Heat budget and thermodynamics at a free surface:

Some theory and numerical implementation (revision 1.0c) ED 1300 BH

Introduction

Heat transfer at a free surface is generally classified according to classical concepts of heat transfer: radiation, convection, conduction, and evaporation. For numerical modeling of water surface heat fluxes, it is convenient to classify heat transfer in terms of its ability to penetrate the water surface. Evaporation, conduction, and long wave radiation are all *surface* heat transfer effects that heat occur only at the surface of the water. Short-wave radiation is a penetrative effect that distributes its heat through a significant range of the water column. This paper will outline the primary models of heat transfer that are being used in the CWR suite of numerical models.

Nomenclature

Heat transfer terms[1]:

Q	heat transfer	W/m^2
Q_H	sensible heat transfer	W/m^2
Q_R	long wave radiation	W/m^2
Q_W	evaporative heat transfer	W/m^2
Q_S	total surface (non-penetrative) heat transfer	W/m^2
Q_r	short wave radiation reflected from bottom of domain	W/m^2
$Q_{S(k)}$	surface heat transfer at top of k^{th} layer	W/m^2
$Q_{S(n)}$	surface heat transfer at free surface	W/m^2
$Q_{S(b-1)}$	surface heat transfer that reaches bottom of domain	W/m^2
$Q_{S(m)}$	surface heat transfer at maximum penetration depth	W/m^2
Q_{sw}	short wave radiation that penetrates surface	W/m^2
$Q_{sw(k)}$	short wave radiation at top of k^{th} layer	W/m^2
$Q_{sw(n)}$	short wave radiation at free surface	W/m^2
$Q_{sw(m)}$	short wave radiation at maximum penetration depth	W/m^2
$Q_{sw(b-1)}$	short wave heat transfer that reaches bottom of domain	W/m^2
$\Delta Q_{S(k)}$	total surface radiation absorbed in the k^{th} layer	W/m^2
$\Delta Q_{sw(k)}$	total short wave radiation absorbed in the k^{th} layer	W/m^2

Coefficients and constants

σ	Stefan-Boltzmann constant,	5.669×10^{-8} W m^{-2} K^{-4}
ε	emissivity	non-dimensional
C_ε	coefficient for emissivity	C^{-2}

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[1] These are in *power* transferred per unit of surface area rather than *energy*.

C_W	bulk coefficient of evaporative heat transfer	non-dimensional
C_H	bulk coefficient of sensible heat transfer	non-dimensional
$C_{(cloud)}$	fractional cloud cover	non-dimensional $0 \leq C_{(cloud)} \leq 1.0$
C_b	fractional Q_S reflected from bottom of domain	non-dimensional $0 \leq C_b \leq 1.0$
C_r	fractional Q_{sw} reflected from bottom of domain	non-dimensional $0 \leq C_r \leq 1.0$
$R_{t(lw)}$	total reflectivity (long wave radiation)	non-dimensional $0 \leq R_t \leq 1.0$
$R_{t(sw)}$	total reflectivity (short wave radiation)	non-dimensional $0 \leq R_t \leq 1.0$
η_e	bulk extinction coefficient: short wave radiation	m^{-1}
η_s	extinction coefficient: surface heat transfer	m^{-1}
η_r	extinction coefficient: bottom reflection	m^{-1}

Other variables

ρ	density	kg/m^3
c_p	specific heat capacity	$J\ kg^{-1}\ C^{-1}$
D	depth of domain	m
e	vapor pressure of water in air	Pa
$e_{(sat)}$	saturated vapor pressure of water in air	Pa
E	evaporative mass flux	kg/s
L	latent heat of evaporation	J/kg
P	atmospheric pressure	Pa
q	specific humidity	non-dimensional
$q_{(sat)}$	specific humidity of saturated air	non-dimensional
R_h	relative humidity	non-dimensional $(0 \leq R_h \leq 1)$
S	height of surface	m
$T_{(K)}$	temperature	K
T	temperature	C
u	velocity	m/s
z	height measured from a baseline with (+) up	m
$\Delta z_{(k)}$	grid thickness of k^{th} layer	m^{-1}

Long wave radiation

The radiant energy emission (long wave or infrared radiation) by a *black body* is (Holman, pg 387, eq 8-3):

$$Q = -\sigma T_{(K)}^{\ 4} \tag{1}$$

where Q is the long wave energy transfer per unit surface area (W/m^2) with a negative value indicating heat transfer out of the surface[2], σ is the Stefan-Boltzman constant[3] (5.669×10^{-8} W

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[2] Our definition of negative energy transfer as the transfer *out* of the water is consistent with a thermodynamic definition of a system (i.e. the surface is the system boundary and transfer out of the system is a loss). However, it should be noted that air-sea interaction studies of oceanographers typically have a system definition that encompasses both the air and the water (the interface as an interior bound). The conventional oceanography definition of energy transfer across the interface is that energy transfer downward (air to sea) is negative, while an upward energy transfer (water to air) is positive (the opposite of our convention).

$\mathrm{m}^{-2}\ \mathrm{K}^{-4}$, Holman, pg. 387) and $T_{(K)}$ is the absolute temperature in Kelvin degrees. For the remainder of this paper, it will be convenient to work in Celsius degrees *(T)* where

$$T_{(K)} = T + 273.2 \tag{2}$$

In engineering heat transfer, radiant energy exchanges between bodies are usually computed through using: (1) *emissivities* (ε) that relate the difference in radiation between real bodies and a black body, (2) shape factors or area ratios that account for the shape of the bodies in the radiation problem, (3) the absorption of radiation in a gas (such as air), and (4) the relative temperature difference (see Holman). For atmospheric and water surface interactions we generally use (1) emissivity, (2) cloud cover, and (3) water surface reflectivity (see TVA). The literature provides several different approaches for applying these empirical factors. In DYRESM (Imberger and Patterson) the long-wave radiation problem is separated into (1) radiant emission from the water, and (2) net radiation from the atmosphere that reaches penetrates the water surface. We will designate these as $Q_{(emitted)}$ and $Q_{(absorbed)}$. The equations used to describe these are:

$$Q_{(emitted)} = -\varepsilon_{(water)}\,\sigma\left(273.2 + T_{(water)}\right)^4 \tag{3}$$

and

$$Q_{(absorbed)} = \varepsilon_{(air)}\,\sigma\left(1 + 0.17\,C_{(cloud)}{}^2\right)\left(273.2 + T_{(air\,2)}\right)^4\left(1 - R_{t(lw)}\right) \tag{4}$$

where $C_{(cloud)}$ is the fractional cloud cover, $T_{(water)}$ is the water surface temperature, $T_{(air\,2)}$ is the air temperature (dry bulb in Celsius degrees) measured two meters above the water surface, and $R_{t(lw)}$ is the total reflectivity of the water surface for long wave radiation.

Equation (3) is found in Imberger and Patterson (eq 8), also in TVA (eq 3.5), and Jacquet, (eq A5.5). Equation (4) is a slightly more generalized form of TVA (eq 3.14), Fischer *et al.,* (eq 6.22), Imberger and Patterson (eq 9), and Jacquet (eq A5.4). All four equations in the literature incorporate the Swinbank (1963) model for the emissivity of air[4]. This incorporation is confusing as it provides a radiation equation that is a sixth power in temperature, which can be mistaken for a typographical error.

The formula attributed to Swinbank (1963) for the emissivity of the air is:

$$\varepsilon_{(air)} = C_\varepsilon\left(273.2 + T_{(air2)}\right)^2 \tag{5}$$

(see TVA, unnumbered equation following eq 3.10), where C_ε is a *dimensional* emperical coefficient C^{-2}. TVA (pg 3.10) gives a *mean value* for C_ε as 0.937×10^{-5}, while Jacquet (pg 172) gives a range of values $0.906 \times 10^{-5} < C_\varepsilon < 0.999 \times 10^{-5}$, and quotes Swinbank's coefficient as 0.938×10^{-5}.

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[3] DYRESM uses a Stefan-Boltzman constant of 2.00411×10^{-7} kJ / (m^2 hr K^4), which converts to 5.56697×10^{-8} W m^{-2} K^{-4}.

[4] Note that Imberger and Patterson contains a typographical error in their eq (9): the temperature is raised to the second power rather than the sixth power.

Net heat transfer through long wave radiation

The net heat transfer through long wave radiation (Q_R) is the sum of the emitted, equation (3), and absorbed, equation (4):

$$Q_R = Q_{(emitted)} + Q_{(absorbed)} \tag{6}$$

Herzfeld (1996) uses a formula for the net long wave radiation heat transfer that can be presented as:

$$Q_R = \left\{ \sigma \, \varepsilon_{(water)} \left(1 - \varepsilon_{(air)}\right) \left(273.2 + T_{(air)}\right)^4 + 4 \varepsilon_{(water)} \, \sigma \left(273.2 + T^3_{(air)}\right) \left(T_{(water)} - T_{(air)}\right) \right\} \left(1 - \beta C_{(cloud)}\right) \tag{7}$$

where different emissivities and temperatures for air and water are used. The coefficient β in the cloud cover term is a function of latitude. Emissivity of air in Herzfeld is computed from:

$$\varepsilon_{(air)} = 0.920 \times 10^{-5} \left(273.2 + T_{(air)}\right)^2 \tag{8}$$

Note that Herzfeld's approach applies the cloud cover correction to both the emission and absorption of long-wave radiation, while the DYRESM approach applies the cloud cover correction only to absorption. The former may be a more accurate scheme.

Numerical implementation

Long wave radiation in is computed from equations (3), (4) and (6) as follows:

$$Q_R = -\varepsilon_{(water)} \, \sigma \left(273.2 + T_{(water)}\right)^4 + \ \varepsilon_{(air)} \, \sigma \left(273.2 + T_{(air\,2)}\right)^4 \left(1 - R_{t(lw)}\right) \left(1 + 0.17 \, C_{(cloud)}{}^2\right) \tag{9}$$

Following previous versions of DYRESM, we use equation (5) for the emissivity of air and the following constants:

- C_ε : 0.937×10^{-5} C^{-2} (Imberger and Patterson, eq 9)
- $\varepsilon_{(water)}$: 0.96 (Imberger and Patterson, below eq 8)[5]
- $R_{t(lw)}$: 0.3 (Imberger and Patterson, below eq 9)[6]
- σ : 5.669×10^{-8} W m^{-2} C^{-4} (Holman, pg. 387)

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[5] Reynolds and Perkins (1977) list the emissivity of pure water as falling in the range 0.95 to 0.963, corresponding to the temperature range of 0° to 100° C. Using linear interpolation, a value appropriate to water at 20° C is 0.9526. However, TVA gives a value of 0.97 (TVA pg 3.5).

[6] TVA (pg 2.16, 2.17) gives a method for estimating total reflectivity of the waters surface based on cloud cover and solar altitude. This may be an improvement on the use of a fixed reflectivity.

Latent Heat of Evaporation

The energy transfer per unit surface area (in W/m^2) due to evaporation (Q_W) can be modeled as the product of the latent heat of evaporation (L) in J/kg and the water vapour flux (E) in kg/s (TVA eq 4.54, Blanc, eq 11, Jacquet, eq A5.6)[7]:

$$Q_W = L\,E \tag{10}$$

The latent heat of evaporation in J/kg (from Blanc 1985, below eq 11) is:

$$L = 4186.8\left(597.31 - 0.56525\,T_{(air\ average)}\right) \tag{11}$$

where the average dry bulb air temperature ($T_{(air\ average)}$) is in Celsius degrees The factor of 4186.8 has the units *J / kcal*. The constant 597.31 has the units *kcal / kg*. The factor 0.56525 has the units *kcal / (kg C)*.

Following Jacquet (pg 172), the latent heat of evaporation (J/kg) is given by

$$L = 4186.8\left(597.1 - 0.57\,T_{(water)}\right) \tag{12}$$

while TVA (eq 4.2) is

$$L = 2500 - 2.39\,T_{(water\ surface)} \times 10^3 \tag{13}$$

Note that Jacquet and TVA use the water surface temperature while Blanc uses the average air temperature. If a model equation for latent heat of evaporation is to be included in any numerical model, this discrepancy should be investigated. However, for practical implementation of a constant latent heat of vaporization, equations (11), (12) and (13) give values for L that are near the value 2.5×10^6 J/kg noted in Gill, (pg 34), and the value of 2.453×10^6 J/kg used in DYRESM.

The water vapor flux (E) model used in Imberger and Patterson (eq 7) is

$$E = C_W\; u_{(wind)}\; \rho_{(air)}\left(q_{(air\ r)} - q_{(surface)}\right) \tag{14}$$

where $u_{(wind)}$ is the wind speed, C_W is the dimensionless bulk transfer coefficient for evaporation (primarily due to wind), $\rho_{(air)}$ is the density of air at the surface in kg/m^3, $q_{(air\ r)}$ is the specific humidity at some reference level in the air, and $q_{(surface)}$ is the specific humidity at the surface. Imberger and Patterson (1981) states that DYRESM uses a C_W of 1.4×10^{-3}. We have defined the above equation such that a negative value indicates a flux out of the water.

An alternative form is given by Jacquet (eq A5.10)

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[7] Some of the literature presents E as a volume flux rather than a mass flux. With this approach, equation (10) would include the density of water.

$$\frac{E}{\rho_{(air)}} = C_{W(J)}\, U_{(wind\,4)} \left(e_{(air\,2)} - e_{(surface)}\right) \qquad [\text{mm/day}] \tag{15}$$

where e are water vapor pressures (saturated at the surface) in millimeters of mercury, $U_{(wind\ 4)}$ is the wind (km / hr) measured 4 meters above the surface, and $C_{W(J)}$ is 7.44×10^{-5}. More detailed and complicated methods can be found in TVA, Blanc, and Herzfeld. The computation of the evaporative flux is arguably the most important and least accurate set of model equations in the free surface heat budget.

We usually do not have data for the specific humidity, so it is convenient to write the specific humidity in terms of vapor pressures and relative humidity. From Reynolds and Perkins (eq 10.33, pg 394)[8], the specific humidity can be written as:

$$q = 0.622\, \frac{e}{P - e} \tag{16}$$

where the dimensionless coefficient 0.622 is obtained as the ratio of the ideal gas constants (or the inverse ratio of molal masses) for air and water vapor, and P is the atmospheric pressure. The dimensionless relative humidity R_h can be written as (Reynolds and Perkins equation 10.34):

$$R_h = \frac{q\,(P - e)}{0.622\, e_{(sat)}} \tag{17}$$

where $e_{(sat)}$ is the saturation vapor pressure. Using equations (16) and (17) we can write:

$$q = R_h\, \frac{0.622\, e_{(sat)}}{P - e} \tag{18}$$

Since the water vapor pressure is small (relative to atmospheric pressure), we can reasonably approximate the specific humidity as:

$$q \approx \frac{0.622\, e_{(sat)}}{P} R_h \tag{19}$$

We can substitute equation (19) into (14) to get the evaporative flux in terms of the relative humidity at a reference altitude and at the free surface. If we do not have a surface value for relative humidity (a common occurrence), then we must make some further assumptions in our model. It is reasonable to assume that the relative humidity is unity at the surface and the saturated vapor pressure at the surface and the reference altitude are approximately equal, so that we can write:

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[8] Note that Reynolds and Perkins (1977) contains a typographical error in equation (10.33), where the ratio of the gas constants R_a/R_w is presented as 0.662. Since the molecular mass of dry air is 28.966 and the molecular mass of water is 18.016 (Gill, pg 597), the gas constant ration is 0.62197. This is correctly shown in Reynolds and Perkins equation (10.34).

$$q_{(air\ r)} - q_{(surface)} \approx \frac{0.622\, e_{(sat)}}{P}\left(R_h - 1\right) \tag{20}$$

Using equations (14) and (20), the evaporative mass flux can be modeled as:

$$E = \frac{0.622}{P} C_W\, u_{(wind)}\, \rho_{(air)}\, e_{(sat)} \left(R_h - 1\right) \tag{21}$$

with the requirements that u is in m/s, ρ is in kg/m^3, $e_{(sat)}$ and P are in Pa. C_w and R_h and 0.622 are dimensionless. As noted previously, the factor 0.622 is derived from the ratio of the ideal gas constants for air and water vapor.

Numerical implementation

The evaporative (latent) heat term is implemented in ELCOM using three approaches. The approach used in a simulation is user-selectable based on the input data available. Where the user has available specific humidity values in the air an at the surface, the appropriate model is:

$$Q_W = L\, C_W\, u_{(wind)}\, \rho_{(air)} \left(q_{(air\ r)} - q_{(surface)}\right) \tag{22}$$

where the latent heat of evaporation is fixed at the value used in DYRESM: 2.453 × 10^6 J / kg (water at 20.4 C°).

If only a specific humidity is available at the reference level, it can be assumed that the surface is near saturation so that the model for the evaporative flux can be written as:

$$E = C_W\, u_{(wind)}\, \rho_{(air)} \left(q_{(air\ r)} - q_{(sat)}\right) \tag{23}$$

The saturation specific humidity can be estimated from

$$q_{(sat)} \approx \frac{0.622}{P} e_{(sat)} \tag{24}$$

The saturation vapor pressure can be approximated from a curve fit to field and laboratory data (Gill, 1982, pg 606):

$$e_{(sat)} = 10^{\left(\frac{0.7859 + 0.03477\, T}{1 + 0.00412\, T} - 3\right)} \tag{25}$$

where the result is the saturation vapor pressure in Pa, and temperatures are in degrees C (valid over a range of +-40 C). Combining equations (23), (24) and (25) gives a model for the evaporative heat flux as:

$$Q_W = L\,C_W\,u_{(wind)}\,\rho_{(air)}\left(q_{(air\,r)} - \frac{0.622\times 10^{\left\{\frac{0.7859+0.03477\,T}{1+0.00412\,T}-3\right\}}}{P}\right)$$

(26)

If we only have a relative humidity value, then from equation (19), the estimate of the specific humidity is

$$q_{(air\,r)} \approx \frac{0.622\,e_{(sat)}}{P}\,R_h$$

(27)

So the third model for evaporative heat flux is

$$Q_W = L\,C_W\,u_{(wind)}\,\rho_{(air)}\,\frac{0.622\times 10^{\left\{\frac{0.7859+0.03477\,T}{1+0.00412\,T}-3\right\}}}{P}\left(R_h - 1\right)$$

(28)

Thus, equations (22), (26) and (28) are a set of three different implementations of the evaporative heat flux model, equation (10).

Sensible heat flux

The energy transfer due to sensible heat flux (i.e. conduction and convection) can be modeled (Imberger and Patterson 1981, eq 7) as:

$$Q_H = C_H\,c_{p\,(air)}\,\rho_{(air)}\,u_{(wind)}\left(T_{(air\,r)} - T_{(water)}\right)$$

(29)

where C_H is the (nondimensional) bulk coefficient of sensible heat transfer, c_p is the specific heat capacity at constant pressure, $T_{(air\,r)}$ is the dry bulb temperature in the air above the water surface at some reference level. This version of the equation maintains the convention that energy transfer out of the water is negative. Imberger and Patterson are not clear on whether the specific heat and density are air or water values, however Fischer *et al.* uses the density and specific heat of air (eq 6.20), as does Gill in (eq 2.4.5).

Jacquet's equation (A5.10) gives the sensible heat transfer as:

$$Q_H = -f\left(\mathrm{Ri}\right)N\,\frac{P}{P_0}\,c_{p\,(air)}\,\rho_{(water)}\,u_{(wind)}\left(T_{(air\,r)} - T_{(water)}\right)$$

(30)

where f is a function of the Richardson number (see Jacquet pg 173), N is a dimensionless evaporation coefficient, P is the atmospheric pressure, and P_0 is the standard atmospheric pressure at sea level. A range of more complicated formulas are provided in TVA and Blanc.

Numerical implementation

Equation (29) will be implemented with $C_H = 1.4 \times 10^{-3}$ as discussed in Imberger and Patterson. The specific heat capacity of air is approximately 1003 J kg^{-1} C^{-1} (Reynolds 1979, pg 4) for typical values of air temperature in the near surface region.

Total surface heat transfer

The surface heat transfer (Q_S), can modeled as the sum of the net radiation heat transfer, the latent heat transfer due to evaporation, and the sensible heat transfer due to conduction and convection (i.e. all the heat transfer across the free surface except short wave radiation):

$$Q_S = Q_R + Q_W + Q_H \tag{31}$$

This surface energy transfer can be assumed to occur over a layer of thickness that is of the order 0.6 to 1.0 meters, with an exponential decay such that[9]:

$$Q_S(z) = Q_S(S)\exp\{-\eta_s(S-z)\} \tag{32}$$

where $Q_S(z)$ is the surface heat energy that has not been absorbed at height z (measured from a coordinate baseline with z positive in the upward direction), $Q_S(S)$ is the surface heat transfer penetrating the water surface, η_s is a bulk extinction coefficient for the surface heat transfer, S is the height of the free surface (measured from the same baseline as z). If we assume that 90% of the surface heat transfer is absorbed in the first 0.6 meters of the domain, then:

$$0.10\, Q_S(S) = Q_S(S)\exp\{-0.6\,\eta_s\} \tag{33}$$

It follows that

$$\eta_s = -\frac{\ln(0.10)}{0.6} = 3.84 \tag{34}$$

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[9] It is generally presumed that convection, conduction and long wave radiation are non-penetrative effects that would appropriately be modeled as a surface boundary condition. However, for geophysical-scale numerical simulations we cannot accurately compute the near-surface turbulent convection in the water that mixes the surface heat transfer down into the near surface region. Thus, if the surface heat transfer is treated simply as a temperature boundary condition, the surface may overheat if the net surface heat transfer is into the domain. Where the surface heat transfer is negative and causes an unstable density profile, a Richardson number mixing model *can* account for some mixing. However, the mixing due to wave and wind generated turbulence (as well as Langmuir circulations) cannot be accounted for in either a Richardson number mixing model or the present 1 meter mixing depth. Note that having the surface heat transfer absorbed arbitrarily in the uppermost grid cell (rather than arbitrarily in the first meter) is undesirable since it results in changing the physical model as the grid size is changed. Our approach is to fix the distance that we expect the surface heat transfer to mix down (via subgrid-scale processes), so that the result is relatively invariant with the grid size. The use of exponential decay to model the distribution of surface heat transfer is a mathematical model that (at this point) does not appear to have any firm backing in the literature. However, without any empirical evidence, this appears to be a reasonable model. A better approach would be to develop a parameterization model that includes wind speed, fetch, duration, waves, and water velocities to obtain a subgrid-scale model for convective mixing near the free surface.

Then at 1.0 meters of depth, then unabsorbed surface heat loss/gain is 2% of the input surface heat energy.

Numerical implementation

The surface heat energy is implemented by integrating down through water column, determining the absorption in each layer. Define the available surface heat transfer energy at the top of the k^{th} layer as $Q_{S(k)}$, and the uppermost layer as the n^{th} layer so that equation (32) can be written as

$$Q_{S(k)} = Q_{S(n)} \exp\left\{ -\eta_s \sum_{i=k+1}^{i=n} \Delta z_{(i)} \right\} \tag{35}$$

where $\Delta z_{(i)}$ is the thickness of the i^{th} layer, and η_s is the bulk extinction coefficient (set to 3.84 to absorb 98% of the surface heat transfer energy in the first meter of the water).

A more convenient method of encoding is to recognize that

$$Q_{S(k)} = Q_{S(k+1)} \exp\left\{ -\eta_s \, \Delta z_{(k+1)} \right\} \tag{36}$$

This is executed for $k = n,m$ (stepping down from the surface layer n by a stride of -1), where m is the cell such that

$$\sum_{k=m+1}^{n} \Delta z_{(k)} \quad < \quad 1.0 \quad \leq \quad \sum_{k=m}^{n} \Delta z_{(k)} \tag{37}$$

This prevents the heat transfer scheme from distributing increasingly small surface heat transfer values through the entire depth of the water column. The surface heat transfer energy absorbed in the k^{th} layer for $m+1 \leq k \leq n$ is:

$$\Delta Q_{S(k)} = Q_{S(k)} - Q_{S(k-1)} \tag{38}$$

The surface heat transfer energy absorbed in the m layer (the lowest layer that has its upper surface less than 1 meter deep) is the remaining energy available:

$$\Delta Q_{S(m)} = Q_{S(m)} \tag{39}$$

Where the depth of the domain is smaller than the penetration of the surface heat transfer (i.e. less than 1 meter), then we evaluate equation (36) for $k = n,b-1$ (stepping down from the surface layer n by a stride of -1), where b is the bottom cell. The surface heat transfer energy remaining after the distribution is $Q_{S(b-1)}$. We do not have any field data or theory that provides appropriate distribution for $Q_{S(b-1)}$, so we will simply assume that a portion of the energy is used to heat the sediments, and the remainder is distributed uniformly throughout the water column. If the total depth of the water column is *D*, we can write (for layer *k*)

$$\Delta Q_{S(k)} = Q_{S(k)} - Q_{S(k-1)} + \left(C_b \, Q_{S(b-1)} \, \frac{\Delta z_{(k)}}{D} \right) \tag{40}$$

where $0 \leq C_b \leq 1.0$ is the fraction of the heat transfer energy at the bottom that is returned to the water column. Until further investigation (or the implementation of a complete sediment heat transfer model), C_b should probably be set to a value near 1.0.

Short wave radiation

The depth of penetration of short wave radiation depends on the net short wave radiation that penetrates the water surface and the bulk extinction coefficient (which is a function of water color, turbidity, plankton concentration, etc.). The equations given in TVA (eq 2.48 and 2.37) and Jacquet (eq A5.2) for the net solar radiation penetrating the water can be written as:

$$Q_{sw}(S) = Q_{(sw\,surface)} \left(1 - 0.65\, C_{(cloud)}{}^{2}\right)\left(1 - R_{t(sw)}\right) \tag{41}$$

where $Q_{(sw\ surface)}$ is the short wave radiation that would reach the surface of the water on a clear day (after atmospheric attenuation, $Q_{sw}(S)$ is the net short wave radiation penetrating the water surface, $C_{(cloud)}$ is the dimensionless fractional cloud cover ($0 \leq C_{(cloud)} \leq 1.0$), and $R_{t(sw)}$ is the dimensionless surface reflectivity for short wave radiation. A method of determining $R_{t(sw)}$ is provided in TVA (pg 2.17). If field data on short wave radiation reaching the surface are available, then the cloud cover term may be eliminated (but not the reflectivity).

The short wave radiation at any depth for a constant bulk extinction coefficient can be found from:

$$Q_{sw}(z) = Q_{sw}(S)\, \exp\left\{-\eta_e\, (S - z)\right\} \tag{42}$$

where $Q_{sw}(z)$ is the short wave radiation absorbed at height z (measured from a coordinate baseline with z positive in the upward direction), $Q_{sw}(S)$ is the net short wave radiation penetrating the water surface, η_e is a bulk extinction coefficient, S is the height of the free surface (measured from the same baseline as z).

Where the short wave radiation reaches the bottom, a complete heat budget model would require: (1) absorption and reflection of the short wave radiation by the sediments, (2) long wave radiation emission from the sediments, and (3) conduction and convection model at the bottom boundary. As a simpler approach, we will consider that any short wave radiation that reaches the bottom boundary is treated by a model similar to that used for the total surface heat transfer near the free surface (i.e. equation 40). Let $Q_{sw}(B)$ represent the short wave radiation that reaches the bottom boundary, and C_r represent the fraction of the short wave radiation that is returned to the water column. Assuming an exponential decay (in the positive z direction), we have

$$Q_r(z) = C_r \; Q_{sw}(B) \exp\{-\eta_r (z - B)\}$$

(43)

where $Q_r(z)$ is the vertical distribution of the heat energy returned to the water column, and η_r is the bulk extinction coefficient for reflected energy.

It is convenient to use the same bulk extinction coefficient used for the total surface heat transfer (i.e. 3.84 m^{-1}). This ensures 98% of the energy returned to the water column is transferred into the first one meter above the bottom.

Numerical implementation

Due to the presence of suspended sediment or phytoplankton, the bulk extinction coefficient (η_e) may change with depth. The short wave radiation at the top of the k^{th} layer is then

$$Q_{sw(k)} = Q_{sw(k+1)} \exp\left\{-\eta_{e(k+1)} \, \Delta z_{(k+1)}\right\}$$

(44)

so that the short wave radiation heat transfer into layer k is

$$\Delta Q_{sw(k)} = Q_{sw(k)} - Q_{sw(k-1)}$$

(45)

To prevent computation of small values of short wave radiation at large depths, we can set a condition for stopping the computation at layer m such that

$$\frac{Q_{sw(m)}}{Q_{sw(n)}} \le 0.02 < \frac{Q_{sw(m+1)}}{Q_{sw(n)}}$$

(46)

where the n layer is the water surface. The remaining short wave radiation, $Q_{sw(m)}$, is considered to be stored in the $m-1$ layer.

Where the bottom is reached before condition in equation (46) is met, the remaining energy $(Q_{sw(b-1)})$ is “reflected”[10] into the water column using an implementation of equation (43):

$$Q_{r(k)} = Q_{r(k-1)} \exp\left\{-\eta_{r(k)} \, \Delta z_{(k)}\right\}$$

(47)

This equation must be integrated up from the bottom. Again, we apply the convention that $Q_{r(k)}$ is the reflected heat transfer energy at the top of the k^{th} layer, so that:

$$Q_{r(b)} = Q_{sw(b-1)} \exp\left\{-\eta_{r(b)} \, \Delta z_{(b)}\right\}$$

(48)

The reflected heat transfer into layer k is

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[10] We are not actually modeling the only the reflection of the short wave radiation, but also the long wave radiation emissions from the sediments and convection and conduction from sediments as they are warmed by the short wave radiation. However, it is convenient to lump all these terms into a “reflected” heat transfer.

$$\Delta Q_{r(k)} = Q_{r(k)} - Q_{r(k-1)} \tag{49}$$

The condition for stopping the computation at layer *m* is

$$\frac{Q_{r(m)}}{Q_{sw(n)}} \leq 0.02 < \frac{Q_{r(m-1)}}{Q_{sw(n)}} \tag{50}$$

The remaining heat transfer energy, $Q_{r(k)}$, is considered to be absorbed in the *m*+1 layer.

It is possible (in a very shallow domain) that the stopping condition in equation (50) may not be met before the free surface is reached with the reflected heat transfer. In such a case, the remaining heat energy, $Q_{r(n)}$, can be distributed evenly over the water column. Thus, a more comprehensive version of equation (49) is:

$$\Delta Q_{r(k)} = Q_{r(k)} - Q_{r(k-1)} + \left(Q_{r(n)} \frac{\Delta z_{(k)}}{D} \right) \tag{51}$$

Where water quality parameters are not invoked, the user can input either a bulk extinction coefficient or a depth to which the light penetrates. In the latter case, the bulk extinction coefficient is computed from:

$$\eta_e = -\frac{\ln(C_v)}{D_v} \tag{52}$$

where D_v is the visible depth (user input) and C_v is the fraction of the short wave radiation that must penetrate to a depth for visibility. Properly setting C_v requires a literature review of Secchi depths.

Change in cell temperature

The total heat transfer *(ΔQ_T)* into a computational cell with location *(i,j,k)* is the sum of the surface heat transfer and the shortwave radiation heat transfer:

$$\Delta Q_{T(i,j,k)} = \Delta Q_{S(i,j,k)} + \Delta Q_{sw(i,j,k)} \tag{53}$$

The relationship between the change in internal energy *(ΔE_T)* in a volume *(V)* and the change in temperature *(ΔT)* is given by:

$$\Delta E_T = \rho \, V \, c_p \, \Delta T \tag{54}$$

The heat transfer used in this paper has been in terms of power per unit area, so the total energy transfer into a computational cell of length Δx and width Δy in time Δt can be given as:

$$\Delta E_T = \Delta Q_T \, \Delta x \, \Delta y \, \Delta t \tag{55}$$

It follows that the temperature change can be written as:

$$\Delta T = \frac{\Delta Q_T \, \Delta x \, \Delta y \, \Delta t}{\rho \, V \, c_p} \tag{56}$$

or, more simply as:

$$\Delta T = \frac{\Delta Q_T \, \Delta t}{\rho \, c_p \, \Delta z} \tag{57}$$

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