Appendix A Ocean Model

The formulation of bulk mixed layer models is based on the observation that the top layer of the ocean is well mixed and is bounded below by a highly stratified pycnocline. The interplay between turbulence energy supplied to the ocean by surface winds and buoyancy forcing provided by surface heat fluxes determines the depth of this well mixed layer. Surface heat (freshwater) fluxes and the exchange of heat (freshwater) from below the mixed layer through entrainment effect the temperature (salinity) of the mixed layer. The solution of the Turbulent Kinetic Energy (TKE) equation to calculate entrainment (or mixed layer depth) is simplified by assuming a uniform distribution of properties throughout the upper layer of the ocean.

This study employs a mixed layer model (MLM) developed by Alexander (1992a) which is based on the classic formulation of Niiler and Kraus (1977) (NK). Temperature, salinity, and mixed layer depth are predicted by the ocean model. The entrainment formulation of Gaspar (1988), which treats the parameterization of the dissipation of TKE differently than NK, was incorporated in the MLM to accommodate multi-year simulations . The dissipation in Niiler and Kraus (1977) is a constant fraction of the creation of TKE, whereas in Gaspar (1988) it depends on rotation and stability.

The ocean model is described in section A1 and the numerical methods and model parameters are discussed in section A2.

A.1 Ocean model

Following Niiler and Kraus (1977), the upper ocean in midlatitudes is represented by a well mixed surface layer with uniform temperature and salinity and a sharp discontinuity in these quantities at the base of the mixed layer. Integrating the continuity equations for heat and salt over the mixed layer depth yields:

$$\frac{\partial T_{om}}{\partial t} = w_e (T_b - T_{om}) / h + \frac{(Q_{tot} - Q_{SWH})}{\rho_0 C_p h} + \frac{v_H}{h} \frac{\partial T_{om}}{\partial z} \bigg|_{z = h}$$
(A1)

$$\frac{\partial S_{om}}{\partial t} = w_e (S_b - S_{om}) / h + \frac{S_{om} (E - P)}{\rho_0 h} + \frac{v_S}{h} \frac{\partial S_{om}}{\partial z} \bigg|_{z = h}$$
(A2)

where *T* is the temperature, *S* the salinity, *t* the time, w_e the entrainment rate, *h* the mixed layer depth, ρ_o the reference density, C_P the specific heat, *z* the vertical coordinate (positive down), *E* the evaporation rate, *P* the precipitation rate, Q_{SWH} the penetrating solar radiation, and $v_H(v_S)$ the molecular diffusion coefficient for heat (salt). Subscripts *om* and *b* represent conditions within and below the mixed layer, respectively. The net *surface* heat flux is given by:

$$Q_{tot} = Q_L + Q_S + Q_{SW} + Q_{LWnet}$$
(A3)

where the fluxes are positive downwards and Q_{SW} is the shortwave radiation, Q_{LWnet} the net longwave radiation, and $Q_{S}(Q_{L})$ is the sensible (latent) heat flux. The heat flux below the surface is due to penetrating solar radiation is calculated up to a depth of 300 meters and is prescribed following Paulson and Simpson (1977):

$$Q_{SWH} = Q_{SW}(R \cdot exp(-z/\xi_1) + (1-R) \cdot exp(-z/\xi_2)).$$
 (A4)

The constants R, ξ_1 and ξ_2 (see Table A-1) depend on the optical water type (see Jerlov 1967) for which values over the N. Atlantic have been obtained from Simonot and Le Treut (1986). At the base of the mixed layer, the water properties T_b and S_b are obtained directly from the layer in which *h* resides; below the mixed layer, temperature and salinity evolve according to:

$$\frac{\partial T}{\partial t} = \frac{1}{\rho_0 C_p} \frac{\partial Q}{\partial z} + \nu_H \frac{\partial^2 T}{\partial z^2}$$
(A5)

$$\frac{\partial \mathbf{S}}{\partial t} = \mathbf{v}_{\mathbf{S}} \frac{\partial^2 \mathbf{S}}{\partial z^2} \tag{A6}$$

There are two additional processes that influence the temperature and salinity within the model: convective overturning and an adjustment to conserve model properties. Convective adjustment occurs when the density of a layer exceeds the density of the layer below. The temperature of both layers is subsequently set to the mass-weighted mean. The conservation of heat, salt and potential energy (Adamec et al., 1981) is ensured by adjusting T_{om} and T_b according to

$$T'_{m} = T_{b} + \frac{(D_{k} - h - D_{m})h(T_{m} - T_{b})}{D_{k}D_{m}}$$
 (A7)

$$T'_{b} = T_{b} + \frac{(h - D_{m})h(T_{m} - T_{b})}{D_{k}(D_{k} - D_{m})}$$
(A8)

where $D_k = \sum_{l=1}^k \Delta z_l$ and $D_m = max(h, D_k - \Delta z_k)$. Salinity is analogously adjusted.

The entrainment rate is derived from vertically integrating the turbulent kinetic energy equation over the mixed layer depth and then parameterizing the resulting terms using the known variables. The formula, common to most mixed layer models, can be expressed as follows:

$$w_{e} = \frac{mu_{*}^{3} - 0.5hB(h) - h\varepsilon}{q^{2} + 0.5(h\Delta b - s\Delta \bar{v})}$$
(A9)

where

$$B(h) = \frac{\alpha g}{\rho_{ref} C_P} \left(Q_{tot} + Q_{SWH} - \frac{2}{h} \int_0^h Q dz \right) + \frac{\beta g S_m}{\rho} (P - E)$$
(A10)

$$\Delta b = \alpha g \Delta T - \beta g \Delta S \tag{A11}$$

 $\Delta = \{()_{om} - ()_{b}\}$ represents the discontinuity at the base of the mixed layer, u_{*}

is the friction velocity, ε the turbulent dissipation rate, \forall the velocity, q^2 the mean turbulent kinetic energy, and *m* and *s* are constants determined from observations. The thermal expansion coefficients α and β are determined from the international equation of state for sea water. The three terms in the numerator of (A9) represent the effects of wind stirring, changes in the buoyancy due to surface fluxes and penetrating solar radiation, and the dissipation of energy within the mixed layer. The terms in the denominator of (A9) are the energy required to agitate entrained water, and the buoyancy jump at the base of the mixed layer. The instability term resulting from the shear across the base of the mixed layer is not included due to the transient nature of this term. The mean turbulent kinetic energy is parameterized according to Kim (1976):

$$q = 9 \cdot \max(10^{-4} m^2 s^{-2}, u_*^2)$$
(A12)

Dissipation is an important process in the mixed layer: several approaches have been used to parameterize this term (cf., Niiler and Kraus 1977; Garwood 1977; Gaspar 1988). We use the formulation of Gaspar, as his model is designed for use in extended integrations (i.e., for integrations longer than a season). In addition, the model with this formulation of entrainment simulates better the depth of the mixed layer in summer. When $w_e \ge 0$, $\frac{dh}{dt} = w_e$ and w_e in (A9) becomes a function of the mixed layer depth, the Monin-Obukov length and the Ekman length scale. When the mixed layer shallows, *h* is solved iteratively until a balance is reached between the wind stirring and the net buoyancy forcing over the depth of the mixed layer.



Figure A-1. Schematic of the (A) mixed layer and (B) convective-diffusive components of the ocean model where τ is the windstress, Q_{tot} the total heat flux at the surface of the ocean, T_m (S_m) the mixed layer temperature (salinity), E the evaporation, P the precipitation, T_b (S_b) the temperature (salinity) in the layer below the mixed layer and h_m the mixed layer depth.

The convective-diffusive (CD) model works in conjunction with the mixed layer model to represent the temperature and salinity in the layers of the ocean below the mixed layer. Figure A-1 presents a schematic of the mixed layer and the CD components of the ocean model. The physical processes represented in the CD model are convective overturning and diffusion, which are discussed earlier in this section.

The CD model consists of 30 unevenly spaced layers starting at the surface and reaching 1000 meters. The vertical resolution is higher at the top of the ocean in order to model better the summer pycnocline. The thicknesses of the 30 model layers starting from the surface are as follows: 10, 5, 5, 5, 5, 5, 5, 10, 10, 10, 10, 10, 10, 10, 10, 10, 20, 20, 20, 50, 50, 50, 100, 100, 100, 100, 100, and 1000 meters. The temperature (salinity) of the layers that are completely in the mixed layer are set to the temperature (salinity) of the mixed layer (Figure A-1). Layers below the mixed layer evolve according to the processes of convective overturning and diffusion except for the bottom layer which has a fixed temperature and salinity.

A.2 Numerical methods, model constraints and initial conditions

The prognostic equations for T_{om} , S_{om} and *h* are solved using a fourth order Runge-Kutta scheme, which requires information at only one previous time step. All prognostic model equations are integrated using a one-day time step. Below the mixed layer, the integration is a forward differencing scheme in time.

The mixed layer depth is constrained to be greater than 10m and less than 850m to ensure computational stability. While long-lived mixed layer depths less than 10m are extremely rare in Nature, there is the potential for the model to simulate such shallow mixed layers in summer, as there are processes that act to keep the mixed layer away from the surface (e.g., surface wave mixing) that are not included in the model. In the hindcast integrations presented in Chapter 3 of this thesis, the mixed layer is initialized with the climatological values of T and S from Levitus (1982) as prepared by Samuels and Cox (1987).

The depths to which solar radiation can penetrate depends on the optical properties of the sea water. Jerlov (1976) classified ocean water according to its clarity, with type I being the clearest. Using the observed distribution of solar irradiance with depth in the ocean, Paulson and Simpson (1977) determined for different water types the coefficients used in Equation A-4 (see Table A-1) to calculate penetrating solar radiation . The distribution of water types used in this study for the North Atlantic was taken from Simenot and Le Treut (1986) and is shown in Table A-2.

Water Type	R	ζ ₁ (m)	ζ ₂ (m)
Ι	.58	.35	23
IA	.62	.6	20
IB	.67	1.	17
II	.77	1.5	14
III	.78	1.4	7.9

Table 2-1. Values of R, ζ_1 , and ζ_2 from Paulson and Simpson (1977) associated with the optical water types defined by Jerlov (1976). R, ζ_1 , and ζ_2 are the percentage of solar radiation absorbed in the upper few meters of the ocean, the attenuation coefficients for above 10 meters and for below 10 meters, respectively

	-98°	-90°	-83°	-75°	-68°	-60°	-53°	-45°	-38°	-30°	-23°	-15°	-8°	0°
60°	@	@	@	@			III	II	III	III	II	II	II	III
56°	@	@	@	@	@	@	III	III	III	III	II	II	III	III
51°	@	@	@	@	@	@	III	III	III	III	III	III	III	@
47°	@	@	@	@	@	III	III	III	III	II	III	III	III	@
42°	@	@	@	@	II	II	II	III	II	II	II	II	@	@
38°	@	@	@	III	II	IB	IB	II	II	IB	IB	IB	@	@
33°	@	@	@	II	IB	@	@							
29°		III	III	II	Ι	IA	IB	IB	IB	IB	IB	IB	@	@
24°		II	II	II	Ι	IA	IA	IA	IB	IB	II	II	@	@
20°	@	IB	II	IB	IB	IB	IA	IA	IB	II	II	@	@	@

Table 2-2. Distribution of water types used in the ocean model for the North Atlantic Ocean taken from Simenot and Le Treuet (1986). Land points are shown with a '@'.The top row indicates the longitude and the first column the latitude of the domain.

Constant	Symbol	Value
ocean reference density	ρ _o	1024.438 kg/m3
specific heat of sea water	C _P	3950 J/kg °K
diffusion coefficient for heat (salt)	$\nu_{H}^{}(\nu_{S}^{})$	$2 \times 10^{-5} \text{ m}^2/\text{s}$

 Table 2-3. Values of constants used in the ocean model.

Constants used in the ocean model are listed in Table A-3.

Sea ice is not predicted but is specified according to the observed climatology of Alexander and Mobley (1976). When sea ice appears it is assumed to cover an entire grid box and the surface fluxes are prescribed as follows: $Q_{tot} = -2.0W \text{ m}^{-2}$, $Q_{sw} = 0$, and taux and tauy are set to one third of their value. In addition, the ocean temperature below the sea ice is set to 271.2 °K, which is the freezing point of ocean water (for S~35 ppt).