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Technical Note

Estimating Effective Light Exposure by Property-Tracking Tracers

Edward Gross [1,2,*], Rusty Holleman [1], Eric Deleersnijder [3] and Eric J. M. Delhez [4]

1 Resource Management Associates, 1756 Picasso Avenue, Suite G, Davis, CA 95618, USA; rusty@rmanet.com
2 Department of Civil and Environmental Engineering, University of California Davis, One Shields Avenue, Davis, CA 95616, USA
3 Institute of Mechanics, Materials and Civil Engineering (IMMC) & Earth and Life Institute (ELI), Université Catholique de Louvain, Bte L4.05.02, Avenue Georges Lemaître 4, 1348 Louvain-la-Neuve, Belgium; eric.deleersnijder@uclouvain.be
4 Department of Aerospace and Mechanics, University of Liège, 4000 Liège, Belgium; e.delhez@uliege.be
* Correspondence: ed@rmanet.com; Tel.: +1-530-564-7043

Abstract: A numerical approach to estimating the mean exposure of a tracer to a scalar property is applied to predict the light exposure of sinking phytoplankton. In our application, effective light exposure is defined as the time integral of a light limitation factor commonly used in phytoplankton models. Solutions from an adjoint approach have previously been published for a set of one-dimensional sinking phytoplankton scenarios. We illustrate that a simple extension to a standard advection–diffusion model produces similar results. Specifically, we present numerical solutions using property tracking in a one-dimensional advection–diffusion model for multiple tracers. Solutions are calculated for a range of eddy diffusivity distributions and compared with the published solutions. The consistency of the numerical solutions with the published solutions provides validation of the property-tracking approach. While the adjoint method solution is much less computationally intensive for the test cases, the property-tracking approach can be applied in multidimensional time-varying applications with an arbitrary distribution of sinking speed, diffusivity, and turbidity for which an adjoint solution has not been developed. Our intention is for this example application and corroboration of the "property-tracking" approach to inspire readers to envision additional applications for this approach.

Keywords: transport; phytoplankton; light exposure; mixed layer; water age; adjoint approach; property exposure

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1. Introduction

Transport time scale estimates are useful in a wide range of ecological studies [1]. One widely used approach to calculate transport time scales is the Constituent-oriented Age and Residence Time Theory (CART, www.climate.be/cart, accessed on 10 March 2024) [2]. This approach has also been applied to estimate exposure time to specific spatial regions, defined as partial age [3]. By analogy to partial age, a "property-tracking" approach has been proposed [4] and applied to phytoplankton modeling [5]. Property tracking is a numerical tracer-based approach to estimate a tracer's mean exposure to different properties. For example, the mean temperature exposure at a specific time and location is the mean temperature encountered by water parcels in transit from a source to that location. The mathematical properties of this approach were documented in [6], which explored several test cases to confirm the consistency of the approach with physical intuition and concluded that their results "lend credence to the novel diagnostic approach" and that "the time is ripe for applying this method to a number of realistic problems".

Following this advice, we simulate integral measures of property exposure for moderately complex test cases with known solutions [7] for the purpose of corroborating the property-tracking approach. Both sets of test cases are one-dimensional with steady conditions of eddy diffusivity and track the experience of sinking phytoplankton. Adjoint model solutions for each have been published for a number of vertical distributions of eddy diffusivity [7]. In the first test case, we estimate exposure time to the euphotic zone. In the second test case, we estimate the "effective light exposure", which is a time-integrated light limitation factor for phytoplankton growth, a key element of typical phytoplankton models [8]. The light exposure of phytoplankton has been studied using Lagrangian modeling approaches [9,10], but never using the property-tracking approach documented here.

In most Lagrangian models, transport and ecological processes are evaluated on a per-particle basis as the particle moves through space [9,11]. A potentially large number of particles are simultaneously modeled in order to resolve mixing and spatial variability. In contrast, our approach makes use of a standard Eulerian advection–diffusion equation to track the age of a tracer and the properties it is exposed to as it moves through space. While the computation is Eulerian, the resulting information reflects the Lagrangian history of the water at a specific location for a given time. In the specific Lagrangian approaches that we will describe, information is incorporated by calculating the age of the tracer from a source and, in some cases, the conditions (e.g., temperature) encountered by the tracer. This approach is conceptually similar to the application of the widely used Streeter–Phelps equation [12] to estimate dissolved-oxygen concentrations in rivers. In both cases, the downstream concentration is estimated from the concentration at a known starting location, the travel time to the downstream location of interest and the specified biogeochemical transformation rates. While even the simplest Eulerian modeling approach requires substantial computation to advect and disperse water quality and ecological constituents, predictions in a Lagrangian model become simple computations [5]. Such approaches are of particular interest for ecological models, as the formulations and ecological rate parameters are often uncertain. Property tracking provides a method to incorporate more information into these Lagrangian models, such as the mean temperature experienced by the tracer [5] or the mean light exposure in a phytoplankton biomass model. More generally, our novel property-tracking approach may be useful for a large range of applications to both correlative analyses and mechanistic Lagrangian modeling of ecological and biogeochemical processes. They are particularly computationally advantageous when the number of observational datapoints predicted by the Lagrangian approach is much less than the number of computations that would be required by a Eulerian model, which scales by the number of points in the computational grid times the number of time steps in the simulation. This efficiency allows the approaches to be used for parameter estimation by optimization or Bayesian inference.

2. Materials and Methods

2.1. Property Exposure

The mathematical properties and foundation of the general approach to calculating age using Constituent-oriented Age and Residence Time Theory (CART, www.climate.be/cart) are described in [1,2,13]. The mathematical properties of a recently developed property exposure calculation approach have been examined, and idealized test cases have been documented [6]. The theoretical foundation for property tracking is summarized in Appendix A. Below, we provide the governing equations of our analysis, and Table 1 lists the variables used in the equations.

To estimate the mean age of water from a specific source in our test cases, we simulated the transport of two conservative tracers in a one-dimensional advection–diffusion model. The first tracer is the concentration from the specific source, governed by

$$\frac{\partial C}{\partial t} + \frac{\partial (wC)}{\partial z} = \frac{\partial}{\partial z}\left(\lambda \frac{\partial C}{\partial z}\right) \tag{1}$$

where C is the tracer concentration, which tags a subset of water in the domain, w is vertical velocity and λ is the vertical eddy diffusivity. The one-dimensional model domain is a vertical water column with coordinate z ranging from 0 at the surface to H at the bed. This scalar advection–diffusion equation is discretized with a fully implicit central difference for the diffusion term and an explicit flux-limiting method using the van Leer limiter [14] for the advection term.

Table 1. Variables in the phytoplankton light exposure analyses with associated units and descriptions.

Variable	Unit	Description
C	g m^{-3}	Concentration of tracer from specific source location
α	d g m^{-3}	Age concentration of tracer
a	d	Mean age of tracer
α_j	d g m^{-3}	Partial age concentration tracking exposure to euphotic zone
a_j	d	Mean partial age representing exposure time to euphotic zone
β	d g m^{-3}	Property age concentration, where property is f_I
b	-	Mean value of tracer exposure to property f_I
P	g m^{-3}	Phytoplankton biomass concentration
M_0	g	Initial phytoplankton biomass
t	d	Time
t_0	d	Time of insertion of biomass in simulation
t_e	d	End time of the simulation
λ	m^2 d^{-1}	Vertical eddy diffusivity
z	m	Vertical coordinate increasing downward from surface
w	m d^{-1}	Vertical (sinking) speed, positive downward
z_0	m	Location of insertion of initial tracer mass
Θ	d	Cumulative exposure time to the euphotic zone
m	m	Surface mixed-layer depth and euphotic zone depth
l	m	Depth of bottom layer with faster sinking
χ	-	Characteristic function of the euphotic layer
f_I	-	Light inhibition factor for phytoplankton growth
I	µmol photons m^{-2} s^{-1}	Light intensity
I_{opt}	µmol photons m^{-2} s^{-1}	Light intensity for optimal phytoplankton growth
I_o	µmol photons m^{-2} s^{-1}	Surface light intensity
k_d	m^{-1}	Light extinction coefficient
Θ_f	d	Effective light exposure time
λ_{bg}	m^2 d^{-1}	Background eddy diffusivity
λ_{max}	m^2 d^{-1}	Maximum increase from background eddy diffusivity
w	m d^{-1}	Vertical (sinking) speed, positive downward
w_s	m d^{-1}	Sinking speed in surface layer
w_b	m d^{-1}	Sinking speed in bottom layer
$\tilde{\Theta}$	d	Predicted exposure time to the euphotic zone
$\tilde{\Theta}_f$	d	Predicted effective light exposure time

The governing equation of age concentration for a one-dimensional application is

$$\frac{\partial \alpha}{\partial t} + \frac{\partial (w\alpha)}{\partial z} = \frac{\partial}{\partial z}\left(\lambda \frac{\partial \alpha}{\partial z}\right) + C \tag{2}$$

where α is the age concentration. Details of the interpretation of α and its derivation are given in Appendix A.

Mean age is calculated as the ratio of the age concentration and the tracer concentration:

$$a = \frac{\alpha}{C}. \tag{3}$$

An analogous approach was applied for partial age [3], which we will later refer to as exposure time to the euphotic zone in our application. The partial age concentration for exposure to a region j (e.g., the euphotic zone) is

$$\frac{\partial \alpha_j}{\partial t} + \frac{\partial (w\alpha_j)}{\partial z} = \frac{\partial}{\partial z}\left(\lambda \frac{\partial \alpha_j}{\partial z}\right) + \chi_j C \tag{4}$$

where $\chi_j = \chi_j(z)$ is 1 for cells in region j and 0 otherwise. Then, the exposure time (partial age) to region j is

$$a_j = \frac{\alpha_j}{C} \tag{5}$$

To quantify the mean exposure of a tracer to a water property ("effective light level" in our application), the property age concentration β is calculated with the equation

$$\frac{\partial \beta}{\partial t} + \frac{\partial (w\beta)}{\partial z} = \frac{\partial}{\partial z}\left(\lambda \frac{\partial \beta}{\partial z}\right) + \psi C \tag{6}$$

where $\psi = \psi(z, t)$ is the instantaneous value of the property.

Then, the mean property encountered by the tracer can be estimated as the ratio of the property age concentration and age concentration,

$$b = \frac{\beta}{\alpha} \tag{7}$$

where b is the mean property encountered by the tracer. The variables used in these equations and the light exposure equations below are summarized in Table 1.

The initial condition and boundary conditions of α, α_j and β were zero everywhere and no flux was allowed through boundaries.

2.2. Exposure Time to the Euphotic Zone

The exposure time of phytoplankton to the euphotic zone is the total time spent in this region and includes both time prior to leaving this layer for the first time and additional time accumulated upon return to the euphotic zone by diffusion. The exposure time analysis of [7] considers sinking phytoplankton released at different depths for different distributions of vertical eddy diffusivity. The concentration field representing phytoplankton biomass is the solution to the initial value problem

$$\frac{\partial P}{\partial t} + \frac{\partial (wP)}{\partial z} = \frac{\partial}{\partial z}(\lambda \frac{\partial P}{\partial z}) \tag{8}$$

$$P(t_0, z) = \delta(z - z_0) \tag{9}$$

where z_0 is the location of the insertion of phytoplankton biomass and $\delta(z - z_0)$ is the Dirac generalized function for modeling a starting point at z = z_0 [7]. In our discretized representation, the release location will correspond to a single computational grid point (cell). The boundary conditions are no flux of phytoplankton at the surface or bed.

$$w(z)P + \lambda(z) \left.\frac{\partial P}{\partial z}\right|_{z=0} = 0 \tag{10}$$

$$\lambda(z) \left.\frac{\partial P}{\partial z}\right|_{z=H} = 0 \tag{11}$$

In the above equations, H is the total depth of the water column. The cumulative exposure time to the euphotic zone is given by

$$\Theta(z_o) = \frac{1}{M_0}\int_{t_0}^{\infty}\int_0^m P(t,z)dzdt \quad (12)$$

where t_0 is the initial time corresponding to the initial phytoplankton location z_o, M_0 is the initial phytoplankton biomass and m is the depth of the euphotic zone. An adjoint method was applied to calculate the exposure time [7]. The ordinary differential equation and boundary conditions of the adjoint method for computing the exposure time are

$$w(z)\frac{d\Theta}{dz} + \frac{d}{dz}\left(\lambda\frac{d\Theta}{dz}\right) + \chi_{[0,m]}(z) = 0 \quad (13)$$

$$\lambda(z)\left.\frac{d\Theta}{dz}\right|_{z=0} = 0 \quad (14)$$

$$w(z)\Theta + \lambda(z)\left.\frac{d\Theta}{dz}\right|_{z=H} = 0 \quad (15)$$

where Θ is the cumulative exposure time and $\chi_{[0,m]}$ is the characteristic function of the euphotic zone.

$$\chi_{[0,m]}(z) = \begin{cases} 1 \text{ for } z \in [0,m] \\ 0 \text{ elsewhere} \end{cases} \quad (16)$$

An analytical solution to the differential problem (13)–(15) is provided by [7]. We will solve for this exposure time using the partial age approach [3], with the characteristic function of Equation (16) as χ_j in Equation (4). This test case can be considered a building block for property tracking where the property is "in the euphotic zone", with a property value of 1 if inside and 0 when outside.

2.3. Effective Light Exposure

Typical phytoplankton models include a light limitation factor that accounts for the dependence of phytoplankton growth on light [8]. Following [7], we will refer to the spatially and time-integrated light limitation factor as the effective light exposure.

$$\Theta_f(z_0) = \frac{1}{M_0}\int_{t_0}^{\infty}\int_0^H P(t,z)f_I(z)dzdt \quad (17)$$

In the above equation, f_I is the light inhibition factor. A specific functional form of this factor is

$$f_I = \frac{I}{I_{opt}}e^{(1-\frac{I}{I_{opt}})} \quad (18)$$

where I is the light intensity and I_{opt} is the optimal light intensity [15]. The light intensity is given by the Beer-Lambert law [7],

$$I = I_o e^{-k_d z} \quad (19)$$

where I_o is the light intensity at the surface and k_d is the light extinction coefficient. The adjoint steady state model for effective light exposure is

$$w(z)\frac{d\Theta_f}{dz} + \frac{d}{dz}\left(\lambda\frac{d\Theta_f}{dz}\right) + f_I(z) = 0 \quad (20)$$

$$\lambda(z)\left.\frac{d\Theta_f}{dz}\right|_{z=0} = 0 \quad (21)$$

$$w(z)\Theta_f + \lambda(z)\,\frac{d\Theta_f}{dz}\bigg|_{z=H} = 0 \tag{22}$$

Note that Equations (20)–(22) for effective light exposure are similar to Equations (13)–(15) for euphotic zone exposure. The primary difference is that the third term of Equation (17) is $\chi_{[0,m]}(z)$, while the third term of Equation (24) is $f_I(z)$. Furthermore, note the similarity between the last term of Equation (4), $\chi_j(z)C$, which becomes $\chi_{[0,m]}(z)P$ in our application, and the last term of Equation (6), $\psi(z)C$, which becomes $f_I(z)P$ in our application. Note that the difference between the two adjoint solutions and the two CART tracer equations is the replacement of the characteristic function, $\chi(z)$, in Equations (4) and (13) with the property of light limitation, $\psi(z) = f_I(z)$, in Equations (6) and (20), illustrating how property tracking is an extension of partial age [3] to a broader class of characteristic functions.

2.4. Numerical Test Cases

The test cases consider a surface mixed layer with larger diffusivity and, below a pycnocline, a region of small background diffusivity. Following the notation in [7], the eddy diffusion distribution for the test cases is defined by the expression

$$\lambda(z) = \begin{cases} \lambda_{bg} + \frac{\lambda_{max}}{2}\left(1 - \cos\left(\frac{2\pi z}{m}\right)\right), & z \le m \\ \lambda_{bg}, & z > m \end{cases} \tag{23}$$

where λ_{bg} is the background diffusivity, and $\lambda_{max} + \lambda_{bg}$ is the maximum diffusivity coefficient at the mid-depth of the surface mixed layer, with a depth m and euphotic zone depth of 30 m in all test cases. Note that for this specific test case, the surface mixed-layer depth (m) is also the euphotic zone depth. Table 2 gives the diffusivity distribution parameters for each test case.

Table 2. Eddy diffusivity distribution parameters used in simulations.

Test Case Name	λ_{bg} ($m^2\ d^{-1}$)	λ_{max} ($m^2\ d^{-1}$)
Base	1	8000
Advective	0	0
Higher background	20	8000
Highest background	60	8000
Lower peak	1	1000
Lowest peak	1	200

The sinking velocity distribution for the test cases is uniform to the bottom of the euphotic zone (m) and transitions linearly to a different constant value as follows:

$$w(z) = \begin{cases} w_s, & z < m \\ w_s + (w_b - w_s)\frac{z-m}{l-m}, & m \le z < l \\ w_b, & z \ge l \end{cases} \tag{24}$$

where l is 100 m, w_s is 4 m d^{-1} and w_b is 8 m d^{-1}. An increase in settling velocity could occur due to the aggregation/flocculation processes of phytoplankton [7]. The total water column depth, H, is 500 m.

The light extinction coefficient was 0.06667 m^{-1} for all scenarios. The euphotic zone depth (m) was defined as 30 m. The constant surface irradiance (I_o) in Equation (19) was assumed to be $1.5I_{opt}$.

The solutions of Equations (13)–(15) and Equations (20)–(22) were obtained by an ordinary differential equation solver in Mathematica version 14.0.

The numerical solutions to the advection–diffusion equations of the property-tracking approach (Equations (1)–(7)) used a spatial step of 0.5 m, a time step of 0.125 days, and a simulation period of 500 days to allow the full settling of phytoplankton on the bed.

The numerical initial conditions were a concentration (C) of 1 in the single vertical cell corresponding to the initial phytoplankton depth and 0 at all other cells. A numerical simulation was performed with the initial mass in a single cell for each of the top 100 cells extending from the surface to a 50 m depth. No-flux boundary conditions were applied at the surface and bed for all tracer fields.

After completing each advection–diffusion integration, the property-tracking-based estimate of total exposure time to the euphotic zone for a single release location was then calculated from the tracer distributions at the ending time t_e of the solution as follows:

$$\tilde{\Theta}(t_e, k_0) = \frac{\sum_{k=0}^{nk} \alpha_j(k)\Delta z}{\sum_{k=0}^{nk} C(k)\Delta z} \quad (25)$$

where $\tilde{\Theta}$ is the exposure time calculated from property tracking, k is the cell index, Δz is the vertical grid spacing and k_0 is the index of the vertical cell with a nonzero initial tracer concentration. The numerator of Equation (25) is the total exposure time (partial) content of the tracer which is normalized by the total tracer mass, assuming a unit area of the vertical model, in the denominator.

Similarly, the property-tracking-based estimate of effective light exposure is

$$\tilde{\Theta}_f(t_e, k_0) = \frac{\sum_{k=0}^{nk} \beta(k)\Delta z}{\sum_{k=0}^{nk} C(k)\Delta z} \quad (26)$$

where $\tilde{\Theta}_f$ is the effective light exposure calculated from property tracking, representing the accumulated light exposure of the phytoplankton biomass. The numerator of Equation (26) is the total effective light exposure content of the tracer which is normalized by the total tracer mass, assuming a unit area of the vertical model.

3. Results

3.1. Exposure Time to the Euphotic Zone

Figure 1 shows consistency between the exposure time calculated by the CART partial age approach [3] described by Equations (4) and (5) and the adjoint solution in Equations (13)–(15) of [7]. This serves as a verification of the implementation of the advection–diffusion solution of partial age (exposure time). The numerical solutions of Equations (4) and (5) were found to have minimal sensitivity to changes in the spatial and temporal resolution of the solution by a factor of 2.

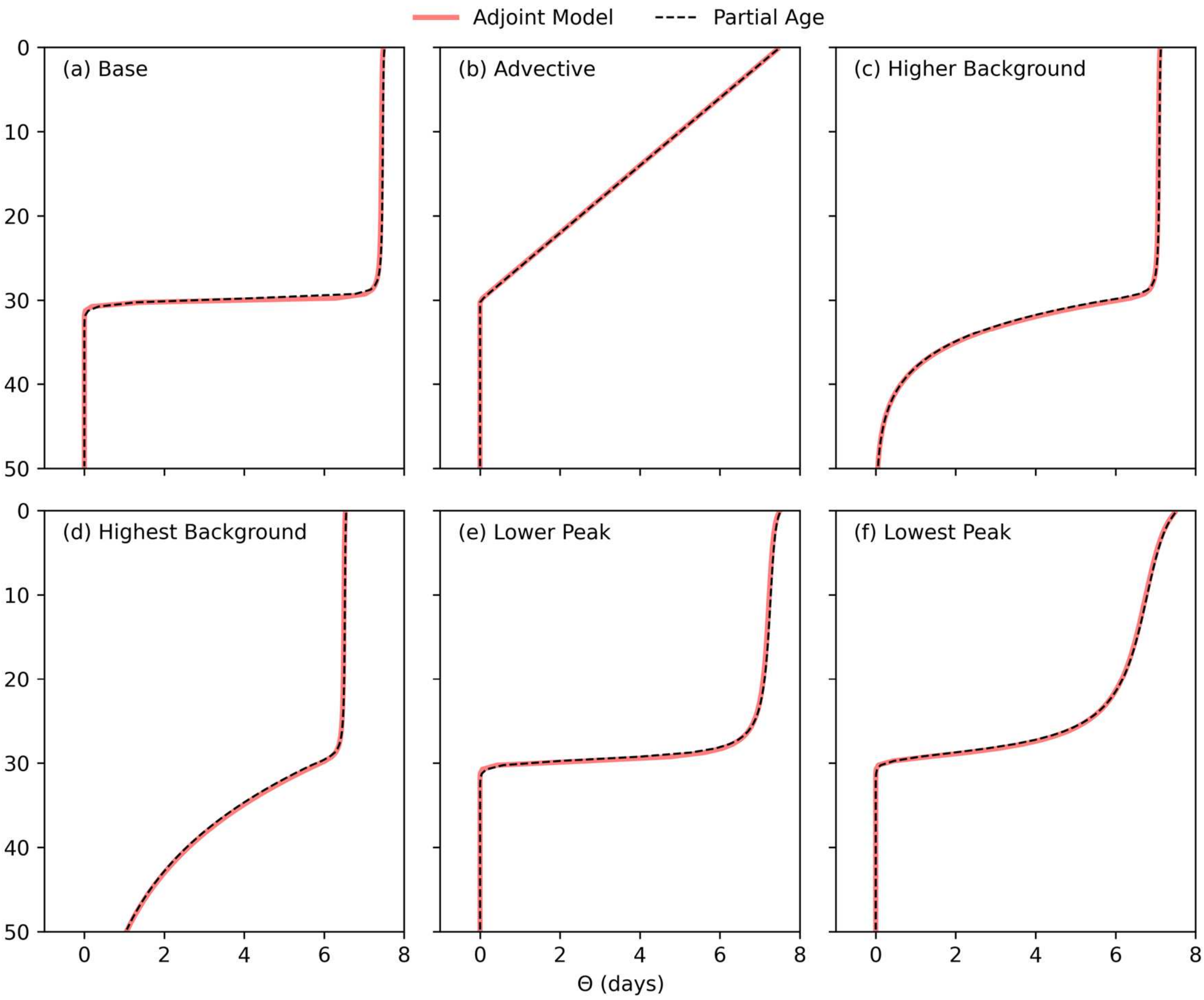

Figure 1. Vertical profiles of exposure time of sinking phytoplankton to the euphotic zone. Wide, light red lines are from the adjoint model solution, while dashed black lines are for the partial age simulations. Parameters for each labeled case are given in Table 2.

3.2. Effective Light Exposure

Figure 2 shows consistency between the integral property exposure calculated by the property-tracking approach [4] described by Equations (6) and (7) and the adjoint solution in Equations (20)–(22). The consistency between the sets of predictions to the published solutions corroborates the property-tracking approach. The ecological meaning of the individual curves in the figure is discussed in [7].

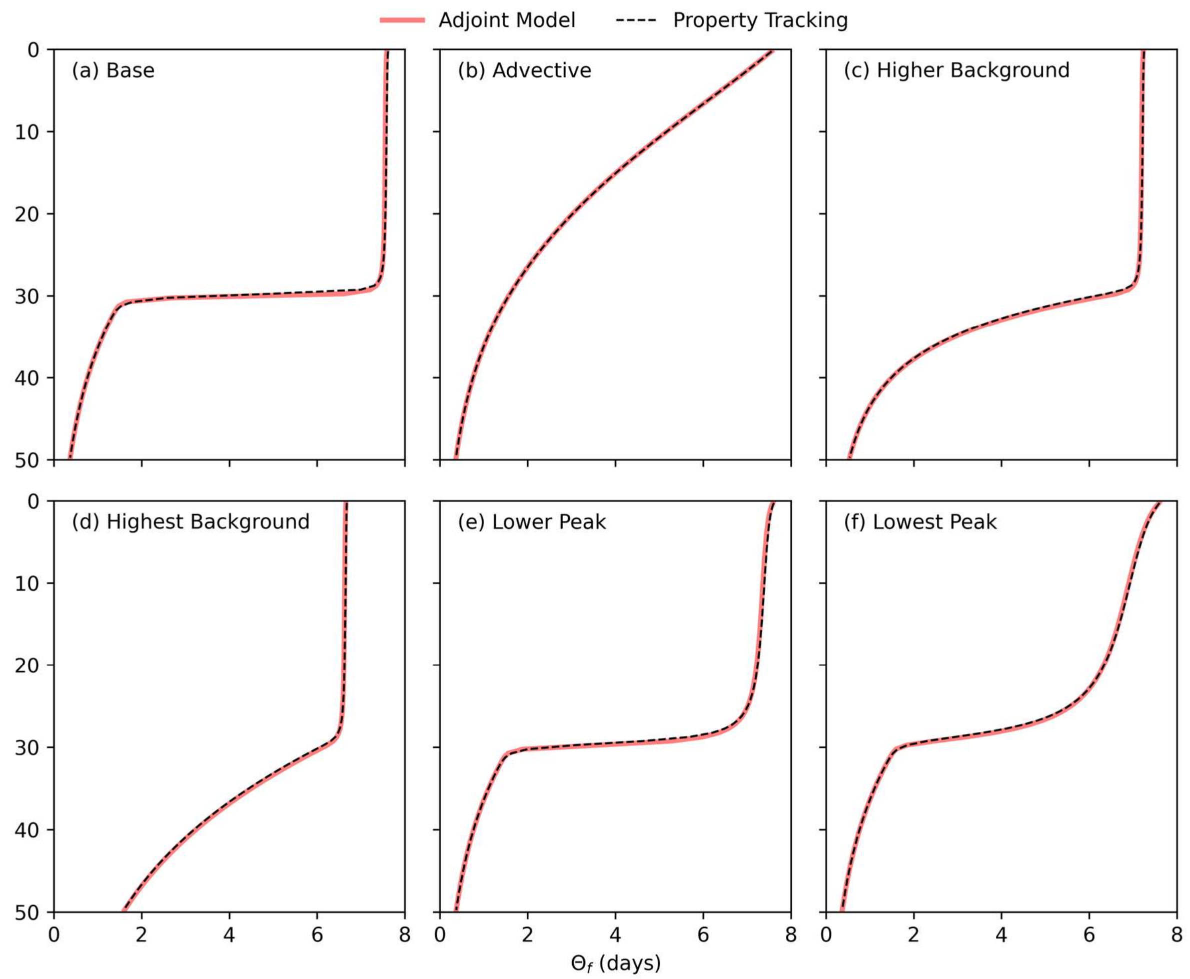

Figure 2. Vertical profiles of effective light exposure of sinking phytoplankton. Wide, light red lines are from the adjoint model solution, while dashed black lines are for the partial age simulations. Parameters for each labeled case are given in Table 2.

4. Discussion

The novel property-tracking approach described in [4] was initially proposed by analogy to the partial age approach of [3] and applied with neither mathematical proof nor comparison to known solutions in [4,5]. Since that time, mathematical analysis and evaluation in simple test cases were provided in [6], which led to the application of property-tracking to increasingly realistic problems.

We applied both the partial age approach of [3] and the property-tracking approach of [4] to estimate exposure time to the euphotic zone and effective light exposure for sinking phytoplankton for several prescribed vertical-diffusivity profiles. While the partial age approach [3] to calculate exposure time is well established, including it in our study provides insight to the similarities between this approach and the property-tracking approach of [4] and highlights the not-coincidental similarities in the corresponding adjoint approaches for the two analyses. The published adjoint solution [7] serves as a reference solution for testing the validity of the property-tracking approach.

The near-perfect match between the numerical solutions using the property-tracking approach of [4] and the published solutions [7] provides strong credence to the novel property-tracking approach [4]. This Lagrangian approach uses a standard advection–diffusion equation to estimate property exposure in contrast to conceptually similar but computationally distinct particle-tracking approaches applied with similar goals [9]. We believe that this approach will be useful for a large range of ecological and biogeochemical applications, building on the application in [5]. In that application, the properties experienced in specific habitats, which could be referred to as partial property exposure, were estimated by a three-dimensional hydrodynamic model. This generalized property tracking in the same way as partial age [3] generalized the CART water age estimation approach of [13].

This approach can be applied in steady or unsteady three-dimensional tracer simulations [5] in addition to the steady one-dimensional application described here. The approach can also be applied to any variables in a hydrodynamic model (depth, temperature, salinity, etc.), exogenous variables (e.g., observed turbidity) and the scalar functions of these variables. Here, we applied it to effective light exposure, which is a function of irradiance. Such transformations allow property-tracking to partially account for the nonlinear effects of properties (temperature, irradiance, etc.) on predicted constituents (e.g., phytoplankton biomass). Furthermore, a wide range of boundary and initial conditions can be applied, as documented for CART approaches in [16], allowing tis approach's applicability to a range of diagnostic and prognostic applications [17]. The property-tracking method as developed and applied thus far calculates only the mean property experienced for a given property (temperature, depth, light exposure, etc.). However, in many cases, the mean property experience of the tracer may not be adequate information. For example, in cases in which complex relationships exist between these properties and ecological or biogeochemical constituents of interest, or the time history of exposure is important, the approach may not be adequate. We anticipate thoroughly exploring and expanding the applicability of property tracking in future work.

5. Conclusions

Time- and position-dependent timescales, such as water age and partial age, can be estimated in the technically mature CART framework [1–3,13]. These timescales can be used in several ways [17], including predictive ecological models [18]. The property-tracking approach of [4] greatly extends the power and utility of these predictive, timescale-based models [5], making them applicable to a broader range of applications. The property-tracking approach was originally proposed by analogy to the CART water age estimation approach [13], without mathematical evidence of validity. Here, we illustrate that property tracking and partial age are nearly identical mathematically but conceptually distinct. We applied this novel property-tracking approach to an ecological application with a known solution and faithfully predicted the exposure time to the euphotic zone and the effective light exposure calculated by an adjoint method [7]. The conceptual simplicity and great computational efficiency of these approaches are appealing for a large range of potential applications, and we have just begun to explore these applications [5].

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Appendix A Summary of Theoretical Aspects of Property-Tracking Approach

The core variable of the age theory is the age distribution function, i.e., the histogram of the ages of the particles present at time t in an elemental control volume located at point $\mathbf{x}$. Then, the concentration and the age concentration and the zeroth- and first-order moments of the aforementioned distribution function are obtained. The mean age is the ratio of the former to the latter.

The property exposure theory is largely inspired by developments related to age [6]. The property for which the mean exposure is to be evaluated is denoted as $\psi(t,\mathbf{x})$. Its precise physical meaning is unimportant in the present Appendix. It is not necessarily a positive definite quantity; it may be assumed that $\psi(t,\mathbf{x})\epsilon]-\infty,\infty[$.

As in the age theory, a distribution function needs to be introduced to develop property-exposure-related equations. Accordingly, the age concentration distribution function, $\eta(t,\mathbf{x},\xi)$, is defined as a histogram of the age concentration of the particles at time t and position $\mathbf{x}$, where ξ is the property exposure—as an independent variable. The age concentration and the property age concentration are the zeroth- and first-order moments of the distribution function, i.e.,

$$\alpha(t,\mathbf{x}) = \int_{-\infty}^{\infty}\eta(t,\mathbf{x},\xi)d\xi, \quad \beta(t,\mathbf{x}) = \int_{-\infty}^{\infty}\eta(t,\mathbf{x},\xi)\xi d\xi \tag{A1}$$

Finally, the mean property encountered by the tracer naturally is $b(t,\mathbf{x}) = \beta(t,\mathbf{x})/\alpha(t,\mathbf{x})$.

From considerations involving no arbitrary assumption [6], the equation for the abovementioned distribution function may be seen to be

$$\frac{\partial\eta}{\partial t} = C\delta[\xi-\psi(t,\mathbf{x})] - \nabla\cdot(\eta\mathbf{v}-\mathbf{K}\cdot\nabla\eta) \tag{A2}$$

where δ is the Dirac delta function (it must be borne in mind that the physical dimension of the Dirac delta function is the inverse of the physical dimension of its argument), whilst $\mathbf{v}(t,\mathbf{x})$ and $\mathbf{K}(t,\mathbf{x})$ are the velocity and the diffusivity tensor, respectively. The first term on the right-hand side of this equation is zero, except for a value of ξ equal to the local value of property ψ. In other words, this source term is active only at the local value of property $\psi(t,\mathbf{x})$, hence the need to have recourse to the Dirac delta function.

Taking the zeroth-order moment of (A2) yields the equation for the age concentration,

$$\frac{\partial\alpha}{\partial t} = C - \nabla\cdot(\alpha\mathbf{v}-\mathbf{K}\cdot\nabla\alpha) \tag{A3}$$

which must be equivalent to that obtained in the framework of the age theory, thereby highlighting the close link between the age and property exposure theories. Then, the first-order moment of (A3) leads to

$$\frac{\partial\beta}{\partial t} = C\psi - \nabla\cdot(\beta\mathbf{v}-\mathbf{K}\cdot\nabla\beta) \tag{A4}$$

The above developments were performed under the assumption that the substance under study is a passive one, i.e., it is subject to no reactive processes. If this is not the case, then relevant source-sink terms must be added to Equations (A2)–(A4) [6], which entails no modification to the terms already included in these equations.

Ref. [4] introduced Equation (A4) on the basis of dimensional analysis and physical intuition and illustrated their ability to address practical issues [4,5]. On the other hand, ref. [6] made an attempt at providing a thorough theoretical underpinning for these equations by seeking inspiration in CART's age theory, which may be regarded as a generalization of the reservoir (i.e., zero-dimensional) theory of [19]. This Appendix is a brief summary of [6].

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