A comparison between the uncertainties in model parameters and in forcing functions: its application to a 3D water quality model.

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Abstract: This paper presents the application of both local and global sensitivity analysis techniques to an estimation of the uncertainty of the output of a 3D reaction-diffusion ecological model, which describes the seasonal dynamics of dissolved Nitrogen and Phosphorous, and that of the phytoplanktonic and zooplanktonic communities in the lagoon of Venice. Two sources of uncertainty were taken into account and compared: 1) uncertainty concerning the parameters of the governing equation; 2) uncertainty concerning the forcing functions. The mean annual concentrations of Dissolved Inorganic Nitrogen, DIN, was regarded as model output, as the current Italian legislation sets a quality target for Total Dissolved Nitrogen in the lagoon of Venice. Local sensitivity analysis was initially used, so as to rank the parameters and provide an initial estimation of the uncertainty, which is due to an imperfect knowledge of the dynamic of the system. This uncertainty was compared with that induced by an imperfect knowledge of the loads of Nitrogen, which represent the main forcing functions. On the basis of the results of the local analysis, the most important parameters and loads were then taken as the sources of uncertainty, in an attempt to assess their relative contribution. The global uncertainty and sensitivity analyses were carried out by means of a sampling-based Monte Carlo method. The results of the subsequent input-output regression analysis suggest that the variance in model output could be partitioned among the sources of uncertainty in accordance with a linear model. Based on this model, 87.8% is due to the uncertainty in the parameters which specify the dynamics of phytoplankton and zooplankton only % of the variance in DIN mean annual concentration is accounted for by the uncertainties in the three main source, while.

Keywords: uncertainty analysis; 3D water-quality models; lagoon of Venice.

1. INTRODUCTION

In 1999, the Italian government issued a new law for the regulation of pollutant loads in water bodies, which is based on the so-called Maximum-Permissible-Loads (MPLs) policy. Within this framework, the relevant Local Authorities should make an inventory of the sources of pollution and then fix the level of emission of each of these activities, so as not to exceed a set of given concentration thresholds within the system, called "Quality Targets", QTs.
The effective implementation of the MPLs policy in a large coastal water body such as the lagoon of Venice is not straightforward, because the actual concentration of a given pollutant in water and sediment is determined by the "controllable" external load, by the "uncontrollable" exchanges with the Adriatic sea and by its auto-purifying capacity. In principle, mathematical models may be of help in the determination of the MPLs, since, in numerical terms, the loads are specified by a set of boundary conditions: numerical models can then be used for determining a functional relationship between the set of boundary conditions and the output variables which have been chosen for comparison with the Quality Targets. Once this task has been accomplished, one can invert this function, in order to estimate the MPLs which are compatible with the target [Pastres et al., 2002].
Furthermore, once the MPLs have been fixed, it is necessary to design a long-term monitoring plan, in order to assess whether the quality target has been reached. At this stage, it becomes important to understand whether the fluctuations in the concentration around the annual mean value, or the systematic deviation from the target are due to a

lack of control in the loads, to fluctuations in the uncontrollable exchanges or to variations in the "auto purifying capacity". This question is not merely academic, since, in the first case, a revision of the MPLs and/or a reinforcement of the control over the pollution sources is required, while, in the other two cases, the aforementioned costly measures are not effective.

In this paper, we focus on this question, in an attempt to make use of a 3D mathematical model in order to assess how the uncertainties in the loads and in the auto purifying capacity of the system can give rise to a total uncertainty in the model output which is to be compared with the quality target.

We illustrate this procedure by using the mean annual concentration of Dissolved Inorganic Nitrogen, DIN_{av}, in the waters of the lagoon of Venice as a case study. Because of its peculiarity, the lagoon of Venice has been thoroughly investigated in the past and a 3D reaction-diffusion water quality model is already available [Pastres et al., 1995, Pastres et al., 2001]. The reaction-diffusion equation (1), is solved using a finite-difference scheme.

$$\partial \boldsymbol{c}(x,y,z,t)/\partial t = \nabla (\boldsymbol{K}(x,y,z) \nabla \boldsymbol{c}(x,y,z,t)) + \boldsymbol{f}(\mathbf{c}(x,y,z),\boldsymbol{\alpha},t) \quad (1)$$

In eq. (1), $\boldsymbol{c}$ is the state vector, $\boldsymbol{K}$ the tensor of eddy diffusivities, $\boldsymbol{f}$ is the reaction term and $\boldsymbol{\alpha}$ the set of 25 site-specific parameters which are presented in Table 1. The model simulates the dynamics of the ecosystem up to the second trophic level by using twelve state variables, among which there are the concentrations of the two main forms of inorganic nitrogen, ammonium and nitrate, and that of inorganic reactive phosphorous: these chemicals are considered to be the main cause of the eutrophication in the lagoon and, therefore, the current legislation has fixed their quality target. At present, the concentration of DIN is above the target, while the concentration of phosphorous is now low, as its use in detergents was prohibited in 1986. Ammonium, NH_4^+, and nitrate, NO_3^-, are carried into the lagoon by its tributaries, and are directly released from the Industrial area of Porto Marghera, on the edge of the lagoon, and from the city of Venice and the nearby islands. The Nitrogen sources are shown in Figure 1. The yearly evolutions of these inputs were modelled using Von Neumann-type, time-dependent, boundary conditions: the fluxes Φ_i are specified using a set of trigonometric polinomia [Pastres et al., 2002], which contain a total of 7x19 coefficients for each chemical. However, only the 19 mean annual values of the loads of Ammonia and Nitrate are considered here as sources of uncertainty. The uncertainty in the auto purifying capacity is assumed to be due to the uncertainties in the 25 parameters in Table 1, which were used to specify the reaction term f in eq. (1), which is described in detail in [Pastres et al. 2001]. Thus, 25+(19x2)=63 potential sources of uncertainty were taken into consideration in the sensitivity and uncertainty analyses.

Table 1. Parameters of the water-quality model.

Parameter	Description	Units and value
k_{gr}	Max. grazing rate of zooplankton	0.04 [h^{-1}]
k_{pz}	Half-saturation constant for phytoplankton	1. [mg C-Phy/L]
k_{mz}	Zooplankton mortality rate	0.006 [h^{-1}]
e_{pz}	Phyto-Zooplankton digestion efficiency	0.5 [dimensionless]
k_{escrez}	Zooplankton excretion rate	0.002 [h^{-1}]
G_{Pmax}	Max phytoplankton growth rate at $T=t_{opt}$	0.12 [h^{-1}]
k_{mp}	Phytoplankton mortality rate	0.005 [h^{-1}]
k_{rp}	Phytoplankton respiration rate	0.004 [h^{-1}]
k_n	Half-saturation constant for nitrogen	0.05 [mg N/L]
k_p	Half-saturation constant for phosphate	0.01 [mg P/L]
K_{nit}	Nitrification rate at 20°C	0.0023 [h^{-1}]
k_{dec}	Organic detritus decay rate at 20° C	0.0048 [h^{-1}]
k_{rear}	Reaeration rate	0.04584 [h^{-1}]
k_{est}	light extinction coefficient	1. [m^{-1}]
E_{splass}	Lassiter e Kearnes exponential coefficient	0.1157 [$°C^{-1}$]
T_{max}	phytoplankton max. temperature	30 [° C]
T_{opt}	Phytoplankton optimal temperature	26 [°C]
I_{op}	Light intensity parameter	50,000 [lux]
r_{ncp}	Nitrogen/Carbon ratio in phytoplankton	0.15 [mg N/mg C
r_{pcp}	Phosphorous/Carbon ratio in phytoplankton	0.023 [mg P/mg C]
r_{oc}	Oxygen/Carbon ratio	2.66 [mg O/mg C]
r_{on}	Oxygen/Nitrogen ratio	4.5 [mg O/mg N]
k_{sed}	Detritus sedimentation rate	0.016 [h^{-1}]
k_{sedP}	Phytoplankton sedimentation rate	0.0016 [h^{-1}]
k_{od}	Half-saturation constant for Oxygen	2. [mg O/L]

2. METHODS

The sensitivity and uncertainty analyses were carried out in two steps. In the first step, the local sensitivities of the model output with respect to all the parameters were computed. Based on the results of the first step, nine "uncertainty factors", i.e. nine sources of uncertainty, were chosen: these were six paramters among the most important ones

in the reaction term and the three most relevant sources of nitrogen. In the second step, a global uncertainty analysis with respect to the uncertainty factors was performed, by using one of the simplest, sampling-based, techniques.

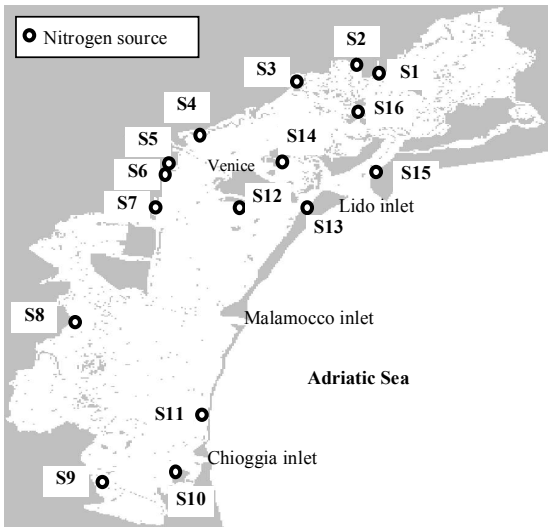

Figure 1 The lagoon of Venice and the sources of Nitrogen.

2.1 Local sensitivity analysis

Local sensitivity analysis of a dynamic system is based on a Taylor series expansion around its "nominal" trajectory, that is the trajectory which is obtained when the estimates, or nominal values, of the parameters are used [Turanyi, 1990]. The effect of a small change of a parameter α_i on the solution of an ODE system:

$$d\mathbf{x}/dt=f(\mathbf{x},\boldsymbol{\alpha},t) \quad (2)$$

can be expressed as:

$$\mathbf{x}(t,\alpha_j + \Delta\alpha_j) = \mathbf{x}(t, \alpha_j) + (\partial\mathbf{x}/\partial\alpha_j)\Delta\alpha_j + \ldots \quad (3)$$

The partial derivatives $\partial x_1/\partial\alpha_{j,} \ldots \partial x_i/\partial\alpha_j$, are called first-order sensitivities or, simply, sensitivities, $S_{ij}(t) = \partial x_i/\partial\alpha_j$ Information about the, approximate, effect of the simultaneous variations in two or more parameters can be straightforwardly obtained by means of eq. (3):

$$\mathbf{x}(t,\boldsymbol{\alpha} + \Delta\boldsymbol{\alpha}) \approx \mathbf{x}(t, \boldsymbol{\alpha}) + \underline{\mathbf{S}}\Delta\boldsymbol{\alpha} \quad (4)$$

where $\underline{\mathbf{S}} = \{S_{ij}\}$ is the sensitivity matrix and $\boldsymbol{\alpha}$ is the vector of the parameters.

The sensitivities provide a measurement of the "importance" of the parameters and, therefore, can be used for ranking them. In order to compare parameters which have different physical dimensions and numerical values, the ranking is usually based on the relative sensitivities, which are defined as $s^r_{ij} = S_{ij}\ (\alpha_i/x_j)$. The definition of sensitivity given above can be extended to a distributed parameter system. The basic equation needed for the computation of the first-order sensitivities of the reaction-diffusion equation (1) reads as [Koda et al., 1979]:

$$\partial\underline{\mathbf{S}}\ (x,y,z,t)/\partial t = \nabla\ (\underline{\mathbf{K}}(x,y,z)\ \nabla\underline{\mathbf{S}}\ (x,y,z,t)) + \underline{\mathbf{JS}} + \{\partial f/\partial\boldsymbol{\alpha}\} \quad (5)$$

where $\mathbf{S}$ is the space-time dependent sensitivity matrix, $\boldsymbol{\alpha}$ the vector of parameters, $\underline{\mathbf{K}}$ is the diffusivity tensor, and $\underline{\mathbf{J}}$ is the Jacobian matrix. Eq. (5) must be solved together with the state equation (1): the so-called "direct method", [Koda et al., 1979], was used in this application. The elements matrices $\mathbf{J}$ and the $\{\partial f/\partial\boldsymbol{\alpha}\}$ were calculated using symbolic calculus: this may appear to be a limitation regarding the extension of this approach to other problems, but such calculations are now performed automatically using a number of software packages, which also give the corresponding piece of Fortran code as an output. Once the sensitivity matrix has been determined, eq (4) provides the basis for an estimation of the variance in the model output [Turanyi et al., 2000], as a function of the standard deviations of the parameters. For example, the variance of a model output Y which is linear function L(x) of the state vector, can be estimated as:

$$\mathrm{Var}(Y) = \mathrm{Var}(L(x)) \approx [L(\underline{\mathbf{S}}\Delta\boldsymbol{\alpha})]^2$$

2.2 Global sensitivity and uncertainty analysis

The main advantage of the local analysis briefly outlined in the previous paragraph is its computational efficiency, which allows one to estimate the sensitivity matrix for large sets of parameters and complex, time-consuming models. However, care must be taken in using the results of the local analysis when ranking the parameters and evaluating the total uncertainty in the model output because the local analysis is based on Taylor series expansion and, therefore, the assumption of linearity between the perturbations of the parameters and the variation of the output may be violated when the whole ranges of variation of the parameters are considered. The aim of the so-called "global" methods of is to estimate the uncertainty of model output and to apportion it to the uncertainty in the "input factors", which may include, besides the parameters, the forcing functions, the boundary and initial conditions, as well as alternative model structures. Global methods are based on the sampling of the distribution function of the input factors and on the repeated execution of the model, in order to determine the distribution of the output: therefore they are, in general, computationally expensive. The uncertainty analysis involves three steps: the selection of the joint distribution of the input

factors, the generation of a sample from the distribution, and the computation of model output, Y, for each element of the sample, in order to estimate the distribution of the output. In the subsequent sensitivity analysis, the variation in the output is apportioned to the different sources.

In this paper, a simple Monte Carlo analysis was employed in order to explore the relationship between the model output and a set of "m" input factors, $X_1,\ldots\ldots X_m$, which were selected on the basis of the results of the local analysis. The factors were assumed to be independently and normally distributed. A sample of 250 elements was generated, using a crude Monte Carlo sampling scheme, and the input-output relationship was fitted by means of a multiple regression model:

$$Y = b_0 + \Sigma_i b_i X_i \qquad (6)$$

The average yearly concentration of DIN in the lagoon was taken as a modul output in our numerical experiment. The coefficients b_i, i=1,m, represent reliable "global" measurements of the sensitivity of model output to the variation of each factor if the regression model (6) explains a large fraction of the variance in model output, that is if the coefficient of determination R_y^2 is close to unity. In this case, if the input factors are independent, the contribution of each factor to the total variance of Y can be taken as proportional to the square of the regression coefficients. The standardized regression coefficients $\beta_i = b_i$ STD(Xi)/STD(Y) were also compute, in order to rank the input factors. In analogy with the relative sensitivities, these coefficients give the change in model output, measured as a fraction of its standard deviation, which follows a change in the input X_j, measured as a fraction of its standard deviation STD(X_j). If the regression model (6) is not adequate, other, more complex, variance-based techniques, such as Sobol or FAST methods [Chan et al., 2000] should be employed, in order to decompose the variance in model output with respect to its sources.

3. RESULTS

The methods, which are outlined in the above section, were applied in sequence to the sensitivity and uncertainty analyses of the distributed parameter 3D finite-difference water-quality model described in the introduction. Eqs. (1) and (5) were solved, in order to compute the nominal trajectory and the sensitivity matrix, whose elements give, at each time and grid point, the sensitivities of all the state variables to the set of 63 parameters.

The evolution of the space-averaged nominal trajectories of the three most important variables, DIN, which is given by the sum of nitrate and ammonia, phytoplankton and zooplankton, is shown in Figure 2. A DIN mean annual concentration of 0.57 g/m^3 was obtained. As one can see, the DIN concentration in the system decreases in the spring and summer, as a result of the decrease in the discharges from the tributaries and of the increase in the assimilation by phytoplankton. Such a seasonal evolution is in qualitative agreement with the one which was observed in the monitoring network which was set up by the Venice Water Authority in September 2000.

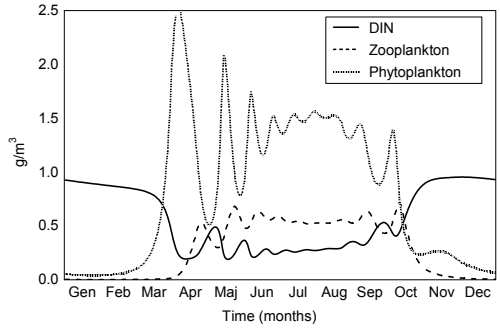

Figure 2. Space-averaged nominal trajectory of DIN [gN/m^3], Phytoplankton [gC/m^3] and Zooplankton [gC/m^3]

The sensitivities of the space-averaged nominal trajectory to any of the parameters, are obtained by averaging the sensitivities over the computational grid. The curve regarding the specific growth rate of phytoplankton, G_{max} is shown in Figure 3. The sensitivity was scaled by dividing by the average DIN annual concentration and multiplying by the nominal value of the parameter. The first relative minimum in Figure 3 shows that an increase in G_{max} causes an anticipation of the spring bloom in the phytoplankton, which results in a decrease in the DIN concentration. Furthermore, such an anticipation shifts the predator-prey oscillations, as it is evidenced by the oscillations of the sensitivity.

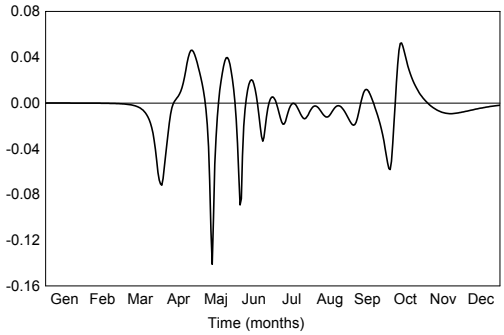

Figure 3. Space-averaged sensitivity of DIN to the specific growth rate of phytoplankton, G_{max}.

The effect of the variation in a given parameter on the mean annual concentration of DIN was then estimated by averaging the sensitivities over space and time. The coefficients thus obtained were multiplied by 1% of the nominal value of the parameter: therefore, they represent estimates of the variations ΔDIN_{av} which are caused by an increase of 1% of each parameter. The results are summarized in Table 2, which shows the values of ΔDIN_{av} above .001. The ranking of the parameters is based on the square of ΔDIN_{av}, third column, and is presented in the fourth column. The sum of squares of the variations ΔDIN_{av} is taken as an overall measure of the influence of the remaining 15 parameters in Tab. (1) which do not appear in the Tab. 2, and of the 38 sources. The results of the local analysis suggest that the mean annual concentration of DIN is more sensitive to small fluctuations in the parameters which govern the predator-prey oscillation than to slight variations in the input of nitrogen. In fact, the ten parameters listed in Table 2 are directly related to the zooplankton and phytoplankton and on the effect of the light and temperature on their evolution.

Table 2. Expected variation in DIN_{av}, relative to a 1% increase in the parameter.

Parameter	ΔDIN_{av}	$(\Delta DIN_{av})^2$	Rank
k_{gr}	2.23E-03	4.97 E-06	4
k_{pz}	-1.08E-03	1.16 E-06	10
k_{mz}	-1.36E-03	1.86 E-06	8
e_{pz}	3.04E-03	9.23 E-06	3
G_{Pmax}	-1.96E-03	3.85 E-06	6
E_{xplass}	2.19E-03	4.82 E-06	5
T_{opt}	1.81E-02	3.28 E-04	1
T_{max}	-3.17E-03	1.01 E-05	2
k_P	2.72 E-4	7.40 E-8	12
I_{op}	5 E-4	2.5 E-7	11
Sum of squares of the remaining 15 parameters.		1.39 E-6	9
Sum of squares of all nitrogen sources		2.49 E-6	7

Based on this preliminary screening, six parameters, k_{gr}, G_{Pmax}, T_{opt}, Explass, Iop and kP, and the three main nitrogen sources, S2, S6 and S9 in Figure 1, were taken as input factors in the following global analysis.

In this first numerical experiment**,** the eight factors were assumed to be independently and normally distributed, with a standard deviation equal to 20% of their nominal value. A Monte Carlo random sampling scheme was employed [Helton et al., 2000] for extracting 250 elements. For each element of the sample, a yearly simulation of the model was repeated, in order to compute the mean annual TIN concentration. Total elapsed time was about five days, on a Digital 533Au WS.

The results of the uncertainty analysis of model output and of the multiple linear regression with respect to the input factors are summarized in Table 3.

The descriptive statistics of the distribution of DIN are given in the first two rows. The standardized regression coefficients, β_i, and the regression coefficients are given in columns two and three respectively. The fourth column shows the rank of the parameters, based on the absolute value of the standardized coefficients. The high value of the coefficient of determination, last row of Table 3, indicates that the linear model explains a large fraction of the output variability. This would make it reasonable to use the linear model in order to obtain a tentative estimation of the relative weight of the uncertainty in the internal parameters and in the forcing functions when determining the variability of the DIN mean annual concentration. The ratio between the contributions of the two groups of input was computed by assuming that the variance in the model output could be partitioned in accordance with eq. 7, which strictly holds for independently distributed variables only.

$$Var(DIN_{av}) \approx \Sigma_i b_i^2 Var(X_i) \qquad (7)$$

The ratio between the two contributions and the total variance was then computed:

$$Var(X_1,X_2,X_3,X_4,X_7,X_9)/Var(DIN_{av}) = 87.8\%$$

$$Var(X_5,X_6,X_8)/Var(DIN_{av}) = 6.4\%$$

The remaining 5.8% of the output variance is not accounted for by the linear model.

Table 3. Summary of the Monte Carlo uncertainty and sensitivity analysis.

Uncertainty analysis			
Model output	Mean value	Standard Deviation	CV%
DIN_{av}	.602	.081	13.4
Sensitivity analysis			
Input factors	β	b	Rank
Intercept		-1.15 E-01	
$X_1 = k_{gr}$	5.72 E-01	5.73 E+00	1
$X_2 = G_{Pmax}$	-5.58 E-01	-2.20 E+00	2
$X_3 = T_{opt}$	4.35 E-01	1.50 E-02	3
$X_4 = E_{xplass}$	1.88 E-01	6.50 E-01	4
X_5 = S2	1.85 E-01	8.45 E-02	5
X_6 = S6	1.44 E-01	4.80 E-02	6
X_7 = Iop	1.35 E-01	1.07 E-06	7
X_8 = S9	9.55 E-02	2.15 E-02	8
$X_9 = k_P$	5.73 E-2	1.63 E+00	9
R^2= .92			

4. CONCLUDING REMARKS

The results presented in the previous section, though preliminary, show that the combination of a local and a global sensitivity analysis may be very effective when dealing with large models. In this paper, the local analysis was essentially used as a screening method. Although other screening methods, of easier implementation, are available, [Campolongo et al., 2000], the local analysis provides extra information, such as the sensitivity curve in Figure 3, which can be used for an understanding of how each parameter affects the trajectory. Such information, and the fact that the sensitivities can be used to compute the gradient of a goal function, are extremely useful when guiding the calibration of the model.

The Monte Carlo uncertainty and sensitivity analyses here presented should be considered as the preliminary phases of a deeper analysis. In fact, the results based on the linear model, eq. (6), should be checked by means of other variance-decomposition methods, such as Fast or Sobol, which are not tied to the linear hypothesis. These techniques also gives indications about the "interaction" of the input factors in determining the model output. In other words, the addition of quadratic or higher order terms to eq. (6) may be needed, in order to explain a larger fraction of the variance. The fact that the linear model gave satisfactory results may also be due to the ranges of variation in the parameters which were tentatively chosen. The range of variation in each parameter should be determined on the basis of the available information and then the numerical experiment should then be repeated, in order to obtain a more realistic estimation of the expected variability in the model output.

However, from the ecological point of view, as well as from the point of view of the management of the water basin, the results strongly suggest that the variability induced by non-controllable fluctuations in the internal dynamics of the system, that is the variations in its auto purifying capacity, may overshadow the variability resulting from the fluctuations in the loads. These fluctuations could be due to uncontrollable factors, such as the amount and distribution of atmospheric precipitation which affects the discharges from the tributaries, or they could be the result of the management strategy. Therefore, it might be difficult to assess whether the adoption of a particular management strategy or set of controls imposed on the pollution sources are actually effective in keeping the system below the water quality target.

5. AKNOWLEDGEMENTS

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