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A simple model of plankton population dynamics coupled with a LES of the surface mixed layer

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Abstract

The concentration of phytoplankton in the sea is affected by biological processes, such as growth/mortality rates, predatory zooplankton concentrations and nutrient levels. Phytoplankton concentrations are also influenced by physical processes, in particular the mixing properties of the local fluid environment. On planktonic scales ($\sim 10-1000 \,\mu$ m) one can assume the local turbulent flow is isotropic, with no distinction between horizontal and vertical mixing. However, agglomerations of phytoplankton into patches are observed on larger scales of up to hundreds of metres, whose formation will be influenced by the anisotropic advection/mixing properties and large-eddy structures prevalent in the surface mixed layer. This paper presents the results of the coupling of a large-eddy simulation (LES) model of the mixed layer with an advection–diffusion system of coupled equations for nitrate–phytoplankton–zooplankton growth due to light levels and ambient nitrate concentration, offset by grazing losses due to the presence of zooplankton. The primary goal of this work is to investigate how the characteristics of the mixed layer turbulence influence the observed distribution of phytoplankton. One novel feature is the incorporation of a 'vortex-force' term in the LES code in order to generate Langmuir circulations. It has been speculated that the enhanced mixing rates associated with 'Langmuir turbulence' play a significant role in regulating planktonic activity. Results derived from the coupled LES–*NPZ* model, run with and without the presence of Langmuir circulations, are presented in order to investigate these ideas. © 2005 Elsevier Ltd. All rights reserved.

Keywords: Large-eddy simulations; Plankton population dynamics; NPZ models; Mixed layer turbulence; Langmuir circulations

1. Introduction

The importance of the physical processes influencing the motion of the sea on the distribution and dynamics of phytoplankton populations is widely recognized (e.g. Denman and Gargett, 1995; Wiafe and Frid, 1996; Bees et al., 1998; Yamazaki et al., 2002). One problem facing researchers in seeking to model these biological–physical interactions is the enormous range of spatial scales involved. Large biologically productive regions are observed on ocean basin scales ~1000 km (e.g. Lewis et al., 1988). Typically these regions are associated with large-scale up-welling zones, which transport nutrients into the surface mixed layer and stimulate phytoplankton photosynthesis (Bryden and Brady, 1985; Franks et al., 1986; McGillicuddy et al., 1995a, b). At the same time individual predator-prey encounters are governed by turbulent motion on the scale of millimetres (Rothschild and Osborn, 1988; Lewis and Pedley, 2000; Lewis, 2003). Reconciling all the biological-physical interactions across such a wide range of scales presents a formidable challenge, which is currently beyond the scope of any model of a planktonic ecosystem. However, the continued advances in computational power and resources, does open up the possibility of studying the influence of physical processes on plankton population dynamics at intermediate scales (tens of metres), namely

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those associated with the large-eddy structures of turbulence in the ocean mixed layer. One well-established empirical feature of plankton populations is their spatial patchiness e.g. Pinel-Alloul (1995), Solow and Steele (1995), Gallager et al. (1996) and Franks and Walstad (1997), on a variety of different scales. The persistence of these patches is somewhat surprising given the high levels of turbulent mixing normally prevalent in the mixed layer. This is particularly so when the most basic assumption is that the mixed layer is biologically homogeneous, i.e. the physical mixing rates are much faster than any biological processes (Fasham et al., 1990). One of the objectives of this paper will be to try and establish the necessary conditions for 'patch' formation, characteristics of their spatial scale and temporal longevity.

In order to attempt to answer some of these questions this paper will present a coupled large-eddy simulation (LES) model of the ocean mixed layer with a simple nitrate-phytoplankton-zooplankton (NPZ)model (Franks, 2002) used to describe plankton dynamics. It has long been thought that mixed layer turbulence exerts a considerable influence on biological productivity (Marrasé et al., 1990; Kiørboe, 1993; MacKenzie et al., 1994), in particular the effects of rapid vertical mixing motions over scales comparable with the mixed layer depth. In order to study such phenomena it is necessary to incorporate a dynamical model that resolves the largest energy containing scales explicitly. Computational limitations currently rule out this sort of resolution via direct numerical simulations (DNS) of the Navier-Stokes equations, and hence LES has been suggested as a substitute, e.g. Franks (1995) and Denman and Gargett (1995). The idea of coupling a biological model of three (or more) components with a physical model of mixed layer is not new, but nearly all previous attempts employ one-dimensional parameterizations of the vertical mixing processes (see for instance Denman and Peña, 1999; Flierl and McGillicuddy, 2002 and references therein). The relative simplicity of such models means they can be employed to study both seasonal and annual variations in the biological populations, at the expense of investigating their spatial variability. The adoption of a fully three-dimensional LES model obviates this drawback, although the expanded spatial domain necessitates that the simulations are restricted to much more modest time-scales (~ 1 day here). Consequently, more emphasis in this work will be to placed on the formation and nature of any horizontal heterogeneity in the biological fields, features which are absent in previous models.

One unusual feature of the LES model employed here is the incorporation of a 'vortex force' term brought about by a coupling of the Stokes-drift velocity associated with surface waves and the local vorticity. This 'vortex force' term is thought to be the mechanism underlying the formation of Langmuir circulations (Craik and Leibovich, 1976), near surface counter rotating roll cells (called Langmuir cells) aligned roughly in the wind direction. Associated with these cells are upand down-welling zones, where levels of vertical mixing are greatly increased. It has been speculated (Woodcock, 1993; Bees et al., 1998) that such enhanced mixing rates, characteristic of 'Langmuir turbulence', will play a significant role in stimulating planktonic activity. In particular, large Langmuir circulations should enhance biological production by rapidly cycling the phytoplankton through the sunlit zone. At the same time, speculation has centred on what influence, if any, the coherent and persistent Langmuir roll cell pattern has on the spatial distribution of the phytoplankton. To this end a number of model runs have been conducted with and without the 'vortex force' term in order to investigate these hypotheses.

The layout of the paper is as follows. Section 2 describes the LES of the mixed layer to be employed and presents some comparisons with published LES work for validation purposes. The biological *NPZ* model is discussed in Section 3 and together with the parameterizations made and the boundary conditions employed in this work. Section 4 presents a series of results derived from runs of the fully coupled biological–physical system, which are the main focus of the paper. Finally, some concluding remarks are presented in Section 5.

2. The LES model of the ocean mixed layer

Skyllingstad and Denbo (1995) and McWilliams et al. (1997) both employed LES in order to study Langmuir circulations. The results of McWilliams et al. (1997) will be used as a benchmark to validate the results of the LES model used here. Briefly, the results of applying both a spatial and temporal filter (over one wave period) to the full Navier–Stokes equations, is a reduced set of equations first derived by Craik and Leibovich (1976), viz.

$$\frac{D\boldsymbol{u}}{Dt} + f\hat{\boldsymbol{k}} \times (\boldsymbol{u} + \boldsymbol{U}_S) = -\frac{\nabla p_S}{\rho_0} - g \frac{\rho'}{\rho_0} \hat{\boldsymbol{k}} + \frac{\boldsymbol{U}_S \times \boldsymbol{\omega}}{\text{vortex force}} + SGS,$$
(1)

$$(D/Dt \equiv \partial/\partial t + u.\nabla)$$
 plus continuity

$$\nabla \boldsymbol{u} = \boldsymbol{0} \tag{2}$$

and energy

$$\frac{D\theta}{Dt} + U_S \cdot \nabla \theta = SGS. \tag{3}$$

Here $u(\mathbf{x}) = [u(\mathbf{x}), v(\mathbf{x}), w(\mathbf{x})] = [u_1, u_2, u_3]$ is the (resolved) turbulent velocity field, $\omega(x) = \nabla \times u(\mathbf{x})$ the vorticity, $\theta(\mathbf{x}) = \theta_r + \theta'(\mathbf{x})$ the temperature field and $\rho(\mathbf{x}) = \rho_0 + \rho'(\mathbf{x})$ the fluid density at position

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 $\mathbf{x} = (x, y, z)$. As in McWilliams et al. (1997) the density is assumed to be proportional to the temperature, such that $\rho'/\rho_0 = \theta'/\theta_r$ where ρ_0 and θ_r are suitable reference density and temperature scales, respectively $(\rho_0 = 1000 \text{ kg m}^{-3} \text{ and } \theta_r = 288.15 \text{ K})$. In addition $p_S =$ $p + \rho_0 [2\mathbf{u}.\mathbf{U}_S + U_S^2]/2$ is a generalized pressure term, gthe acceleration due to gravity, f the Coriolis frequency $(f = 10^{-4} \text{ s}^{-1} \text{ here})$, and \mathbf{U}_S is the Stokes drift velocity. The latter is estimated by assuming that the ocean consists of steady, monochromatic deep-water waves (which for convenience will be assumed to propagate in the positive x direction) of the form

$$\eta = a \cos(kx - \sigma t),\tag{4}$$

where $\eta(x, t)$ is the position of the free surface (z = 0)being the average surface height) *a* the wave amplitude, *k* the wavenumber and $\sigma = (gk)^{1/2}$ the wave frequency. The Stokes drift associated with such a wave is $U_S = (U_S e^{2kz}, 0, 0)$ where $U_S = \sigma ka^2$ (Philips, 1977).

The sub-grid scales (SGSs) terms used to close the set of equations are not shown explicitly. Basically a standard Smagorinsky (1963) scheme is employed, in which the Reynolds stresses $\overline{u'_iu'_j}$ (where overbar denotes the filtering operation) are related to the non-isotropic part of the rate of the resolved strain tensor S_{ij}

$$\overline{u_i'u_j'} = -\upsilon_T S_{ij} = -\upsilon_T \left[\left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} \right) - \frac{2}{3} \,\delta_{ij} \nabla \boldsymbol{.} \boldsymbol{u} \right], \tag{5}$$

by means of an eddy viscosity v_T . Note the distinction between q' denoting the unresolved part of a scalar quantity $q_{total} = \bar{q} + q'$, $(\bar{q} = q$ being the resolved part after the application of the spatial and temporal filter) and q'' used later to denote a fluctuation in the resolved scalar quantity q derived from the filtered Eqs. (1)–(3). Likewise the turbulent buoyancy fluxes can be modelled in terms of v_T , viz.

$$\overline{u_i'\theta'} = \frac{v_T}{Pr} \frac{\partial\theta}{\partial x_i},\tag{6}$$

where Pr is a turbulent Prandtl number. Typically in LES the turbulent kinetic energy equation is not solved explicitly, and instead the SGS energy dissipation rate ε is defined in terms of a velocity scale U and a length scale L by $\varepsilon = U^3/L$. Assuming $v_T = UL = L^{4/3}\varepsilon^{1/3}$ and the energy dissipation rate equates to the shear production $-\overline{u'_iu'_i}S_{ij}/2$, one obtains

$$v_T(\mathbf{x}) = CL^2 \sqrt{\frac{S_{ij}S_{ij}}{2}} = CL^2 S(\mathbf{x}), \tag{7}$$

where C is an O(1) constant. The art of LES is to make appropriate choices for C and L to satisfy the surface boundary conditions (e.g. Sullivan et al., 1994).

In these simulations (following McWilliams et al., 1997) a fixed wind stress of $\tau = 0.037 \text{ Nm}^{-2}$ (corresponding to a wind speed of about 5 m s^{-1}) is applied in

the positive x direction, so that

$$\left. \frac{\partial u}{\partial z} \right|_{z=0} = \frac{\tau}{\rho_0} = U_*^2, \tag{8}$$

where $U_* = 6.1 \times 10^{-3} \text{m s}^{-1}$ is a friction velocity. In addition, the boundary layer was assumed to be slightly convective, with a turbulent buoyancy flux $w'\theta' = -1.2 \times 10^{-6} \text{ K m s}^{-1}$, which implies a Monin–Obukhov length, defined here to be

$$L_{Mon} = \frac{17.3 U_*^3 \theta_r}{q \mathbf{k} \overline{w' \theta'}} \tag{9}$$

of -240 m as in McWilliams et al. (1997) (Here $k \approx 0.4$ is von Kármán's constant and $(\alpha \theta_r)^{-1} \approx 17.3$, with the thermal expansion coefficient $\alpha = 2 \times 10^{-4} \text{ K}^{-1}$ again as used by McWilliams et al., 1997.) Near the surface $u \approx$ $U_* \log(z + z_0)/k$, where z_0 is a sea surface roughness length, and $S \approx \partial u/\partial z$, allowing one to postulate a suitable form for *L* using Eqs. (7) and (8). Following Mason and Sykes (1982) it can be shown that

$$\frac{1}{L^2} = \left(\frac{C^{1/2}\phi_m(z/L_{Mon})}{k(z+z_0)}\right)^2 + \frac{1}{L_0^2},\tag{10}$$

where ϕ_m is the Monin–Obukhov similarity function defined such that $\partial u/\partial z = U_*\phi_m[(z+z_0)/L_{Mon}]/k(z+z_0)$ in the surface layer and L_0 is the upper limit of L. Here L_0 is a resolution scale, set to be 1 m throughout these simulations (In practice, varying L_0 found between 1 and 3 m had little influence on the results.) The Craik–Leibovich equations (1)–(3) and the modified surface boundary condition (8) were incorporated into the UK Meteorological Office LES code (which utilizes the closure relations (5)–(7) and (10)), described in much more detail in Wood et al. (1999) (including calculations of *C*). Other boundary conditions imposed on the flow were horizontal periodicity, w = 0 at the surface, and w = 0, zero stress and zero heat flux at the bottom of the boundary layer.

In order to validate the changes made, a number of preliminary runs were carried out in order to attempt to replicate the published results of McWilliams et al. (1997). Hence the selected run parameterizations mirror their work very closely. The Craik-Leibovich equations were solved over a domain $120 \times 120 \text{ m}^2$ horizontally and to a mixed layer depth $z_{ML} = 33 \,\mathrm{m}$ on a grid of $40 \times 40 \times 75$. This implies basic resolution scales of $\Delta x = \Delta y = 3$ m and $\Delta z = 0.45$ m (although the vertical grid was staggered, so the vertical resolution was greater near the surface) similar to McWilliams et al. (1997). One crucial difference is that the latter incorporated a stably stratified region in their model extending from z = -33 to -90 m, below the surface mixed layer. This required the imposition of an outward wave radiation condition at the bottom (Klemp and Duran, 1983), which proved impossible to incorporate satisfactorily in

this model. However, as one is primarily interested in reproducing the characteristics of the turbulent mixed layer and given that McWilliams et al. (1997) results show that the velocity field is virtually zero below 33 m, this omission is unlikely to prove significant in practice. Two basic simulations were performed, the first using the wave parameters $U_S = 0.068 \,\mathrm{m \, s^{-1}}$ (Langmuir No. $La = (U_*/U_S)^{1/2} = 0.3)$ and $k = 0.105 \text{ m}^{-1}$ of McWilliams et al. (1997). Initially this run was allowed to spinup from rest for a period $\tau_{spin} = 5000 \, \text{s}$, until a quasiequilibrium state was reached. Second a shear turbulence run was performed, with the Stokes drift set to zero ($La = \infty$) and spin-up time $\tau_{spin} = 60\,000\,\text{s}$. Subsequently, a number of different turbulent statistics were collected, averaged over both time and space (horizontally across the x-y plane) (The symbol $\langle \rangle$ will be used to denote such averaging.) The typical averaging time was 60 000 s, which is equivalent to $\sim 13T_E$, where T_E is a large-eddy turnover time-scale (For this work it will be defined by $T_E = L_E^{2/3}/\epsilon^{1/3}$, where L_E is a large-eddy scale. At a depth of z = -30 m, $L_E \approx 30$, $\langle \epsilon \rangle \sim 1 \times$ $10^{-8} \,\mathrm{m^2 \, s^{-3}}$ and $T_E \approx 4500 \,\mathrm{s.}$)

Fig. 1 shows a comparison of the mean horizontal velocities $\langle u \rangle$ and $\langle v \rangle$ obtained using the modified Met Office code and the results published in McWilliams et al. (1997) (specifically the S/0.3 and S/ ∞ runs of that paper). The results agree pretty well, the main characteristic being that the mean flow is directed south-southwest throughout the mixed layer ($\langle u \rangle$ and $\langle v \rangle$ are both negative except close to the surface) when the Stokes drift is present (Fig. 1a), compared with the 'shear turbulence case when the near-surface flow is more closely aligned with the easterly wind direction (Fig. 1b). The current deflection away from the easterly wind direction exhibited by the Langmuir simulation is considerable more than the 45° or so predicted by standard lamina Ekman theory. It is a direct result of the wave-induced Stokes drift coupling with the Coriolis force to produce a wave stress in the interior of the flow which deflects the mean current counter-clockwise, typically by more than 75° just below the surface. Observations of current flows (Price and Sundermeyer, 1999) confirm that such high-value current deflection angles are a characteristic feature of the Stokes-Ekman layer (Lewis and Belcher, 2004).

Fig. 2 shows a comparison of the total shear-stress profiles (both the resolved and unresolved parts derived from the closure relation (5)) $\langle u''w'' \rangle + \overline{u'w'}$ and $\langle v''w'' \rangle + \overline{v'w'}$, normalized by U_*^2 . The former is constrained by boundary condition (8) to be unity at the surface. The agreement is good although the $\langle v''w'' \rangle + \overline{v'w'}$ values are slightly less than those obtained by McWilliams et al. (1997) in both cases. Generally, the magnitudes of these shear stresses are larger for the Langmuir run (Fig. 2a) than the 'shear turbulence run' (Fig. 2b), highlighting



Fig. 1. Time and spatially (horizontally across the x-y plane) averaged horizontal velocity profiles $\langle u \rangle$ and $\langle v \rangle$. The solid lines are the results derived from the current LES code. The corresponding profiles from McWilliams et al. (1997) are also shown as $* * * * \equiv \langle u \rangle$ and $+ + + + \equiv \langle v \rangle$. (a) is for the Langmuir simulation with $U_S = 0.068 \text{ m s}^{-1}$, and (b) is for the case when $U_S = 0$.

the enhanced levels of turbulent mixing, which are a feature of Langmuir turbulence.

Fig. 3 shows a comparison of the mean velocity variance profiles $\langle u''^2 \rangle$, $\langle v''^2 \rangle$ and $\langle w''^2 \rangle$ for the two different runs. Fig. 3a illustrates the anisotropic nature of Langmuir turbulence in that $\langle u''^2 \rangle \leq \langle v''^2 \rangle \sim \langle w''^2 \rangle$ throughout most of the mixed layer. Physically this is due to the tilting and stretching of elements of vertical

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Fig. 2. Total averaged shear stress profiles $\langle u''w'' \rangle + \overline{u'w'}$ and $\langle v''w'' \rangle + \overline{v'w'}$, normalized by U_*^2 . Solid lines are derived from the current LES code. The corresponding profiles from McWilliams et al. (1997) are also shown as $* * * \equiv \langle u''w'' \rangle + \overline{u'w'}$ and $+ + + \pm \langle v''w' \rangle + \overline{v'w'}$. (a) is for the Langmuir simulation with $U_S = 0.068 \text{ m s}^{-1}$, and (b) is for the case when $U_S = 0$.

vorticity by the Stokes drift of the wave (Teixeira and Belcher, 2002) along the direction of wave propagation. This leads to the formation of Langmuir cells, the series of counter-rotating vortices aligned with the wind direction, which are characteristic of this form of turbulence. It also leads to an intensification of the turbulence in the directions perpendicular to the direction of wave propagation, hence the domination of $\langle v''^2 \rangle$ and $\langle w''^2 \rangle$ over $\langle u''^2 \rangle$. Notice too that $\langle w''^2 \rangle$ remains large throughout the mixed layer indicating the presence of the Langmuir cells leads to enhanced levels of vertical mixing. By contrast for the shear turbulence run (Fig. 3b), the variances are more isotropic in nature and the magnitudes reduced, particularly for $\langle w''^2 \rangle$ when Langmuir cells are absent.

The organization of these cells is confirmed by taking horizontal sections of the instantaneous vertical velocity at different depths, as shown in Figs. 11d, 12d and 13d (actually taken from simulations of the coupled biological-physical model, but the physical parameters are identical to the model discussed above). For a Langmuir simulation (Figs. 11d and 12d) the typical cellular pattern of alternating up- and down-welling zones (dark and light strips), elongated in the wind/wave direction (x-axis) is immediately apparent. The zones are particularly narrow near the surface (Fig. 11d), and tend to exhibit a slight south easterly trend (which increases with depth). The down-welling zones are more intense and narrower than the corresponding up-welling ones. Results derived from a purely shear driven turbulence run (Fig. 13d) show that the intensity of the up- and down-welling zones is much reduced (although there is still a certain elongation in the wind direction). These patterns closely resemble the corresponding figures of Skyllingstad and Denbo (1995) and McWilliams et al. (1997).

Finally, Fig. 4 shows the profile of the mean kinetic energy dissipation rate $\langle \varepsilon(z) \rangle$ for the two simulations. This quantity is derived from the resolved scale turbulent kinetic energy budget equation

$$\frac{1}{2} \frac{d\langle u_i''^2 \rangle}{dt} = -\frac{1}{2} \frac{d\langle w'' u_i''^2 \rangle}{dz} - \frac{1}{\rho_0} \frac{d\langle w'' p'' \rangle}{dz} - \langle u'' w'' \rangle \frac{d\langle u \rangle}{dz} - \langle v'' w'' \rangle \frac{d\langle v \rangle}{dz} - \langle u'' w'' \rangle \frac{dU_S}{dz} + \alpha g \langle \theta'' w'' \rangle - \langle \varepsilon \rangle.$$
(11)

Eq. (11) can be derived from Eq. (1) by standard methods of Reynolds decomposition and horizontal averaging (e.g. Hinze, 1975). The terms on the righthand side represent turbulent transport, pressure working, shear production, Stokes production, buoyancy production and SGS dissipation. At equilibrium, the left-hand side is zero and one can estimate $\langle \epsilon(z) \rangle$ from the balance of the other terms. In practice, for the shear turbulence run the shear production terms dominate, but in Langmuir turbulence the Stokes production combines with an increased pressure working term to produce raised levels of turbulent kinetic energy. This results in enhanced levels of $\langle \epsilon(z) \rangle$, particularly near the



Fig. 3. Time-averaged velocity variance profiles $\langle u''^2 \rangle$, $\langle v''^2 \rangle$ and $\langle w''^2 \rangle$, normalised by U_*^2 . Solid lines are derived from the current LES code. The corresponding profiles from McWilliams et al. (1997) are also shown as $* * * = \langle u''^2 \rangle$, $+ + + + = \langle v''^2 \rangle$ and $\wedge \wedge \wedge = \langle w''^2 \rangle$. (a) is for the Langmuir simulation with $U_S = 0.068 \text{ m s}^{-1}$, and (b) is for the case when $U_S = 0$.

surface, as illustrated in Fig. 4. Experimental observations of this phenomenon are described in Terray et al. (1996). The overall agreement with the results of McWilliams et al. (1997) demonstrates the satisfactory nature of the LES code.

3. The biological model

The biological model incorporated into the LES code is basically a three-state *NPZ* model of plankton population dynamics of a type widely used in the biological literature, e.g. Kiefer and

Atkinson (1984), Franks (1995), Edwards and Brindley (1996) and Edwards et al. (2000). It consists of three advection–diffusion equations for the concentrations of nitrate $N^*(\mathbf{x}, t)$, phytoplankton $P^*(\mathbf{x}, t)$ and zooplankton $Z^*(\mathbf{x}, t)$ (the sizes of the micro-organisms are assumed to be sufficiently small, $<10^{-4}$ m, to justify a continuum hypothesis and the treatment of their concentrations as scalar fields) of the form

$$\frac{DN}{Dt} + U_S \cdot \nabla N = D_{TN} \nabla^2 N - N \text{ uptake by } P$$
$$+ N \text{ recycled from } P \text{ growth,} \qquad (12)$$



Fig. 4. Mean kinetic energy dissipation rate profiles $\langle \varepsilon(z) \rangle$, normalized by $U_*^3/z_{ML} \approx 7 \times 10^{-9} \text{ m}^2 \text{ s}^{-3}$. The solid lines are derived from the current LES code. The corresponding profiles from McWilliams et al. (1997) are also shown as + + + + for the Langmuir simulation with $U_S = 0.068 \text{ m s}^{-1}$, and * * * * for the shear turbulence simulation with $U_S = 0$.

$$\frac{DP}{Dt} + U_S \cdot \nabla P = D_{TP} \nabla^2 P + P \text{ growth from } N$$
$$-Z \text{ grazing loss,} \tag{13}$$

$$\frac{DZ}{Dt} + U_S \cdot \nabla Z = D_{TZ} \nabla^2 Z + Z \text{ growth grazing } P$$
$$-Z \text{ mortality,} \tag{14}$$

where u is the instantaneous (LES) turbulent velocity field and $D_{TN/P/Z}$ turbulent eddy diffusivities. Here, the equations for the scalar fields have been non-dimensionalized such that $N = N^*/N_0$, $P = P^*/P_0$ and Z = Z^*/Z_0 , where N_0 (kg m⁻³), P_0 (cells/m⁻³) and Z_0 (cells/m⁻³) are suitable (constant) reference scales. Alongside the advection/diffusion terms in Eqs. (12)–(14) there are a number of source/sink terms, which take place on small SGSs, which are derived from the biology. Their form, and the associated boundary conditions, will be discussed in the following subsections. Most of the formulations are based on the work of Baird and Emsley (1999) and, consequently, only brief details of their derivation are given. Exceptions are the equations for nitrate uptake (not original, but some modifications are needed to allow coupling into the LES) and the phytoplankton grazing loss (original) which are discussed in rather more detail. Specific variations of this class of biological model have been successfully employed to replicate observations of a wide variety of planktonic ecosystems on many

different length scales (see the review of Franks (2002) for a summary of examples). Hence, it is the most natural type of biological model to incorporate with the more sophisticated LES of the mixed layer discussed in the previous section.

3.1. Nitrate uptake by phytoplankton

The basic equation for the flux of nitrate Q_N , into a spherical phytoplankton cell of radius r_P , takes the form (Baird and Emsley, 1999)

$$Q_N(z)$$

$$= \begin{cases} 4\pi r_p Sh_{turbulent}(z)D_N \\ \times N^*(1 - N_S/N^*), & N_S/N^* < 1, \\ 0 & \text{otherwise.} \end{cases}$$
(15)

Here D_N is the molecular diffusivity of nitrate (~ $10^{-9} \,\mathrm{m^2 \, s^{-1}}$), N_S is the nitrate concentration at the cell's surface and N^* the ambient nitrate concentration level. The non-dimensional Sherwood number $Sh_{turbulent} \ge 1$ is a measure of the ratio of the total nitrate flux at the cell's surface in the presence of relative fluid motion (which has the effect of increasing the local nitrate concentration gradients and hence the flux into the cell) to the flux obtained through diffusion alone (when Sh = 1). The value of Sh is itself determined by the dimensionless Péclet number Pe which measures the relative strength of advective transport to diffusive transport over a particular length scale r. In general it takes the form

$$Pe = \frac{Ur}{D_N},\tag{16}$$

where U is a particular velocity scale, characterizing the swimming speed/fluid motion near the cell. When $Pe \ll 1$ diffusion is the main transport mechanism, whilst when $Pe \gg 1$ advection predominates.

In these simulations the phytoplankton cells are assumed to be non-motile, but the ambient fluid is turbulent, characterized by its associated turbulent kinetic energy dissipation rate $\langle \varepsilon \rangle$. The first theoretical study of the phenomenon of mass transport in turbulent flows was carried out by Batchelor (1980). Karp-Boss et al. (1996), summarizing Batchelor's work, suggest that for small cells with $r_P < \eta$ (where $\eta = (v^3/\langle \varepsilon \rangle)^{1/4}$ is the Kolmogorov microscale, v being the kinematic viscosity of sea water $\sim 10^{-6} \text{ m}^2 \text{ s}^{-1}$), a suitable definition for a turbulent Péclet number is given by

$$Pe_{turbulent} = \frac{r_p U_{turbulent}}{D_N}, \text{ where } U_{turbulent} = \left(\frac{\langle \varepsilon \rangle}{\upsilon}\right)^{1/2} r_P.$$
(17)

. ...

They go on to suggest that the associated turbulent Sh number can be estimated from $Pe_{turbulent}$ via

the equation

$$Sh_{turbulent} = \begin{cases} 1 + 0.29Pe_{turbulent}^{1/2}, \\ 0.5 \left[1.969 + 0.15Pe_{turbulent}^{1/2} + 0.344Pe_{turbulent}^{1/3} \right] \\ 0.55Pe_{turbulent}^{1/3}, \end{cases}$$

where Eq. (18b) represents an average of two suggested interpolation schemes. The expressions that appear in Eq. (18) are based on theoretical results of nutrient uptake in a pure (non-rotating) shear flow. Unfortunately, there is very little empirical evidence of uptake in turbulent flows that could be used to validate these predictions. The functional dependence of Q_N on depth z, explicit in Eq. (15), derives from the depth dependence of $\langle \varepsilon(z) \rangle$ (as illustrated in Fig. 4), via Eqs. (17) and (18). In practice, for a phytoplankton cell of radius $r_p =$ 10^{-5} m employed here, $Pe_{turbulent}(z) < 0.08$ for all $\langle \varepsilon(z) \rangle$, and only Eqs. (18a,b) are relevant in calculating $Sh_{turbulent}(z)$.

It remains to estimate the relative surface nitrate concentration N_S/N^* . In a turbulent flow it is very difficult to make practical estimates. However, it is recognized that the uptake rate of any cell will be limited by its physiological state, in particular the nitrate reserves R_N (kg/cell⁻¹) stored in the cell at any one time. In Baird and Emsley's (1999) biological model, the total nutrient (nitrate) reserves available to the phytoplankton were carried as a fourth scalar field in addition to the N, P and Z fields employed here. The additional computational demands of the LES of the mixed layer precludes the possibility of calculating R_N explicitly here, and hence the term needs to modelled. The most common assumption is that R_N and N_S are linearly related (although in a subsequent paper, Baird et al. (2001), more complicated nonlinear relationships are studied), in which case the term $(1 - R_N/R_N^{\text{max}})$ can be substituted for $(1 - N_S/N^*)$ in Eq. (15), where R_N^{max} is a measure of the maximum storage capacity of a single cell.

The problem now is to estimate R_N/R_N^{max} . The usual procedure is to assume the system reaches a steady state of mass balance, in which nitrate uptake is equal to consumption through growth. In a turbulent flow the system is never actually steady, so the validity of such an assumption is less clear. However, it seems reasonable to assume that there exists some fixed ambient nitrate

$$Pe_{turbulent} \leq 0.01,$$

$$0.01 < Pe_{turbulent} < 100,$$
 (18a,b,c)

$$Pe_{turbulent} \geq 100,$$

concentration level N_0 at which a mass balance is reached and

$$4\pi r_p Sh_{turbulent}(z) D_N N_0 \left(1 - \frac{R_{N_0}(z)}{R_N^{\max}}\right) = \mu_P^{\max} \frac{R_{N_0}(z)}{R_N^{\max}} (s_N + R_{N_0}(z)).$$
(19)

Here μ_P^{max} is the maximum phytoplankton growth rate, s_N (kg/cell⁻¹) is a nitrate stoichiometry coefficient, essentially quantifying the minimal amount needed for a cell to be viable and $R_{N_0}(z)$ represents the average stored reserves at this ambient concentration level N_0 . The term $(s_N + R_{N_0}(z))$ on the left-hand side of Eq. (19) reflects the fact that some nitrate is needed to maintain a cell's upkeep, whilst some is used in the production of daughter cells (Baird et al., 2001). The value of N_0 was chosen to reflect the average nitrate concentration of the thermocline (where the flow is relatively quiescent and a steady-state mass balance is likely to be attained), 2×10^{-3} mol nitrogen m⁻³ \equiv estimated to be $2.8 \times 10^{-5} \text{ kg m}^{-3}$ in Fasham et al. (1990). Eq. (19) is a quadratic in $R_{N_0}(z)$, which can easily be solved to give

$$\frac{R_{N_0}(z)}{R_N^{\max}} \approx 1 - \frac{R_N^{\max} \mu_P^{\max}}{4\pi r_P D_N Sh(z) N_0}.$$
(20)

Having established $R_{N_0}(z)/R_N^{\text{max}}$ when $N = N_0$, it is necessary to estimate its value for general nitrate concentration levels. With no empirical evidence from turbulent flows to go on, the simplest choice is to assume a linear relationship based on Eq. (20), namely

$$\frac{R_N(\mathbf{x},t)}{R_N^{\max}} = \begin{cases} \frac{R_{N_0}(z)}{R_N^{\max}} \left[\frac{N^*(\mathbf{x},t)}{N_0} \right] & \text{assuming this is } \leqslant 1, \\ 1 & \text{otherwise.} \end{cases}$$
(21)

All the above analysis applies for a single phytoplankton cell. Hence, the final form of the nitrate uptake term in Eq. (12) for an ambient phytoplankton concentration $P^*(\mathbf{x}, t)$ will be

$$N \text{ uptake by } P = \begin{cases} 4\pi r_P Sh(z) D_N N(\mathbf{x}, t) \left[1 - \frac{R_N(\mathbf{x}, t)}{R_N^{\max}} \right] P^*(\mathbf{x}, t) & \text{if } 0 \leq \frac{R_N}{R_N^{\max}} \leq 1 \\ 0 & \text{if } \frac{R_N}{R_N^{\max}} > 1 \end{cases}$$
(22)

3.2. Nitrate recycled

Inefficiency of phytoplankton growth usually leads to a recycling of nitrate back into the ocean. Following Baird and Emsley (1999) this term was modelled by

Nitrate recycled =
$$(1 - \beta_E) \frac{s_N P^*(\mathbf{x}, t)}{N_0} \times \left[\mu_P^{\max} e^{\alpha z} \min\left(1, \frac{R_N(\mathbf{x}, t)}{R_N^{\max}}\right) \right].$$
 (23)

The term in square brackets essentially represents the growth rate of the phytoplankton, regulated by the average nitrate reserves in a cell $R_N(\mathbf{x}, t)$ and the local light intensity level available for photosynthesis. Generally this is assumed to decay exponentially with depth, with the light attenuation coefficient due to water $\alpha = 0.04 \,\mathrm{m^{-1}}$ (Fasham et al., 1990). The dimensionless parameter $\beta_E \in [0, 1]$ is just a reflection of the efficiency of the phytoplankton growth process of the species under consideration. Typically, for the parameter values employed here the recycling term is some ten times smaller than the uptake term.

3.3. Phytoplankton growth

This term is essentially the analogue of the nitraterecycled term above. Potentially phytoplankton growth is determined by μ_P^{max} , but is regulated by light levels, cellular nitrate reserves and growth efficiency. Following Baird and Emsley (1999) one has

$$P \text{ growth} = \beta_E \min\left[1, \frac{R_N(\boldsymbol{x}, t)}{R_N^{\max}}\right] e^{\alpha z} \mu_P^{\max} P(\boldsymbol{x}, t).$$
(24)

3.4. Grazing loss

Estimates of grazing loss due to zooplankton predation depend essentially on two parameters, the encounter rate between zooplankton and phytoplankton cells, and the probability of capture given an encounter. Encounter rate depends on the product of the prey density, the square of the predator's contact radius R(assuming that a predator's perception field is spherical) and a relative velocity scale, which depends upon the swimming capabilities of the micro-organisms concerned. Turbulence has the effect of increasing encounter rate (Rothschild and Osborn, 1988), by adding a term to the relative velocity scale that is proportional to $\langle \varepsilon \rangle R^{1/3}$. Lewis and Pedley (2000), by means of theoretical analysis and backed by numerical simulations, established the following formula for the turbulent encounter rate:

$$ER = \langle f_v(U(R), R, n, \tau) \rangle 4\rho_P R^2 \sqrt{\frac{\pi}{2}} \sigma_U(R).$$
(25)

Here, ρ_P is the prey density (assumed uniform in those calculations) and the relative velocity scale satisfies

$$\sigma_U^2(R) = \frac{4}{3} \int_0^\infty E(k) \left[1 - \frac{\sin(kR)}{kR} \right] \mathrm{d}k + \sigma_H^2 + \sigma_P^2, \qquad (26)$$

assuming the predator and prey swimming speeds are drawn from Gaussian distributions of zero mean, with standard deviations σ_P and σ_H , respectively. E(k) is the turbulent kinetic energy spectrum (Batchelor, 1953), which in the inertial subrange takes the form (Tennekes and Lumley, 1972)

$$E(k) = \frac{3}{2} \langle \varepsilon \rangle^{2/3} k^{-5/3}, \tag{27}$$

giving rise to the $R^{1/3}$ dependence of σ_U . The volume fraction term $\langle f_{U}(U(R), \hat{R}, n, \tau) \rangle$ is a number between zero and one, which estimates the relative encounter volume a predator maps out following an irregular path (which depends on τ a time-scale reflecting how long it takes to make a distinct change of direction, which in turn depends on the relative strengths of its swimming speed and the flow field and n the number of direction changes in a given time period), as opposed to moving in a straight line. For the latter $\langle f_V \rangle = 1$, but following an irregular path means that, on average, a predator will tend to linger and revisit previously searched areas (encounter volume is reduced because there is overlap between moves), reducing encounters and $\langle f_V \rangle < 1$. For a predator with a given search strategy, estimates of $\langle f_V \rangle$ can be made by Monte Carlo simulations (Lewis and Pedley, 2000).

In Lewis and Pedley (2001) these ideas were extended to look at how often an encountered prey might be captured. This is a complicated problem, depending upon the speed and reaction of the predator in question, as well as the escape capabilities of the prey. Rather than try and model the behaviour of any particular species a more general and simplified approach to the capture problem was adopted, which would hopefully prove applicable to a wide range of predator-prey interactions. The main idea was to assume that on encountering a prey, a predator has only a certain limited time interval available in which to make a capture attempt. This interval was taken to be the time a prey would naturally transverse the predator's perception sphere, assuming no predator reaction. In turn, one can relate this time to the closest approach between the predator and prey r_m , again assuming that does not attempt to facilitate a capture. The predation rate can then be derived from Eq. (25) in the form

$$PR = \rho_P 4 \sqrt{\frac{\pi}{2}} \int_0^R \left\{ -\frac{\mathrm{d}p_{cap}}{\mathrm{d}r_m} \right\} r_m^2 \langle f_v(U(r_m), r_m, n, \tau) \rangle \sigma(r_m) \,\mathrm{d}r_m,$$
(28)

where $p_{cap}(r_m)$ is the probability of capture when the closest approach distance is r_m . A variety of possible functional forms could be substituted into Eq. (30) for

 $p_{cap}(r_m)$. One possibility highlighted in Lewis and Pedley (2001) is to set

$$p_{cap}(r_m) = \frac{\langle t(r_m) \rangle^{\beta}}{\langle t(r_m) \rangle^{\beta} + T_R^{\beta}}.$$
(29)

Here $\langle t(r_m) \rangle$ is the average time a prey takes to transverse a predator's perception sphere assuming a closet approach of r_m , T_R is a time-scale encapsulating the trade off between how fast the predator can react, fixate and lunge at its prey, and the latter's escape capabilities; and β is a shape parameter. Lewis and Pedley (2001) give full details of how $\langle t(r_m) \rangle$ can be calculated, depending upon the prey's path across the perception sphere. Comparisons with numerical simulations suggested that a path composed of a circular arc was best and this approach was adopted here. If T_R small relative to $\langle t(r_m) \rangle$ the predator will be an efficient feeder, and efficiency will decrease as T_R increases.

Two problems remain. First, to specify the relative velocity scale $\sigma_U(r_m)$ to give suitable values over the range $r_m \in [0, R]$, rather than just $r_m = R$ as was the case in Eq. (25). This can be done by setting (Monin and Yaglom, 1975)

$$\sigma_U^2(r_m) = \frac{c_1 r_m^2}{1 + c_2 r_m^{4/3}} + \sigma_P^2 + \sigma_H^2$$
(30)

with $c_1 = \frac{1}{9}$ and

$$c_2 = \frac{[c_1 R^2 / (\sigma_U^2(R) - \sigma_H^2 - \sigma_P^2) - 1]}{R^{4/3}},$$
(31)

which ensures Eq. (30) gives the correct value of σ_U at $r_m = R$. Second, the calculation of the volume fraction over a range of r_m by Monte Carlo simulation is computationally expensive. In order to avoid this a simple linear interpolation was employed in Eq. (30), linking the value $\langle f_v \rangle = 1$ at $r_m = 0$ to the value at $r_m = R$, viz.

$$\langle f_v(U(r_m), r_m, n, \tau) \rangle = \left\{ 1 + \frac{r_m}{R} [\langle f_v(U(R), R, n, \tau) \rangle - 1] \right\}.$$
(32)

Typical values of $\langle f_V(U(R), R, n, \tau) \rangle$, for a range of turbulent regimes and swimming behaviours, lie in the range 0.5–0.8, and a value of 0.7 was used for all the simulations discussed here. Hence, the final form for the grazing loss term in Eq. (13) for local phytoplankton density $P^*(\mathbf{x}, t)$ and local zooplankton density $Z^*(\mathbf{x}, t)$ is

Grazing loss =
$$Z^*(\mathbf{x}, t) \frac{P^*(\mathbf{x}, t)}{P_0} 4\sqrt{\frac{\pi}{2}}$$

 $\times \int_0^R \left\{-\frac{\mathrm{d}p_{cap}}{\mathrm{d}r_m}\right\} r_m^2 \left[1 - 0.3 \frac{r_m}{R}\right] \sigma_U(r_m) \,\mathrm{d}r_m.$
(33)

It should be pointed out that the calculations behind Eqs. (28) and (33) assume the local turbulent regime is homogeneous, isotropic and statistically stationary. Planktonic contact scales $\sim 1-40 \times 10^{-3}$ m lie well below the limit of the large-eddy scale resolution, and on these small scales such an assumption is reasonable. Of course on the larger explicitly resolved scales, particularly near the surface, the turbulent regime is far from isotropic (as illustrated in Fig. 3). A more serious drawback is the assumption that the predator's perception field is spherical. Browman and Skiftesvik (1996) point out that many predatory zooplankton species have perception fields that resemble forward facing wedges. Such a restricted perception field will inevitably reduce the number of prey encounters significantly. Experimental observations, highlighted in Galbraith et al. (2004), also suggest that the enhancement of encounter rate by the turbulent flow is likely to be less significant for predators with this type of perception field, than those with full all round 'vision'. Hence, it is very probable that the predation rate predicted by Eqs. (28) and (33) is too large for most zooplankton species. Although the problem of encounter rate for predators with limited perception fields has been studied theoretically (Lewis, 2003), the author is not aware of any studies of capture probabilities (which are fundamental to any estimate of predation rate), in turbulent conditions, for such predators. Consequently, the results based on spherical perception fields described here are retained, until something better can be substituted.

3.5. Zooplankton growth through grazing

This term essentially depends on how the grazing term discussed in the previous section manifests itself in the production of new zooplankton cells. Assuming a yield Y of new predator cells per prey cell captured, then the growth rate derived from grazing can be calculated simply by multiplying Y by the predation rate (28). However, for this work it was assumed that the zooplankton growth could not exceed some fixed maximum value μ_Z^{max} . Consequently, the zooplankton growth rate term used in Eq. (14) takes the form

$$Z \text{ growth} = \min\left[\mu_Z^{\max}, YP^*(\mathbf{x}, t)4\sqrt{\frac{\pi}{2}} \times \int_0^R \left\{-\frac{\mathrm{d}p_{cap}}{\mathrm{d}r_m}\right\} r_m^2 \left(1 - 0.3\frac{r_m}{R}\right) \mathrm{d}r_m\right] \frac{Z^*(\mathbf{x}, t)}{Z_0}.$$
(34)

3.6. Mortality rate

Zooplankton growth was assumed to be limited by a mortality rate term given by

$$\mu_{Z \ death} \frac{Z^*(\boldsymbol{x}, t)}{Z_0},\tag{35}$$

in Eq. (14). Fasham et al. (1990) gives a value of 0.05 per day (~ $6 \times 10^{-7} \text{ s}^{-1}$) for $\mu_Z \text{ death}$ and this value was used here (Franks et al., 1986 give values for $\mu_Z \text{ death}$ some 2–3 times larger, which would tend to regulate the relatively rapid growth in Z that is a feature of the simulations described in Section 4.) This parameter includes both natural and predator mortality, and in practice will depend largely on the particular zooplankton species in question. It may also exhibit a seasonal variation.

3.7. Diffusive terms

The magnitude of these terms is regulated by the sizes of the turbulent eddy diffusion coefficients $D_{TN/P/Z}$ for nitrate, phytoplankton and zooplankton, respectively. Diffusion on molecular scales tends to smooth out concentration gradients in a solute scalar field. It is conventional to think of this as a scalar transport process (from parts of the fluid at high scalar concentration to those parts at low concentrations) and to express the effectiveness of this process relative to the molecular momentum transport (in the sense that any shearing motion of the flow transports momentum across a fluid element in the flow) by means of a dimensionless Schmidt number

$$Sc = \frac{v}{D},$$
 (36)

where D is the molecular diffusivity. In a turbulent flow, the Reynolds stresses are frequently assumed to act like viscous stresses, i.e. their magnitudes are directly proportional to the velocity gradient. This idea forms the basis of the closure model discussed in Section 2, Eq. (5). Although the validity of such an assumption is open to debate, it is conventional (e.g. McComb, 1991) to characterize turbulent transport of a scalar field in terms of the gradient of mean concentrations, and introduce an analogous equation to Eqs. (5) and (6), such that

$$\overline{\Gamma' u'_i} = D_{T\Gamma} \frac{\partial \Gamma}{\partial x_i} \quad (\Gamma = N, P, Z).$$
(37)

The relative strength of the turbulent transport of momentum and scalar is summarized by means of a turbulent Schmidt number

$$Sc_{turbulent} = \frac{v_T(\mathbf{x})}{D_{T\Gamma}(\mathbf{x})} \quad (\Gamma = N, P, Z).$$
(38)

Recently, there have been a number of papers using DNS to examine the phenomena of scalar transport and dispersion in isotropic turbulence for a wide range of Schmidt numbers, e.g. Yeung (2001) and Brethouwer et al. (2003). However, in DNS it is possible to obtain much higher spatial resolution (down to the Kolmogorov and Batchelor microscales), whereas for LES the resolution scale is only $\sim (\Delta x \Delta y \Delta z)^{1/3} \approx 1.59$ m. Em-

ploying a Schmidt number greater than one would imply that the scalar fields contain more small-scale structure than the velocity fields, which cannot be justified for this resolution. So logically it only makes sense to consider $Sc_{turbulent} < 1$. For LES, Sullivan et al. (1994) suggest a relation between v_T and D_{TT} of the form

$$Sc_{turbulent} = \frac{\upsilon_T}{D_{T\Gamma}} = \frac{1}{(1 + 2L_0/\Delta)},\tag{39}$$

where $\Delta^3 = (3\Delta x/2)(3\Delta y/2)\Delta z$. Here, $\Delta \approx 2$ and $L_0 = 1$ which implies $Sc_{turbulent} \approx 1/2$, and this value was used for all three scalar fields in the biological model.

3.8. Boundary conditions and parameter values

Eqs. (12)–(14) can only be solved subject to various boundary conditions. Horizontal periodicity and zero surface flux conditions were imposed, i.e.

$$\left. \frac{\partial \Gamma}{\partial z} \right|_{z=0} = 0 \quad (\Gamma = N, P, Z).$$
(40)

At the lower boundary the equations were solved subject to certain prescribed fluxes into and out of the mixed layer, i.e.

$$\frac{\upsilon_T}{Sc_{turbulent}} \left. \frac{\partial \Gamma}{\partial z} \right|_{z_{ML} = -50 \text{ m}} = \langle w\Gamma \rangle \quad (\Gamma = N, P, Z).$$
(41)

Nitrate stocks can be replenished from nutrient rich deep water of the permanent thermocline. Wind forcing drives major up-welling gyres, ensuring that on average the mixed layer receives a steady supply of nutrients which phytoplankton can use to photosynthezise. Williams and Follows (1998) estimate the vertical flux of nitrate by this means can reach a maximum of $2 \times$ 10^{-8} mol N m⁻² s⁻¹ (equivalent to $\langle wN^* \rangle = -2.8 \times$ $10^{-10} \,\mathrm{kg}\,\mathrm{m}^{-2}\,\mathrm{s}^{-1}$ assuming 1 mol of $N \equiv 0.014 \,\mathrm{kg}$, and negative because $z_{ML} < 0$) and this value was used for the simulations here. Nitrate can also cross the thermocline by diffusion. Fasham et al. (1990) estimates the net vertical flux of nitrate by this method to be about $2.3 \times$ 10^{-9} mol N m⁻² s⁻¹. For these intermediate scale simulations no provision is made for the type of large-scale wind-driven vertical mixing described in Williams and Follows (1998). Indeed the water column is relatively quiescent at the mixed layer boundary (see Figs. 1-3), so it is possible that diffusion is the more appropriate replenishment mechanism. Consequently, the value $\langle wN^* \rangle = -2.8 \times 10^{-10} \text{ kg m}^{-2} \text{ s}^{-1}$ maybe somewhat too large, although the results of the simulations suggest this is not a critical parameter in regulating the planktonic population levels.

The fluxes of P and Z are more problematic. Following Baird and Emsley (1999) it was assumed that all the micro-organisms were denser than the surrounding fluid and hence are subject to a gravitational force. This means in the absence of fluid flow (or swimming) they will have a tendency to settle at some terminal sinking velocity U_{sink} . One can estimate U_{sink} from a force balance between gravity and the friction exerted on a cell by the surrounding fluid, which gives

$$gV(\rho_{P/Z} - \rho_0) = C_D \mu U_{sink}.$$
(42)

Here V is the volume of a cell, $\rho_{P/Z}$ the cell density, C_D a drag coefficient and the viscosity of water $\mu = 1 \times 10^{-3} \text{ kg m}^{-1} \text{ s}^{-1}$. For spherical cells $C_D = 6\pi r_{P/Z}$ where $r_{P/Z}$ is the cell radius and

$$U_{sink} = \frac{2gr_{P/Z}(\rho_{P/Z} - \rho_0)}{9\mu}.$$
 (43)

The outward flux is then given by the product of the normalized cell concentration and U_{sink} . For these simulations it will be assumed that living cells can maintain their relative position in the water column (either by swimming or some other mechanism) and that only a small proportion $\phi_{\Gamma}^{dead} \ll 1$ of dead cells will settle in the manner outlined. Hence the outward flux boundary conditions employed were

$$\frac{\upsilon_T}{Sc_{turbulent}} \left. \frac{\partial \Gamma}{\partial z} \right|_{z_{ML} = -50} = U_{sink} \phi_{\Gamma}^{dead} \Gamma_{z_{ML} = -50} \quad (\Gamma = P \text{ or } Z).$$
(44)

Table 1 shows a list of the baseline parameter values used for the LES–*NPZ* model simulations to be discussed in the next section. The vast majority will remain constant for all the simulations. The background concentrations (equivalent to 0.02 ml^{-1} for the zooplankton and 5 ml^{-1} for the phytoplankton) are relatively dilute. Many of the other parameters are taken from the results published in Baird and Emsley (1999), or derived from relationships postulated by Hansen et al. (1997). It should be pointed out that the average zooplankton swimming speed σ_Z only plays a

Table 1 Biological parameter values used in the LES-*NPZ* model role in the capture probability function (29)–(31), not in the general motion of the scalar field. Essentially the assumption is that the zooplankton adopts an 'ambush'type predation strategy, only engaging in active swimming after perceiving a nearby prey.

4. Results

4.1. Simulations performed

Simulations of the coupled LES-NPZ model were carried out for two contrasting turbulence regimes. In the first, a Stokes-Ekman mixed layer was generated, incorporating the vortex force term as discussed in Section 2 (with identical parameter values, except that for the coupled model the mixed layer depth was extended to 50 m from 33 m). Runs of the biological model subject to this 'Langmuir turbulence' regime were compared to a second set of simulations carried out in a regular turbulent mixed layer (shear turbulence) with the vortex force term switched off. On each occasion the boundary layer was spun up from rest for a time τ_{spin} , before the various biological scalar fields were added (the initial distributions of the scalar fields were uniform, with initial values N_0 for N^* , $P_0/2$ for P^* and $Z_0/2$ for Z^* , respectively).

The most critical parameter in the biological model regulating the planktonic population levels is zooplankton predation. For these runs two different types of predator were studied, an efficient one with a characteristic reaction time $T_R = 5$ s and an inefficient one with $T_R = 15$ s (In general a predator's reaction time is usually somewhat faster than this, but T_R must also take into account a potential prey's escape response, which will reduce predatory efficiency.) Fig. 5a shows the magnitude of the predation rate for these two types of

Parameter and symbol	Numerical value	Parameter and symbol	Numerical value
Background Z concentration Z_0	2×10^4 cells m ⁻³	Contact radius R ^c	$2 \times 10^{-3} \mathrm{m}$
Background P concentration P_0	5×10^6 cells m ⁻³	Z reaction time T_R	5 and 15 s
Background $N^{\rm a}$ concentration N_0	$2.8 \times 10^{-5} \mathrm{kg}\mathrm{m}^{-3}$	Capture probability ^d parameter β	2
Z cell radius r_Z	$5 \times 10^{-5} \text{m} \equiv V_Z = 5.2 \times 10^{-13} \text{ m}^3$	Volume fraction $\langle f_V \rangle^{\rm e}$	0.7
<i>P</i> cell radius r_P	$1 \times 10^{-5} \mathrm{m} \equiv V_P = 4.2 \times 10^{-15} \mathrm{m}^3$	^b Yield Y	$0.003 \sim 0.33 V_P / V_Z$
Density of water ρ_0	$1000 \text{kg} \text{m}^{-3}$	<i>P</i> growth efficiency β_E^{f}	0.75
<i>P</i> cell density ρ_P	$1.002\rho_0$	Light attenuation coefficient α^a	$0.04{ m m}^{-1}$
Z cell density ρ_Z	$1.02\rho_0$	Proportion of dead <i>P</i> cells ϕ_P^{dead}	10 ⁻³
<i>P</i> maximum ^b growth rate μ_P^{max}	$2.5 \times 10^{-5} \mathrm{s}^{-1} \sim 2.4 \times 10^{-8} V_P^{-0.21}$	Proportion of dead Z cells ϕ_Z^{dead}	10^{-5}
Z maximum ^b growth rate μ_Z^{max}	$1.0 \times 10^{-5} \mathrm{s}^{-1} \sim 2.4 \times 10^{-8} V_Z^{-0.21}$	Nitrate stoichiometry coefficient s_N^g	$2.7 \times 10^{-14} \mathrm{kg} \mathrm{cell}^{-1} \sim \frac{1.38 \times 10^3 V_P}{3}$
Z death rate $\mu_{Z \ death}^{a}$	$6 \times 10^{-7} \mathrm{s}^{-1}$	Nitrate flux into mixed layer $\langle wN^* \rangle^h$	$-2.8 \times 10^{-10} \mathrm{kg}\mathrm{m}^{-2}\mathrm{s}^{-1}$
Z swimming speed σ_{z}^{b}	$5 \times 10^{-5} \mathrm{m s^{-1}} \sim 1.97 \times 10^{-2} V_{-2}^{0.2}$		

(*Sources*: ^a Fasham et al., 1990; ^b Hansen et al., 1997; ^c Muelbert et al., 1994; ^d Lewis and Pedley, 2001; ^e Lewis and Pedley, 2000; ^f Baird and Emsley, 1999; ^g Straile, 1997; ^h Williams and Follows, 1998).



Fig. 5. Predation rate profiles derived from Eqs. (30)–(34) over the 50 m boundary layer used for the coupled LES–*NPZ* model simulations. The profiles show the predation rate for the 'efficient' predator when $T_R = 5$ s and those for the 'inefficient' predator when $T_R = 15$ s. (a) is for the Langmuir turbulence regime ($U_S = 0.068 \text{ m s}^{-1}$) and (b) the shear turbulence regime ($U_S = 0$). Also shown is the predation level for the 'efficient' predator in a 'No Flow' regime, when the energy dissipation rate is set to a very low uniform value of $6.8 \times 10^{-12} \text{ m}^2 \text{ s}^{-3}$.

predator in Langmuir turbulence, whilst Fig. 5b presents the equivalent data in the shear turbulence regime. The results depend crucially on the variation of $\langle \varepsilon \rangle$ with z as shown in Fig. 4 (the only difference being that in the 50 m boundary layer the dissipation rate is about 10% smaller in the upper layers, but dies off more slowly at greater depths). In Langmuir turbulence the efficient predator is able to maintain a very high predation rate, particularly close to the surface. By contrast the inefficient predator's predation rate falls off close to the surface. The local turbulent intensity is simply too high for it to capture any of the numerous prey it



Fig. 6. Time-averaged normalized mean concentration profiles $m_P(z, T)$ and $m_Z(z, T)$ (a); and time-averaged concentration intensity profiles $I_N^2(z, T)$, $I_P^2(z, T)$ and $I_Z^2(z, T)$ (b); from the uncoupled NPZ model simulation run. (Here 'TIME' refers to the time after spin-up when the scalar biological fields were added to the boundary layer, with initially Z = P = 0.5 at t = 0). The averages were calculated at various intermediate times shown at the bottom of (a). The intensity averages, which are calculated at the same times, evolve from left to right on (b).

encounters. In shear turbulence, where the dissipation rates are reduced, the efficient predator does less well overall, but the inefficient predator does better near the surface. Although prey encounters are reduced, it has more time to react and perform a capture.

An initial run of the biological model alone was performed, simply to test out the parameter values listed in Table 1. The predation level for this 'No flow' simulation was set to a constant value of $6.7 \times 10^{-10} \text{ m}^3 \text{ s}^{-1}$ (equivalent to a very low-energy dissipation rate of $6.8 \times 10^{-12} \text{ m}^2 \text{ s}^{-3}$) throughout the mixed layer. Fig. 6a shows the evolution of the time-averaged mean $m_{\Gamma}(z, T)$ of the zoo and phytoplankton concentration fields, defined by

$$m_{\Gamma}(z,T) = \frac{1}{T} \int_0^T \langle \Gamma(x,t) \rangle \,\mathrm{d}t \quad (\Gamma = P \text{ or } Z) \tag{45}$$

against depth, over a typical simulation period of 70 000 s. (A time period of $70\,000 \,\mathrm{s} \sim 20 \,\mathrm{h}$ is a very short time-scale when considering the evolution of plankton populations. Ideally one would like to study the population dynamics over periods of weeks, or even months but the coupled model is computationally expensive, and this was the best that could be achieved with the resources available. In any event the reality is that the boundary conditions will constantly fluctuate over longer time periods, for which as yet the model makes no provision.) As one can see near the surface the light levels are sufficient for the phytoplankton to grow at a rate which offsets the zooplankton predation. However, at greater depths with less light phytoplankton growth is insufficient to offset predation and the population declines. The relatively low value of μ_Z death means that the zooplankton population grows at all depths (faster near the surface where there is more prey), and will continue to do so until the phytoplankton concentration falls to about 10% of its initial value. Fig. 6b shows the vertical profile of the relative timeaveraged concentration intensity

$$I_{\Gamma}^{2}(z,T) = \frac{1/T \int_{0}^{T} \langle (\Gamma - \langle \Gamma \rangle)^{2} \rangle \,\mathrm{d}t}{m_{\Gamma}^{2}(z,T)} \quad (\Gamma = N, P \text{ or } Z)$$

$$(46)$$

for all three concentration fields under consideration. The values remain near zero at all times, indicating there is virtually no x-y spatial heterogeneity in the distributions of these fields.

The results of six basic simulations of the coupled LES-NPZ model will be presented. The essential

Table 2 Key parameters distinguishing the simulations of the LES-*NPZ* Model

Run number	T_R (s)	μ_P^{\max} (s ⁻¹)	Langmuir No. La
321	15	2.5×10^{-5}	∞
322	15	2.5×10^{-5}	0.3
323	5	2.5×10^{-5}	0.3
324	5	2.5×10^{-5}	∞
325	5	5×10^{-5}	∞
326	5	5×10^{-5}	0.3

differences between these runs are highlighted in Table 2.

Three of the simulations, (runs 322, 323 and 325) studied the population dynamics in a Langmuir turbulence regime, whilst the others were for a purely shear turbulence mixed layer. In two of the simulations (runs 321 to 322) the inefficient predator was used and in two others (runs 323 to 324) the efficient predator was substituted. Finally, as the presence of the efficient predator tended to deplete the local phytoplankton concentration rapidly, two further simulations (runs 326) were performed in which the growth rate μ_P^{max} was doubled, to try and offset this effect.

4.2. Vertical profiles of the temporal evolution of the scalar fields

Figs. 7a-f show the vertical profiles of the timeaveraged mean (45) of the P and Z concentrations for all six simulations (the time-averaged mean of the nitrate N hardly varied from its initial value of unity throughout). In all cases, the enhanced zooplankton predation (compared to the 'no flow' regime) outweighs the new phytoplankton growth, causing the former population to increase and the latter to decrease. However, the rate of phytoplankton decline varies considerably. For the relatively slow inefficient predator (Fig. 7a run 321) it takes about 65 000 s for $m_P(z, T)$ to fall by 10%, whereas for the efficient predator in Langmuir turbulence this time-scale is only $\sim 19000 \, s$ (Fig. 7c run 323). Even doubling the phytoplankton growth rate (Fig. 7f run 326) only slows this depletion time-scale to around 23000 s. What is clear is that the turbulent mixing ensures that the mean concentration profiles for both zoo and phytoplankton are virtually uniformly distributed throughout the mixed layer, in contrast to the 'no flow' simulation in Fig. 6a. There are some slight variations. As the inefficient predator struggles to catch prey near the surface, the phytoplankton do relatively well here, and consequently $dm_P/dz > 0$ (Figs. 7a and b). By contrast the efficient predator consumes many prey near the surface, more than offsetting increased phytoplankton growth due to enhanced light intensity, and consequently $dm_P/dz < 0$ (Figs. 7c-f).

Figs. 8a–f show the corresponding vertically profiles of the time-averaged concentration intensities (46). The first thing to note is that the values exhibited in these diagrams are much larger than for the 'no flow' simulation results (Fig. 6b), by as much as twenty times in some cases. The intensities grow as time increases (the profiles evolve from left-to-right), but the overall values still remain relatively small. Even in the case of run 324 (Fig. 8d) when the intensity is largest, values of $I_P^2 \sim$ 2.0×10^{-4} only equate to a variation $\sim 1.5\%$ between the largest and smallest concentration values over the



Fig. 7. Time-averaged normalized mean concentration profiles $m_P(z, T)$ and $m_Z(z, T)$ for the six simulations of the coupled LES–*NPZ* model outlined in Table 2. The averages are calculated at various intermediate times shown at the bottom of each profile on the figures. All show phytoplankton depletion and zooplankton growth, although the time-scales of each depend upon the nature of the boundary layer turbulence and the predator efficiency.



Fig. 8. Time-averaged concentration intensity profiles $I_N^2(z, T)$, $I_P^2(z, T)$ and $I_Z^2(z, T)$ for the six simulations of the coupled LES–*NPZ* model outlined in Table 2. The averages are calculated at the same intermediate times as for the corresponding diagrams of Fig. 7. All the profiles evolve from left-to-right. Note the much larger scale used in (d) and (e).

x-y plane. So in no sense can one say that the model is demonstrating any patch formation (for these timeaveraged statistics), where typically one might expect variations of perhaps 1000% between regions of low and high concentration (with I^2 values perhaps 1000 times large than these, Pinel-Alloul, 1995). Although Fig. 8 shows a steady increase in both $I_Z^2(z,T)$ and $I_P^2(z,T)$ with time, a much longer simulation (essentially run 324 continued up to $T = 200\,000\,\text{s}$) show that this increase is only sustained for $I_P^2(z, T)$. The values of $I_Z^2(z, T)$ tend to peak at around ~ 2.0×10^{-4} when $T = 100\,000$ s and then decline to about 1.3×10^{-4} by the end of the simulation. The value of $I_P^2(z,T)$ continues to grow (as $m_P(z,T)$ decreases), to reach a maximum value of ~ 9.4×10^{-4} at $z = -22.6 \,\mathrm{m}$ when $T = 200\,000 \,\mathrm{s}$. The (perhaps more relevant) instantaneous values of I_P^2 are larger than this. For instance, after 200 000 s the instantaneous value of I_P^2 at $z = -13.8 \,\mathrm{m}$ was $2.5 \times$ 10^{-3} , equating to a variation ~ 20% between the largest and smallest concentration values at this depth.

Nevertheless despite this lack of evidence of significant patch formation, the figures do show some interesting trends. Predictably the simulations conducted under shear turbulence conditions (Figs. 8a, d and e) show more variations than those conducted under Langmuir turbulence, where the enhanced mixing tends to smooth out concentration fluctuations. However, other factors are important as well. For the phytoplankton the growth rate is influential, with low levels of μ_P^{max} corresponding to relatively high-intensity levels. For the zooplankton predatory efficiency is important, the relatively high-intensity levels being associated with the efficient predator. High local concentrations of efficient predators tend to deplete the local phytoplankton population relatively quickly. If μ_P^{max} is low the phytoplankton population cannot respond to these losses very quickly, resulting in correlated regions of relatively low P and high Z concentration, compared to the average background. Hence, the high values of $I_z^2(z,T)$ and $I_P^2(z,T)$ displayed in the shear turbulence simulation 324, where $T_R = 5$ and $\mu_P^{\text{max}} = 2.5 \times 10^{-5} \text{ s}^{-1}$. It is also interesting to note that all the $I_Z^2(z, T)$ and $I_P^2(z, T)$ profiles in Fig. 8 are convex in shape, with a maximum at around $z \sim -20$ m. It is not surprising that the intensity levels are low near the surface, where turbulent mixing will be strongest. At the same time the low phytoplankton growth and lower zooplankton predation levels below 40 m, seem to inhibit the formation of spatial heterogeneities in the concentration fields at these depths. Rather the model predicts that spatial variation (limited though it is here) in the concentration fields is most likely to be observed at intermediate depths, where the turbulence levels are not so high as to lead to rapid mixing and the biological fields are still relatively dynamic.

4.3. Vertical flux profiles and concentration correlations

Figs. 9a–f show the time-averaged vertical flux profiles of the three concentration fields for the various simulations. In the upper 15 m or so of the boundary layer turbulent transport mechanisms dominate leading to relatively high flux values here. There is always a net downward transport of zooplankton from the surface, because this is where zooplankton predation is highest and consequently where zooplankton growth is best. The exception is run 322 (Fig. 9b) where the inefficient predator struggles to capture prey in the highly turbulent Langmuir regime.

The low predation rates associated with the inefficient predator means that the phytoplankton grow relatively well in the uppermost layers. As a result there is a net transport of P down from the surface into the interior of the boundary layer for these simulations (Figs. 9a and b). The strength of this flux is enhanced by the strong down-wellings associated with the Langmuir turbulence regime (Fig. 9b). By contrast the efficient predator is able to capture prey near the surface, depleting the local P concentration, which results in a negative dP/dz concentration profile (Figs. 7c–f). Consequently the flux of phytoplankton is reversed for these simulations (Figs. 9c–f).

At lower levels, below about 40 m, the turbulent regimes are relatively quiescent and the interactions of the three biological fields are more important in determining the observed fluxes. The imposed flux boundary condition (41) at the bottom of the computational domain ensures that nitrate-rich water tends to be entrained upwards. However, a high nitrate flux promotes higher levels of phytoplankton growth, which in turn results in a depletion of the local nitrate concentration through increased absorption. Hence the negative values of $\langle w''N'' \rangle$ observed 40 m. The sign of $\langle w''P'' \rangle$ depends on below whether the zooplankton predator can take advantage of the higher phytoplankton growth at the up-wellings The efficient predator can do so and the excess phytoplankton growth is offset by greater zooplankton growth and predation, resulting in $\langle w''P''\rangle$ being negative too (Figs. 9c-f). The inefficient predator cannot take advantage so quickly and consequently the sign of $\langle w''P'' \rangle$ is reversed (Figs. 9a and b). The magnitude of these fluxes is surprisingly large considering the value of $\langle w''^2 \rangle$ is about ten times smaller at these depths than it is at 10 m. The overall lack of mixing in this region enhances the contrasts between areas of relatively high and low growth of the biological fields (as illustrated in Fig. 8, which shows the intensity levels are much larger below 40 m than above 10 m), leading to relatively high flux values. All the Figs. 9a-f show that the overall net concentration fluxes tend to cancel each other out at a depth of



Fig. 9. Time-averaged vertical flux profiles $\langle w''N'' \rangle$, $\langle w''P'' \rangle$ and $\langle w''Z'' \rangle$, normalized by U_* , for the six simulations of the coupled LES–*NPZ* model outlined in Table 2. The averages are calculated at the same intermediate times as for the corresponding diagrams of Fig. 7. The magnitude of the flux values increases from zero with time.



Fig. 10. Time-averaged profiles of the concentration correlations $\langle Z''N'' \rangle$, $\langle P''N'' \rangle$ and $\langle P''Z'' \rangle$, for the six simulations of the coupled LES–*NPZ* model outlined in Table 2. The averages are calculated at the same intermediate times as for the corresponding diagrams of Fig. 7. The magnitude of the correlations increases from zero with time.



Fig. 11. Horizontal contour plots of the biological scalar fields (a) Z, (b) P, (c) N and (d) vertical velocity field w, at a depth z = -3.41 m, taken from the Langmuir turbulence run 323 some 61 217 s after spin-up. Relatively high zooplankton concentrations are situated at down-wellings, whilst phytoplankton survive best in up-wellings.

around 20 m, which is precisely the level where $I_Z^2(z, T)$ and $I_P^2(z, T)$ attain there maximum values (Fig. 8).

Fig. 10, which shows the time-averaged vertical profiles of the correlations of the biological fields, reemphasizes the trends highlighted above. The enhanced mixing prevalent in the Langmuir turbulence regime tends to reduce the magnitude of the correlations (Figs. 10b, c and f) as compared to those conducted in shear turbulence (Figs. 10a, d and e). Relatively large concentrations of phytoplankton tend to deplete the local nitrate concentration field and grow quickly. However, in the presence of the efficient zooplankton predator this growth is more than offset by predation losses (notice how $\langle P''Z'' \rangle$ evolves quickest with time) resulting in a negative $\langle P''Z''\rangle$ correlation and $\langle P''N''\rangle > 0$ (Figs. 10c–f). If the predator is inefficient, this extra phytoplankton growth is sustained and the signs of $\langle P''Z''\rangle$ and $\langle P''N''\rangle$ are reversed (Figs. 10a and b).

4.4. Horizontal instantaneous scalar field distributions

Fig. 11 displays some instantaneous horizontal sections of the Z, P and N scalar fields (Figs. 11a-c, respectively) together with the corresponding instantaneous w velocity field (Fig. 11d), all recorded at a depth of z = -3.4 m, taken from the Langmuir simulation 323. The characteristic Langmuir turbulence pattern of alternating up and down-welling zones is immediately apparent. Down-wellings from the surface (where the efficient predator grows fastest) mean relatively higher zooplankton concentrations in these regions (e.g. the areas centred on y = 25 m, x = -20 m and y = -20 m, $x = -10 \,\mathrm{m}$ of Fig. 11a), which deplete the local phytoplankton population here (Fig. 11b). The phytoplankton tend to thrive best in up-welling regions (such as the area centred on y = -15 m, x = 20 m) sustained by higher nitrate levels brought up from below and benefiting from the relative absence of zooplankton. There is some evidence that zones of high/low concentration are elongated in the wave direction (along the xaxis). Confirmation of this fact can be discerned from calculations of the corresponding longitudinal (x-axis) and traverse (y-axis) integral length scales, defined by

$$L_{x\Gamma}(z,t) = \int_{0}^{X} \frac{\langle (\Gamma(x,y,z,t) - \langle \Gamma \rangle) (\Gamma(x+r,y,z,t) - \langle \Gamma \rangle) \rangle}{\langle (\Gamma - \langle \Gamma \rangle)^{2} \rangle} dr,$$
(47a)

$$= \int_{0}^{Y} \frac{\langle (\Gamma(x, y, z, t) - \langle \Gamma \rangle) (\Gamma(x, y + r, z, t) - \langle \Gamma \rangle) \rangle}{\langle (\Gamma - \langle \Gamma \rangle)^{2} \rangle} dr,$$
(47b)

Table 3 Integral length scales at different depths in Langmuir turbulence (Run 323)

Integral length scales (in metres) at a depth of $z = -3.4 \text{ m}$								
Time t / s	L_{xw}	L_{yw}	L_{xZ}	L_{yZ}	L_{xP}	L_{yP}		
20 041	14.9	2.7	17.6	9.5	18.7	10.3		
30 1 1 6	16.7	2.1	17.0	11.8	17.6	12.4		
40 045	17.4	2.3	32.7	12.7	34.1	12.8		
50 044	17.6	1.3	19.2	13.0	19.0	13.1		
61 217	14.1	2.1	25.0	10.6	25.4	10.5		
Integral length scales (in metres) at a depth of $z = -13.8 \mathrm{m}$								
20 041	19.7	9.9	17.3	11.7	17.4	12.0		
30116	16.5	10.5	13.4	15.4	13.7	15.3		
40 045	14.3	11.1	16.7	11.7	16.7	11.8		
50 044	13.0	10.3	15.6	16.8	15.5	16.7		
61 217	19.0	7.1	17.4	9.1	17.4	9.1		

respectively (for $\Gamma = Z, P$ or w; and the integration ranges in Eq. (47) are restricted so that integrands are positive), which are shown in Table 3.

As can be seen from the table, at a depth of z =-3.4 m the longitudinal integral length scales for both zooplankton L_{xZ} and phytoplankton L_{xP} are almost twice the size of the corresponding transverse length scales L_{vZ} and L_{vP} , mirroring, to a certain extent, the Langmuir cell structure. However, the intensification of the levels of turbulence transverse to the direction of wave propagation (as evidenced in the larger values of $\langle v''^2 \rangle$ compared to $\langle u''^2 \rangle$ shown in Fig. 3a) means that there is increased mixing in the y direction. Consequently, the dominance of the L_x integral scale over L_y for the biological fields, is much less than the value of $L_{xw}/L_{yw} \sim 8$ exhibited by the vertical velocity, and the plankton 'patches' show a more elliptical (or ellipsoidal if viewed in 3D) pattern than the long thin Langmuir cells. Hence at this relatively shallow depth, the association of up-wellings with high phytoplankton concentrations is somewhat blurred. Possibly other aggregation mechanisms, not included here, may result in modifications to this pattern. However, as Pinel-Alloul (1995) points out, many species zooplankton tend to swim relatively little horizontally, but can move more than 10 m vertically in response to diel changes in light level, so one might still expect to see this pattern repeated in field observations.

Fig. 12 shows the corresponding instantaneous cross sections 10 m lower down. At this depth the up/downwelling zones have to a certain extent merged and become broader span-wise. As a consequence the elongated vortex structure downwind is less readily apparent and the distributions of the scalar fields exhibit a more circular (or oblate spheroidal in 3D) horizontal pattern. This is reflected in the small differences in the longitudinal and transverse integral length scales shown





Fig. 13. Horizontal contour plots of the biological scalar fields (a) Z, (b) P, (c) N and (d) vertical velocity field w, at a depth z = -13.8 m, taken from the shear turbulence run 324 some 40 114 s after spin-up. Note the different scale used in (d) compared to Fig. 12d. Relatively high zooplankton concentrations are situated at down-wellings, whilst phytoplankton survive best in up-wellings.

in the bottom part of Table 3, and is characteristic of a more isotropic turbulent regime at this depth (Fig. 3a). Again relatively high zooplankton concentrations, associated with down-wellings, tend to deplete the local phytoplankton population in these areas. Meanwhile the phytoplankton thrive in up-wellings (e.g. in the area x =10 m, y = 0 m, Fig. 12b), where nitrate is relatively plentiful and zooplankton concentrations are reduced. Similar characteristics are exhibited in Fig. 13, which shows the corresponding diagrams from simulation 324 conducted in shear turbulence. The correlations between the P and Z distributions and the up- and down-welling zones are much more striking, despite the fact the intensity of the w velocity field is reduced (cf. Figs. 12d and 13d). The reduced scale of turbulent mixing in this regime as compared to the Langmuir simulation (cf. Figs. 2 and 3) means that it is the up-welling of nitrate from below which principally determines the spatial pattern of the phytoplankton field. As one can see from the scales of these graphs, the magnitudes of the differences between the highest and lowest concentrations are not great (perhaps 5% for P, 4% for Z). Interestingly these variations in the biological fields exhibited here are consistent with equilibrium perturbations found by Flierl and McGillicuddy (2002), when they subjected their mesoscale biological-physical model to an up-welling event caused by an eddy translation. However, they are generally much smaller than the variations cited as evidence of real patchiness (Folt and Burns, 1999).

5. Conclusions

This paper presents the development of a fully integrated biological-physical model of the dynamics of plankton populations. It comprises a three-dimensional LES of the turbulent mixed layer coupled to a standard NPZ-type model of plankton population dynamics. Previously, each of these component parts have been used separately to successfully (with some modifications) replicate the physical behaviour of, and ecological system within, the surface mixed layer (McWilliams et al., 1997; Baird and Emsley, 1999). In one sense the results of this coupling can been seen as negative, in that the model does not predict the kind of spatial patchiness frequently observed in the distribution of zoo and phytoplankton concentrations (Pinel-Alloul, 1995; Folt and Burns, 1999). However, this is not necessarily too surprising for two reasons. First experimental observations in the coastal zone, recorded by Tiselius (1998), show that copepods tend to group together in food layers during calm conditions, but become dispersed when strong winds stir up the mixed layer. These observations are in line with the model predictions made

here, that when subject to strong wind forcing, the mixed layer is biologically homogeneous with the physical mixing rates dominating the biological processes. Second, at present the model does not contain, as yet, any mechanism, physical or biological, for significant aggregations to occur. Reigada et al. (2003) demonstrated that zooplankton patchiness can arise in a synthetic turbulent-like flow field as a result of differences in the inertial properties of a zooplankton cell from the surrounding fluid. Typically if the zooplankton cell is denser than the surrounding fluid, aggregations of zooplankton will tend to occur in low vorticity regions of the flow (e.g. Sundaram and Collins, 1997). Reigada et al. (2003) were able to show that this accumulation of zooplankton in regions of low vorticity led to phytoplankton blooms inside turbulent eddies, as a result of the relative absence of predators.

The most likely biological mechanism of patch formation (on the intermediate length scales relevant to these simulations) is the swimming behaviour of zooplankton. Observations of zooplankton swimming speeds vary greatly from species to species, e.g. Daphnia magna's overall swimming speed varies from $4-16 \times 10^{-3} \,\mathrm{m \, s^{-1}}$ (Young and Getty, 1987), cod larvae from $2-10 \times 10^{-3} \,\mathrm{m \, s^{-1}}$ Galbraith et al. (2004), whilst the copepod Diaptomus sicilis idles at around $1 \times 10^{-3} \,\mathrm{m \, s^{-1}}$ or jump at a speed of $20 \times$ $10^{-3} \,\mathrm{m \, s^{-1}}$, depending on whether it is foraging for prey or escaping a predator (Bundy et al., 1998). Swimming strategies are equally diverse. One common behaviour, observed for many species of zooplankton, is diel vertical migration (e.g. Young and Watt, 1996), in which the organism migrates to the surface in order to feed at night and descends to deeper levels during the day to avoid visual predators such as fish. Many species of copepod can swim up chemical gradients in order to find patches of phytoplankton e.g. Van Gool and Ringelberg (1996), whilst others can follow pheromone trails in order to find mates (van Duren and Videler, 1996). All these different behaviours will, in all probability, lead to zooplankton aggregations of one sort or another. However, what is clear from the magnitude of the swimming speeds mentioned, is that in windy conditions aggregations due to swimming behaviour are unlikely to occur in the upper reaches of the mixed layer, simply because the levels of turbulent mixing near the surface would be too intense (cf. Figs. 2, 3 and 11 in this paper, and Sullivan et al., 2004). Consequently, it seems more likely that zooplankton swimming would see an enhancement of the convex concentration variance profiles shown in Fig. 8, with the maximum 'patchiness' to be found in the middle of the mixed layer. The results of incorporating various physical and biological aggregation mechanisms into

the current model in order to investigate their significance under turbulent conditions will be the subject of a future paper.

Even without a direct mechanism for generating aggregations, the instantaneous concentration fields shown in Figs. 11–13 hint that there is likely to be a strong correlation between their spatial distribution, and regions of local up- and down-welling (as well as local vorticity for 'heavy' cells). Experimental evidence supporting this supposition is presented by Malinen et al. (2001), who report that following the onset of upwellings associated with wind-generated Langmuir circulations, clouds of phantom midge larvae can be observed being advected to the surface from below the mixed layer where they like to take refuge from fish predators. The most crucial biological parameter in determining the spatial distribution of the planktonic scalar fields is the zooplankton predation level (see Fig. 5). In these simulations, the zooplankton are seen to deplete the phytoplankton (regardless of the latter's growth) relatively rapidly, which suggests the current predation levels are too high. Of course one could reduce predation levels still further either by reducing R(e.g. a reduction in contact radius by a factor 2 reduces predation levels to a point where continuous phytoplankton growth is obtained) or by making the predator less efficient. Regarding the latter it is not so much the value of $T_R \sim 5$ s which is erroneous (the observations of Bundy et al. (1998) for copepods show if anything that T_R is a little faster than this) but rather the assumption that predator's perception field is spherical. Consequently, the predicted number of encounters (and hence the predation rate) is too large. The importance of obtaining better estimates of the predation rate is underlined by the fact the signs of the correlations $\langle w''P'' \rangle$ and $\langle P''Z'' \rangle$ are reversed for the two types of predator used here (cf. Figs. 9 and 10 for simulations 321 and 322 with those of simulations 323 and 324), which in turn alters the spatial distribution of the scalar fields with respect to the position of the up- and down-wellings. Given that the predation rate of a zooplankton with a non-spherical perception field will depend on its relative orientation to the prey it encounters, which may be influenced by various taxi, such a light levels, gravitational torques, or simply the vorticity of the flow field itself, making better predation estimates will not be easy.

What is certain is that developments of this type of coupled LES–*NPZ* model discussed here can only be made in conjunction with more observations of planktonic behaviour under turbulent conditions. New developments in experimental methodology, such as those described in Webster et al. (2004), will probably be needed. This in turn will require greater collaboration between modellers and experimentalists concerning what can be predicted and what can be measured.

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References

- Baird, M.E., Emsley, S.M., 1999. Towards a mechanistic model of plankton population dynamics. J. Plankton Res. 21, 85–126.
- Baird, M.E., Emsley, S.M., McGlade, J.M., 2001. Modelling the interacting effects of nutrient uptake, light capture and temperature on phytoplankton growth. J. Plankton Res. 23, 829–840.
- Batchelor, G.K., 1953. The Theory of Homogeneous Turbulence. Cambridge University Press, Cambridge, UK.
- Batchelor, G.K., 1980. Mass transfer from small particles in a turbulent fluid. J. Fluid Mech. 98, 609–623.
- Bees, M.A., Mezic, I., McGlade, J., 1998. Planktonic interactions and chaotic advection in Langmuir circulations. Math. Comput. Simul. 44, 527–544.
- Brethouwer, G., Hunt, J.C.R., Nieuwstadt, F.T.M., 2003. Microstructure and Lagrangian statistics of the scalar field with a mean gradient in isotropic turbulence. J. Fluid Mech. 474, 193–225.
- Browman, H.I., Skiftesvik, A.B., 1996. Effects of turbulence on the predation cycle of fish larvae: comments on some of the issues. Mar. Ecol. Prog. Ser. 139, 309–312.
- Bryden, H.L., Brady, E.C., 1985. Diagnostic model of three-dimensional circulation in the upper equatorial Pacific Ocean. J. Phys. Oceanogr. 15, 1255–1273.
- Bundy, M.H., Gross, T.F., Vanderploeg, H.A., Strickler, J.R., 1998. Perception of inert particles by calanoid copepods: behavioural observations and a numerical model. J. Plankton Res. 20, 2129–2152.
- Craik, A.D.D., Leibovich, S., 1976. A rational model for Langmuir circulations. J. Fluid Mech. 73, 401–426.
- Denman, K.L., Gargett, A.E., 1995. Biological–physical interactions in the upper ocean: the role of vertical and small-scale transport processes. Annu. Rev. Fluid Mech. 27, 225–255.
- Denman, K.L., Peña, M.L., 1999. A coupled 1-D biological/physical model of the northeast subarctic Pacific Ocean with iron limitation. Deep-Sea Res. II 46, 2877–2908.
- Edwards, A.M., Brindley, J., 1996. Oscillatory behaviour in a threecomponent plankton population model. Dyn. Stabil. Syst. 11, 347–370.
- Edwards, C.A., Powell, T.A., Batchelder, H.P., 2000. The stability of an NPZ model subject to realistic levels of vertical mixing. J. Mar. Res. 58, 37–60.
- Fasham, M.J.R., Ducklow, H.W., McKelvie, S.M., 1990. A nitrogenbased model of plankton dynamics in the oceanic mixed layer. J. Mar. Res. 48, 591–639.
- Flierl, G., McGillicuddy, D.J., 2002. Mesoscale and submesoscale physical-biological interactions. In: Robinson, A.R., McCarthy, J.J., Rothschild, B.J. (Eds.), The Sea, vol. 12. Wiley, New York, pp. 113–185.
- Folt, C.L., Burns, C.W., 1999. Biological drivers of zooplankton patchiness. Trends Ecol. Evol. 14, 300–305.
- Franks, P.J.S., 1995. Coupled physical-biological models in oceanography. Rev. Geophys. (Suppl. July) 1177–1187.
- Franks, P.J.S., 2002. NPZ models of plankton dynamics: their construction, coupling to physics and application. J. Oceanogr. 58, 379–387.

- Franks, P.J.S., Walstad, L.J., 1997. Plankton patches at fronts: a model of formation and response to wind events. J. Mar. Res. 55, 1–29.
- Franks, P.J.S., Wroblewski, J.S., Flierl, G.R., 1986. Behaviour of a simple plankton model with food-level acclimation by herbivores. Mar. Biol. 91, 121–129.
- Galbraith, P.S., Browman, H.I., Raccca, R.G., Skiftesvik, A.B., Saint-Pierre, J.F. 2004. The effect of turbulence on the energetics of foraging in Atlantic cod (*Gadus morhua*) larvae. Mar. Ecol. Prog. Ser. 281, 241–257.
- Gallager, S.M., Davies, C.S., Epstein, A.W., Solow, A., Beardsley, R.C., 1996. High-resolution observations of plankton spatial distributions correlated with hydrography in the Great South Channel, Georges Bank. Deep-Sea Res. II 43, 1627–1663.
- Hansen, P.J., Bjornsen, P.K., Hansen, B.W., 1997. Zooplankton grazing and growth: scaling within the 2–2000 micro m body size range. Limnol. Oceanogr. 42, 687–704.
- Hinze, J.O., 1975. Turbulence. McGraw-Hill, New York, USA.
- Karp-Boss, K., Boss, E., Jumars, P.A., 1996. Nutrient fluxes to planktonic osmotrophs in the presence of fluid motion. Oceanogr. Mar. Biol. Annu. Rev. 34, 71–107.
- Kiefer, D.A., Atkinson, C.A., 1984. Cycling of nitrogen by phytoplankton: a hypothetical description based upon efficiency of energy conversion. J. Mar. Res. 42, 655–675.
- Kiørboe, T., 1993. Turbulence, phytoplankton cell size and the structure of pelagic food webs. Adv. Mar. Biol. 29, 1–72.
- Klemp, J., Duran, D., 1983. An upper boundary condition permitting internal gravity wave radiation in numerical mesoscale models. Mon. Weather Rev. 11, 430–444.
- Lewis, D.M., 2003. Planktonic contact rates in homogeneous isotropic turbulence: the case of predators with limited fields of sensory perception. J. Theor. Biol. 222, 73–97.
- Lewis, D.M., Belcher, S.E., 2004. Time-dependent, coupled, Ekman boundary layer solutions incorporating Stokes drift. Dyn. Atmos. Oceans 37, 313–351.
- Lewis, D.M., Pedley, T.J., 2000. Planktonic contact rates in homogeneous isotropic turbulence: theoretical predictions and kinematic simulation. J. Theor. Biol. 205, 377–408.
- Lewis, D.M., Pedley, T.J., 2001. The influence of turbulence on plankton predation strategies. J. Theor. Biol. 210, 347–365.
- Lewis, M.R., Kuring, N., Yentsch, C., 1988. Global patterns of ocean transparency: implications for the new production of the open ocean. J. Geophys. Res. 93, 6847–6856.
- MacKenzie, B.R., Miller, T.J., Cyr, S., Leggett, W.C., 1994. Evidence for a domeshaped relationship between turbulence and larval fish ingestion rates. Limnol Oceanogr. 39, 1790–1799.
- Malinen, T., Horppila, J., Liljendahl-Nurminen, A., 2001. Langmuir circulations disturb the low-oxygen refuge of phantom midge larvae. Limnol Oceanogr. 43, 689–692.
- Marrasé, C., Costello, J.H., Granata, T., Strickler, J.R., 1990. Grazing in a turbulent environment: energy dissipation, encounter rates and efficacy of feeding currents in *Centropages hamatus*. Proc. Natl. Acad. Sci. USA 87, 1653–1657.
- Mason, P.J., Sykes, R.I., 1982. A two-dimensional numerical study of horizontal roll vortices in an inversion capped planetary boundary layer. Q. J. Roy. Meteorol. Soc. 108, 801–823.
- McComb, W.D., 1991. The Physics of Fluid Turbulence. Oxford University Press, Oxford, UK.
- McGillicuddy, D.J., McCarthy, J.J., Robinson, A.R., 1995a. Coupled physical and biological modelling of the spring bloom in the North Atlantic (i): model formulation and 1D bloom processes. Deep-Sea Res. 42, 1313–1357.
- McGillicuddy, D.J., McCarthy, J.J., Robinson, A.R., 1995b. Coupled physical and biological modelling of the spring bloom in the North

Atlantic (ii): 3D bloom and post bloom processes. Deep-Sea Res. 42, 1359–1398.

- McWilliams, J.C., Sullivan, P.P., Moeng, C.H., 1997. Langmuir turbulence in the ocean. J. Fluid Mech. 334, 1–30.
- Monin, P., Yaglom, A.M., 1975. Statistical Fluid Mechanics, vol. 2. MIT Press, Cambridge, MA, USA.
- Muelbert, J.H., Lewis, M.R., Kelley, D.E., 1994. The importance of small-scale turbulence in the feeding of herring larvae. J. Plankton Res. 16, 927–944.
- Philips, O.M., 1977. The Dynamics of the Upper Ocean. Cambridge University Press, Cambridge, UK.
- Pinel-Alloul, B., 1995. Spatial heterogeneity as a multiscale characteristic of zooplankton community. Hydrobiologia 300/ 301, 17–42.
- Price, J.F., Sundermeyer, M.A., 1999. Stratified Ekman layers. J. Geophys. Res. 104, 20467–20494.
- Reigada, R., Hillary, R.M., Bees, M.A., Sancho, J.M., Sagués, F., 2003. Plankton blooms induced by turbulent flows. Proc. R. Soc. London B 270, 875–880.
- Rothschild, B.J., Osborn, T.R., 1988. Small-scale turbulence and plankton contact rates. J. Plankton Res. 10, 465–474.
- Skyllingstad, E.D., Denbo, D.W., 1995. An ocean large-eddy simulation of Langmuir circulations and convection in the surface mixed layer. J. Geophys. Res. 100, 8501–8522.
- Smagorinsky, J., 1963. General circulation experiments with the primitive equations, I: the basic experiment. Mon. Weather Rev. 91, 99–164.
- Solow, A., Steele, H., 1995. Scales of plankton patchiness—biomass versus demography. J. Plankton Res. 17, 1669–1677.
- Straile, D., 1997. Gross growth efficiencies of protozoan and metazoan zooplankton and their dependence on food concentration, predator-prey ratio and taxonomic group. Limnol. Oceanogr. 42, 1375–1385.
- Sullivan, P.P., McWilliams, J.C., Moeng, C.H., 1994. A subgrid-scale model for large-eddy simulation of planetary boundary layer flows. Bound.-Layer Met. 71, 247–276.
- Sullivan, P.P., McWilliams, J.C., Kendall Melville, W., 2004. The oceanic boundary layer driven by wave breaking with stochastic variability, Part 1: direct numerical simulations. J. Fluid Mech. 507, 143–174.
- Sundaram, S., Collins, L.R., 1997. Collision statistics in an isotropic particle-laden turbulent suspension, Part 1: direct numerical simulations. J. Fluid Mech. 335, 75–109.
- Tennekes, H., Lumley, J., 1972. A First Course in Turbulence. MIT Press, Cambridge, MA, USA.
- Terray, E.A., Donelan, M.A., Agrawal, Y.C., Drennan, W.M., Kahna, K.K., Williams, A.J., Huang, P.A., Kilaigorodskii, S.A., 1996. Estimates of kinetics energy dissipation under breaking waves. J. Phys. Oceanogr. 26, 792–807.
- Teixeira, M.A.C., Belcher, S.E., 2002. On the distortion of turbulence by a progressive surface wave. J. Fluid Mech. 458, 229–267.
- Tiselius, P., 1998. An *in situ* video camera for plankton studies: design and preliminary observations. Mar. Ecol. Prog. Ser. 164, 293–299.
- van Duren, L.A., Videler, J.J., 1996. The trade-off between feeding, mate seeking and predator avoidance in copepods: behavioural responses and chemical cues. J. Plankton Res. 18, 805–818.
- Van Gool, E., Ringelberg, J., 1996. Swimming of *Daphnia galeata* × *hyalina* in response to changing light intensities and predator kairomone. In: Lenz, P.H., et al. (Eds.), Zooplankton: Sensory Ecology and Physiology. Gordon and Breach, London, pp. 399–405.
- Webster, D.R., Brathwaite, A., Yen, J., 2004. A novel laboratory apparatus for simulating isotropic oceanic turbulence at low Reynolds number. Limnol. Oceanogr.: Methods 2, 1–12.

- Wiafe, G., Frid, C.L.J., 1996. Short-term temporal variation in coastal zooplankton communities: the relative importance of physical and biological mechanisms. J. Plankton Res. 18, 1485–1501.
- Williams, R.G., Follows, M.J., 1998. The Ekman transfer of nutrients and maintenance of new production over the North Atlantic. Deep-Sea Res. I 45, 461–489.
- Wood, N., Hewer, F., Hobson, M., 1999. BLASIUS Version 3.03: Documentation of a model of flow over hills. Available by writing to Andy Brown, UK Met Office FitzRoy Road Exeter Devon EX1 3PB, UK (a postscript file can be downloaded from www.met.rdg.ac.uk/~marc/blasius/).
- Woodcock, A.H., 1993. Winds subsurface pelagic *Sargassium* and Langmuir circulations. J. Exp. Mar. Biol. Ecol. 170, 117–125.
- Yamazaki, H., Mackas, D.L., Denman, K.L., 2002. Coupling smallscale physical processes with biology. In: Robinson, A.R., McCarthy, J.J., Rothschild, B.J. (Eds.), The Sea, vol. 12. Wiley, New York, pp. 51–112.
- Yeung, P.K., 2001. Lagrangian characteristics of turbulence and scalar transport in direct numerical simulations. J. Fluid Mech. 427, 241–274.
- Young, S., Getty, C., 1987. Visually guided feeding behaviour in the filter feeding cladoceran, *Daphnia magna*. Anim. Behav. 35, 541–548.
- Young, S., Watt, P.J., 1996. Daily and seasonal vertical migration rhythms in *Daphnia*. Freshwater Biol. 36, 17–22.