{Q_{ds}^n \phi_{ds}^n - Q_{us}^n \phi_{us}^n}{\Delta x} + \frac{\Gamma_{ds} A_{ds} \frac{\partial \phi^*}{\partial x_{ds}} - \Gamma_{us} A_{us} \frac{\partial \phi^*}{\partial x_{us}}}{\Delta x}$$

Cross multiplying,

$$(A_i^{n+1} \phi_i^{n+1} - A_i^n \phi_i^n) \Delta x = -(Q_{ds}^n \phi_{ds}^n - Q_{us}^n \phi_{us}^n) (\Delta t) + \left(\Gamma_{ds} A_{ds} \frac{\partial \phi^*}{\partial x_{ds}} - \Gamma_{us} A_{us} \frac{\partial \phi^*}{\partial x_{us}} \right) \Delta t$$

Where an asterisk * indicates the time-averaged value at a cell face, or its derivative.

Integrating across each cell over a time step and grouping into the three terms: mass accumulation; mass advection and mass diffusion:

$$\int_{\frac{-\Delta x_c}{2}}^{\frac{\Delta x_c}{2}} (A_c^{n+1} \phi_c^{n+1} - A_c^n \phi_c^n) dx =$$

Mass Accumulation

$$\int_0^{\Delta t} (\mathcal{Q}_{us}^n \phi_{us}^n - \mathcal{Q}_{ds}^n \phi_{ds}^n) dt + \int_0^{\Delta t} \left(\Gamma_{ds} A_{ds} \frac{\partial \phi^*}{\partial x_{ds}} - \Gamma_{us} A_{us} \frac{\partial \phi^*}{\partial x_{us}} \right) dt$$

Advection
Diffusion

The three integrals are solved with three different methods. The Mass Accumulation integral is solved numerically using a Simpson's Rule approximation. The Mass Advection integral is solved using a modified form of the QUICKEST approach. The Mass Diffusion integral is solved using a divided difference approach. Once all three are solved, terms are then collected from both sides of the equation and lumped into expressions to be solved for the concentration of the cell at the current time step.

3.5 Solution for the Mass Accumulation Term

$$\text{Accumulation} = \int_{\frac{-\Delta x_c}{2}}^{\frac{\Delta x_c}{2}} (A_c^{n+1} \phi_c^{n+1} - A_c^n \phi_c^n) d\zeta$$

The product of area and concentration is integrated between the upstream and downstream faces.

Time steps are integrated separately,

$$\text{Accumulation} = \underbrace{\int_{\frac{-\Delta x_c}{2}}^{\frac{\Delta x_c}{2}} A_c^{n+1} \phi_c^{n+1} d\zeta}_{\text{current time step}} - \underbrace{\int_{\frac{-\Delta x_c}{2}}^{\frac{\Delta x_c}{2}} A_c^n \phi_c^n d\zeta}_{\text{previous time step}}$$

4 Stability for One Dimensional Water Quality Modeling: Courant and Peclet Considerations

At the beginning of each computation, the model computes a new time step.

Each new time step is the largest time that satisfies all three conditions:

- Timestep satisfies the Courant condition for all water quality cells
- Timestep satisfies the Peclet condition for all water quality cells
- Timestep is less than or equal to the User Defined Maximum

4.1 Equivalent Path Length

In order to compute the Courant and Peclet conditions, an expression of the distance that flow moves through a particular water quality cell must be defined.

In this computational framework, where each water quality cell is characterized by an upstream face area, a downstream face area, and a volume, an equivalent path length, Δx_e , is computed from the volume of the cell and the face area of the upstream face.

$$\Delta x_e = \frac{V}{A_{us}}$$

Symbol	Description	Units
Δx_e	equivalent flow path	meters
V	volume of water quality cell	m ³
A_{us}	area of upstream face	m ²

4.2 The Courant Number

The Courant Number is a dimensionless measure, of the distance over which a constituent is advected through the computational grid.

$$C_r = u \frac{\Delta t}{\Delta x}$$

where

Symbol	Description	Units
C_r	Courant Number	unitless
u	velocity across upstream face of water quality cell	ms^{-1}
Δt	time step	seconds
Δx	length of water quality cell	meters

In order to maintain numerical stability, the water quality engine does not allow the Courant Number to exceed 0.9.

The water quality model chooses a time step that will satisfy this (Courant) condition for all water quality cell face velocity - water quality cell length pairs.

Remember that the time step is chosen to maintain the Courant condition for all cell velocities, and at all times. This means that a single small water quality cell in any part of the geometry could force the model to apply a short time step. This could result in a long run time.

It is wise to examine your water quality cell geometry, identifying locations where cross sections have been closely spaced. One place where this may occur is around hydraulic structures. Closely spaced hydrodynamic cross sections result in correspondingly small water quality cells. Small water quality cells force short time steps and long run times.

Keep in mind that water quality cells may be adjusted, by increasing the minimum water quality cell length. Choosing a larger minimum water quality cell length asks the model to merge water quality cells, until the minimum water quality cell length is attained.

4.3 The Peclet Number

The Peclet Number is a measure of the distance over which a constituent is diffused through the computational grid.

$$P = \frac{\Gamma \Delta t}{\Delta x^2}$$

where

Symbol	Description	Units
P	Peclet Number	unitless
Γ	Diffusion Coefficient	ms^{-2}
Δt	time step	seconds

Symbol	Description	Units
Δx	length of water quality cell	meters

In order to maintain numerical stability, the water quality engine does not allow the Peclet Number to exceed 0.3.

The water quality model chooses a time step that will satisfy this (Peclet) condition for all water quality cell face dispersion coefficient - water quality cell length pairs. Keep in mind that the larger the Diffusion Coefficient, the shorter the resulting time step.

4.3.1 Computation of the Dispersion Coefficient

The diffusion coefficient may be set by the user, as a constant, or it may be computed as a function of cell face velocity, average cell width, shear velocity, and average channel depth.

$$\Gamma = M \, 0.011 \, \frac{\bar{u}^2 W^2}{y u^*}$$

Symbol	Description	Units
Γ	Dispersion Coefficient	m s^{-2}
M	user defined multiplier	unitless
u	cell face velocity	m s^{-1}
W	average cell surface width	meters
y	average cell depth	meters
u^*	cell face shear velocity	m s^{-1}

5 Oxygen Reaeration

Oxygen reaeration refers to the transfer of oxygen across the air-water interface. This transfer is affected by the difference in DO concentrations between the air and water and by the turbulence in the film of water adjacent to the surface. The turbulence in that thin film may be caused by wind shear or shear produced by water currents. Oxygen reaeration rate (k_a) is commonly estimated from hydraulic parameters and wind speed.

$$k_a(T) = \frac{k_{aw}(T)}{h} + k_{ah}(T)$$

Symbol	Description	Units
$k_a(T)$	Oxygen reaeration rate	1/day
$k_{aw}(T)$	Wind derived oxygen reaeration velocity	m/day
$k_{ah}(T)$	Flow derived oxygen reaeration rate	1/day
h	Water depth	m

5.1 Flow derived oxygen reaeration rate equations

Numerous formulations have been developed to estimate oxygen reaeration rates. Most of the oxygen reaeration equations in the literature were derived from relatively small sets of laboratory or field data. Eight flow derived oxygen reaeration equation are included in the model. The oxygen reaeration rate calculated from these equations is referenced to 20 C and is adjusted to local water temperature using the Arrhenius Equation. Reaeration rates may also be defined as constants by the user.

No	Method	Equation	Applicability
1	User Defined	k_{ah} Entered by user (under Parameters tab)	Applies to all water quality cells with a region
2	O'Connor and Dobbins (1958) Natural streams	$k_{ah} = \frac{3.93 u^{0.5}}{h^{1.5}}$	$0.3 \leq h \leq 9$

No	Method	Equation	Applicability
3	Owens et al (1964) Natural streams	$k_{ah} = \frac{5.32 u^{0.67}}{h^{1.85}}$	$0 \leq h \leq 3.3$
4	Churchill et al. (1962) Natural streams	$k_{ah} = \frac{5.026 u}{h^{1.67}}$	$0 \leq h \leq 3.3 \text{ m}$
5	Covar (1976) Combines three equations above.	$k_{ah} = \frac{5.32 u^{0.67}}{h^{1.85}}$ Owens et al (1964)	$h < 0.61 \text{ m}$
		$k_{ah} = \frac{3.93 u^{0.5}}{h^{1.5}}$ O'Connor and Dobbins (1958)	$h > 0.61 \text{ m}$
		$k_{ah} = \frac{5.026 u}{h^{1.67}}$ (Churchill et al. 1962)	
6	Melching and Flores (1999) Pool and riffle streams	$k_{ah} = 517(u s_l)^{0.524} Q^{-0.242}$	$Q < 0.556 \text{ m}^3/\text{s}$
		$k_{ah} = 596(u s_l)^{0.528} Q^{-0.136}$	$Q \geq 0.556 \text{ m}^3/\text{s}$
7	Melching and Flores (1999) Channel control systems	$k_{ah} = 88(u s_l)^{0.313} h^{-0.353}$	$Q < 0.556 \text{ m}^3/\text{s}$
		$k_{ah} = 142(u s_l)^{0.333} h^{-0.66} B_t^{-0.243}$	$Q \geq 0.556 \text{ m}^3/\text{s}$
8	Tsivoglou and Neal (1976)	$k_{ah} = 31183 u s_l$	$0.0283 < Q < 0.425 \text{ m}^3/\text{s}$
		$k_{ah} = 15308 u s_l$	$0.425 \leq Q \leq 84.938 \text{ m}^3/\text{s}$

No	Method	Equation	Applicability
9	Thackston and Dawson (2001)	$k_{ah} = 2.16 \left(1 + 9 F_d^{0.25} \right) \frac{u_*}{h}$ $F_d = \frac{u}{\sqrt{\frac{g A_c}{B_t}}}$ $u_* = \sqrt{g R_h s_l}$	
<p> u = water velocity (m/s) h = water depth (m) s_l = channel slope B_t = top width of channel (m) R_h = channel hydraulic radius (m) A_c = channel cross-sectional area (m) </p>			

5.2 Wind derived oxygen reaeration rate equations

No	Method	Equation	Applicability
1	User defined	k_{aw} Entered by user (under Parameters tab)	Applies to all water quality cells with a region
2	Broecker et al. (1978)	$k_{aw} = 0.864 W$	
3	Gelda et al. (1996)	$k_{aw} = \alpha W^\beta$ $\alpha = 0.2 \quad \beta = 1.0$ $\alpha = 0.057 \quad \beta = 2.0$	$W < 3.5 \text{ ms}^{-1}$ $W > 3.5 \text{ ms}^{-1}$
4	Banks and Herrera (1977)	$k_{aw}(T) = 0.728 U_{w10}^{0.5} - 0.317 U_{w10} + 0.0372 U_{w10}^2$	
5	Wanninkhof et al. (1991)	$k_{aw}(T) = 0.728 U_{w10}^{1.64}$	
6	Chen, Kanwisher (1963)	$k_{aw} = \frac{D_{o2}}{(200 - 60W^{0.5}) 10^{-6}}$	

N o	Method	Equation	Applicability
7	Cole and Buchak (1993)	$k_{aw} = 0.5 + 0.05 W^2$	
8	Banks (1975)	$k_{aw} = 0.363\sqrt{W}$ $k_{aw} = 0.0277 W^2$	$W < 5.5 \text{ m s}^{-1}$ $W > 5.5 \text{ m s}^{-1}$
9	Smith (1978)	$k_{aw} = 0.64 + 0.128 W^2$	
10	Liss (1973)	$k_{aw} = 0.156 W^{0.63}$	$W \leq 4.1 \text{ m s}^{-1}$ $W > 4.1 \text{ m s}^{-1}$
11	Downing and Truesdale (1955)	$k_{aw} = 0.0276 W^2$	
12	Kanwisher (1963)	$k_{aw} = 0.0432 W^2$	
13	Yu et al. (1977)	$k_{aw} = 0.319 W$	
14	Weiler (1974)	$k_{aw} = 0.398$ $k_{aw} = 0.155 W^2$	$W < 1.6 \text{ m s}^{-1}$ $W \geq 1.6 \text{ m s}^{-1}$
W = wind speed measured at 2 meters above the water surface U_{w10} = wind speed measured at 10 meters above the water surface (m s^{-1}) D_{o2} =Molecular diffusivity of oxygen ($D_{o2} = 2.19 \text{ E}^{-9} \text{ m}^2 \text{ s}^{-1}$ at 20°C)			

5.3 References

Churchill, M.A., H.L. Elmore, and R.A. Buckingham. 1962. The Prediction of Stream Reaeration Rates, ASCE, *Journal Sanitary Engineering Division*, Vol. No. 88, SA4, pp. 1-46.

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6 Dissolved Oxygen Saturation (DOs)

In order to compute reaeration rates, dissolved oxygen at saturation (DO_s) must be computed. DO_s is initially computed as a function of temperature. It is then corrected for variations in atmospheric pressure and salinity.

6.1 Dissolved Oxygen at Saturation as function of temperature

DO_s as a function of temperature alone is calculated using the equation provided in APHA (1992) and also Brown and Barnwell (1987). For typical natural water in temperate climates, DO_{sat} ranges from 6.413 mg/L at 40C to 14.621 mg/L at 0C.

$$\ln DO_s = -139.34411 + \frac{1.575701 \times 10^5}{T_{wk}} - \frac{6.642308 \times 10^7}{T_{wk}^2} + \frac{1.243800 \times 10^{10}}{T_{wk}^3} - \frac{8.62194 \times 10^{11}}{T_{wk}^4}$$

Symbol	Description	Units
DO_s	Dissolved oxygen at saturation	mg /L
T_{wk}	Water temperature	K

6.1.1 Correction for Atmospheric Pressure

Correction for atmospheric pressure is made using the relationship developed by Benson and Krause (1984),

$$DO_s = DO_s p_{atm} \frac{(1 - \frac{p_{wv}}{p_{atm}})(1 - \alpha p_{atm})}{(1 - p_{wv})(1 - \alpha)}$$

Symbol	Description	Units
p_{atm}	Local atmospheric pressure	atm
p_{wv}	Partial pressure of water vapor	atm

6.1.1.1 Correction Coefficient

The correction coefficient is a function of water temperature,

$$\alpha = 0.000975 - 1.426 \times 10^{-5} T_w + 6.436 \times 10^{-8} T_w^2$$

Symbol	Description	Units
T_w	Water temperature	C

6.1.1.2 Vapor Pressure

Vapor pressure is computed as a function of water temperature,

$$p_{wv} = \exp \left(11.8571 - \frac{3840.70}{T_{wk}} - \frac{216961}{T_{wk}^2} \right)$$

6.1.2 Correction for Salinity

Dissolved Oxygen saturation may be correct for salinity based on the equations given by APHA (1992)

$$\ln DO_s = \ln DO_s - Salt \left(1.7674 \times 10^{-2} - \frac{1.07454 \times 10}{T_{wk}} + \frac{2.1407 \times 10^3}{T_{wk}^2} \right)$$

Symbol	Description	Units
$Salt$	Salinity	ppt

6.1.2.1 Salinity

Salinity is the total of all non-carbonate salts dissolved in water, usually expressed in parts per thousand (ppt). Salinity is an important measurement in seawater or in estuaries where freshwater from rivers and streams mixes with salty ocean water. Because most anions in seawater or brackish water are chloride ions, salinity may be estimated from chloride concentration using the equation below. Note that while salinity and chloride are proportional in seawater, this equation is not accurate in freshwater (MDNR 2009).

$$Salt = 0.03 + 0.0018066 Cl$$

Symbol	Description	Units
Cl	chloride concentration	mg – Cl/L

6.2 Oxygen Saturation Level (DO%)

The oxygen saturation level (DO%) is defined as

$$DO(\%) = 100 \frac{DO}{DO_s}$$

6.3 References

APHA (1992)

Benson and Krause (1984)

Brown and Barnwell (1987) The Enhanced Stream Water Quality Models QUAL2E and QUAL2E-UNCAS: Documentation and user Manual EPA/600/3-81/007.

MNDR (2009)

7 Sediment Oxygen Demand (SOD)

Sediment oxygen demand (SOD) is the rate of oxygen consumption exerted by degradation and mixing processes in the benthic sediments.

SOD is expressed as a zero-order reaction rate ($gO_2/m^2/day$) and is a user-specified parameter.

Positive flux is from sediment to water. Negative flux is from water to sediment.

Reference	SOD $gO_2/m^2/day$	Location	Conditions
USEPA (1985)	0.5-2.0	Laboratory Experiments	
NCASI (1978)	2.0 - 33	Four Eastern U.S. rivers Downstream of paper mill discharge	In-situ respirometer, light, stirred, dark 22-27 °C
NCASI (1978)	0.9-14.1	Four Eastern U.S. rivers Downstream of paper mill discharge	In-situ respirometer, tunnel respirometer, light, stirred, dark 22-27 °C
NCASI (1979)	0.1-1.4	Four Eastern U.S. rivers Downstream of paper mill discharge	In-situ respirometer, stirred, dark 9-16 °C $\theta = 1.08$
Butts and Evens (1978)	0.27-9.8	Northern Illinois rivers 89 Stations	In-situ respirometer, stirred, 1-3 hrs dark 5-31 °C
Chiaro and Burke (1980)	0.1-5.3	Eastern Michigan rivers 6 Stations	In-situ respirometer, stirred, 15-27 hr dark 19-25 °C $\theta = 1.08$
Hunter et al. (1973)	1.1-12.8	New Jersey rivers 10 Stations	In-situ respirometer, dark, 30 min - 8hr, stirred 22-27 °C

Reference	SOD $gO_2 / m^2 / day$	Location	Conditions
Edberg and Hofsten (1973)	0.3-1.4	Swedish rivers	In-situ respirometer, light, stirred 0-10 °C
James (1974)	4.6-44	Streams	Oxygen mass balance

7.1 References

Butts and Evans, 1978
 Chiaro and Burke, 1980
 Edberg and Hofsten, 1973
 Hunter et al. 1973
 James, 1974
 Manivanan, 2008
 NCASI, 1978
 NCASI, 1979
 USEPA, 1985