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# PREFACE

This report is one of a series describing IIASA research into approaches for comparing alternative models that could be applied to the establishment of control policies to meet water-quality standards. In addition to model evaluation, this project has focused on problems of optimization and conflict resolution in large river basins.

# ABSTRACT

Sensitivity theory is applied in this paper to a class of generalized Streeter-Phelps models in order to predict the variations induced in BOD by the variations of some parameters characterizing the river system.

The paper shows how simple and elegant this technique is, and at the same time proves that many relatively complex phenomena can be explained by Streeter-Phelps models.

## Sensitivity Analysis of Streeter-Phelps Models

#### INTRODUCTION

The aim of this paper is twofold. First we show how the sensitivity of a given river-quality model can be analyzed by means of the so-called sensitivity theory. For this we first survey the main ideas of sensitivity theory and then as an exercise apply it to simple Streeter-Phelps models. Second, we point out that the result of this study proves that Streeter-Phelps models are flexible and abound with relevant consequences if one knows how to analyze them.

#### A SIMPLE TECHNIQUE FOR SENSITIVITY ANALYSIS

Here, we discuss how a given model is influenced by the variations of some of its main parameters (sensitivity analysis). This can be done in two different ways depending upon the purpose of the sensitivity analysis. One way is to simulate the system several times for different parameter values that cover the expected range of parameter variations and then compare the different solutions. The second way consists in calculating, at a nominal parameter value, the derivatives of the system solution with respect to the parameter. If the purpose of the sensitivity analysis is, for example, to make sure that an oxygen standard is not violated if temperature or flow rate varies over a certain range, one can show by decision-theoretical arguments that the first type of sensitivity analysis should be preferred (Stehfest, 1975a). If the sensitivity is to be discussed in general, without reference to a particular application, calculation of the derivative is most appropriate, because the result can be presented more succinctly than in the other case. Therefore, this approach is used in the following for a sensitivity discussion of the Streeter-Phelps model. Before doing this, however, we

briefly present the elements of this type of sensitivity analysis (see, for example, Cruz, 1973).

Assume that a continuous, lumped parameter system is described by the vector differential equation

$$\dot{\mathbf{x}}(t) = \mathbf{f}(\mathbf{x}(t), \theta, t) , \qquad (1)$$

where x is an n-th order vector and  $\theta$  is a constant parameter with nominal value  $\overline{\theta}$ , and let the initial state x<sub>0</sub> of the system depend upon the parameter, i.e.

$$\mathbf{x}_{O} = \mathbf{x}_{O}(\theta)$$
  $(\overline{\mathbf{x}}_{O} = \mathbf{x}_{O}(\overline{\theta}))$  . (2)

The solution of Eq. (1) with the initial condition (2) is a function

$$\mathbf{x} = \mathbf{x}(\mathbf{t}, \boldsymbol{\theta})$$

which, under very general conditions, can be expanded in series in the neighborhood of the nominal value of the parameter, i.e.

$$\mathbf{x}(t,\theta) = \overline{\mathbf{x}}(t) + \left[\frac{\partial \mathbf{x}(t,\theta)}{\partial \theta}\right]_{\overline{\theta}} (\theta - \overline{\theta}) + \cdots,$$

where  $\bar{\mathbf{x}}(t) = \mathbf{x}(t,\bar{\theta})$  is the nominal solution. The vector  $[\partial \mathbf{x}/\partial \theta]_{\bar{\theta}}$ , namely the derivative of the state vector with respect to the parameter, is called the *sensitivity vector* (or sensitiv-ity *coefficient*) and from now on will be denoted by s, i.e.

$$s(t) = \left[\frac{\partial x}{\partial \theta}\right]_{\overline{\theta}}$$

Thus the perturbed solution of Eq. (1) can be easily obtained as

$$\mathbf{x}(t,\theta) \stackrel{\sim}{=} \mathbf{x}(t) + \mathbf{s}(t)(\theta - \overline{\theta})$$

once the sensitivity vector is known.

When there are many parameters  $\theta_1, \theta_2, \ldots, \theta_q$ , the knowledge of the sensitivity vectors  $s_1, s_2, \ldots, s_q$  allows the association of specific characteristics of the system behavior with particular parameters. If, for example, the nominal solution  $\bar{x}(t)$  of a first-order system is the one shown in Figure 1, where  $s_1(t)$ and  $s_2(t)$  are the sensitivity coefficients of x with respect to two parameters  $\theta_1$  and  $\theta_2$ , one can say that the first parameter is responsible for the overshoot of  $\bar{x}$  while the second is responsible for the asymptotic behavior of the system. This characterization of the parameters very often turns out to be of great importance in the validation of the structure of a model; in fact some of the best-known methods of parameter estimation are based on manipulation of the sensitivity vectors.



Figure 1. Nominal solution  $\bar{\mathbf{x}}$  and sensitivity coefficients  $s_1$  and  $s_2$ .

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By taking the total derivative of Eq. (1) it can be concluded that the sensitivity vector s(t) satisfies the following vector differential equation:

$$\dot{\mathbf{s}} = \left[\frac{\partial \mathbf{f}(\mathbf{x}, \overline{\theta}, \mathbf{t})}{\partial \mathbf{x}}\right]_{\overline{\mathbf{x}}} + \left[\frac{\partial \mathbf{f}(\overline{\mathbf{x}}, \theta, \mathbf{t})}{\partial \theta}\right]_{\overline{\theta}}$$
(3)

with initial conditions

$$\mathbf{s}_{\mathbf{O}} = \begin{bmatrix} \frac{\partial \mathbf{x}_{\mathbf{O}}}{\partial \theta} \end{bmatrix}_{\overline{\mathbf{0}}} \qquad (4)$$

Thus, the sensitivity vector is the state vector of the system (3), called *sensitivity system*, which is always a linear system, even if system (1) is nonlinear. Because of this property the sensitivity vectors can often be analytically determined. In any case, they can always be computed by means of simulation following the scheme shown in Figure 2.



Figure 2. Computation of sensitivity vectors.

In the following we apply this methodology to some very particular but interesting sensitivity problems of river pollution. The model we use is the well-known Streeter-Phelps model or some suitable modification of it. To simplify the discussion we deal with the parameters one at a time. Obviously, this does not imply that our results are not general, since in the case of many parameters  $\theta_1, \theta_2, \ldots$  the perturbed solution of Eq. (1) can be simply obtained as

$$\mathbf{x}(t, \theta_1, \theta_2, \ldots) = \overline{\mathbf{x}}(t) + \mathbf{s}_1(\theta_1 - \overline{\theta}_1) + \mathbf{s}_2(t)(\theta_2 - \overline{\theta}_2) + \ldots,$$

where  $s_1(t), s_2(t), \ldots$  are the sensitivity vectors.

## BOD VARIATIONS

Let us first analyze the effects of a variation of the BOD load discharged into the river at a particular point. By writing the Streeter-Phelps model in flow time  $\tau$  we obtain that the system is described by

$$\dot{b} = -k_1 b$$
  
 $\dot{c} = -k_1 b + k_2 (c_s - c)$ ,

where b and c stand for BOD and DO,  $c_s$  is the oxygen saturation level and  $k_1$  and  $k_2$  are the characteristic parameters (BOD decay and re-aeration coefficients, respectively) of the model. The initial conditions are

$$b_0 = \bar{b}_0 + \theta$$
  $c_0 = \bar{c}_0$ 

if we assume that the oxygen content of the effluent is negligible. Thus, the sensitivity system is given by

$$\dot{s}_{b} = -k_{l}s_{b}$$
(5a)

$$\dot{s}_{c} = -k_{1}s_{b} - k_{2}s_{c}$$
 (5b)

and its initial conditions are

$$\mathbf{s}_{\mathbf{b}_{\mathbf{O}}} = \begin{bmatrix} \frac{\partial \mathbf{b}_{\mathbf{O}}}{\partial \theta} \end{bmatrix}_{\overline{\theta}} = 1 \qquad \mathbf{s}_{\mathbf{C}_{\mathbf{O}}} = 0$$

The solution of Eq. (5a) with  $s_{b_0} = 1$  is given by

$$s_b(\tau) = e^{-k_1 \tau}$$
,

which can be introduced in Eq. (5b) together with  $s_0 = 0$ , thus giving

$$s_{c}(\tau) = k_{1} \frac{e^{-k_{1}\tau} - e^{-k_{2}\tau}}{k_{1} - k_{2}}$$
 (6)

The sensitivity coefficient  ${\rm s}_{\rm C}$  given by Eq. (6) is always negative, as shown in Figure 3, and has a minimum for

$$\tau^{\star} = \frac{\ln(k_2/k_1)}{k_2 - k_1} \quad . \tag{7}$$

This means that a positive perturbation of the BOD load at a point on the river implies that all the river downstream from



Figure 3. The sensitivity of dissolved oxygen concentration to BOD load.

that point becomes worse as far as its oxygen content is concerned. This is the conclusion one can derive from the Streeter-Phelps model which does not represent a priori the behavior of a real river. Indeed, it can be shown (see, for instance, Stehfest, 1975b) that because of the mechanisms of the food chain, it could sometimes be expected that the conditions of the river are bettered at some particular point by an increase of the BOD load.

## FLOW VARIATIONS

Let us now suppose that we are interested in predicting the variations induced in BOD and DO in a stream by variations of flow rate (see, for example, Loucks and Jacoby, 1972). Of course we cannot consider flow time as the independent variable and we must therefore write the Streeter-Phelps model in the form

$$\frac{d\mathbf{b}}{d\ell} = - K_1(\mathbf{Q})\mathbf{b}$$

$$\frac{d\mathbf{c}}{d\ell} = - K_1(\mathbf{Q})\mathbf{b} + K_2(\mathbf{Q})(\mathbf{c}_s - \mathbf{c}) , \qquad (8)$$

where l is distance, Q is flow rate and the two new characteristic parameters are given by

$$K_1 = k_1(Q) / v(Q)$$
  $K_2 = k_2(Q) / v(Q)$ 

v(Q) being the average stream velocity.

As far as the initial conditions are concerned, let us suppose that the water coming into the reach under consideration is perfectly oxygenated and with zero BOD. Thus, after mixing with the effluent discharge in point  $\ell = 0$  we have

$$b_{O} = b_{O}(Q) \qquad c_{O} = c_{S},$$

so that the initial conditions of the sensitivity vector turn out to be given by

$$\mathbf{s}_{\mathbf{b}_{\mathbf{O}}} = \mathbf{b}_{\mathbf{O}}' = \left[\frac{\partial \mathbf{b}_{\mathbf{O}}}{\partial \mathbf{Q}}\right]_{\mathbf{\overline{Q}}} < 0 , \quad \mathbf{s}_{\mathbf{C}_{\mathbf{O}}} = 0 ,$$

while the sensitivity system (3) is given by

$$\frac{ds_{b}}{dl} = -\kappa_{1}s_{b} - \kappa_{1}'\bar{b}$$

$$\frac{ds_{c}}{dl} = -\kappa_{1}s_{b} - \kappa_{2}s_{c} - \kappa_{1}'\bar{b} + \kappa_{2}'(c_{s} - \bar{c}) ,$$
(9)

where parameters  $K_1$  and  $K_2$  are evaluated in nominal conditions  $(Q = \bar{Q})$  and the ' means derivative with respect to the parameter, i.e.

The solution of Eqs. (8,9) can easily be found and the sensitivity coefficients  $s_{\rm b}$  and  $s_{\rm c}$  are given by

$$s_{b}(\ell) = (b_{0} - K_{1}\bar{b}_{0}\ell)e^{-K_{1}\ell}$$
  
$$s_{c}(\ell) = A(e^{-K_{1}\ell} - e^{-K_{2}\ell}) + B\ell(K_{1}e^{-K_{1}\ell} - K_{2}e^{-K_{2}\ell})$$

where

$$A = \left[ -\kappa_{1}\dot{b}_{0} - \kappa_{1}'\ddot{b}_{0} + \frac{\kappa_{1}\ddot{b}_{0}}{\kappa_{2} - \kappa_{1}} (\kappa_{2}' - \kappa_{1}') \right] \frac{1}{\kappa_{2} - \kappa_{1}}$$

$$B = \frac{\kappa_{1}\ddot{b}_{0}}{\kappa_{2} - \kappa_{1}} .$$

The sensitivity coefficient  $s_b$  is negative for all values of lwhile a typical situation for  $s_c$  is shown in Figure 4. The derivative of  $s_c$  at the initial point l = 0 is always positive since  $K'_1 < 0$ , and this implies that in the part of the reach immediately downstream from the effluent point, the oxygen concentration is an increasing function of flow rate. On the contrary, if we consider points that are sufficiently downstream we may obtain exactly the opposite result as shown in the example in Figure 4. Nevertheless, roughly speaking we can conclude that the higher the values of the flow rate, the better the global conditions of the river, since the improvement due to an increment of flow rate is obtained where the oxygen conditions are worse; this fact is actually the motivation for the use of low-flow augmentation (see Loucks and Jacoby, 1972) in river-quality control.



Figure 4. The sensitivity of dissolved oxygen concentration to flow rate.

#### TEMPERATURE VARIATIONS

Let us now discuss the influence of the temperature on the dissolved oxygen of a river. To simplify the discussion let us assume we are discharging a given amount of BOD at a particular point of a perfectly clean and oxygenated river. Moreover, suppose that the steady-state (equilibrium) temperature T of the water is constant in space. Thus, the initial conditions of the stretch are given and depend upon the temperature T of the water since the oxygen saturation level  $c_s$  is a decreasing function of T. Under these assumptions the system is described by

$$\dot{\mathbf{b}} = -\mathbf{k}_{1}(\mathbf{T})\mathbf{b} \tag{10a}$$

$$c = -k_1(T)b + k_2(T)(c_2(T) - c)$$
, (10b)

where the independent variable is again flow time  $\tau$ . The initial conditions of system (10) are

$$b_{o} = \overline{b}_{o}$$
  $c_{o} = c_{s}(T)$ .

The corresponding sensitivity system is given by

$$\dot{s}_{b} = -k_{1}s_{b} - k_{1}'\bar{b}$$
$$\dot{s}_{c} = -k_{1}s_{b} - k_{2}s_{c} - k_{1}'\bar{b} + (k_{2}c_{s})' - k_{2}'\bar{c}$$

with initial conditions

$$s_{b_0} = 0$$
  $s_{c_0} = c'_s$ ,

where ' as before means derivative with respect to T. The solution of the sensitivity system is given by

$$\begin{split} \mathbf{s}_{b}(\tau) &= -\mathbf{k}_{1}^{\prime} \mathbf{\bar{b}}_{o} \tau \mathbf{e}^{-\mathbf{k}_{1} \tau} \\ \mathbf{s}_{c}(\tau) &= \mathbf{c}_{s}^{\prime} + \frac{\mathbf{k}_{1} \mathbf{k}_{2}^{\prime} - \mathbf{k}_{1}^{\prime} \mathbf{k}_{2}}{(\mathbf{k}_{2} - \mathbf{k}_{1})^{2}} \mathbf{\bar{b}}_{o} (\mathbf{e}^{-\mathbf{k}_{1} \tau} - \mathbf{e}^{-\mathbf{k}_{2} \tau}) + \\ &+ \frac{\mathbf{k}_{1}}{\mathbf{k}_{2} - \mathbf{k}_{1}} \mathbf{\bar{b}}_{o} \tau (\mathbf{k}_{1}^{\prime} \mathbf{e}^{-\mathbf{k}_{1} \tau} - \mathbf{k}_{2}^{\prime} \mathbf{e}^{-\mathbf{k}_{2} \tau}) \quad . \end{split}$$

From this expression it follows that

$$\dot{s}_{c}(0) = -k_{1}' \ddot{b}_{o}$$
  $s_{c}(\infty) = s_{c} = c'_{s}$ ;

and since  $k'_1 < 0$  and  $c'_s < 0$ , one obtains that the DO sensitivity coefficient s<sub>c</sub> is always characterized by the following three properties:

$$s_{c}(0) < 0$$
  $\dot{s}_{c}(0) < 0$   $\dot{s}_{c}(\infty) < 0$ 

Two possible sensitivity curves  $s_c$  are shown in Figure 5, the first one (a) being all negative and the second one (b) showing that along a segment of the river (segment AB) the conditions are bettered by an increment of the temperature. This surprising fact can be explained by noticing that curve (b) could be obtained under the assumption that re-aeration can be drastically improved by increasing the temperature. Nevertheless, even under these hypothetical conditions the dominant effect is a decrease of the dissolved oxygen concentration with the temperature of the water; and this is why in order to be safe, high temperature conditions are often selected as the reference conditions in the design of wastewater treatment plants or other river pollution control facilities.



Figure 5. The sensitivity of dissolved oxygen concentration to temperature.

#### HEAT DISCHARGE

As a final example we now discuss in very simple and perhaps crude terms the effects that heat pollution has on the biochemical process. This matter has been discussed for a long time, and it is somehow surprising that some of the main conclusions on which people agree today were already contained in the Streeter-Phelps model.

Let us make reference to the case illustrated in Figure 6a where a river with a flow rate  $Q_1$  and temperature  $T^*_O$  receives a heat discharge with a flow rate  $Q_2$  and temperature

 $(T_{O}^{*} + \frac{Q_{1}}{Q_{1}} + \frac{Q_{2}}{Q_{1}}\Delta T_{O})$ . Then after mixing (at the point l = 0) we obtain a flow rate  $Q = Q_{1} + Q_{2}$  and a temperature  $T_{O}^{*} + \Delta T_{O}$ . The variation  $\Delta T_{O}$  induced in the river by the heat discharge is our parameter and its normal value  $\overline{\Delta T}_{O}$  is zero, meaning that the nominal conditions refer to the case in which there is no heat discharge. Moreover, we assume that the BOD concentration of the discharge is the same as that of the river, while where oxygen is concerned we assume that both the river and the discharge are in saturated conditions, as shown in Figure 6b, so that the initial conditions are

$$T_{o} = T_{o}^{*} + \Delta T_{o}$$
  

$$b_{o} = b_{o}^{*}$$
  

$$c_{o} = \frac{Q_{1}}{Q_{1} + Q_{2}} c_{s}(T_{o}^{*}) + \frac{Q_{2}}{Q_{1} + Q_{2}} c_{s}(T_{o}^{*} + \frac{Q_{1} + Q_{2}}{Q_{2}} \Delta T_{o}) \cdot$$

The temperature of the water must now be added as an extra state variable to the simple Streeter-Phelps model considered so far, and the model becomes





$$\dot{T} = f(T)$$
 (lla)

$$\dot{\mathbf{b}} = -\mathbf{k}_{1}(\mathbf{T})\mathbf{b} \tag{11b}$$

$$\dot{c} = -k_1(T)b + k_2(T)(c_s(T) - c)$$
 (11c)

with initial nominal conditions

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$$\overline{T}_{O} = T^{*}_{O} \qquad \overline{b}_{O} = b^{*}_{O} \qquad \overline{c}_{O} = c_{S}(T^{*}_{O}) \quad \cdot$$

Thus the sensitivity system is given by

$$\dot{s}_{T} = f's_{T}$$
 (12a)

$$\dot{s}_{b} = -k_{1}'\bar{b}s_{T} - k_{1}s_{b}$$
 (12b)

$$\dot{s}_{b} = (-k_{1}'\bar{b} + k_{2}'c_{s} + k_{2}c_{s}' - k_{2}'\bar{c})s_{T} - k_{1}s_{b} - k_{2}s_{c} ,(12c)$$

where  $f' = \begin{bmatrix} \frac{\partial f}{\partial T} \end{bmatrix}_{\overline{T}}$  and the initial conditions are

$$s_{T_0} = 1$$
  $s_{b_0} = 0$   $s_{c_0} = c'_s$ 

Eqs. (11, 12) can be easily solved since they are of triangular structure. If we assume that  $T_{O} = T_{O}^{*}$  is a constant solution of Eq. (11a) we can solve this system of equations analytically, and the solution gives the three sensitivity coefficients

$$s_{T} = e^{f'\tau}$$

$$s_{b} = \frac{k_{1}'}{f'} \bar{b}_{o} e^{-k_{1}\tau} (1 - e^{f'\tau})$$

$$s_{c} = A e^{-k_{1}\tau} + Be^{-k_{2}\tau} + C e^{f'\tau} + D e^{(f-k_{1}')\tau} + E e^{(f - k_{2}')\tau}$$

•

where the constants A, B,..., E are given by

$$\begin{split} \lambda &= \frac{k_1 k_2'}{(k_2 - k_1) f'} \bar{b}_0 \\ B &= -\frac{k_2 c_s'}{k_2 - f'} - \frac{k_1 k_2'}{(k_2 - k_1 - f'') f'} \bar{b}_0 + \frac{k_1' k_2}{(k_2 - k_1) (k_2 - k_1 - f'')} \bar{b}_0 + c_s' \\ C &= \frac{k_2 c_s'}{k_2 - f'} \\ D &= \left[ \frac{k_1 k_2'}{k_2 - k_1} - (1 + \frac{k_1}{f''}) k_1' \right] \frac{\bar{b}_0}{k_2 - k_1 - f''} \\ E &= \frac{k_1 k_2'}{(k_2 - k_1) f''} \bar{b}_0 \quad . \end{split}$$

The corresponding sensitivity curves are shown in Figure 7 for realistic values of the parameters, and the main conclusion is that the oxygen concentration is lowered everywhere and in particular around the minimum of the DO curve. Nevertheless, the perturbation introduced by the heat discharge is absorbed along the river, and this is the main distinction between the case of temperature perturbation and the preceding one.

## CONCLUDING REMARKS

Sensitivity theory has been used in this paper to analyze a class of water-quality models (Streeter-Phelps models). Load variations, flow rate variations and temperature variations have been considered, as has the interactions between heat pollution and biodegradable pollution. The results are of general applicability and are presented in a very simple analytical form. The main limitation of the study could be the fact that sensitivity theory makes reference only to small perturbations of the parameters. Nevertheless, the direct comparison with the simulation



Figure 7. Sensitivity coefficients of temperature, BOD and DO to heat discharge.

study carried out by Lin et al. (1973) has shown that the results obtained in this paper are largely satisfactory for realistic variations of the parameters of river-quality models.

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