Computing optimum estuarine residual fluxes with a multiparameter inverse method (OERFIM): application to the Ria de Vigo (NW Spain)

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Abstract. OERFIM is a two-dimensional (2-D) multiparameter inverse method for calculating estuarine residual fluxes and net ecosystem production rates in estuaries and coastal inlets. OERFIM retains the optimum solution for a weighted system of property conservation equations following the mean squares criterion. The properties involved are volume, salinity, temperature, nutrients (NH4+, NO2-, NO3-, and PO43-), dissolved oxygen, and inorganic carbon. Derived variables such as NO, CO, PO, NCO, and PCO are also considered. OERFIM lies between optimum multiparameter analysis and inverse general ocean circulation models. The simplicity of the method allows for derivation of analytical solutions and a clear exposition of the estuarine box models evolution. From the pioneer, just determined Knudsen method to the overdetermined models such as OERFIM. The theoretical analysis also provides a coherent presentation of analytical errors and their relation to the weights entering the equations. We validate the method with field data from the coastal upwelling system of the “Ria de Vigo”, demonstrating that OERFIM results are suitable to understand the solution structure and, therefore, the whole system itself.

1. Introduction

Over the last 25 years, inverse methods have been a key tool for the understanding of (1) the steady state general ocean circulation [Wunsch, 1977, 1978; Mercier, 1986; Grose et al., 1994], and (2) the complex mixing of water masses in the oceans [Tomczak, 1981; Thompson and Edwards, 1981; Mackas et al., 1987]. Conservation of mass/volume, salinity, and temperature are combined with some dynamic equations (thermal wind relation, vorticity conservation, Bernoulli equation, etc.) to solve the ocean circulation inverse problem. The determination of the level of no motion is the main intricacy of the method [Fiadeiro and Veronis, 1982]. The conventional set of linear mixing equations involving the thermohaline properties, dissolved oxygen (O2), and nutrient salts (NO3-, HPO42-, and H4SiO4) are used in the case of the water mass mixing problem. Contrary to the thermohaline properties, dissolved oxygen and nutrient distributions are affected to some extent by organic matter mineralization processes [Redfield et al., 1963]. The effect of mineralization can be overcome in the case of deep ocean waters mixing in a restricted area. However, when thermocline waters are considered or basin-scale mixing problems have to be solved, the nonconservative nature of the chemical tracers should be considered. A new term, accounting for the mineralization processes, has to be added to the set of linear equations [Kasstenso and Tomczak, 1997], or the conservative chemical tracers “NO” (= O2 + RNOX NO3) and “PO” (= O2 + RPOX HPO42-) introduced by Broecker [1974] should replace O2, NO3-, and HPO42-. RN and RP are stoichiometric coefficients, constant with depth and basin [Anderson and Sarmiento, 1994]. Despite the previous classification, some authors have introduced chemical tracers to solve the ocean circulation problem [Wunsch, 1988; Maré et al., 1997], whereas others have proposed using dynamic equations (conservation of vorticity) for water mass mixing problems [Tomczak, 1999].

The circulation and mixing of water bodies in partially mixed estuaries and coastal inlets have been traditionally solved using estuarine box models [Officer, 1980]. They are just particular inverse problems. Classical estuarine box models are based on the equations of mass/volume and salinity conservation to describe the circulation of continental and ocean waters within the study system. We present here a simple inverse method (OERFIM), which also includes temperature and the chemical tracers, to obtain the two-dimensional residual horizontal water fluxes in partially mixed estuaries and coastal inlets. The resultant overdetermined system of linear equations is solved on the basis of the least squares criterion, the most extended in ocean circulation [Wunsch, 1996] and optimum multiparameter (OMP) analysis of water mass mixing inverse methods [Tomczak, 1999]. The relative simplicity of the problem (only two water bodies are mixing) allows us to partly avoid the complicated numerical machinery developed to solve inverse problems [Wunsch, and Minster, 1982; Tarantola and Valette, 1982] and shows the connection between classical estuarine box models and recent inverse methods. Therefore as in Wunsch’s “eclectic ocean model”, our system of equations merges the available physical and chemical information.

In this paper we describe the method (section 2), derive the diverse box model approaches to estuarine circulation in the literature as particular cases of our general formulation (section 3), study the robustness of the estimations (section 4), and apply the method to study the exchange fluxes in the “Ría de Vigo”, a large coastal inlet in NW Spain (section 5).
Figure 1. (a) Map of the "Ria de Vigo" (NW Spain), our study case, with the five sampling sites visited during September 1990 (solid circles) and the position of the remote monitoring buoy with suspended current meter and thermistor chain (solid star). The position of the meteorological observatories at Cape Finisterre and Vigo airport are also indicated. (b) Section across the main channel of the ria showing the study box with an open boundary at station 3. Abbreviations are as follows: $Q_R$, river discharge; $E$, evaporation rate; $P$, rainfall; $H$, atmospheric heat flux; $F_{O_2}$, atmospheric oxygen flux; $F_{CO_2}$, atmospheric carbon flux; and $Q_s$ and $Q_b$, surface and bottom horizontal fluxes at the open boundary.
2. Inverse Method

The study partially mixed system is segmented in a certain number of enclosed volumes, known as "boxes", delimited by vertical sections perpendicular to the main axis of the system, known as "walls" (Figure 1a). The surrounding lands and the atmosphere also bound the boxes. A 2-D circulation pattern is assumed: The boxes are divided into two layers (surface and bottom), flowing in opposite directions (Figure 1b). The limit between the surface and bottom layer (level of no horizontal motion) is the gravity center of the boundary, that is, the depth where the actual density coincides with the average density of the boundary [Rosón et al., 1997]. Equations of volume, heat (temperature), salinity, dissolved oxygen, inorganic carbon, and nutrient salt conservation are written for each box. Fluxes across all the boundaries, including continental inputs and air-sea exchange fluxes, are considered. In addition, net ecosystem production (NEP) rates, that is, the production of autotrophs minus the respiration of autotrophs and all heterotrophs within the box [Smith and Hollibaugh, 1997], are also included in the case of the nonconservative dissolved oxygen, inorganic carbon, and nutrient budgets. OERFIM computes optimum residual horizontal surface and bottom fluxes at the walls (QH and QB), as well as NEP rates within the boxes, between two consecutive surveys. Optimum vertical advection (QV) and turbulent diffusion (Mz) fluxes between the surface and bottom layer of each box can also be calculated. Application of OERFIM requires the direct measurement or the indirect estimation of the series of input variables listed below, which describe the thermohaline and chemical characteristics of each boundary and box.

2.1. Measured Variables

Full-depth profiles of salinity (S), temperature (T), dissolved oxygen (O2), nitrate (NO3), phosphate (PO4), and two of the four carbon system variables (pH, total alkalinity (TA), total inorganic carbon (CT), and CO2 pressure (pCO2)) are required. Ammonium (NH4+) and nitrite (NO2-) measurements are advisable in ecosystems where they contribute significantly to N nutrient variability. In addition, all these parameters have to be determined in the freshwater tributaries to the system. The temporal and spatial density of the sampling program will depend on the level of resolution required by the study problem. In parallel to the hydrographic program, key meteorological data such as local wind components (Wx, Wy), continental runoff (Qa) precipitation rates (P), humidity (h), cloudiness (N), and air temperature (Ta) must be collected throughout the sampling period.

2.2. Variables Calculated From Collected Data

NEP rates of dissolved oxygen (ΔO2COR) and inorganic carbon (ΔC(TCOR)), nitrogen (ΔNt) and phosphorus (ΔPt) are linked by the Redfield's relationships:

\[ \Delta O_{2,\text{COR}} = -R_e \times \Delta C_{\text{TCOR}} = -R_n \times \Delta N_t = -R_p \times \Delta P_t, \]

\[ \Delta C_{\text{TCOR}} = C_{\text{TCOR}} - C_t = \frac{1}{2} \left( TA + NO_3^- + O_2 + 0.45 \times NO_2^- - NH_4^+ \right). \]

O2COR is independent of the N nutrient form and the precipitation/dissolution of CaCO3. Therefore the calculated O2COR and C(TCOR) should be used instead of the directly measured O2 and C(T).

Integration of the differential expressions in equation (1) leads to a corrected version of Broecker's original "NO" (NOCOR), "PO" (POCOR), and "CO" (COCOR) parameters:

\[ NO_{\text{COR}} = O_{2,\text{COR}} + R_n \times N_t, \]

\[ PO_{\text{COR}} = O_{2,\text{COR}} + R_t \times P_t, \]

\[ CO_{\text{COR}} = O_{2,\text{COR}} + R_e \times C_T. \]

NOCOR, POCOR, and COCOR are conservative parameters, independent of the synthesis/degradation of organic matter and the precipitation/dissolution of CaCO3 occurring within the boxes. The conservation of these parameters is compromised by the inalterability of RC, RN, and RP, that is, the composition of the products of synthesis and early degradation of phytoplankton. NOCOR, POCOR, and COCOR are valid for most applications. In any case, deviations from the average composition used to be related to a transient excess production (consumption) of carbohydrates under N nutrient limitation conditions. Fraoya et al. [1992, 1999] corrected the
effect of an excess production (consumption) of carbohydrates with the conservative NCO and PCO parameters, linear combinations of NOCOR, PCOR, and COCOR:

\[
NCO = NO_{COR} \times \left(1 - \frac{1}{R_c}\right) + CO_{COR} \times \frac{1}{R_c},
\]

(7)

\[
PCO = PO_{COR} \times \left(1 - \frac{1}{R_c}\right) + CO_{COR} \times \frac{1}{R_c},
\]

(8)

Exchange fluxes across the air–sea interface require the calculation of the evaporation term \(E\), which enters the volume budget, the net heat entry from the atmosphere \((H)\), which enters the temperature budget, and the net \(O_2\), \(CO_2\), and nutrient entry from the atmosphere, which enter the corresponding tracer budgets. Parametric equations for \(E = f(h, W, T_s, S_b, H = f(h, W, T_s, S_b, N)\) are available in the literature [e.g., Alvarez-Salgado et al., 2001]. Although the atmospheric nutrient input can be neglected in most applications, \(O_2\) and \(CO_2\) fluxes \((F_{O2} \text{ and } F_{CO2})\) should be calculated with the following equations (in mol s\(^{-1}\)):

\[
F_{O2} = k_{O2} \times (O_{SAT} - O_2) \times A,
\]

(9)

\[
F_{CO2} = k_{CO2} \times S_{CO2} \times (p_{CO2_{ATM}} - p_{CO2_{SAT}}) \times A,
\]

(10)

where \(k_{O2}\) and \(k_{CO2}\) are the \(O_2\) and \(CO_2\) piston velocities (m s\(^{-1}\)), calculated from local winds \((W, W_p, W_f)\) following Wolff and Thorpe's [1991] and Kester's [1975] equations, respectively. \(S_{CO2}\) is the solubility of \(CO_2\) in seawater (mmol m\(^{-3}\)), calculated from salinity and temperature with the equation of UNESCO [1985]. \(O_{SAT}\) is the oxygen concentration at saturation in surface waters (mmol m\(^{-3}\)), calculated from salinity and temperature with the equation of UNESCO [1985]. The parameter \(p_{CO2_{ATM}}\) is the \(CO_2\) pressure in the atmosphere (atm), \(O_{SAT}\) and \(p_{CO2_{SAT}}\) are oxygen (mol m\(^{-3}\)) and \(CO_2\) (atm) levels in surface waters. \(A\) is the surface area of the box (m\(^2\)). For the case of the conservative chemical parameters, the net entry of \(NO_{COR} (F_{NO})\) and \(PO_{COR} (F_{PO})\) equals the net entry of \(O_2 (F_{O2})\) if nutrient inputs are neglected. The net entry of \(CO_{COR}\) is \(F_{CO2} = F_{O2} + F_{CO2}\).

Finally, \(F_{NO} = F_{PO} = F_{O2} + F_{CO2}\).

### 2.3. Overdetermined System of Linear Equations

In order to simplify the presentation of the system of linear equations, they will be written for a box with a unique open boundary (Figure 1b). This box extends from the inner reaches of the estuary to the wall where the horizontal exchange fluxes have to be calculated. A NEP rate is simultaneously obtained for the box. Subsequently, an equivalent system of linear equations can be written for the bottom layer of the box in order to obtain the vertical fluxes and the bottom NEP. Then, the surface NEP can be calculated by subtracting the bottom NEP from the box NEP. Finally, several boxes can be defined, depending on the location of the wall along the estuary, and the vertical fluxes and NEP for the volume enclosed between two walls can be obtained by the difference of the corresponding vertical and NEP rates. Therefore although the circulation of partially mixed estuaries and coastal inlets is a 2-D problem, it can be solved step by step, starting from a 0-D system with a unique open boundary, moving to a 1-D system with two layers, and then, considering a 2-D system with several boxes. We present here the detailed solution for the first step, the 0-D system.

The equations of volume, heat (temperature), salt, \(O_{2\text{COR}}, C_{\text{COR}}, N_T\), and \(P_r\) conservation for any box with an unique open boundary are as follows:

\[
\frac{Q_S - Q_B - Q_R}{Q_x} - P + E = r_{Q_2},
\]

(11)

\[
\frac{Q_xT_S - Q_BT_B - Q_RT_R - H}{Q_x} - P + T_A + V \times \frac{\Delta T}{\Delta t} = r_{T_2},
\]

(12)

\[
\frac{Q_xS_S - Q_BT_B + V \times \frac{\Delta S}{\Delta t}}{Q_x} = r_{S_2},
\]

(13)

\[
\frac{Q_xO2_S - Q_BT_B - Q_RT_R - F_{O2}}{Q_x} - P + O_{2A} + V \times \frac{\Delta O2}{\Delta t} = r_{O2},
\]

(14)

\[
\frac{Q_xN2_S - Q_BT_B - Q_RT_R - F_{N2}}{Q_x} - P + N2A + V \times \frac{\Delta N2}{\Delta t} = r_{N2},
\]

(15)

\[
\frac{Q_xP2_S - Q_BT_B - Q_RT_R - F_{P2}}{Q_x} - P + P2A + V \times \frac{\Delta P2}{\Delta t} = r_{P2},
\]

(16)

\[
\frac{Q_xS2_S - Q_BT_B + V \times \frac{\Delta S}{\Delta t}}{Q_x} = r_{S2},
\]

(17)

where \(Q_S\) and \(Q_B\) (m s\(^{-1}\)) are the average residual surface and bottom horizontal fluxes across the open boundary of the box between two consecutive surveys. \(Q_x\), \(P,\) and \(E\) (m s\(^{-1}\)) are the average continental runoff, precipitation and evaporation in the box between two consecutive surveys. \(T_S\), \(T_B\), \(T_R\), and \(T_A\) (°C) are the average temperature of the surface and bottom flows across the open boundary of the box, the river flow, and the atmosphere between two consecutive surveys. \(\Delta T\) and \(\Delta t\) (°C s\(^{-1}\)) is the net rate of change in the heat content (temperature) of the box between two consecutive surveys. For the case of the \(S, O_2\text{COR}, C_{\text{COR}}, N_T,\) and \(P_r\) conservation equations, the meaning of the corresponding variables is the same as for \(T\). \(V\) is the volume of the box. \(H\) (m \(^3\) m\(^{-3}\) s\(^{-1}\)), \(F_{O2}\) (mol O\(_2\) s\(^{-1}\)), and \(F_{CO2}\) (mol C s\(^{-1}\)) are the average heat, \(O_2\), and \(CO_2\) exchange fluxes across the air–sea interface between two consecutive surveys. Finally, \(NEP\) (mol O\(_2\) s\(^{-1}\)) is the average net ecosystem production within the box between two consecutive surveys. Obviously, this term only appears in the equations of the nonconservative chemical parameters.

Some reasonable assumptions are implicit in this system of equations: (1) The volume of the box is constant because a mean tidal volume is considered. (2) The average heat flux across the surface layer of the open boundary, \(Q_xT_S\), is simplified as the product of \(Q_x\) \(T_S\). The same is applicable to the bottom layer, and the river and precipitation fluxes. It is also valid for salinity, \(O_{2\text{COR}}, C_{\text{COR}}, N_T,\) and \(P_r\). The simplification is based on the extreme variability of waters fluxes compared with property changes in most estuarine and coastal systems. (3) The salinity of continental water and
The average temperature, salinity, $O_{SCOR}$, $C_{TCOR}$, $N_T$, and $P_T$ of the surface and bottom layer of the wall and the box are obtained by numeric integration of measured profiles, considering the geometric characteristics of the estuary. $Q_s$, $P_s$, $T_s$, and $T_b$, and the chemical composition of the river flow are known from direct measurements (section 2.1). $H$, $F_{CO}$, and $F_{CO}$, are also estimated from measured variables (section 2.2). Therefore the system of seven linear equations has only three unknowns: $Q_s$, $Q_b$, and NEP. Hereinafter, the overbar used to indicate average values of any variable between two consecutive surveys will be removed.

Since the system is overdetermined, the solution ($Q_s$, $Q_b$, and NEP) that minimizes the weighted sum of squared residuals of the seven equations ($\sum_j r_j^2 \times w_j^2$) can be retained. The $r_i$ are the residuals of the volume ($\rho_s$, m$^3$ s$^{-1}$), heat ($r_h$, $^\circ$C s$^{-1}$), salt ($r_s$, kg s$^{-1}$) $O_{SCOR}$, ($r_{CO}$), $C_{TCOR}$ ($r_{CO}$), $N_T$ ($r_{NT}$), and $P_T$ ($r_{PT}$, mol s$^{-1}$) budgets, partly caused by the simplifications above. The $w_i$ are factors that (1) weight the conservation equations on the basis of the relative analytical accuracy of every measured parameter and (2) normalize the residuals to a common dimension (m$^3$ s$^{-1}$). The corresponding factor for the heat budget is

$$w_T = \frac{T_b - T_s}{\varepsilon_T} \left( \frac{1}{\sum_{j=1}^{n} (T_b - T_s)^2} \right)^{\frac{1}{2}} = \frac{T_b - T_s}{\varepsilon_T} \times \xi_T^{-1}.$$

The weighting term $T_b - T_s$ indicates the number of times that the temperature gradient at the wall exceeds the accuracy of the determination of temperature. The normalizing term $\xi_T = (\sum_{j=1}^{n} (T_b - T_s)^2)^{\frac{1}{2}}$ is the square root of the squared temperature gradient at the study wall averaged over the whole set of time intervals considered ($n$). Equivalent normalizing-weighting terms can be written for $S$, $O_{SCOR}$, $C_{TCOR}$, $N_T$, and $P_T$. Finally, a large value of the factor for the volume budget ($\varepsilon_T >$ tidal prism volume) is preferred to satisfy the desirable condition that the volume is accurately conserved ($\varepsilon_T = 0$).

$O_{SCOR}$, $C_{TCOR}$, $N_T$, and $P_T$ can be substituted by the conservative chemical parameters $CO_{COR}$, $NO_{COR}$, and $PO_{COR}$. Equations (14) to (17) should be replaced by

$$Q_s \times CO_3 - Q_b \times CO_3 - Q_s \times CO_3 - P \times CO_3$$

$$- (F_{CO} + R_s \times F_{CO_2}) + V \times \frac{\Delta CO}{\Delta t} = r_{CO},$$

$$Q_s \times NO_3 - Q_b \times NO_3 - Q_s \times NO_3 - P \times NO_3$$

$$- F_{O_3} + V \times \frac{\Delta NO}{\Delta t} = r_{NO},$$

$$Q_s \times PO_4 - Q_b \times PO_4 - Q_s \times PO_4 - P \times PO_4$$

$$- F_{O_3} + V \times \frac{\Delta PO}{\Delta t} = r_{PO}.$$
obtain water fluxes from salinity distributions, assuming volume and salt conservation. The unique solution for this system of two equations (equations (11) and (13)) with two unknowns, \((Q_s)_h\) and \((Q_b)_h\), is

\[
(Q_s)_h = \frac{(Q_s + P - E) \times S_b - S_b}{S_b - S_s}, \quad (24)
\]

\[
(Q_b)_h = (Q_s)_h - (Q_s + P - E). \quad (25)
\]

Equivalent systems of two equations with two unknowns can be solved to obtain water fluxes from temperature distributions, assuming volume and heat conservation (equations (11) and (12)):

\[
(Q_s)_t = \frac{[(Q_s + P - E) \times T_b - Q_s \times T_b - P \times T_s - H + V \times \frac{\Delta T}{\Delta t}] \times (T_b - T_s)}{(T_b - T_s)}, \quad (26)
\]

\[
(Q_b)_t = (Q_s)_t - (Q_s + P - E), \quad (27)
\]

and from the different conservative chemical variables: CCor (equations (11) and (19)), NOCor (equations (11) and (20)) and POCor (equations (11) and (21)) or NCO (equations (11) and (22)) and PCO (equations (11) and (23)). For the exemplar case of PCO the solution is

\[
(Q_s)_{PCO} = ((Q_s + P - E) \times PCO_a - Q_s \times PCO_a - P \times PCO_a - (F_{CO2} + F_{CO2}) \times PCO_a - V \times PCO_a), \quad (28)
\]

\[
(Q_b)_{PCO} = (Q_s)_{PCO} - (Q_s + P - E). \quad (29)
\]


Rosón et al. [1997] presented for the first time a mass–heat weighted 2-D box model. They used parallel salinity and temperature distributions under the assumptions of volume, heat, and salt conservation. They obtained the solution for this system of three equations ((11), (12) and (13)) with two unknowns that minimizes the sum of weighted square residuals. In addition, they also considered that volume is accurately conserved \((Q_v = 0)\). Under these conditions

\[
r_s \times \frac{S_b - S_s}{T_b - T_s} \times \left(\frac{S_b - S_s}{T_b - T_s}\right)^2 + r_s = 0, \quad (30)
\]

and the analytical expressions for the optimum values of \((Q_s)_{hs,r}\) and \((Q_b)_{hs,r}\) are

\[
(Q_s)_{hs,r} = (Q_s)_h \times f + (Q_s)_h \times (1 - f), \quad (31)
\]

\[
(Q_b)_{hs,r} = (Q_s)_{hs,r} - (Q_s + P - E), \quad (32)
\]

with

\[
f = \frac{(S_b - S_s)^2}{(T_b - T_s)^2 \times \left(\frac{w_s}{w_s}\right)^2}, \quad (33)
\]

Rosón et al. [1997] defined \(w_s\) and \(w_T\) just as normalizing factors:

\[
w_s = \left(\frac{\sum(S_b - S_s)^2}{n}\right)^{1/2}, \quad (34)
\]

\[
w_T = \left(\frac{\sum(T_b - T_s)^2}{n}\right)^{1/2}. \quad (35)
\]

Therefore the final expression of \(f\) for this case is

\[
f = \frac{(S_b - S_s)^2}{(T_b - T_s)^2 \times \left(\frac{w_s}{w_s}\right)^2}, \quad (36)
\]

\[
(S_b - S_s)^2 + (T_b - T_s)^2 \times \left(\frac{w_s}{w_s}\right)^2
\]

The factor \(f\), which varies between 0.0 and 1.0, indicates the relative contribution of the salt, \((Q_s)_r\), and temperature, \((Q_T)_r\), solutions to the optimum salt–heat weighted solution, \((Q_s)_{hs,T}\). Figure 2a shows the 1987–1996 time series of \((S_b - S_s)\) and \((T_b - T_s)\) in the central segment of the "Ria de Vigo" (NW Spain), station 3 in our study case (Figure 1a). The corresponding time series of \(f\) (Figure 2b) was calculated with (36). Values of \(f\) close to 1.0 are obtained during the winter months, when the salinity gradient is quite pronounced and the temperature gradient homogenizes. On the contrary, values of \(f\) close to 0.0 are obtained during the summer period, when continental runoff is limited and the temperature gradient maximizes. Steep transitions from extreme values of \(f\) are observed during spring and autumn.

Using appropriate \(w_T\) (equation (18)) and \(w_s\) normalizing–weighting factors, \(f\) would have the following expression:

\[
f = \frac{\sum(S_b - S_s)^2}{\sum(T_b - T_s)^2 \times \left(\frac{w_s}{w_s}\right)^2}, \quad (37)
\]

\[
(S_b - S_s)^2 + (T_b - T_s)^2 \times \left(\frac{w_s}{w_s}\right)^2
\]

which produces more abrupt transitions between extreme values of \(f\) (Figure 2c), because the influence of vertical gradients in the calculation of \(f\) is now elevated to the fourth power. The values of \(f\) calculated with equations (36) and (37) are compared in Figure 2d.

3.3. OERFIM Solutions for the Thermohaline and Conservative Chemical Variables

Optimum horizontal residual fluxes, obtained from temperature, salinity, CCor, NOCor, and POCor distributions (equations (11), (12), (13), (19), (20) and (21)), using the appropriate normalizing–weighting factors and assuming that the volume is accurately conserved, display the following analytical expressions:

\[
(Q_s) = \sum_{i=1}^{n}(Q_s) \times f_i, \quad (38)
\]

\[
(Q_b) = Q_s - (Q_s + P - E), \quad (39)
\]

with
Figure 2. Time series of (a) $S_b - S_s$ and $T_b - T_s$, (b) the factor $f$ calculated with equation (36), $f_{36}$, (c) the factor $f$ calculated with equation (37), $f_{37}$, and (d) $f_{36}$ versus $f_{37}$ for station 3 ("Ria de Vigo", Figure 1), visited twice a week between 1987 and 1996.
\[ f_i = \left( \frac{b_i - a_i}{2} \right)^2 \times w_i^2 \]
\[ \sum_{i=1}^{n} \left( \frac{b_i - a_i}{2} \right)^2 \times w_i^2 \]

Equivalent analytical expressions are obtained for the case of volume, salinity, temperature, NCO, and PCO conservation through the system of seven equations and three unknowns, which is a 7x3 matrix containing the chemical properties of Qs and Qa and the net ecosystem production rates (NEP). The optimum solution for the system of equations (11)–(17) can be expressed in matrix form as follows:

\[ Q = (A^T \times W^2 \times A)^{-1} \times (A^T \times W^2 \times B) \]

where \( Q \) is a 3x1 matrix containing the optimum multiparametric solution of this system of seven equations; \( A \) is a 3x7 diagonal matrix containing the known river, air-sea exchange, and accumulation parameters involved in the calculation of the individual errors with any pair of conservative variables. For the case of the general salt-heat weighted solution, the error of the estimation, \( \varepsilon_Q \), is

\[ \varepsilon_Q = \varepsilon_S + \varepsilon_{\Delta T} + \varepsilon_{\Delta S} + \varepsilon_{Qs} + \varepsilon_{Qa} \]

where \( \varepsilon_S \) and \( \varepsilon_{\Delta T} \) are the errors of the estimation of \( S \) or \( T \), and \( \Delta S / \Delta T \). The proper error can be approached following the procedure of Maamaatuaiahutapu [Matsukawa and Suzuki, 1985]. The proper error of the estimation (\( \varepsilon_Q \)) is

\[ \varepsilon_Q = \sum_{i=1}^{n} \varepsilon_Q \times f_i \]

An equivalent expression can be written for the mass–heat–NCO–PCO optimum solution.
et al. [1992] for the optimum multiparameter analysis of water mass composition. A number of perturbed systems of equations (11)-(17) can be obtained by random modification of the measured variables within the limits of the oceanographic errors of their estimations. One thousand perturbed systems can be produced, and 1000 different optimum solutions obtained. We obtain an average solution \( \langle PQ, Q \rangle \) from the perturbed data and a proper error equal to the standard deviation \( \sigma = \sigma_0 \) of the 1000 solutions.

Figure 3 shows an exercise of comparison of \( \langle Q_s \rangle \) obtained with equation (42) and \( \delta_{Q_s} \) by perturbation of equations (11) and (13) using the 1987-1996 time series of \( S_s \), \( S_b \), and \( Q_s \) values for the “Ria de Vigo” (Figure 2). It should be noted that in this case \( S_s \) and \( S_b \) are not average values over the surface and bottom layer but just single values in the surface (5 m) and bottom (40 m). \( \Delta S/\Delta t \) is calculated as the \( (S_s + S_b)/2 \) difference between two consecutive sampling dates (3-4 days), that is, it is the salinity change in the boundary rather than in the box. Finally \( P-E \) has been set to zero and \( \delta_{Q_s} = 0.02 \), that is, 20% of \( \lambda_s \) or 5 times \( \epsilon_s \). Despite all these simplifications, the message from Figure 3 is clear: The proper error \( \delta_{Q_s} \) is very well correlated with the maximum expected error \( \delta_{Q_s} \) and represents about 1/4 of its value.

5. Study Case of the “Ria de Vigo” (NW Spain). Description of a Complete Upwelling-Downwelling Event in September 1990

Optimum residual fluxes and NEP rates were estimated by running OERFIM with a set of empirical data collected during a series of five consecutive surveys of the coastal upwelling system of the “Ria de Vigo” (NW Spain) in September 1990. All the required variables were measured during the surveys. In addition, surface currents were measured with a current meter, allowing validation of the calculated optimum fluxes with empirical data. OERFIM retained the solution that best describes (in a weighted least squares sense) the observed short-time scale (2-4 days) changes in the distributions of selected thermohaline and chemical tracers during a complete coastal upwelling-downwelling cycle in the NW Iberian upwelling system.
5.1. Study Area

The "Ria de Vigo" is a large (2.76 km$^3$) V-shaped coastal inlet freely connected with the adjacent shelf of NW Spain (Figure 1a), the northern boundary of the NW African/Iberian Upwelling System. Coastal winds at our latitudes (42°-43°N) are upwelling-favorable from April–May to September–October [Wooster et al., 1976; Bakan and Nelson, 1991] and tend to occur as a succession of stress/relaxation events with a marked periodicity of 10–20 days [Alvarez-Salgado et al., 1993]. The "Ria de Vigo" behaves as an inshore extension of the continental shelf during the upwelling season, with the advantage that circulation can be successfully resolved with a 2-D approach [Prego and Fraga, 1992; Alvarez-Salgado et al., 2001].

For the purposes of this work, the study box extends from the upper reaches of the embayment (San Simon Bay, the estuary of the river Oitaben–Verdugo) to the middle ria (station 3), where the surface current meter was deployed (Figure 1a). This box is 0.53 km$^2$ large and presents a unique open boundary at station 3 (Figure 1b). The open boundary is divided into a surface and a bottom layer by the pycnocline. The thermohaline and chemical properties of the surface and bottom layer are calculated considering the full–depth vertical profiles collected at station 3, assuming that the embayment is transversally uniform (2-D approach). The thermohaline and chemical characteristics of the box are obtained considering measurements at stations 1, 2, and 3, as well as the geometry of the ria.

5.2. Data Set

The data used to run OERFIM came from three sources (Figure 1a): (1) the meteorological station at the airport of Vigo, (2) the buoy deployed at station 3 from September 11 to 27, 1990, and (3) the five hydrographic surveys to visit stations 1, 2, and 3 on September 14, 18, 20, 24, and 27, 1990, aboard R/V Explorador. Stations 4 and 5 were also occupied, but they will not be used in this paper.

The meteorological station at the airport provided data on rainfall ($P$, m$^3$ s$^{-1}$) and cloudiness ($N$, oktas). Cloudiness is necessary to calculate the heat exchange flux across the sea surface following Álvarez-Salgado et al. [2001]. Continental runoff ($Q_C$) was computed from precipitation following Rias et al. [1992].

The buoy at station 3 provided local winds ($W_x$ and $W_y$) with an Aanderaa 2740 sensor, seawater temperature at 11 depths from a thermistor chain, and surface current velocities from a RCM7 current meter. The current meter was deployed at 3.7 m, and the thermistor sensors were deployed at 2, 3.6, 4.5, 8.1, 9.5, 13.5, 14.5, 18, 19.5, 23.5 and 24.5 m. Therefore the last one was about 18 m above the bottom.

At the hydrographic stations, full–depth continuous conductivity and temperature profiles were recorded with a calibrated CTD SBE-25. Salinity was calculated from the CTD–conductivity record with the equation of UNESCO [1985]. The accuracy of CTD salinity and temperature was ±0.005 psu and ±0.005°C respectively. Dissolved oxygen, N, nutrients, phosphate, pH and alkalinity were measured at five to seven selected depths throughout the water column at each station. Dissolved oxygen was analyzed by Winkler potentiometric end point titration, with an estimated analytical error ($\delta_{o2}$) of ±1 μmol kg$^{-1}$. Potentiometric pH was measured on the NBS scale with the classical 7.414 phosphate buffer ($\delta_{PH}$ = ±0.005) following the Pérez and Fraga [1987a] technique. Total alkalinity was determined by titration to pH 4.4 with 0.13 N hydrochloric acid ($\delta_{TA}$ = ±2 μmol kg$^{-1}$), according to the potentiometric endpoint method of Pérez and Fraga [1987b]. Total inorganic carbon (C$_T$) was calculated from pH and TA using the carbon system equation and the acid constants of Mehrbach et al. [1973]. The estimated $\delta_{C_T}$ was ±4 μmol kg$^{-1}$. Nutrients were determined by segmented flow analysis following Hansen and Grasshoff [1983] with some small improvements [Mouriño and Fraga, 1985; Alvarez-Salgado et al., 1992]. The corresponding analytical errors were $\delta_{NO2}=±0.02$ μmol kg$^{-1}$, $\delta_{NO3}=±0.1$ μmol kg$^{-1}$, $\delta_{NH4}=±0.05$ μmol kg$^{-1}$, $\delta_{SiO4}=±0.05$ μmol kg$^{-1}$ and $\delta_{PO4} = ±0.01$ μmol kg$^{-1}$. Air temperature ($T_a$, °C) and relative humidity (h, %) were taken from the ship to calculate the evaporation flux $E = f(h, W_x, T_a, T_s, S_s)$ (m$^3$ s$^{-1}$) with a parametric equation [Alvarez-Salgado et al., 2001].

Table 1 summarizes the meteorological, thermohaline, and chemical data for the three boundaries (continent, atmosphere, and wall) and the volume of the study box necessary to run the conservative and nonconservative versions of OERFIM. Four periods are considered, September 14–18, 18–20, 20–24, and 24–27, 1990.

5.3. Hydrographic Scenario in the Ria de Vigo During September 1990

As for any coastal upwelling system, the offshore Ekman transport ($-$Q$_x$) is the main forcing agent of the residual circulation in the "Ria de Vigo" [Alvarez-Salgado et al., 2000; Pardo et al., 2001]. Ekman transport values were obtained from wind data at the Cape Finisterre meteorological station (Figure 1a) and the equation of Wooster et al. [1976],

$$-Q_x = -\rho_{aw} \times C_D \times \frac{W_x^2 + W_y^2 \times W_y}{f \times \rho_a},$$

where $\rho_{aw}$ is the density of air, 1.22 kg m$^{-3}$ at 15°C; $C_D$ is an empirical drag coefficient (dimensionless), 1.3 $10^{-3}$ according to Hidy [1972]; $f$ is the Coriolis parameter, 9.946 $10^{-5}$ s$^{-1}$ at 43°N latitude; $\rho_{aw}$ is the density of seawater, ~1025 kg m$^{-3}$, and $W_x$ and $W_y$ in m s$^{-1}$ are the south–north and west–east components of the coastal winds at Cape Finisterre. Local winds provided by the buoy are not representative for the wind patterns off the "Ria de Vigo", because the embayment is well protected by the surrounding mountains, more than 400 m high.

Figure 4 presents an excellent picture of the succeeding hydrographic scenarios in the 'Ria de Vigo' during the second fortnight of September 1990, at the time of the transition from upwelling-favorable northerly winds to downwelling-favourable southerly winds. Figure 4a shows the time course of the offshore Ekman transport (3 days running mean). An evolution is clearly observed from a situation of wind calm on September 14 to an upwelling peak on September 17, a subsequent upwelling relaxation to September 24 and, finally, a strong downwelling event that culminates on September 27 1990. Figure 4b shows the response of the water column to coastal winds. The 14°-15°C isotherms paralleled the time evolution of $-Q_x$ from September 14 to 24. The subsequent downwelling event allows the downward penetration of surface water warmer than 17°C up to 20 m depth. Finally, Figure 4c completes the picture, showing the progressive
Table 1. Data Set to Run OERFIM Box Model in the “Ría de Vigo” During September 1990.

### Continental Runoff Tracer Values

<table>
<thead>
<tr>
<th>Interval</th>
<th>$S_r$</th>
<th>$T_r$</th>
<th>$N_{TR}$</th>
<th>$P_{TR}$</th>
<th>$C_{PCOR}$</th>
<th>$O_{PCOR}$</th>
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<td>mmol m$^{-3}$</td>
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### Tracer Box Time Derivatives

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<td>°C m$^{-3}$ s$^{-1}$</td>
<td>Mmol s$^{-1}$</td>
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<td>mmol m$^{-3}$</td>
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### Atmosphere–Sea Exchange Fluxes and Continental Runoff

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<th>$F_{CO_2}$</th>
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<td>10.6</td>
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The data were filtered with a 3 day running mean. Therefore tidal effects were completely erased prior to calculating the progressive vector. The direction of the observed currents is quasi-parallel to the main axis of the ria, supporting the 2-D approach. In agreement with the time evolutions of $-Q_x$ and temperature, from September 12 to 15 warm shelf surface water entered the ria up to station 3. From September 15 to 21 the warm surface waters flowed out of the ria and the temperature of the embayment decreased to its minimum.
Figure 4. (a) Offshore Ekman transport ($-Q_x$) calculated with winds at the Cape Finisterre meteorological station and filtered with a 3 day running mean ($m^3 s^{-1} km^{-1}$). (b) Time evolution of the temperature profile at station 3 from thermistor chain record ($^\circ$C). (c) Progressive vector diagram for the near-surface (3.7 m deep) current meter at station 3 during the study period in September 1990. The velocity data were filtered with a 3 day running mean. The numbers indicate the day of September (00:00 hours).
because of wind-driven upwelling. Finally, from September 21 to 27 the surface circulation reversed again in response to the upwelling relaxation and subsequent strong downwelling.

5.4 Results From the Conservative Version of OERFIM
(S, T, NCO, and PCO)

Optimum \( Q_s \) and \( Q_b \) values were calculated using the required data (Table 1) to solve the system of equations (38)–(40), the analytical errors being \( \epsilon_s = 0.005^\circ C \), \( \epsilon_s = 0.005 \) psu, and \( \epsilon_{NCO} = \epsilon_{PCO} = 7.4 \) pmol kg\(^{-1}\). The oceanographic errors of the estimation, \( O_{Qs} \) and \( O_{Qb} \), were obtained with equation (46) with \( O_{\epsilon} = 0.2 \times \epsilon_i \) (\( i = S, T, NCO \) and \( PCO \)). Twenty percent of \( \epsilon_i \) seems a reasonable oceanographic error, since the spatial and temporal hydrographic variability of the “Ria de Vigo” affects essentially the vertical rather than the horizontal profiles of the thermohaline and chemical variables. The representativeness error for the other variables, river and atmosphere fluxes, was set to 10% of the corresponding measured/estimated value of the variable The results are presented in Table 2. In addition, the average \( (PQ_s, PQ_b) \) and standard deviation \( (\delta_{PQ_s}, \delta_{PQ_b}) \) of the set of 1000 solutions obtained with the perturbation method (section 4.2) are also summarized in Table 2. It is clear that the maximum expected errors are about 4 times the proper error, as in Figure 3.

Figure 5a shows the time evolution of \( f_s \), indicating that \( Q_s \) and \( Q_b \) in the study case depended mainly on the temperature budget. Values of \( f_s, f_{NCO} \) and \( f_{PCO} \) are so low that the solution retained by the conservative version of OERFIM does not differ substantially from the solution arising from equations (26) and (27). The reason behind the observed behavior is the horizontal variability of salinity and PCO, and salinity compared with temperature, as suggested by Table 1. Since continental runoff was quite limited (<11 m\(^3\) s\(^{-1}\)), the ria was primarily occupied by cold and salty Eastern North Atlantic Central Water (ENACW) with constant NCO and PCO concentrations. Heat exchange across the sea surface \( (H) \) contributes to warm the surface layer, enhancing the temperature gradient but producing no effect on the salinity, NCO, and PCO profiles. These tracers acquire more relevance for the calculation of optimum estuarine fluxes when continental runoff is higher, as occurs during the winter in the “Ria de Vigo” or throughout the year in most of the estuaries of large rivers.

5.5 Results From Nonconservative Version of OERFIM
(S, T, O\(_{2COR}\), C\(_{TORS}\), N\(_T\), and P\(_T\))

Optimum horizontal residual fluxes \( (Q_s, Q_b) \) were obtained again at station 3 by solving the overdetermined system of equations (11)–(17) as indicated in section 3.4 (equation (41)). In addition, optimum net ecosystem production rates within the study box \( (NEP) \) were simultaneously obtained. The required data are summarized in Table 1, and the corresponding results are presented in Table 3. Matrices \( A \) and \( B \) were randomly perturbed 1000 times within the error limits of the measured/estimated variables, and again \( O_{\epsilon} = 0.2 \times \epsilon_i \) with \( i = S, T, O_{2COR}, C_{TORS}, N_T, \) and \( P_T \), and 10% of the measured/estimated value for the rest of variables. The \( w \) terms of the diagonal matrix \( W \) were calculated with \( \epsilon_s = 0.005^\circ C, \epsilon_s = 0.005 \) psu, \( \epsilon_{N} = 0.1 \) pmol kg\(^{-1}\), \( \epsilon_{O2} = 0.01 \) pmol kg\(^{-1}\), \( \epsilon_{CORS} = 4.5 \) pmol kg\(^{-1}\) and \( \epsilon_{PCORS} = 1.1 \) pmol kg\(^{-1}\). The corresponding average \( (\delta_{PQ_s}, \delta_{PQ_b}, \delta_{NEP}) \) and standard deviation \( (\delta_{PQ_s}, \delta_{PQ_b}, \delta_{NEP}) \) of the 1000 solutions are also presented in Table 3.

Although \( f_i \) values for the nonconservative version of OERFIM have not been derived, pseudo values of \( f_i \) can be calculated for \( O_{2COR}, C_{TORS}, N_T, \) and \( P_T \) with equation (40). Despite the pronounced vertical gradients of the nonconservative variables (Table 1), the retained solution is again controlled by the extreme temperature gradients (Figure 5b). However, for the September 24–27 period the contribution of \( O_{2COR}, N_T, \) and \( P_T \) became more important because of the relative thermal homogenization caused by strong downwelling events (Figure 4b) and the enhanced gradients of the non conservative tracers (Table 1). In any case, \( Q_s \) and \( Q_b \) are not substantially different from the values obtained with the conservative version of OERFIM. Obviously, the major differences are obtained for the last study period.

The obtained NEP rates are coherent with the expected time evolution during an upwelling–downwelling sequence. NEP is negative, that is, respiration exceeds production, during the spin-up phase of upwelling. It become practically nil during the upwelling climax and increased dramatically, that is, production exceeded respiration, during the subsequent upwelling relaxation. Finally, respiration is again dominant under downwelling conditions. The lag time between NEP and upwelling is related to the low initial phytoplankton biomass in recently upwelled water [Brown and Field, 1986] and the large flushing rates (Table 3), which do not allow complete transition from slow to fast phytoplankton growth in response to the new high nutrient and light conditions [Zimmerman et al., 1987]. On the other hand, downwelling periods usually are dominated by respiration processes [Pérez et al., 2000].

5.6. Comparison of Optimum Fluxes and Measured Surface Current.

The reasonable errors of the residual fluxes and net ecosystem production rates (Table 3) prove the robustness of

<p>| Table 2. Results From OERFIM Box Model With Conservative Equations (NCO and PCO) in the “Ria de Vigo” During September 1990. |</p>
<table>
<thead>
<tr>
<th>Days</th>
<th>( Q_s )</th>
<th>( O_{Qs} )</th>
<th>( Q_b )</th>
<th>( O_{Qb} )</th>
<th>( G_s )</th>
<th>( PQ_s )</th>
<th>( Q_{NEP} )</th>
<th>( PQ_{NEP} )</th>
<th>( \delta_{PQ_s} )</th>
<th>( \delta_{PQ_b} )</th>
<th>( \delta_{PNEP} )</th>
</tr>
</thead>
<tbody>
<tr>
<td>14–18</td>
<td>675</td>
<td>±161</td>
<td>671</td>
<td>±161</td>
<td>100</td>
<td>679</td>
<td>±47</td>
<td>675</td>
<td>±47</td>
<td></td>
<td></td>
</tr>
<tr>
<td>18–20</td>
<td>991</td>
<td>±253</td>
<td>986</td>
<td>±254</td>
<td>62</td>
<td>992</td>
<td>±74</td>
<td>987</td>
<td>±74</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>
the solutions retained by OERFIM. In addition, we have the opportunity to test the accuracy of the estimation of $Q_s$ by comparing the retained solution ($PQ_s$), converted to velocity ($PV_s$) considering the cross section of the surface layer of the wall, with the measured surface currents at station 3 (Figure 6). The agreement is good, though for the September 18–20 period OERFIM underestimates the outgoing velocity under intense upwelling conditions when the 2-D approach could be weaker. In any case, it should be considered that results from direct current measurements indicate water displacements at a

Table 3. Results From OERFIM Box Model With Nonconservative Equations ($N_f, P_f, C_{tor}, O_{cor}$) in the “Ria de Vigo” During September 1990.

<table>
<thead>
<tr>
<th>Interval</th>
<th>$Q_{sn}$</th>
<th>$Q_{bh}$</th>
<th>NEP,</th>
<th>$G$,</th>
<th>$PQ_{sn}$</th>
<th>$PQ_{bh}$</th>
<th>$\delta_{P_{Qn}}$</th>
<th>$\delta_{P_{Qh}}$</th>
<th>$P_{N_{E}}$,</th>
<th>$\delta_{P_{N_{E}}}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>days</td>
<td>m$^3$s$^{-1}$</td>
<td>m$^3$s$^{-1}$</td>
<td>gCm$^2$d$^{-1}$</td>
<td>m$^3$s$^{-1}$</td>
<td>m$^3$s$^{-1}$</td>
<td>m$^3$s$^{-1}$</td>
<td>gCm$^2$d$^{-1}$</td>
<td>gCm$^2$d$^{-1}$</td>
<td>gCm$^2$d$^{-1}$</td>
<td>gCm$^2$d$^{-1}$</td>
</tr>
<tr>
<td>14–18</td>
<td>675</td>
<td>671</td>
<td>-0.38</td>
<td>118</td>
<td>677</td>
<td>745</td>
<td>±45</td>
<td>±45</td>
<td>-0.37</td>
<td>±0.08</td>
</tr>
<tr>
<td>18–20</td>
<td>991</td>
<td>986</td>
<td>0.03</td>
<td>65</td>
<td>994</td>
<td>990</td>
<td>±74</td>
<td>±74</td>
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<td>±0.08</td>
</tr>
<tr>
<td>20–24</td>
<td>-756</td>
<td>-764</td>
<td>0.94</td>
<td>149</td>
<td>-759</td>
<td>-767</td>
<td>±102</td>
<td>±102</td>
<td>0.93</td>
<td>±0.16</td>
</tr>
<tr>
<td>24–27</td>
<td>-441</td>
<td>-452</td>
<td>-0.29</td>
<td>273</td>
<td>-434</td>
<td>-444</td>
<td>±75</td>
<td>±75</td>
<td>-0.28</td>
<td>±0.14</td>
</tr>
</tbody>
</table>
Figure 6. Comparison between surface OERFIM velocities solutions and surface RCM7 current meter average velocities perpendicular to the box wall at station 3.

6. Conclusions

OERFIM is an optimum multiparameter update of the classical box models, which is revealed to be a useful research tool for the simultaneous estimation of residual fluxes and net ecosystem production (NEP) rates in partially mixed estuaries, coastal inlets, and enclosed seas. Compared with classical box models, OERFIM combines all the thermohaline and chemical information usually available from the abundant hydrographic studies of these relevant marine systems to obtain optimum, appropriately weighted, solutions, not only of residual fluxes but of NEP rates too. Knowledge of the analytical solutions of OERFIM allows us to define a specific normalizing–weighting factor \( w_i \) instead of using sophisticated procedures such as single-value decomposition, tapered least squares, or other numerical methods [Wunsch, 1996]. In any case, the normalizing factor \( w_i \), mimics the classical weighting factor used in the literature about inverse methods: the variance of the residuals. Moreover, OERFIM pays particular attention to the reliability of the results, incorporating a rigorous assessment of the analytical, oceanographic, and perturbed errors of the system of balance equations and their intricate relationships. It is concluded that the perturbed error is the more appropriate parameter to assess the consistency of the solutions produced by OERFIM because of the averaging effect of all terms and properties involved in the calculation of the individual error of each thermohaline and chemical variable. This also is also a substantial improvement compared with the classical box models, which usually consider only one state variable (salinity or temperature).

Finally, the first step of OERFIM, the 0-D solution, is applied to a set of field data collected in the Ría de Vigo, a coastal inlet off NW Spain affected by intermittent upwelling/downwelling events. The optimum solution provided by OERFIM is reasonably accurate and reliable regarding either the water fluxes or the NEP rates. Estimated residual fluxes compare fairly well with the concurrent current meter record and the uncertainty of the solution (the perturbed error) stays within an acceptable interval. It is also shown that OERFIM provides useful information on the structure of the solution from the \( f \) factors.

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References


