

Local sensitivity analysis of a distributed parameters water quality model

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A local sensitivity analysis is presented of a 1D water-quality reaction-diffusion model. The model describes the seasonal evolution of one of the deepest channels of the lagoon of Venice, that is affected by nutrient loads from the industrial area and heat emission from a power plant. Its state variables are: water temperature, concentrations of reduced and oxidized nitrogen, Reactive Phosphorous (RP), phytoplankton, and zooplankton densities, Dissolved Oxygen (DO) and Biological Oxygen Demand (BOD). Attention has been focused on the identifiability and the ranking of the parameters related to primary production in different mixing conditions. © 1997 Elsevier Science Limited.

1 INTRODUCTION

Sensitivity and uncertainty analyses have become standard tools in water-quality modelling [1], but they have been mainly applied to lumped parameters models, which do not enable one to describe the evolution of a complex system, such as a coastal basin. In such systems, the morphology of the bathymetry leads to a spatial differentiation which can be modelled only by combining the chemical and biochemical reactions with transport processes in the mass-balance equations. As a result, a system is described by a set of partial differential equations that must be solved numerically.

The interest in the applications of these complex models to the management of coastal areas is growing, also because the availability of fast computers has lowered the costs of numerical simulations. However, their complexity might also be a source of difficulties, e.g., in the calibration/validation stage, and, sometimes, the results may be misleading, because it can be problematic to relate cause and effects, i.e., input and output, and to assess the uncertainty in the output.

Sensitivity analysis can be of great help in tackling the above questions, as, besides giving useful insights into the mechanisms of the model, it can be usefully employed for a correct calibration of the model on the basis of field data. Further, it can also give a first estimate of the uncertainty of the model output, given the uncertainties of the inputs. The computational demand of these programs might discourage a global

analysis, but a large amount of information is provided also by a local analysis, which can be carried out more quickly.

The theory of local sensitivity analysis of the advection-diffusion-reaction equation is very advanced, and many working examples can be found, especially for problems of combustion and air-pollution [2–4]. However, in the field of water-quality modelling, the applications seem to lag behind the theory, and, to the authors' knowledge, no case-study can be found in the literature.

This paper represents an attempt to fill this gap, presenting a first-order local sensitivity analysis of a 1D water-quality model. The reaction-diffusion equation is solved with an explicit finite-difference scheme. A simple derivation of the sensitivity equation for the case dealt with in the paper is also given, in order to stimulate a wider application of this method.

2 METHODS

Taking into account the aim of this study, the sensitivity equations will be derived for a finite-difference model, as in [5] and for the simplest case of simultaneous variation of a given parameter in every cell of a fixed domain. A detailed discussion of the general case, which involves the solution of integro-differential equations to obtain the Green functions of the problem, is given in [6].

The model equation, written in vector form, reads:

$$\frac{\partial c}{\partial t} = \frac{\partial(K_x c / \partial x)}{\partial x} + f \quad (1)$$

where K_x is a space varying diffusivity, c is the state vector and f is a non linear vector function which expresses the local rate of change due to sources and sinks and to the chemical and biochemical transformations.

After discretization of the spatial domain in n_x cells, the dimensions of the state space of the dynamic system become $n_x \times n_v$ and those of the parameter vector become $n_x \times n_p$, where n_v is the number of state variables and n_p the number of parameters in each cell. Therefore, the dimensions of the augmented state vector become $n_x \times (n_v + n_p)$ and one should solve $n_x^2 \times n_p$ vector differential equations like eqn (2) in order to estimate the effects of variation in any parameter in any cell of the spatial domain:

$$\begin{aligned} \frac{dS_{ix,jx,ip}}{dt} &= \frac{\partial f_{ix}}{\partial c_{ix}} S_{ix,kx,ip} + \frac{\partial f_{ix}}{\partial p_{jx,ip}} \\ &+ D_{ix-1}(S_{ix-1,jx,ip} - S_{ix,jx,ip}) \\ &+ D_{ix}(S_{ix+1,jx,ip} - S_{ix,jx,ip}). \end{aligned} \quad (2)$$

In eqn (2), $S_{ix,jx,ip}$ represents the sensitivity of the state variables at the grid point ix , in respect of the parameter ip in the grid point jx . D_{ix} , expressed in [t^{-1}], is a dispersion coefficient which takes into account the spatial step. Nevertheless, in most ecological applications, the same local rate of change f_{ix} and the same vector of parameters p_{ix} are used throughout the spatial domain and one is usually concerned with estimating the changes of the trajectory caused by the simultaneous variation of a given component $p_{ix,ip}$ of p_{ix} in every cell. In this case, the overall effect can be estimated by summing up the individual effects. For a given parameter, after collecting the local Jacobian matrix and noting that the explicit partial derivatives vanish for $jx \neq ix$, one obtains:

$$\begin{aligned} \frac{dS_{ix,ip}}{dt} &= \frac{\partial f_{ix}}{\partial c_{ix}} S_{ix,ip} + \frac{\partial f_{ix}}{\partial p_{ix,ip}} \\ &+ D_{ix-1}(S_{ix-1,ip} - S_{ix,ip}) \\ &+ D_{ix}(S_{ix+1,ip} - S_{ix,ip}) \end{aligned} \quad (3)$$

where $S_{ix,ip} = \sum_{jx=1}^{n_x} S_{ix,jx,ip}$ is the overall sensitivity.

Once the sensitivity equations have been analytically derived for the model equations without diffusion, the solution of eqn (3) is straightforward and computationally convenient, because each overall

sensitivity can be treated like the state vector in the transport subprogram.

3 RESULTS AND DISCUSSION

This method has been applied to a 1-D, depth averaged, finite difference model that follows the seasonal evolution of seven state variables (Phytoplankton and Zooplankton densities, Ammonium, Nitrate and Reactive Phosphorous concentrations, Organic Detritus and Dissolved Oxygen). The model has been developed during a long term multidisciplinary project, aimed at defining a 3D combined transport-water quality model for the central part of the lagoon of Venice [7, 8]. The local rates of change and functional expressions are presented in Table 1. Parameters which have been taken into consideration in the sensitivity analysis are marked in bold in Table 2. The system is forced by a continuous load of nutrients (Nitrogen and Phosphorous) and a light-temperature temporal pattern which reproduces the average meteorological conditions of one of the main channels of the lagoon of Venice. The channel, which connects the Industrial area with the mouth of Malamocco, is included in a monitoring network, see Fig. 1, where monthly samplings of temperature, Ammonia, Nitrate, Total Phosphorous and Chlorophyll, related to the density of phytoplankton, have been made since 1986, providing a consistent time series of water quality data [9]. It is well mixed by tidal agitation, which is accounted for by a vector of turbulent diffusivities. In this first attempt, diffusivities, denoted by K_x , have been kept constant in the spatial domain and have been empirically estimated, so that the concentrations of the nutrients is of the same order of magnitude as the observed ones. A closed boundary condition has been set at the upper end of the canal. The values at the open boundary have been obtained by a statistical analysis of the times series of St. 12, which is representative of the lagoon-sea interface.

The dynamic of the system is illustrated in Fig. 2, which shows the yearly evolution of the densities of zooplankton and phytoplankton and of the concentrations of the three macronutrients at the source cell, St. 7 in Fig. 1, obtained with a diffusivity of $600 \text{ m}^2/\text{sec}$. Phytoplankton starts blooming at the beginning of March, day 60, when water temperature and incident light allow an increase of the photosynthetic activity. Its growth is not limited by the availability of ammonia, which is nearly constant and well above the half-saturation constant for nitrogen, $K_N = 0.05 \text{ mgN/l}$, even when phytoplankton reaches its maximum density. The other nitrogen form, NO_x^- and Reactive Phosphorous, are also always well above their limiting threshold. Therefore, in this model, the

Table 1. Equations and functional expressions

State variables	
[Z] Zooplankton (mgC/1)	[RP] Reactive Phosphorous conc. (mgP/1)
[P] Phytoplankton density (mgC/1)	[BOD] Biochem. Ox. Demand (mgO/1)
[NH ₄ ⁺] Ammonium conc. (mgN/1)	[DO] Dissolved Oxygen conc. (mgO/1)
[NO _x ⁻] Nitrate + Nitrite conc. (mgN/1)	
Source/sink rates within each cell	
	$\frac{d[Z]}{dt} = \vartheta(T) \cdot \{E_{ff} \cdot K_{grz} \cdot f([P]) - K_{mz}\} \cdot [Z]$ (1)
	$\frac{d[P]}{dt} = \{G_p(\bullet) = \vartheta(T) \cdot (K_{mp} + K_{rp})\} \cdot [P] - \vartheta(T) \cdot K_{grz} \cdot f([P]) \cdot [Z]$ (2)
	$\frac{d[NH_4^+]}{dt} = R_{NC} \cdot \vartheta(T) \cdot \{K_{rp} \cdot [P] + (1 - E_{ff}) \cdot K_{grz} \cdot f([P]) \cdot [Z]\} + - \vartheta(T) \cdot K_{nit} \cdot [NH_4^+] / [N_{tot}] \cdot R_{NC} \cdot G_p(\bullet) \cdot [P] + L_{NH}$ (3)
	$\frac{d[NO_x^-]}{dt} = \vartheta(T) \cdot K_{nit} \cdot [NH_4^+] - ([NO_x^-] / [N_{tot}]) \cdot R_{NC} \cdot G_p(\bullet) \cdot [P] + L_{NO}$ (4)
	$\frac{d[RP]}{dt} = R_{PC} \cdot \vartheta(T) \cdot \{K_{rp} \cdot [P] + (1 - E_{ff}) \cdot K_{grz} \cdot f([P]) \cdot [Z]\} - R_{PC} \cdot G_p(\bullet) \cdot [P] + L_P$ (5)
	$\frac{d[BOD]}{dt} = -\vartheta(T) K_{dec} \cdot [BOD] + L_{BOD}$ (6)
	$\frac{d[DO]}{dt} = R_{OC} \cdot (G_p(\bullet) - \vartheta(T) \cdot K_{rp}) \cdot [P] - \vartheta(T) \cdot K_{dec} [BOD] \pm R_{ON} \cdot (K_{nit} \cdot \vartheta(T) \cdot [NH_4^+] + K_{rear} \cdot \Delta_{DO})$ (7)
Functional expression	
$G_p(\bullet) = \mu(T) \cdot f_p([N_{tot}]) \cdot f_p([RP]) \cdot f_p(I) \mu(T) = G_{max} \cdot [(T_m - T) / (T_m - T_o)]^{b(T_m - T_o)} \exp[b(T - T_o)]$ with	
T = water temperature; $f_p([N_{tot}]) = ([N_{tot}] / K_N + [N_{tot}]) / [N_{tot}] = [NH_4^+] + [NO_x^-]$;	
$f_p([RP]) = [RP] / (K_p + [RP])$;	
$f_p(I) = I / (I + I_{op})$; with I = light intensity = $I_o \exp\{-K_{est}h\}$ (h = depth);	
$\vartheta(T) = 1.07^{(T-20)}$	
$f([P]) = [P] / (K_{PZ} + [P])$	
$\Delta_{DO} = [DO]_{sat} - [DO]$ = Oxygen deficit	
$[DO]_{sat} = 14.6244 - 0.36713 \cdot T + 0.0044972 \cdot T^2 - 0.0966 \cdot S + 0.00005 \cdot TS$	
$L_{HH}, L_{NO}, L_P, L_{BOD}$: input rates	

density of phytoplankton is mainly controlled by zooplankton predation, which causes the typical succession of peaks of the predator prey dynamic, but is also influenced by the dispersion. In fact, the gradients of plankton densities between the source and the boundary become higher when the two populations are at their relative maxima, causing an increase in the flux through the open boundary. The weight of these two factors, dispersion and predation, in controlling the primary production, changes by varying the diffusivity constant, as will be seen in the next sections.

3.1 Tuning importance and identifiability of parameters

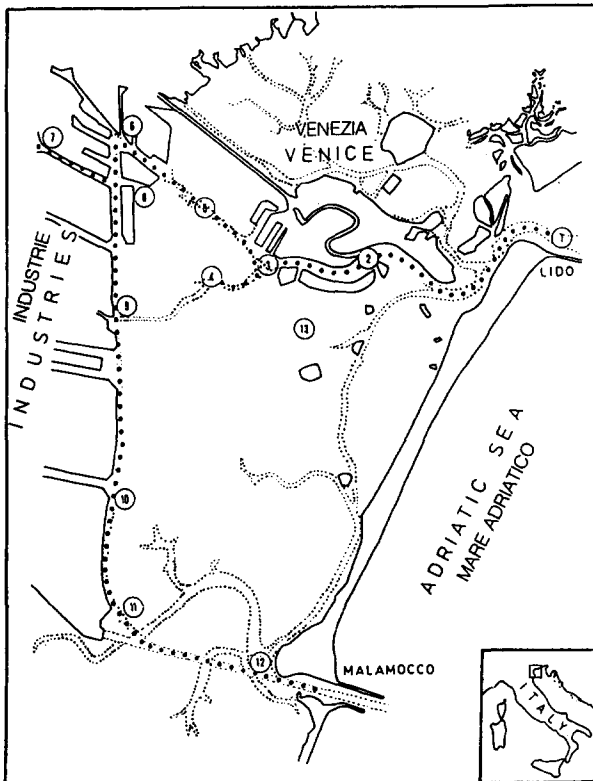
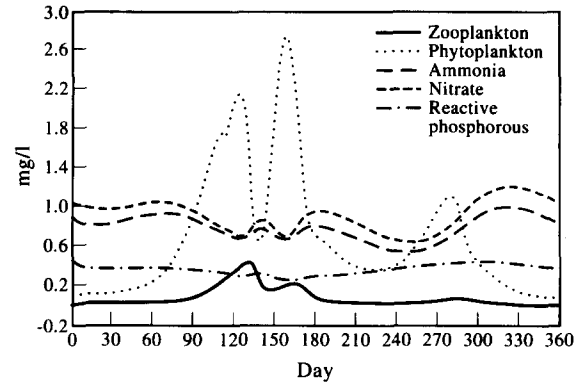
The calibration of water quality models against field data is often difficult, because the number of processes to be modelled, and therefore the number of

parameters to be estimated, is large, compared with the information provided by field investigations. Further, variations of two or more parameters around their nominal values might have quite similar, or quite opposite, effects on the output variables. In this case, the parameters can not be identified, that is their calibration is either impossible or lead to very uncertain estimates, even against a good set of field data [1]. Sensitivity analysis gives one the possibility to investigate both the tuning importance of each parameter and the identifiability of a set of parameters before collecting the data, in order to understand how much information can be gained through an experimental campaign in which l ($l \leq nv$) output variables are sampled at ns sampling station at times nt .

The tuning importance of a single parameter, that is the sensitivity of model output to a small change of its

Table 2. Parameters of the model. Parameters in bold are considered in the sensitivity analysis

Parameters for Zooplankton	
G_{max}	= 0.1 max specific growth rate (h^{-1})
K_{rP}	= 0.003 respiration rate (h^{-1})
K_{mP}	= 0.003 mortality rate (h^{-1})
K_N	= 0.05 half-saturation for N (mgN/l)
K_P	= 0.01 half saturation for Reactive Phosphorous (mgP/l)
I_0	= 5500 half saturation irradiance level (lux)
T_m	= 28 temperature inhibition threshold growth ($^{\circ}C$)
T_0	= 20 optimal temperature for growth ($^{\circ}C$)
b	= 0.11 exponential coefficient
R_{NC}	= 0.15 stoichiometric ratio
R_{PC}	= 0.023 stoichiometric ratio
Parameters for Phytoplankton	
K_{gr}	= 0.06 grazing rate (h^{-1})
K_{mz}	= 0.007 mortality rate (h^{-1})
E_{ff}	= 0.6 grazing efficiency
K_{pZ}	= 0.5 grazing half-saturation (mgC/l)
Other Parameters	
K_{nit}	= 0.0023 nitrification rate (h^{-1})
K_{dec}	= 0.0048 decay rate (h^{-1})
K_{rear}	= 0.045 reareation rate (h^{-1})
K_{est}	= 0.4 water extinction coefficients (m^{-1})
S	= 30 average salinity of the Venice lagoon (PSU)
R_{ON}	= 4.5 stoichiometric ratio
R_{OC}	= 2.66 stoichiometric ratio

**Fig. 1. Sampling network.****Fig. 2. Yearly evolution of the main state variables for $K_x = 600 m^2/sec$.**

value, and groups of parameters whose identification is impossible or extremely difficult, can be determined by analysing the square matrix $s^T s$ [9]. The matrix s is a np columns by $l \times ns \times nt$ rows matrix, formed by nt blocks. Each block s_k is composed by $l \times ns$ row by np columns, and represents the sensitivity to the output at time t_k at the ns sampling points: an element of each block is given by the relative sensitivities $s_{iv, is, ip}$ of the variable c_i to a change of the parameter p_{ip} , defined as:

$$s_{iv, is, ip}(t_k) = S_{iv, is, ip}(t_k) p_{ip} / c_{iv}(t_k). \quad (4)$$

In this paper, the possibility of calibrating the model by taking for a year daily samples of Chlorophyll *a*, proportional to the density of phytoplankton, ammonia, nitrate and phosphorous at one of the stations labelled as 7, 9 and 11 in Fig. 1, has been investigated. In this case, the matrix s is composed by 365 blocks, each formed by 4 rows and 15 columns, representing the relative sensitivities of the four variables sampled at a given cell.

The diagonal elements of the matrix $s^T s$ are related to the effect of the variation of a single parameter on the output, as they are proportional to the distance, weighted by the inverse of the state variables, between the nominal trajectory and the one obtain by changing a single parameter [10]. In scalar form, they can be written as:

$$\delta_{ip}^2 = \sum_{it=1}^{nt} \sum_{is=1}^{ns} \sum_{iw=1}^1 (S_{iv, ix, ip}^2(it)). \quad (5)$$

Their magnitude gives an idea of the tuning importance of a single parameter, but does not give any information about the possibility of identifying the set, or a subset, of parameters. The indexes δ_{ip}^2 have been computed for diffusivities of 720, 600, 480 m^2/sec , in order to study the effects of different mixing conditions. Results are shown in Fig. 3a-c, respectively. Sensitivities in the three stations are very similar at the highest diffusivity, Fig. 3a, while the

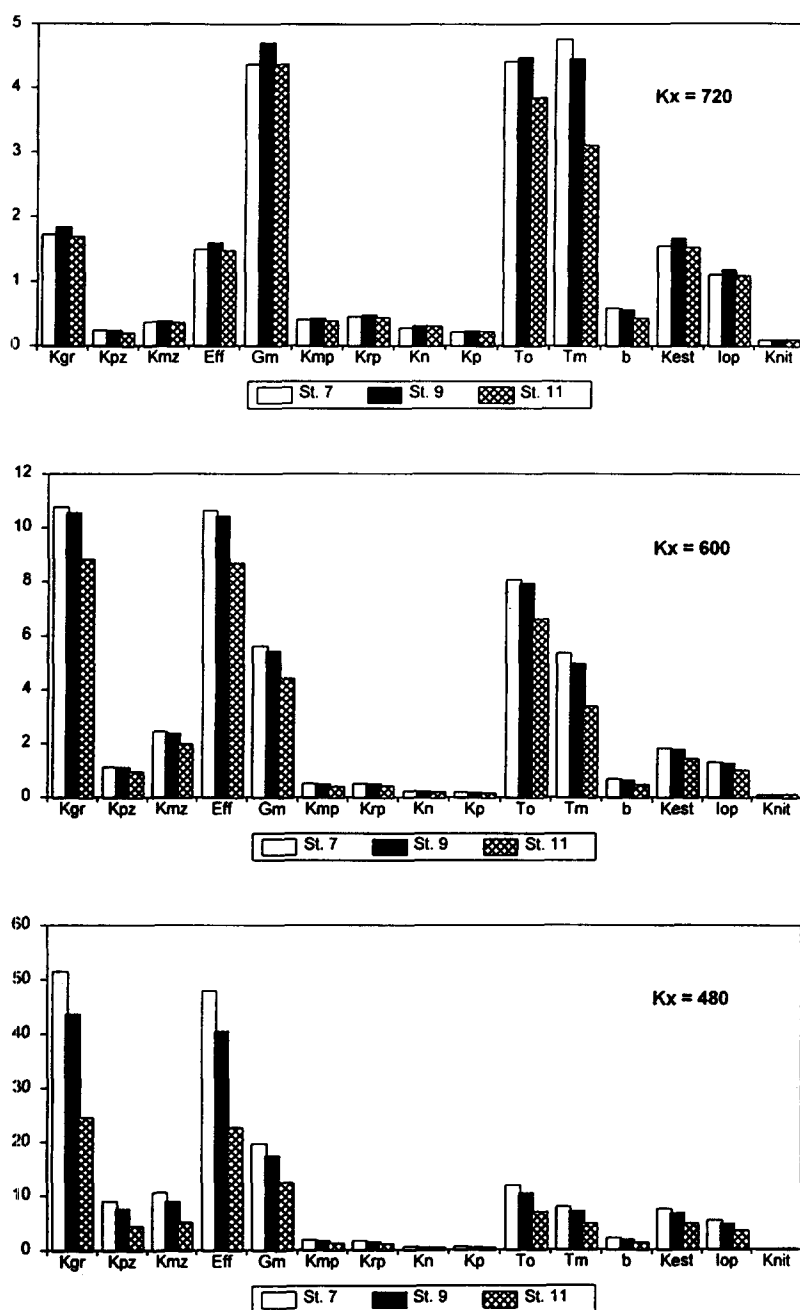


Fig. 3. Diagonal elements of the matrix of relative sensitivities, divided by the number of blocks (365).

source cell, St. 7, is the most sensitive and St. 11, the closest to the open boundary, is clearly the least sensitive when the dispersion is lower, Fig. 3c. Sensitivities of the half saturation constants, K_N and K_P , are low in all cases: this means that the primary production is not severely limited by the lack of nutrients, Nitrogen and Phosphorus, in these three simulations. Further, K_N and K_P are less important than the parameters linked with the efficiency of the phytoplanktonic pool in respect of the water temperature, T_o , T_m , b , and to the incident radiation, I_o and K_{est} . This indicates that this system is more sensitive to small fluctuations of the climate or the

acclimatization of the species, than to small variations of the nutrient loads, regardless of the mixing conditions.

Besides these common features, a comparison of the three situations shows important differences. At the highest diffusivity, Fig. 3a, the maximum specific growth rate of phytoplankton, G_{max} , T_o and T_m are the most important parameters: this indicates that the predator-prey interaction does not affect appreciably the development of the phytoplanktonic community, because the strong dilution lowers the density of zooplankton.

At the intermediate diffusivity, Fig. 3b, the output

becomes extremely sensitive to the grazing, K_{gr} and efficiency, E_{ff} , of zooplankton, suggesting that the evolution of phytoplankton is strongly controlled by the predator-prey interaction. This is confirmed by the fact that the mortality of zooplankton, K_{mZ} and the half-saturation constant, K_{PZ} , also exert a higher influence than the, somewhat, corresponding parameters in the first trophic level, K_{mP} , K_{rP} , K_P , K_N . The tuning importance of the optimal temperature of phytoplankton growth, T_o increases and oversteps that of G_{max} .

At the lowest diffusivity, Fig. 3c, the tuning importance of the first four parameters, linked with zooplankton activity, further increases in respect to that of the other parameters, and the difference between the sensitivities in the three stations are more marked.

Information about the identifiability of parameters can be obtained by computing the eigenvalues and the eigenvector of the matrix $s^T s$: parameters with very similar relative sensitivities have approximately the same loadings in the most important eigenvectors, while the correspondent eigenvalue is related with the tuning importance of the group of parameters which dominate the eigenvector [10]. Nevertheless, such analysis does not reveal the presence of groups of parameters with correlated relative sensitivities of different magnitudes: the same percentile variations of such parameters has qualitatively similar effects on the output. In this case, an attempt at calibrating at the same time parameters belonging to the same group would lead to a very slow convergence of the numerical method, if any. The groups can be determined by a principal component analysis of the correlation matrix ρ_s obtained by autoscaling the

matrix $s^T s$, by dividing the elements of a given row and column by the square root of the diagonal ones.

Results of the principal component analysis of $s^T s$ and of ρ_s are presented in Tables 3–5 for the three diffusivities. The tables show the loadings in the first four eigenvectors: these are, by far, the most important and account for more than 99% of the trace of the matrix. The analysis has been made on the source cell, which is the most sensitive. Parameters have been regrouped according with their ecological role and the suggestions given by their tuning importance, in order to make clearer the discussion of the results. Parameters linked with zooplankton activity (K_{gr} , K_{FP} , K_{mZ} , E_{ff}) are in Group A, those linked with phytoplanktonic dynamic are in Group B (G_{max} , K_{mF} , K_{rF} , K_N , K_P , I_o , and K_{est}), except for the three parameters that relate the photosynthetic activity to water temperature, which form Group C. Nitrification constant, K_{nit} , does not affect the dynamic of the two biological state variables, and constitutes Group D.

At the highest diffusivity, Table 3, the first eigenvector of $s^T s$ is mostly influenced by the parameters of Group C, optimal and maximum temperature, T_o and T_m , with nearly equal loads, and by G_{max} , also with a similar weight. T_m and G_{max} are also important in the second component, while the third one is dominated only by the temperature parameters: this means that they have a marked effect on the evolution of the system and that this effect is different from that of G_{max} . Loadings of the parameters of Group A, linked with zooplankton dynamic, are high only in the fourth eigenvector for K_{gr} , and E_{ff} ; this confirms that, in this mixing condition, predator-prey interaction is not important.

Table 3. Principal components of $s^T s$ and ρ_s for $K_x = 720$

	S'S				ρ_s				
	%	PC1 70.25	PC2 93.01	PC3 99.70	PC4 99.92	PC1 77.18	PC2 88.54	PC3 95.21	PC4 98.76
A									
	K_{gr}	0.2091	0.2092	-0.0249	-0.6318	0.984	-0.0675	-0.0008	0.1178
	K_{PZ}	-0.0231	-0.0296	-0.0496	0.0175	-0.879	0.2065	0.0223	0.4115
	K_{mP}	-0.0459	-0.0366	0.0162	0.1463	-0.977	-0.0289	0.0004	-0.1676
	E_{ff}	0.1806	0.1761	-0.0671	-0.6199	0.973	-0.0497	0.0046	0.1879
	G_{max}	-0.5002	-0.6367	-0.2236	-0.2926	-0.9779	0.1943	-0.0049	0.0209
B									
	K_{mP}	0.0478	0.0505	0.0367	0.0010	0.9845	-0.1205	-0.0010	-0.1145
	K_{rP}	0.0582	0.0440	0.0201	0.0482	0.9949	0.0205	-0.0245	-0.0329
	K_N	0.0321	0.0387	-0.0040	0.0253	0.9699	-0.1575	0.0105	0.1277
	K_P	0.0247	0.0284	-0.0016	-0.0241	0.9790	-0.1322	0.0099	0.1179
	I_o	0.1683	0.2354	0.1221	0.1750	-0.7029	-0.5945	-0.0132	-0.3652
	K_{est}	0.1202	0.1681	0.0872	0.1250	0.9637	-0.2430	0.0022	-0.0899
	T_o	-0.5612	0.2199	0.7787	-0.1635	0.9637	-0.2430	0.0022	-0.0899
C									
	T_m	-0.5483	0.6138	-0.5561	0.0397	-0.5305	-0.7974	0.0087	0.2315
	b	0.0722	-0.0447	0.0464	-0.1761	0.6945	0.6716	-0.0086	-0.1937
D									
	K_{nit}	0.0003	0.0001	0.0000	0.0080	0.0139	0.0059	0.9996	-0.0213

Table 4. Principal components of $s^T s$ and ρ_s for $K_x = 600$

		S'S				ρ_s			
		PC1	PC2	PC3	PC4	PC1	PC2	PC3	PC4
%		79.31	89.84	97.51	99.93	47.96	78.61	90.50	97.17
A	K_{gr}	0.6237	-0.0339	-0.1921	0.2783	-0.3378	0.9204	-0.1756	0.0042
	K_{PZ}	-0.0463	-0.0847	0.0902	-0.0861	-0.3227	-0.8798	0.2498	-0.0066
	K_{mP}	-0.1392	0.0395	-0.0166	-0.0976	0.4580	-0.8735	0.0677	-0.0043
	E_{ff}	0.6170	-0.1153	-0.1268	0.2401	-0.3914	0.9009	-0.1671	0.0029
	G_{max}	0.0863	-0.7667	0.4777	-0.1069	-0.9937	-0.1020	0.0245	0.0036
B	K_{mP}	-0.0105	0.0708	-0.0312	0.0283	0.9880	0.0114	0.1269	-0.0004
	K_{rP}	-0.0019	0.0785	-0.0286	0.0070	0.9374	0.3105	0.1298	0.0201
	K_N	0.0002	0.0331	-0.0219	-0.0052	0.9166	0.3615	-0.1061	-0.0043
	K_P	-0.0005	0.0271	-0.0175	-0.0012	0.9377	0.3077	-0.0768	-0.0047
	I_o	-0.0376	0.2388	-0.1388	0.0956	0.9912	0.0041	0.0482	-0.0025
C	K_{est}	-0.0269	0.1706	-0.0991	0.0683	0.991225	0.0041	0.0482	-0.0025
	T_o	-0.4351	-0.2995	-0.1622	0.8284	0.2076	-0.9083	-0.0314	0.0036
	T_m	-0.0985	-0.4463	-0.8012	-0.3604	0.0359	-0.4139	-0.8789	0.0003
	b	0.0086	0.0295	0.1022	0.0756	-0.2025	0.2402	0.9187	0.0005
	K_{nit}	0.0001	0.0003	0.0001	0.0001	-0.0004	0.0156	0.0001	-0.9998

The first eigenvector of the correlation matrix shows that the sensitivities of parameters of group B are strongly correlated, because their loadings are very similar. An example of perfectly correlated sensitivities is given by I_o and K_{est} , which has the same loading in all the eigenvectors: these parameters could not be identified, even if daily data of four out of 8 state variables would be available. Further, Group A is well correlated with Group B: this means that it would be nearly impossible to calibrate parameters linked with zooplankton activity that, besides being of little tuning importance, have sensitivities qualitatively similar to those of Group B. The third eigenvector is dominated by the nitrification constant K_{nit} : this is a case of a parameter of little tuning importance,

because its loadings in the eigenvectors of the non-scaled matrix are very low, whose independent effects on model output are revealed by the principal components of the autoscaled matrix.

The importance of the second trophic level clearly emerges at the intermediate diffusivity, Table 4, as the grazing parameters, K_{gr} and E_{ff} , become the most important in the first eigenvector of $s^T s$, with nearly equal loadings. The optimal temperature, T_o , is also important in this eigenvector, as if its effect on model output was in resonance with that of parameters of Group A: this aspect will be clearer in the next section. The second component is still strongly influenced by G_{max} , with T_m and T_o not negligible: these two parameters have here distinct effects on the

Table 5. Principal components of $s^T s$ and ρ_s for $K_x = 480$

		S'S				ρ_s			
		PC1	PC2	PC3	PC4	PC1	PC2	PC3	PC4
%		89.55	99.13	99.88	99.99	56.99	89.08	95.74	99.50
A	K_{gr}	0.7131	-0.0041	-0.0316	-0.0580	0.2361	-0.9708	0.0001	-0.0110
	K_{PZ}	-0.1232	-0.0222	-0.0006	0.0386	-0.2943	0.9539	-0.0008	0.0092
	K_{mP}	-0.1463	-0.0100	-0.0039	0.0452	-0.2597	0.9638	-0.0002	0.0157
	E_{ff}	0.6634	-0.0670	-0.0297	-0.0742	0.2059	-0.9776	-0.0002	-0.0135
	G_{max}	-0.0895	-0.7848	-0.0511	-0.4297	-0.9931	0.0962	-0.0003	-0.0576
B	K_{mP}	0.0039	0.0776	0.0109	0.0268	0.9949	0.0866	0.0012	0.0424
	K_{rP}	0.0077	0.0658	0.0249	0.0421	0.9933	-0.1005	0.0053	-0.0214
	K_N	0.0029	0.0237	0.0038	0.0183	0.9911	-0.1145	-0.0002	0.0349
	K_P	0.0028	0.0233	0.0017	0.0126	0.9908	-0.1169	0.0001	0.0543
	I_o	0.0150	0.3109	0.0046	0.1272	0.9925	0.0918	0.0008	0.0760
C	K_{est}	0.0107	0.2221	0.0033	0.0909	0.9925	0.0918	0.0008	0.0760
	T_o	-0.0779	0.3960	-0.6140	-0.6757	0.6280	0.6469	0.0067	0.3898
	T_m	0.0127	-0.2434	-0.7821	0.5645	-0.7250	-0.3144	0.0037	0.6024
	b	-0.0149	0.0737	0.0771	-0.0192	0.6924	0.6983	-0.0000	-0.1641
	K_{nit}	0.0000	0.0001	0.0003	0.0000	0.0103	0.0019	-0.9999	0.0049

dynamic of the system, as their loads are clearly different, in particular T_m , which is the most important in the third eigenvector. The analysis of the correlation matrix shows that parameters of groups A, B, are well distinct and dominate respectively the first and second component. Further, it confirms that T_o and T_m could be independently identified, as their loadings are high, respectively, in the second and third component.

At the lowest diffusivity, Table 5, the importance of the first component of $s^T s$ is even higher, 89% of the trace: the high loadings of the parameters of group A in this component shows that the predator-prey interaction controls almost entirely the dynamic of the system. The second component is again dominated by G_{max} , representative of Group A, while the third still demonstrates the autonomous role of the parameters of Group C, even though the third eigenvector is associated with a small fraction of the trace (0.7%). The correlation matrix supports the above deductions. In fact, the composition of the first and second components show a clear distinction between Groups A and B, while the fact that loading of Group C are important in the first component indicates that their sensitivities are more similar to those of Group A, in comparison with the intermediate diffusivity.

3.2 Analysis of relative sensitivities

The analysis of the matrix of relative sensitivities gives an idea of the average effects of small variations of parameters within the time-window considered in the simulation, but it is also of interest to check the time behaviour of the sensitivities. In fact, parameters which are extremely important for a very short time might not be revealed by the statistical analysis presented in the above section. It could also be important to investigate the time-behaviour of the sensitivities of parameters that are indicated as highly, but not perfectly, correlated from a statistical view point. In these cases, a more detailed analysis of the relative sensitivities might tell if the parameters have distinct effects in a particular sub-period.

The considerations made in the previous section suggest that the most important parameters with independent effects on model output are the maximum grazing, K_{gr} , the maximum specific growth rate of phytoplankton, G_{max} , and its optimal, T_o , and maximum temperature, T_m . The efficiency of assimilation, E_{ff} , also has great tuning importance, but its sensitivity is very well correlated with that of K_{gr} , as their loadings are roughly equal in the principal components of the sensitivity matrix: for this reason it will not be discussed. The relative sensitivities of phytoplankton, the most important output variable, in respect of K_{gr} , G_{max} , T_o and T_m are plotted, respectively, in Fig. 4a–d for $K_x = 720$, continuous line, and $K_x = 600$, dotted line.

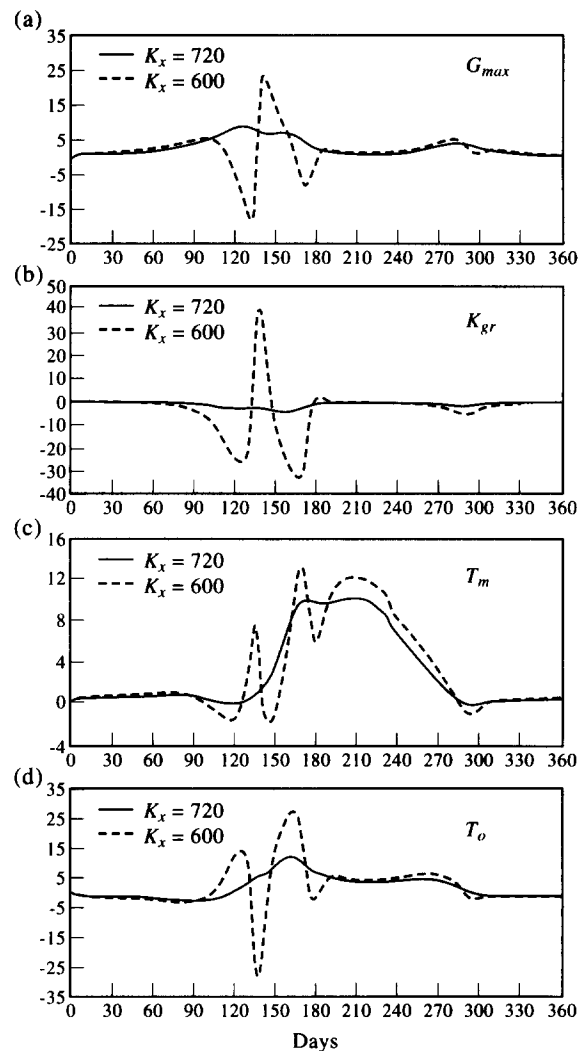


Fig. 4. Relative sensitivities of the four most important parameters, (a) G_{max} , (b) K_{gr} , (c) T_o , (d) T_m , at $K_x = 720 \text{ m}^2/\text{sec}$, continuous line, and $K_x = 600 \text{ m}^2/\text{sec}$, dotted line.

As might be expected, all sensitivities are low in autumn and winter, when the biological activity slows down. Of greater interest, sensitivities to K_{gr} and G_{max} are low also during the summer, as it has already been noted in a sensitivity study [11] of lumped-parameters model with a similar structure. On the contrary, in the same period, the importance of T_m is at a maximum, and that of T_o is not negligible: this difference explains why their sensitivities emerge as distinct from those of Group B in the principal component analysis. The sensitivity of T_m is positive and high during the summer because this parameter is a measure of the tolerance of the phytoplankton to high temperatures: an increase of T_m means an higher photosynthetic rate during the hottest season.

Sensitivities to all parameters change considerably when the diffusivity is varied, as clearly appears from

a comparison of the two curves presented in Fig. 4a and 4b for K_{gr} and G_{max} . At the highest diffusivity, continuous line in Fig. 4, the sensitivity of G_{max} is always positive: this means that an increase in the maximum specific growth rate causes an increase in the standing crop, but does not affect the position of the peaks of biomass. The effect of a decrease in K_{gr} , whose sensitivity is always negative, continuous line in Fig. 4b, is qualitatively the same, as revealed by the similar loading of these parameters in Table 3, but quantitatively less important. This confirms that the predation is not important and that the identification of related parameters would be very difficult in this condition.

The picture is completely different for $K_x = 600 \text{ m}^2/\text{sec}$, when the predation becomes important. In this case, a slight modification of the parameters which control the predator-prey interaction, causes a significant shift in the oscillations of the system, which is revealed by the rapid change of sign of the sensitivity of K_{gr} in Fig. 4a. Besides that, the fact that the integral of the sensitivity is clearly negative indicates that an increased grazing pressure diminishes the average density of phytoplankton. The shape of the sensitivity of the optimal temperature, T_o , looks quite similar to the opposite of the sensitivity of K_{gr} , in particular until the end of the spring (day 180). The previous statistical analysis gives a quantitative support to this similarity, as the absolute values of the loadings of T_o in the first component of $s^T s$ and in the second of ρ_s are similar to the loadings of K_{gr} . The optimal temperature is extremely important because it regulates the response of phytoplankton to the sudden temperature increase that occurs in the spring: a lower optimal temperature means that phytoplankton starts blooming earlier and, therefore, the predator-prey dynamic is anticipated. At this diffusivity, an increase in the predation, K_{gr} , or a decrease in T_o shift backward the two peaks of phytoplankton of Fig. 2 in a similar way. The effect of an increase in G_{max} becomes more complex and less predictable on the basis of common sense, because of the predator-prey interaction. As can be seen in Fig. 4b, sensitivity in the early spring is slightly positive, which means that the first peak of phytoplankton in Fig. 2 would be higher if G_{max} were augmented. Again, this has a feedback on the population of zooplankton, which develops more rapidly and causes a sudden decrease in the population of the first trophic level, as is evidenced by the change of sign of the sensitivity. The following rapid oscillations of the sensitivity show that the next peak is shifted backward. As a result, an increase in G_{max} shifts backward the two peaks, but does not increase appreciably the average density of phytoplankton, as the integral of the sensitivity is only slightly positive.

4 CONCLUSIONS

Sensitivity analysis of this distributed parameter model has demonstrated that the entity of the dispersion should be taken into consideration when planning experimental campaigns aimed at identifying and calibrating a model. Identifiability and tuning importance of parameters generally decrease as the diffusivity increases, indicating that trophic processes, though important, are difficult to characterize in open coastal water basins that exchanges actively with the sea. In the eutrophic conditions, and with average climatic forcing functions, considered here, the model is sensitive to a few parameters, all related to a direct, G_{max} , T_m , T_o , or indirect, K_{gr} , limitation of phytoplankton growth. Parameters linked with phytoplankton decay, K_{mP} and K_{rP} , and those which express the limitations due to the availability of macronutrients, K_N and K_P , and light, I_o and K_{est} , are of less tuning importance and, also, their sensitivities are always well correlated with that of G_{max} . Therefore, in the sampling scenario here considered, it would be impossible to calibrate any of them together with G_{max} , regardless of the mixing conditions. As a consequence, parameters of Group C, except G_{max} , and related formulations and processes can be removed from the structure of the model when treating cases similar to the one presented here. The importance of the parameters related to the activity of the zooplanktonic community increases as the diffusivity decreases, indicating that the system is controlled by the predator prey interaction.

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