A Multiple Organic Pollutant Simulation/Optimization Model of Industrial and Municipal Wastewater Loading to a Riverine Environment

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Abstract. A simulation/optimization model in a multiple pollutant framework is developed to aid policy analysis of least cost approaches to wastewater management that maintain downstream ambient quality levels. The objective is to choose treatment levels for several industrial and municipal sites and for three organic pollutants that minimize the combined cost of wastewater treatment of 5-day biological oxygen demand, nitrogen, and phosphorus over the sites in order to achieve chosen ambient quality standards. Treatment costs and downstream ambient quality impacts vary with each site and pollutant. A subroutine is developed for a river water quality simulation model that provides the marginal downstream ambient quality impacts, or the Jacobian matrix, of each pollutant. The Jacobian matrix must be recalculated for each iterative treatment solution of the optimization model until equilibrium is reached. The Jacobian matrix varies due to the non-linear interaction of nitrogen and phosphorus in the production of algae, affecting dissolved oxygen levels. The necessity of recalculating the Jacobian matrix is demonstrated using, first, a hypothetical example, then using a case study of the Nitra River Basin in Slovakia. The robustness of the solution procedure is tested by varying the initial pollution abatement levels.

1. Introduction

Wastewaters discharged into rivers have a variety of impacts on water quality. Water quality has impacts on fisheries, irrigated agriculture yields, water intake treatment costs for cities, human health, recreation and aesthetic values, as well as other impacts. The principal sources of river pollution are municipal (both point and non-point), industrial and agricultural. Water quality is affected both by organic pollutants such as biological oxygen demand, phosphorus and nitrogen, and by inorganic, often toxic, pollutants such as heavy metals. Each of these pollutants has different impacts and requires different treatment methods. This paper considers only organic pollutants.

Dissolved oxygen (DO) is the primary indicator of the general health of a river system, in part because fish need oxygen to survive. DO is affected by many organic pollutants. Biological oxygen demand (BOD) is organic matter that uses dissolved oxygen from the river as it decays[1]. The effect of BOD on DO is well known and simple. Municipal wastewater and agricultural sources are particularly significant contributors of BOD. It is the most common pollutant and typically the least expensive to remove from wastewater. Traditionally, only BOD has been considered in water quality management. Two other organic pollutants, nitrogen (N) and phosphorus (P), are present in most wastewater sources, especially agricultural. They both affect water quality by contributing to algae growth. Algae can cause water clarity problems and also affect DO concentrations directly. Nitrogen also affects DO levels directly because the transformation of organic nitrogen to its hydrated forms uses DO.

Models incorporating river water quality and optimization modeling have generally focused on the simple linear relationship between DO and BOD, as expressed by the Streeter-Phelps equation (Streeter and Phelps, 1925). Such models have not addressed other important organic pollutants such as nitrates and phosphates, although these pollutants are modeled empirically in several ways in water quality modeling [Thomann and Mueller, 1987]. Many water quality simulation models have incorporated these empirical processes. However, such models are not capable of policy analysis of various wastewater treatment strategies. Existing models for policy analysis consider only a single pollutant. Such models fail to address the interaction of organic pollutants and consequent appropriate wastewater treatment policies. For example, Schleich et al. [1996] considered cost implications of reducing nitrogen loading using a linear programming model.

The development of a simulation/optimization model capable of policy analysis involving several organic pollutants is a useful advance. The discharge and resulting downstream presence of nitrogen, phosphorus and BOD are important to include in the modeling process because they are present in most types of wastewater and runoff into streams and rivers. Agricultural runoff has particularly high levels of nitrogen and phosphorus because they are primary ingredients in fertilizer. This is very important because agricultural non-point sources are the most common source of river pollution throughout the world, both in the developed and the developing world. The simulation/optimization model for river water

[1] The rate of decay is based upon 5-day BOD laboratory tests (BOD_5) (Chapra, 1997).

quality developed here is similar to that developed by Gorelick et al. [1984] for aquifer reclamation design.

A management model is developed to consider management objectives such as single and multiple pollutant least cost approaches and uniform nutrient reduction targets. The least cost models choose percentage reductions in pollutant wasteloads at each of the sites in order to minimize the total treatment cost of meeting chosen downstream ambient quality standards.

The usefulness of the multiple pollutant simulation/optimization model is demonstrated by comparing results among models in which: (1) only BOD abatement is considered; (2) BOD, P and N abatement are considered without regard to their biological and chemical interaction; and (3) BOD, P and N abatement are considered including their interaction. Finally, the robustness of the iterative solving procedure is demonstrated. The model is applied first to the hypothetical 'Fluss River' maquette, followed by an application to the Nitra River Basin in Slovakia. Optimization models are solved using GAMS/MINOS optimization software [Brooke, Kendrick and Meeraus, 1992].

2. Water Quality / Pollutant Transport Model

The water quality simulation model is QUAL2E [Brown and Barnwell, 1987], which is used here for in-stream simulation of reaeration, oxidation of carbonaceous waste material, oxidation of nitrogenous waste material, oxygen demand from sediments, oxygen use by algae for respiration, algae production by photosynthesis, sedimentation of carbonaceous waste material and nitrogenous waste material, photosynthesis and respiration. An additional module is developed and added to QUAL2E that calculates the marginal effect of increasing a pollutant load on downstream DO levels. The matrix formed by calculating this gradient for each different type of pollutant and each different pollution emitting site is called the Jacobian matrix. The module also passes information to and from the optimization model. The Jacobian matrix is passed to the optimization model, and the matrix of post-treatment wasteload levels, calculated by the optimization model, is passed to the simulation model. Single pollutant (BOD) and multiple pollutant (BOD, P and N) cases of water quality modeling are given. The derivation of the Jacobian matrix in each case and its importance in developing solution methods are presented.

2.1 Single Pollutant Modeling

As noted above, models in the literature have generally focused on the relationship between DO and BOD. This relationship is a reasonable starting position for water quality modeling. BOD is generally the most common river pollutant. Its treatment processes are well known and relatively cost effective in comparison with treatment of other organic pollutants. It is also well used in modeling because the relationship is well known and simple. The Streeter-Phelps equation gives the response of DO concentration (AQ) at each river reach to a BOD load concentration (E_0, in mg O/liter) (Streeter and Phelps, 1925). Also required are the DO saturation concentration (AQ_s), the initial DO concentration (AQ_0), the effective deoxygenation rate (K_d, in t^{-1}), the volumetric reaeration coefficient (K_a , in t^{-1}), and the overall BOD loss rate (K_r, in t^{-1}). K_r is based on the depth, area, flow, and temperature of the river. All concentrations are in milligrams per liter. This equation drives the well known illustration of DO "sag" (Figure 1). "Emitting site" is the source from which wastewater pollution enters the river (the y axis, in Figure 1). "Monitoring point" is the downstream location at which DO is measured (Point A, in Figure 1). The equation may be calculated for each emitting site (*i*) and every downstream monitoring point (*j*).

$$AQ_j = AQ_{s,j} - \left[(AQ_{s,j} - AQ_{0,j}) \cdot \exp(-K_a \cdot t_j)\right] - \left\{\frac{K_d}{K_a - K_r}\left[\exp(-K_r \cdot t_j) - \exp(-K_a \cdot t_j)\right]\right\} E_{0,i} \qquad (1)$$

The marginal downstream impact, referring to the marginal reduction in dissolved oxygen due to a one unit increase in a pollutant from an emitting site, at monitoring point (*j*) of BOD loading from site (*i*) may be found through the derivative with respect to the BOD load.

$$\frac{\partial AQ_j}{\partial E_{0,i}} = \left\{\frac{K_d}{K_a - K_r}\left[\exp(-K_r \cdot t_j) - \exp(-K_a \cdot t_j)\right]\right\} \qquad (2)$$

This term is constant for each (*i,j*). The marginal impact is independent of the size of the load and of the size of loads from other sites. The collected matrix of these marginal impacts over all (*i*) and (*j*) is the Jacobian matrix. The impacts, then, from several emitting sites may simply be added to determine the collective downstream impact on dissolved oxygen levels.

$$\left[\mathbf{J}_{mn}\right] = \frac{\partial \mathrm{AQ}_j}{\partial \mathrm{E}_{0,i}} \quad \text{for all } i = 1 \text{ to m and all } j = 1 \text{ to n} \tag{3}$$

The first two terms of equation (1) may be collected as the DO concentration that would exist if no BOD emissions entered the stream (AQB). The last term gives the impact on DO due to BOD emissions from site (*i*). Expanding to include several BOD emitting sites only requires adding on a term measuring impact on DO due to BOD for each separate emitting site. Each impact is found by multiplying the marginal impact of a pollutant at a site (J_{ijk}, in {mg DO/liter}/{kg BOD/yr}) by the annual pollutant load from that site (E_{ik}, now expressed in kilograms of BOD per year). These impacts are summed across emitters. This gives a form that will be used by the optimization model.

$$\mathrm{AQ}_j = \mathrm{AQB}_j - \sum_{i=1}^{m} (\mathrm{J}_{ij} \cdot \mathrm{E}_{0,i}) \quad ; \text{for all monitoring points } j = 1 \text{ to n} \tag{4}$$

2.2 Multiple Pollutant Modeling

Modeling complexity increases when additional pollutants are considered. BOD, several forms of nitrogen, two forms of phosphorus, algae[2] and dissolved oxygen interact (Figure 2). A modified form of the Streeter-Phelps equation dictates how these elements affect DO concentration (adapted from Thomann and Mueller, 1987).

$$\mathrm{AQ} = \left(\mathrm{AQ}_s + (\mathrm{AQ}_s - \mathrm{AQ}_0)\exp(-\mathrm{K}_a t)\right) \tag{5}$$

$$- \left\{\left(\frac{\mathrm{K}_d}{\mathrm{K}_a - \mathrm{K}_r}\right)\left[\exp(-\mathrm{K}_r \cdot t) - \exp(-\mathrm{K}_a \cdot t)\right]\right\}\mathrm{E}_0 - \left\{\left(\frac{a_2 b_2}{\mathrm{K}_a - a_2 b_2}\right)\left[\exp(-a_2 b_2 t) - \exp(-\mathrm{K}_a t)\right]\right\}\mathrm{E}_1$$

$$- \left\{\left(\frac{a_3 b_3}{\mathrm{K}_a - a_3 b_3}\right)\left[\exp(-a_3 b_3 t) - \exp(-\mathrm{K}_a \cdot t)\right]\right\}\mathrm{E}_2 + \left\{\left[1 - \exp(-\mathrm{K}_a t)\right]\left(\frac{p_a}{\mathrm{K}_a}\right) - \left[1 - \exp(-\mathrm{K}_a t)\right]\left(\frac{R}{\mathrm{K}_a}\right)\right\}$$

where

K_d	effective deoxygenation rate (t^{-1})
K_a	volumetric reaeration coefficient (t^{-1})
K_r	overall BOD loss rate (t^{-1})
a_2	rate of oxygen use per ammonia nitrogen oxidation (mg O / mg N)
b_2	ammonia oxidation rate coefficient (t^{-1})
E_1	ammonia nitrogen concentration (mg N / liter)
a_3	rate of oxygen use per nitrite nitrogen oxidation (mg O / mg N)
b_3	nitrite oxidation rate coefficient (t^{-1})
E_2	nitrite nitrogen concentration (mg N / liter)
p_a	average gross photosynthetic production of DO (mg O / liter day)
R	average respiration (mg O / liter day)

Algae growth is a non-linear function of the inputs of ammonia nitrogen, nitrate, and dissolved phosphorus (henceforth, “phosphorus”). Using a grouped measure of nitrogen, both nitrogen and phosphorus are necessary in the production of chlorophyll, in an approximate ratio of seven to two, respectively, by weight. Algae has a non-linear growth path when one of these inputs is increased and the other held constant. In some situations, one of the pollutants is a limiting factor in algae growth.

The production of oxygen by algae is governed by the ratio of DO produced per unit of algal photosynthesis, r_{oa} (mg O / mg chl *a)*[2]; the algae growth rate, K_g (t^{-1}); and the algal biomass concentration, *a* (mg chl *a* / liter).

$$p_a = r_{oa} K_g a \tag{6}$$

The algal growth rate is dependent upon nutrient limitations (ϕ_N), light limitations (ϕ_L), and the temperature-corrected (T, ^oC) maximum growth rate under optimal conditions ($k_{g,T}$).

$K_g = k_{g,T}\ \phi_N\ \phi_L$ (7)

$k_{g,T} = G_{max}\,(1.066)^{T-20}$

G_{max} maximum growth rate of algae (t^{-1})

Concerning ϕ_N, separate limitation terms are developed for each nutrient involved. For ammonia nitrogen, nitrite nitrogen, and phosphorus, respectively, these are

$$\phi_{E1} = \frac{E_1}{k_{sE1}+E_1},\quad \phi_{E2} = \frac{E_2}{k_{sE2}+E_2},\ \text{and}\quad \phi_{E3} = \frac{E_3}{k_{sE3}+E_3} \tag{8}$$

where E_1, E_2, and E_3 are the concentrations of each nutrient (mg / liter), and k is the half-saturation constant in each case (mg / liter). It is possible for either of the forms of nitrogen to be limiting. For simplicity and due to data limitations, for the remainder of this paper ammonia nitrogen (henceforth, "nitrogen") will be considered the relevant limiting form of nitrogen.[3] Several approaches to modeling the combined effects of multiple nutrients exist in the literature. The most commonly accepted formulation is

$\phi_N = \min\,(\phi_{E1},\phi_{E3})$ (9)

The use of oxygen by algae is governed by the ratio of DO uptake per unit of algae respired, a_{op} (mg O / mg chl *a*); the algae respiration rate, k_{ra} (t^{-1}); the algae concentration, *a* (mg chl *a* / liter), and a temperature adjustment factor. Grazing losses are omitted.

$R = a_{op}\ k_{ra}\ (1.08)^{T-20}\ a$ (10)

The three dimensional Jacobian matrix for all (*i,j,k*) is composed of the set of elements

$$\frac{\partial AQ_j}{\partial E_{0,i}} = \left\{\frac{K_d}{K_a - K_r}\left[\exp\,(-K_r \cdot t_j) - \exp\,(-K_a \cdot t_j)\right]\right\}\ \text{for BOD loads,} \tag{11}$$

$$\frac{\partial AQ}{\partial E_{1,i}} = -\left\{\left(\frac{a_2 b_2}{K_a - a_2 b_2}\right)\left[\exp(-a_2 b_2\, t) - \exp(-K_a\, t)\right]\right\}$$

$$+\left(\frac{1-\exp(-K_a\, t)}{K_a}\right) r_{oa}\, G_{max}\,(1.066)^{T-20}\ \phi_L\ a\ \frac{\partial\ \phi_N}{\partial E_{1,i}}\quad \text{for nitrogen loads, and} \tag{12}$$

$$\frac{\partial AQ_j}{\partial E_{3,i}} = \left(\frac{1-\exp(-K_a\, t)}{K_a}\right) r_{oa}\, G_{max}\,(1.066)^{T-20}\ \phi_L\ a\ \frac{\partial\ \phi_N}{\partial E_{3,i}}\quad \text{for phosphorus loads} \tag{13}$$

The complete Jacobian may be represented as

$$\left[\mathbf{J}_{mnp}\right] = \left[\frac{\partial AQ_j}{\partial E_{ik}}\right]\ \text{for all sites i = 1 to m, monitoring points j = 1 to n, and pollutants k = 1 to p}$$

The effects of nitrogen and phosphorus on algae growth cause some elements of the Jacobian to depend on the nitrogen and phosphorus loads. The marginal downstream impact of nitrogen loading from a site **depends** on the size of the nitrogen load, the phosphorus load emitted from the site, and the nitrogen and phosphorus loads of all other sites as well. This means that each element value is only valid very near the mix of pollutant loads at which it was calculated. As a result, the Jacobian must be recalculated at each state of the system.

The variability of the marginal effects on DO is illustrated for the emission range of one site in two pollutants (Figure 3). Suppose the load has a high initial concentration of N and a low initial concentration of P (point B). The DO impact of early reductions in nitrogen will be minimal, because nitrogen is in excess and phosphorus acts as the limiting agent. As nitrogen reductions continue,

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[2] Algae concentrations are measured by chlorophyll concentration (chl-*a*).

[3] Whether ammonia, nitrite, or both forms of nitrogen are used does not affect the non-linearity of the algae growth process nor the implications on the Jacobian matrix.

however, the impact on DO increases, as the excess nitrogen is removed. Eventually, nitrogen becomes the limiting factor and DO impacts rise further.

The importance of the variable Jacobian matrix is that the effects of the pollutants from all of the sources on a given monitoring site cannot be accurately separated. The impact of each polluter's emissions on DO levels is dependent on the effluent activities of the others.

Equation (5) may be restated by collecting terms and simplifying to a form readily applicable to the optimization model. Ambient quality is still found by determining the maximum possible quality level and subtracting all impacts on dissolved oxygen levels. The first two terms may be collected as AQB, as before. Multiple emitters are now considered as well. The remaining terms describe each emitters' impacts on DO, differentiated by pollution and emitting site.

$$AQ_j = AQB_j - \sum_{i=1}^{m}\sum_{k=1}^{p}\left(J_{ijk}\,(\mathbf{X}_{mp})\cdot(E_{ik}(X_{ik}))\right) \text{ for all monitoring points } j = 1 \text{ to } n \qquad (14)$$

3. Optimization Model

This paper expands on previous studies by including in the optimization model the impacts of and treatment of BOD, nitrogen and phosphorus from municipal and industrial sites. As shown above, the effects of the pollutants from all of the sources on a given monitoring site cannot be accurately separated. The impact of each polluter's emissions on DO levels is dependent on the effluent activities of the others.

The principal form of the optimization model minimizes the combined annualized cost (C, in dollars per year) of wastewater load abatement (A, in kg pollutant / day) of biological oxygen demand (BOD), ammonium nitrogen (N), and dissolved phosphorus (P) at each of the emitting sites so that ambient quality standards are maintained. The decision variables are the percentage abatements (X) of each of the pollutants at each of the polluting sites. These values are simpler than abatement quantities for exposition and comparison. Cost also depends on the effluent flow requiring treatment (Q, in cubic meters per year). Q is considered fixed for this model. The objective is then:

$$\underset{X_{11},\ldots X_{mp}}{\text{Minimize}} \sum_{i=1}^{m}\sum_{k=1}^{p} C_{ik}\,(A_{ik}\,(X_{ik}), Q_i) \qquad (15)$$

The model is constrained to meet chosen ambient quality standards (AQS, in mg O / liter) for each downstream monitoring point. The use of ambient quality standards means that downstream damages are not included in the model endogenously. Rather, ambient quality levels below the standard are considered arbitrarily to allow "too much" damage, indicating that the amount of damage occurring at the AQS levels is "just right." The use of these values should properly be replaced by damage functions.

Ambient quality (AQ, in mg O / liter) is measured by the dissolved oxygen concentration. AQ at each monitoring point is calculated by equation (13) as developed in the section above. Each pollutant load depends on the percentage abatement chosen, and may be expressed as a maximum (unabated) pollution load minus abatement $(\bar{E}_{ik} - A_{ik}\,(X_{ik}))$. The constraining equations are then:

$$AQ_j = AQB_j - \sum_{i=1}^{m}\sum_{k=1}^{p}(J_{ijk}\,(\mathbf{X}_{mp})\cdot(\bar{E}_{ik} - A_{ik}\,(X_{ik}))) \geq AQS_j \text{ for all monitoring points } j = 1 \text{ to } n \qquad (16)$$

As discussed above, the Jacobian matrix is dependent on all of the pollution loads, represented by the matrix of pollutant percentage abatements (**X)**.

It is also possible to constrain the input loads directly, as is considered under nutrient reduction targets policies. This allows useful comparisons with such policy options.

$$E_{ik} \leq \tilde{E}_{ik} \text{ for all emitting sites } i \text{ and pollutants } k \qquad (17)$$

Annualized costs include both construction and maintenance[4]. The cost functions are assumed to be quadratic and continuous[5], to vary among sites and pollutants, and are based (in the Nitra River Basin study) on engineering estimates for each site. Load abatement (A) and percentage abatement (X) are also assumed to be continuous over the relevant ranges.

4. Solution Method

The method used to solve the optimization problem and constraints is an iterative procedure based on local numerical linearized estimates of the elements of the Jacobian matrix. For any chosen starting level of pollution emissions from each of the sites, the simulation model calculates the elements of the Jacobian matrix valid for that emission matrix. A solution set of pollution abatement levels is then found by the optimization model. If the solution set is not identical to the initial level of pollution emissions, however (as is likely on the first iteration), then the Jacobian parameters that created the solution are no longer valid. The relative impacts of each of the pollutant emissions has changed by moving to the first solution. The Jacobian matrix must then be recalculated. Accordingly, the first solution is returned to the simulation model for reevaluation of the Jacobian, which in turn is used to create a second solution matrix. The iterative procedure continues until the solution returned by the solver is identical[6] to the previous solution; that is, the Jacobian elements are confirmed as valid. Figure 4 illustrates how the calculation of the Jacobian matrix changes as the solver creates each new possible abatement solution set.

5. Two Polluter, One Monitoring Point, Three Pollutant Model Hypothetical Illustration

An initial demonstration of the model illustrates how the presence of multiple, interactive pollutants affects water quality and the relative impacts of emissions. Figure 5 illustrates the hypothetical Fluss River case. Two industrial sites, Mature Manure (MM) and Lovely Laundry (LL), discharge pollution. Three pollutants enter the river: BOD, dissolved phosphorus (P) and ammonia nitrogen (N) (each in kg / yr). Water quality (mg O / liter) is measured downstream at the Wave Quake monitoring point (WQ). When no discharges enter the river, the DO level is known to be 9.0 at this point.

MM discharges a load per year that consists of 10 BOD, 1 P, and 20 N. If MM were the only emitter, there would be an excess of nitrogen. Phosphorus would be the limiting agent in the production of algae in the river. If MM added more nitrogen, the impact on the DO level at WQ point would be minimal. This is reflected in the small Jacobian element ($J_{MM(N)}$) for MM with respect to pollutant N. Conversely, if MM added more phosphorus, this would have a large impact on the downstream DO level, because the phosphorus load is so small. This is reflected in the large $J_{MM(P)}$ for MM with respect to pollutant P. The same logic applies for the phosphorus dominated wasteload of site LL.

If the quality impacts of the two dischargers were independent, the total DO reduction could be found by simply adding the independent impacts $\sum_k (J_{MM(k)} \cdot E_{MM(k)} + J_{LL(k)} \cdot E_{LL(k)})$. The DO level would be reduced to 3.75 (Table 1).

Table 1 Water Quality in Fluss River: Independent Loads

	Mature Manure			Lovely Laundry		
	BOD	P	N	BOD	P	N
Pollutant load (E)	10	1	20	10	18	2
Marginal impact (J)	0.15	0.25	0.02	0.18	0.05	0.20
DO Reduction (J E)	-1.5	-0.25	-0.4	-1.8	-0.9	-0.4
DO Level	9.0 - 1.5 - 0.25 - 0.4 - 1.8 - 0.9 - 0.4 = **3.75**					

[4] A treatment plant effective life span of 40 years and a discount rate of 10 percent (applied to maintenance costs) are assumed.
[5] This assumption oversimplifies the discrete nature of treatment technologies and will be the subject of future work.
[6] More accurately, until the solution changes to a degree that is within acceptable tolerance.

The effects must be considered jointly, however, because the nitrogen and phosphorus pollution loads from the two dischargers interact. The Jacobian matrix is affected by this interaction. Much of the excess nitrogen from MM combines with much of the excess phosphorus from LL. The relative impact of extra nitrogen from MM ($J_{MM(N)}$) is increased, because the former N excess has been largely used in algae production. The relative impact of extra phosphorus from MM ($J_{MM(P)}$) decreases, because LL has discharged a lot of phosphorus, meaning that phosphorus is much less limiting (if at all) in the production of algae. The Jacobian elements for LL adjust by the same logic at the same time.

The DO reduction including the interactive effects is still found by adding the impacts $\sum_k (J_{MM(k)}(\mathbf{X}) \cdot E_{MM(k)} + J_{LL(k)}(\mathbf{X}) \cdot E_{LL(k)})$. The only difference is that the pollutant interactions cause the Jacobian elements to change. When interactive impacts are included, the DO level is reduced to 1.36, which is much lower than the hypothetical DO level that would result if no interaction occurred (Table 2).

Table 2 Water Quality in Fluss River: Interactive Loads

	Mature Manure			Lovely Laundry		
	BOD	P	N	BOD	P	N
Pollutant load (E)	10	1	20	10	18	2
Marginal impact (J)	0.15	0.08	0.11	0.18	0.10	0.13
DO Reduction (J E)	-1.5	-0.08	-2.2	-1.8	-1.8	-0.26
DO Level	9.0 - 1.5 - 0.08 - 2.2 - 1.8 - 1.8 - 0.26 = **1.36**					

A least cost problem is solved in three different ways in order to demonstrate the need for the variable Jacobian approach. The three approaches are (1) only BOD abatement is considered; (2) abatement of BOD, P and N is considered, using only the fixed Jacobian matrix, that is, the Jacobian matrix that corresponds to the initial wasteloads, with no abatement in place; and (3) abatement of BOD, P and N is considered, using an iterative procedure with a variable Jacobian matrix to achieve a result with locally precise parameters.

Cost curves are necessary to determine how much abatement of each pollutant will cost at each of the discharging plants (Table 3). The ratio of costs between the pollutants is roughly based on actual wastewater treatment technologies. Total costs at each site are the sum of the costs of abating each pollutant.

Table 3 Discharger Treatment Cost Curves

Pollutant	Mature Manure	Lovely Laundry
BOD	$C_{MM(B)} = 0.6 * X_{MM(B)}^2$	$C_{LL(B)} = 0.45 * X_{LL(B)}^2$
Phosphorus	$C_{MM(P)} = 1.8 * X_{MM(P)}^2$	$C_{LL(P)} = 1.35 * X_{LL(P)}^2$
Nitrogen	$C_{MM(N)} = 3.0 * X_{MM(N)}^2$	$C_{LL(N)} = 2.25 * X_{LL(N)}^2$

A solution allowing only BOD abatement is valuable because such an approach is often advocated and used, particularly in the literature, due to the difficulty of solving multiple pollutant models. Solving this problem and comparing it with multiple pollutant abatement solutions will provide insight concerning the degree of inefficiency that the single pollutant solution creates.

The Jacobian matrix used includes elements for each of the pollutants, because exclusion of P and N from the matrix would not properly capture all DO impacts. Only abatement of BOD is considered in the first example, however, irrespective of the marginal costs of abatement of P and N.

In the first approach, the model chooses BOD pollution percentage abatement levels (X) at the two sites in order to minimize treatment cost, subject to a certain DO concentration being met.

$$\text{Minimize Cost} = 0.6 * X_{MM(B)}^2 + 0.45 * X_{LL(B)}^2 \tag{18}$$

$$\text{subject to DO} = 9.0 - (0.15 * E_{MM(B)}) - (0.08 * 1) - (0.11 * 20) - (0.18 * E_{LL(B)}) - (0.10 * 18) - (0.13 * 2) > 4.5$$

Note that the abatement levels of phosphorus and nitrogen are fixed at zero by construction, and therefore are excluded as decision variables. Abatement enters the constraint by determining the emission level linearly, according to $E = (\bar{E} - (X * \bar{E}))$, where $\bar{E}$ is the maximum (unabated) emission level. The solution pollution abatement levels are 89.3 percent for MM and 100 percent for LL, at a total cost of $ 9288. With this solution, the dissolved oxygen level improves to the required level, but only by removing all of the BOD emitted as effluent by site LL and nearly all of the BOD emitted by site MM.

The second approach considers pollution abatement for all three pollutants (B, P and N) in solving the same least cost problem.

$$\begin{aligned}\text{Minimize Cost} = {} & 0.6 * X_{MM(B)}^2 + 1.8 * X_{MM(P)}^2 + 3.0 * X_{MM(N)}^2 \\ & + 0.45 * X_{LL(B)}^2 + 1.35 * X_{LL(P)}^2 + 2.25 * X_{LL(N)}^2\end{aligned} \tag{19}$$

$$\begin{aligned}\text{subject to DO} = {} & 9.0 - (0.15 * E_{MM(B)}) - (0.08 * E_{MM(P)}) - (0.11 * E_{MM(N)}) \\ & - (0.18 * E_{LL(B)}) - (0.10 * E_{LL(P)}) - (0.13 * E_{LL(N)}) > 4.5\end{aligned}$$

The same Jacobian matrix is used. Note that this Jacobian is correct <u>only</u> when no abatement of P or N occurs at either discharger. If P or N abatement occurs, the Jacobian matrix will change. Here, the possibility is considered that the fixed Jacobian provides an adequate approximate solution. The solution pollution abatement levels for MM are 52.3, 0.9, and 15.4 percent for BOD, P, and N respectively, and are 83.8, 27.9, and 2.4 percent for LL. The total cost is $ 6574. The multiple pollutant fixed Jacobian solution is less costly than the first approach of BOD-only treatment, because lower cost improvements to water quality are chosen in the second approach through abating P and N. These improvements were not considered in the first approach.

The third approach solves the same least cost problem using an iterative procedure that adjusts the Jacobian matrix values.

$$\begin{aligned}\text{Minimize Cost} = {} & 0.6 * X_{MM(B)}^2 + 1.8 * X_{MM(P)}^2 + 3.0 * X_{MM(N)}^2 \\ & + 0.45 * X_{LL(B)}^2 + 1.35 * X_{LL(P)}^2 + 2.25 * X_{LL(N)}^2\end{aligned} \tag{20}$$

$$\begin{aligned}\text{subject to DO} = {} & 9.0 - (J_{MM(B)}(\mathbf{X}) * E_{MM(B)}) - (J_{MM(P)}(\mathbf{X}) * E_{MM(P)}) \\ & - (J_{MM(N)}(\mathbf{X}) * E_{MM(N)}) - (J_{LL(B)}(\mathbf{X}) * E_{LL(B)}) \\ & - (J_{LL(P)}(\mathbf{X}) * E_{LL(P)}) - (J_{LL(N)}(\mathbf{X}) * E_{LL(N)}) > 4.5\end{aligned}$$

The Jacobian matrix values are now variable. The initial Jacobian matrix values used correspond to no abatement (that is, the values used in the previous approach). Using these values, the constraint is:

$$\begin{aligned}\text{subject to DO} = {} & 9.0 - (0.15 * E_{MM(B)}) - (0.08 * E_{MM(P)}) - (0.11 * E_{MM(N)}) \\ & - (0.18 * E_{LL(B)}) - (0.10 * E_{LL(P)}) - (0.13 * E_{LL(N)}) > 4.5\end{aligned} \tag{21}$$

The solution provided using the initial Jacobian matrix is given above. However, at this solution set, the Jacobian is no longer correct. It is necessary to determine new, corrected Jacobian values corresponding to the first solution abatement set. These are provided by the water quality model.

Abatement of phosphorus by LL reduces the amount of phosphorus in the river, therefore decreasing the downstream impact of extra nitrogen from MM ($J_{MM(N)}$) to 0.08. In the same way, reductions in nitrogen emissions from MM decrease the downstream impact of extra phosphorus from LL ($J_{LL(P)}$) to 0.09. At these new Jacobian values, the old solution set is no longer optimal, because the impacts are lower than expected. The DO level is higher than the required standard, causing the total cost of abatement to be greater than necessary. The problem must be solved again using the new Jacobian matrix. The next iteration is then:

$$\text{Minimize Cost} = 0.6 * X_{MM(B)}^2 + 1.8 * X_{MM(P)}^2 + 3.0 * X_{MM(N)}^2 + 0.45 * X_{LL(B)}^2 + 1.35 * X_{LL(P)}^2 + 2.25 * X_{LL(N)}^2 \quad (22)$$

$$\text{subject to DO} = 9.0 - (J_{MM(B)}(\mathbf{X}) * E_{MM(B)}) - (J_{MM(P)}(\mathbf{X}) * E_{MM(P)}) - (J_{MM(N)}(\mathbf{X}) * E_{MM(N)}) - (J_{LL(B)}(\mathbf{X}) * E_{LL(B)}) - (J_{LL(P)}(\mathbf{X}) * E_{LL(P)}) - (J_{LL(N)}(\mathbf{X}) * E_{LL(N)}) > 4.5$$

The transfer coefficients have changed. Substituting the new values (in bold) the constraint becomes:

$$\text{subject to DO} = 9.0 - (0.15 * E_{MM(B)}) - (0.08 * E_{MM(P)}) - (\mathbf{0.08} * E_{MM(N)}) - (0.18 * E_{LL(B)}) - (\mathbf{0.09} * E_{LL(P)}) - (0.13 * E_{LL(N)}) > 4.5 \quad (23)$$

The second iteration solution abatement levels for MM are 42.8, 0.8, and 9.1 percent for BOD, P, and N respectively, and are 68.5, 20.6, and 2.0 for LL. The total cost is $ 4042.

The process of finding a solution, determining how this affects the transfer coefficients, and solving again continues until the transfer coefficients remain the same, which in turn means that the ambient quality and the total cost remain the same. Figure 6 shows the path of the transfer coefficients and solutions through each step as the process continues. As shown in Figure 6, the final solution abatement levels for MM for pollutants B, P and N are 46.1, 0.8, and 10.9 percent, respectively, and are 73.8, 23.1, and 2.1 percent for LL. The total cost is $4818.

A direct comparison of the three solutions (Figure 7) reveals that the BOD-only abatement solution costs 41 percent more than the fixed Jacobian matrix result, and 93 percent more than the correct, variable Jacobian solution. The fixed Jacobian solution approximation, in turn, costs 36 percent more than the variable Jacobian solution. These differences are significant. The assumption that BOD treatment alone is an adequate replacement for a multiple pollutant solution is poorly placed. Likewise, the assumption that the initial fixed estimate of the marginal impacts from multiple pollutant sources is an adequate approximation to the true, varying values of these impacts is shown to be inappropriate.

6. Application to the Nitra River Basin, Slovakia

The usefulness of the iterative model is demonstrated empirically using an actual case study of the Nitra River Basin in Slovakia. A comparison is made between solutions using a fixed Jacobian matrix and a variable Jacobian matrix. The solution procedure is shown to be robust to variation in initial parameter values.

The Nitra is a tributary of the Vah river, which in turn is a tributary of the Danube river, entering downstream of Bratislava, Slovakia. The catchment area is slightly more than 5000 square kilometers and has about 600,000 inhabitants. It is 171 kilometers in length and has a mean flow at the mouth of 25 cubic meters per second. The total amount of BOD discharged into the river system is greater than 10,000 metric tons per year. Municipal wastewater treatment plant effluent accounts for approximately 70 percent of this amount (Somlýody and Paulsen, 1992). Twelve monitoring points, sixteen effluent emitting sites and seven tributaries over 126 kilometers of river miles are incorporated. Particularly significant DO depletion occurs during low flow conditions, which may occur in late summer or autumn. Models were developed for January, April, August and October flow conditions, considering low, average and high flow conditions for each of these months. These scenarios allow comparative analysis of policy effects on the seasonal hydrologic cycle.

A comparison of two solutions is given in Table 4. The two approaches are (1) abatement of BOD, P and N is considered, using only the fixed Jacobian matrix, that is, the Jacobian matrix that corresponds to the initial wasteloads, with no abatement in place; and (2) abatement of BOD, P and N is considered, using an iterative procedure with a variable Jacobian matrix to achieve a result with locally precise parameters. Ten-year low flow October conditions are used (the year with the lowest monthly mean flow). October often has the lowest mean flow for the Nitra. Solutions are found for a range of imposed ambient quality standards. The difference between these solutions varies between 17 and 61 percent with the ambient quality standard imposed. Each of these differences indicates how much error is involved in the approximation provided by the fixed set of impact coefficients. It is obvious that these cost differences, which range from $185,000 to $41 million are very significant, particularly in a country with such limited resources as Slovakia.

Table 4 October Minimum Flow Least Cost Solutions (costs in $1000s)

Ambient Quality Standard (mg O/L)	Initial (Fixed Jacobian) Solution	Final (Variable Jacobian) Solution	Percentage Difference Between Solutions
2.6	765	950	19.5%
2.8	1781	2167	17.8%
3.0	3193	3828	16.6%
3.2	5331	13697	61.1%
3.4	20894	35124	40.5%
3.6	101067	141844	28.7%
3.8	140490	169584	17.2%
4.0	141270	170479	17.1%

What is wrong with the fixed Jacobian solution? It appears to provide an abatement solution that meets the chosen dissolved oxygen standards and to do so at a lower cost than the variable Jacobian solution that includes interactive effects of the pollutants. This fixed Jacobian estimated solution, however, does not produce the ambient quality results that it predicts. By using linear estimates of the coefficients, it overestimates the effectiveness of the chosen abatement set. Figure 8 contrasts the expected dissolved oxygen outcome with the actual outcome, as well as the variable Jacobian solution outcome. The actual fixed Jacobian outcome violates the chosen DO standard in two different reaches of the river, including the last 15 kilometers, in which the second largest city of the region is located. An appendix of site-specific abatement solutions for both the variable and fixed Jacobian cases is available from the author.

7. Robustness of Solution Procedure

Two issues are addressed. First, it is possible to have several more than one set of abatement solutions, each of which meets the ambient quality standards and costs the same. Second, it is possible concerning cost for multiple local optima to exist; that is, to have solutions that are only best in comparison with the other immediate choices (i.e., marginal changes), but not better than solutions that are significantly different. It is necessary to show that the least cost result of each problem is a unique result. This is shown by solving each problem from two extreme initial abatement sets: no abatement and full abatement.

In a textbook approach, iterative solutions are found by iterating until the choice variable is fixed within a chosen level of tolerance. The choice variable in this problem, however, is a matrix of percentage abatement values. Determining when this matrix becomes “fixed” is intractable. However, cost is the value that is actually of greater interest, and, as a single value, may be solved within a chosen tolerance. This, however, allows the possibility that more than one distinctly different set of percentage abatement values may fulfill the water quality standards at approximately the same cost. Such a possibility is not cause for concern, rather, simply evidence that multiple equilibria may exist, providing a number of options for policymakers. Although such multiple solution sets are possible, none were observed in the empirical solutions of this study.

It is possible to show analytically the certainty of a locally optimal solution to the least cost problem using a variable Jacobian matrix (available in an appendix from the author). However, many such local optima may exist. Therefore an empirical test of the robustness of the local solution is necessary in order to establish it empirically as a global optimum.

A simple method to test robustness is to solve the problem using extreme initial abatement conditions and to compare the results for convergence. The least cost problem is first solved using initial conditions of no abatement at all sites. The problem is then solved using opposite initial conditions of complete abatement at all sites. The correct total cost value is approached from below when the solution procedure begins using the existing situation, that is, zero abatement at all sites (accounting for preexisting treatment). Zero abatement has no cost. The early cost estimates therefore underestimate the correct cost. In contrast, the correct total cost value is approached from above when the solution procedure begins using full abatement at all sites. The early cost estimates in this case overestimate actual cost. This test was conducted for a range of ambient quality standards.

Figure 9 shows solutions for a 3.0 mg O / liter ambient quality standard for the October low flow case. Least cost solutions provided by each iteration are shown for two situations: beginning with no abatement, and beginning with full abatement. In this and all other scenarios and for each ambient quality standard, the solution cost values from above and below converge. Empirically, the cost solutions are shown to be unique.

The number of iterations necessary to converge on a cost solution varied considerably, ranging from one to ten iterations. Each iteration required approximately 1.5 minutes to solve at 66 MHz on a PC. This relatively rapid process indicates that the significant number of computations involved no longer seems to prohibit the use of such a method.

8. Summary

The simulation/optimization model presented determines the optimal percentage of pollution abatement of multiple pollutants from industrial and municipal sources that will meet downstream ambient quality constraints at the least cost. In order to do so, the marginal downstream effects of each of the pollutants from each source must be determined. These impacts depend on the actual pollution loads, due to the interdependent nature of algae production (and hence of oxygen production) by nitrogen and phosphorus. The impacts must then be recalculated for each possible solution set of pollution loads until an equilibrium solution is reached. A river water quality simulation model is called upon during each iteration to provide the matrix of these impacts, the Jacobian matrix, for each pollutant type and source.

The degree of error involved in treating the Jacobian matrix as fixed was demonstrated using both a hypothetical Fluss River example and an actual study of the Nitra River Basin in Slovakia. The results indicated the need for the iterative model, as the errors provided by fixed Jacobian approximation are very large. The robustness of the solving procedure was tested using the Nitra River Basin model by solving various least cost problems using opposite initial assumptions concerning abatement. It was shown that the values from the two procedures converged, empirically indicating the existence of a global optimum.

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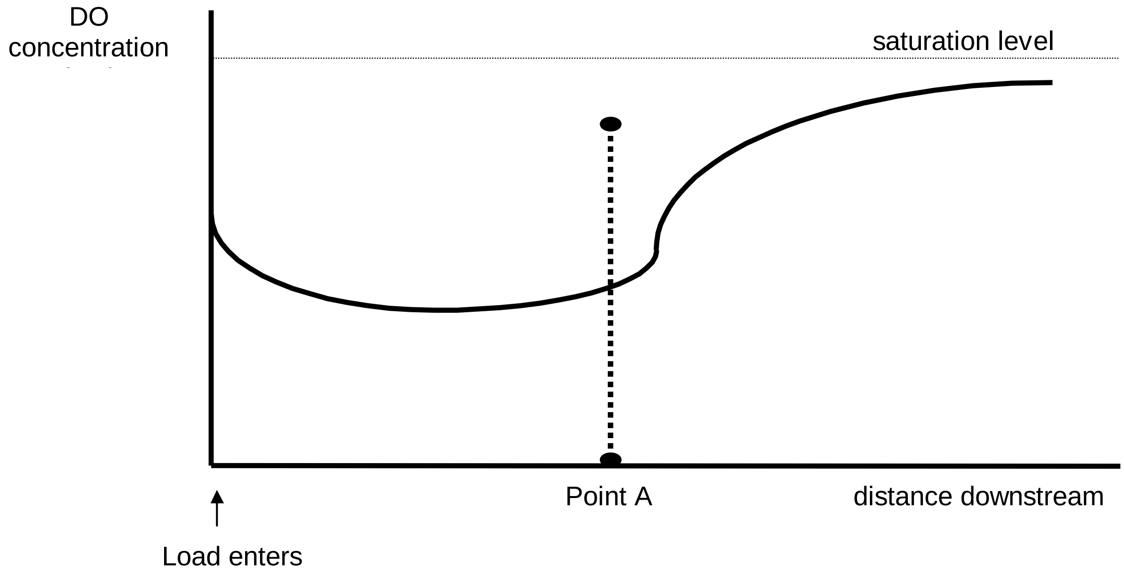


Figure 1 Dissolved Oxygen Sag

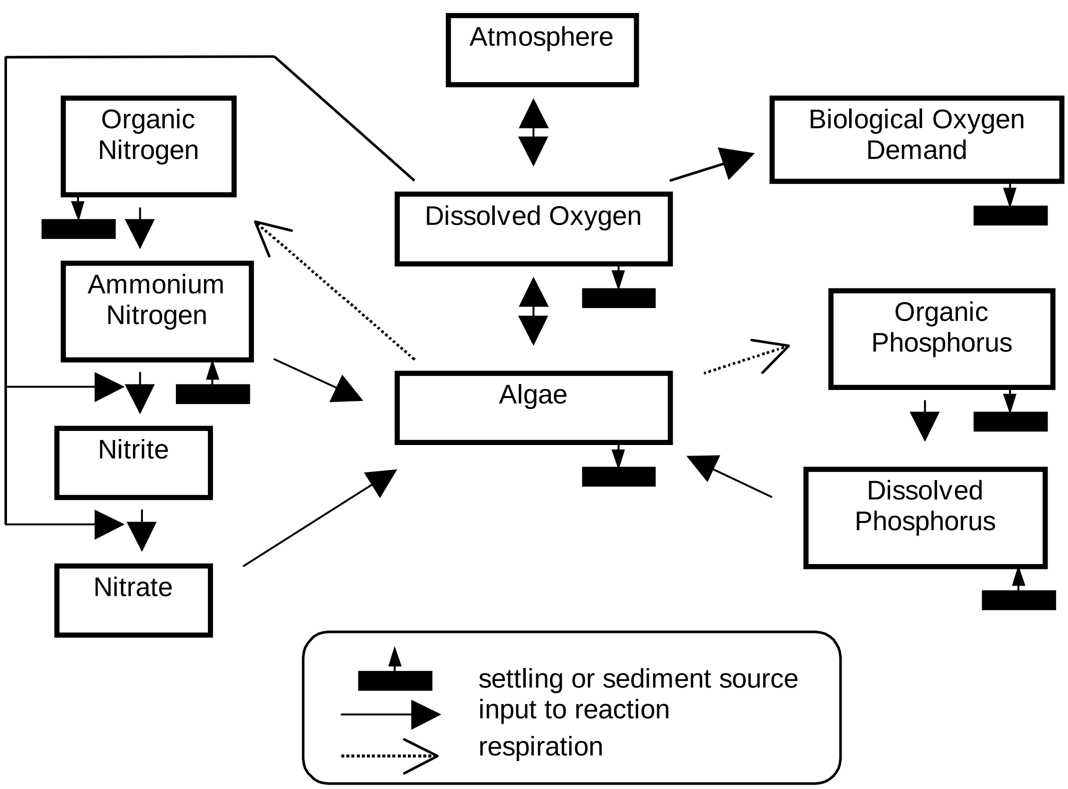


Figure 2 Multiple Pollutant Constituent Interactions Affecting Dissolved Oxygen Level

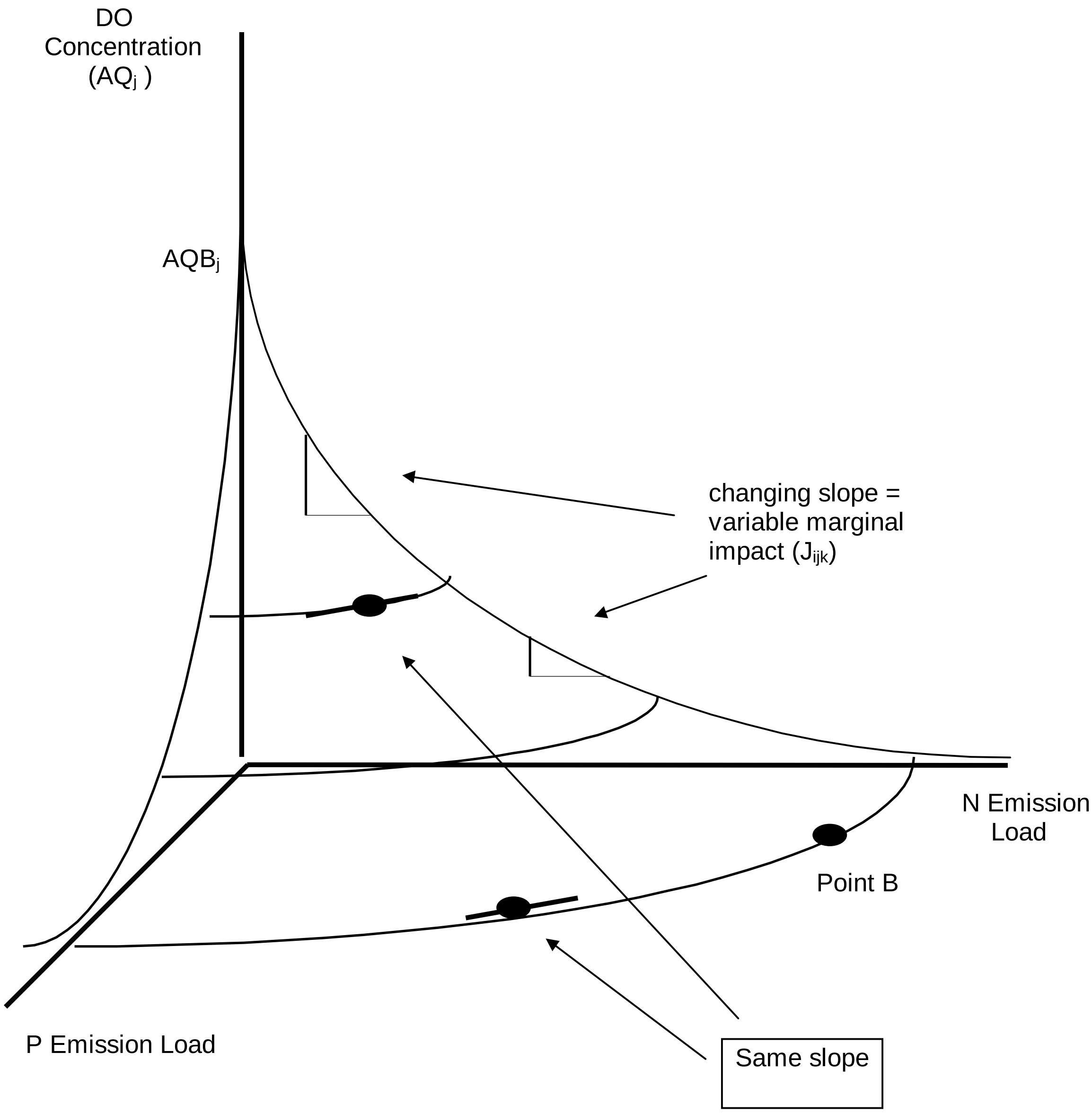
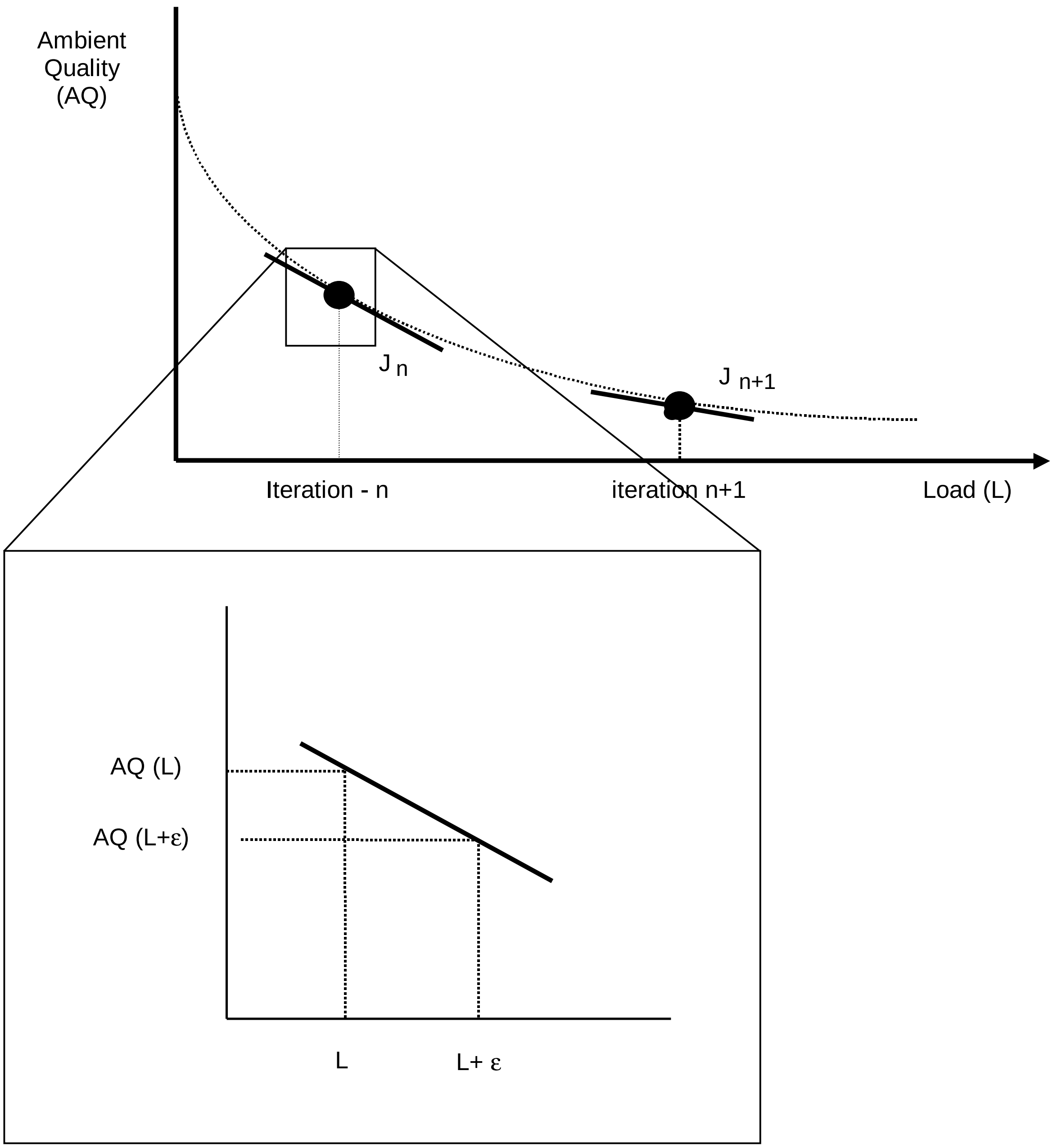


Figure 3 Non-Linear Relationship Between Nitrogen and Phosphorus Emissions and DO Level: One Emitter (*i*)



$$\mathbf{J} = \frac{\{\mathbf{AQ\ (L} + \varepsilon\mathbf{)\ -\ AQ\ (L)}\}}{\{\mathbf{(L} + \varepsilon\mathbf{)\ -\ (L)}\}}$$

$$\lim_{\varepsilon \to 0} \mathbf{J} = \frac{\partial\, \mathbf{AQ(L)}}{\partial\, \mathbf{L}}$$

Figure 4 Methodology Used to Calculate Jacobian Matrix

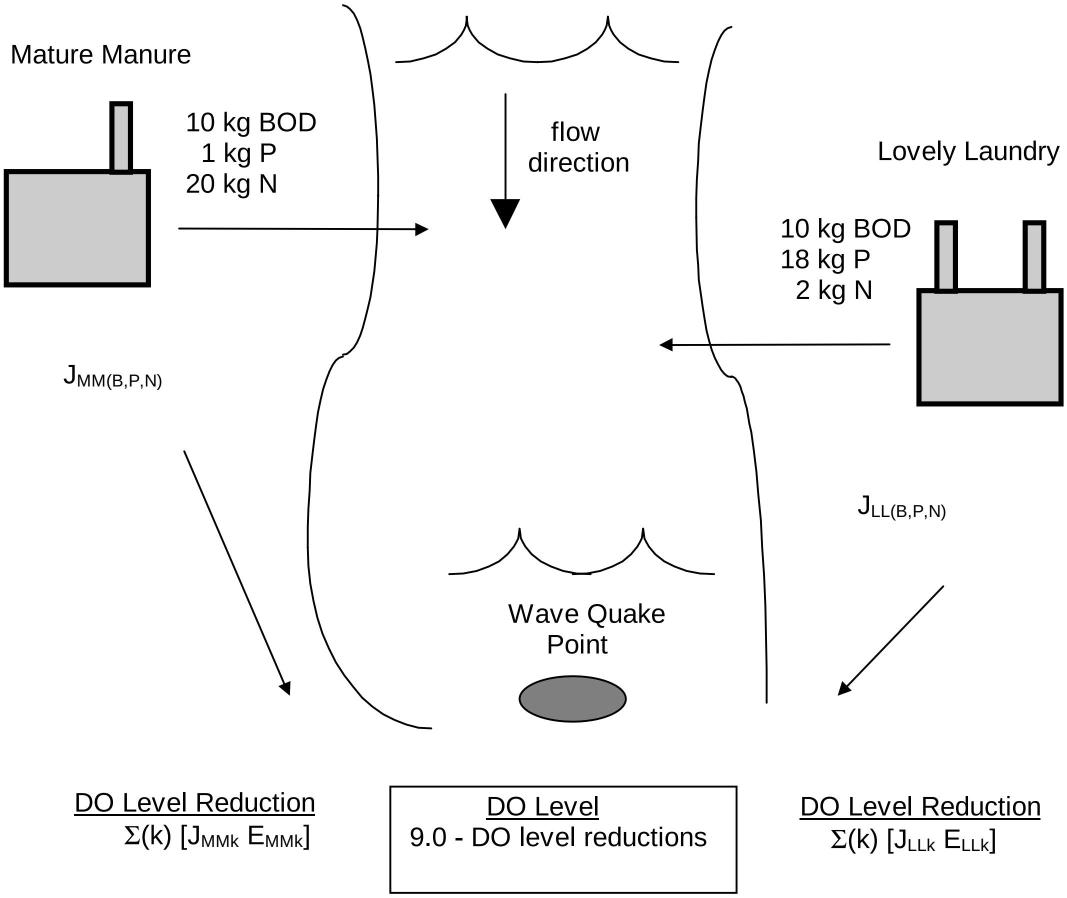


Figure 5 Water Quality in Hypothetical Fluss River Illustration

Initial Jacobian Matrix Values

$J_{MM}(B) = 0.15$ $J_{LL}(B) = 0.18$
$J_{MM}(P) = 0.08$ $J_{LL}(P) = 0.10$
$J_{MM}(N) = 0.11$ $J_{LL}(N) = 0.13$

1st Solution

$X_{MM}(B) = 52.3\%$ $X_{LL}(B) = 83.8\%$
$X_{MM}(P) = 0.9\%$ $X_{LL}(P) = 27.9\%$
$X_{MM}(N) = 15.4\%$ $X_{LL}(N) = 2.4\%$

Total Cost: $ 6574

1st Adjustment to Jacobian Matrix

$J_{MM}(B) = 0.15$ $J_{LL}(B) = 0.18$
$J_{MM}(P) = 0.08$ $J_{LL}(P) = \mathbf{0.09}$
$J_{MM}(N) = \mathbf{0.08}$ $J_{LL}(N) = 0.13$

AQ = 5.13 Overtreatment

2nd Solution

$X_{MM}(B) = 42.8\%$ $X_{LL}(B) = 68.5\%$
$X_{MM}(P) = 0.8\%$ $X_{LL}(P) = 20.6\%$
$X_{MM}(N) = 9.1\%$ $X_{LL}(N) = 2.0\%$

Total Cost: $ 4042

2nd Adjustment to Jacobian Matrix

$J_{MM}(B) = 0.15$ $J_{LL}(B) = 0.18$
$J_{MM}(P) = 0.08$ $J_{LL}(P) = \mathbf{0.095}$
$J_{MM}(N) = \mathbf{0.09}$ $J_{LL}(N) = 0.13$

AQ = 4.25 Undertreatment

3rd Solution

$X_{MM}(B) = 46.6\%$ $X_{LL}(B) = 74.5\%$
$X_{MM}(P) = 0.8\%$ $X_{LL}(P) = 23.6\%$
$X_{MM}(N) = 11.2\%$ $X_{LL}(N) = 2.2\%$

Total Cost: $ 4935

3rd Adjustment to Jacobian Matrix

$J_{MM}(B) = 0.15$ $J_{LL}(B) = 0.18$
$J_{MM}(P) = 0.08$ $J_{LL}(P) = \mathbf{0.094}$
$J_{MM}(N) = \mathbf{0.089}$ $J_{LL}(N) = 0.13$

AQ = 4.53 Overtreatment

4th Solution

$X_{MM}(B) = 46.1\%$ $X_{LL}(B) = 73.8\%$
$X_{MM}(P) = 0.8\%$ $X_{LL}(P) = 23.1\%$
$X_{MM}(N) = 10.9\%$ $X_{LL}(N) = 2.1\%$

Total Cost: $ 4818

No Further Adjustment to Jacobian Matrix

$J_{MM}(B) = 0.15$ $J_{LL}(B) = 0.18$
$J_{MM}(P) = 0.08$ $J_{LL}(P) = \mathbf{0.094}$
$J_{MM}(N) = \mathbf{0.089}$ $J_{LL}(N) = 0.13$

AQ = 4.50 Quality Standard Met

Figure 6 Iteration to Solution of Hypothetical Fluss River Problem

BOD-Only Abatement Solution	Fixed Jacobian Matrix Solution	Variable Jacobian Matrix Solution
$X_{MM}(B)$ = 89.3%	$X_{MM}(B)$ = 52.3%	$X_{MM}(B)$ = 46.1%
$X_{LL}(B)$ = 100%	$X_{LL}(B)$ = 83.8%	$X_{LL}(B)$ = 73.8%
$X_{MM}(P)$ = 0%	$X_{MM}(P)$ = 0.9%	$X_{MM}(P)$ = 0.8%
$X_{LL}(P)$ = 0%	$X_{LL}(P)$ = 27.9%	$X_{LL}(P)$ = 23.1%
$X_{MM}(N)$ = 0%	$X_{MM}(N)$ = 15.4%	$X_{MM}(N)$ = 10.9%
$X_{LL}(N)$ = 0%	$X_{LL}(N)$ = 2.4%	$X_{LL}(N)$ = 2.1%
Total Cost: $ 9288	Total Cost: $ 6574	Total Cost: $ 4818

Figure 7 Comparison of Different Solutions for Hypothetical Fluss River Problem

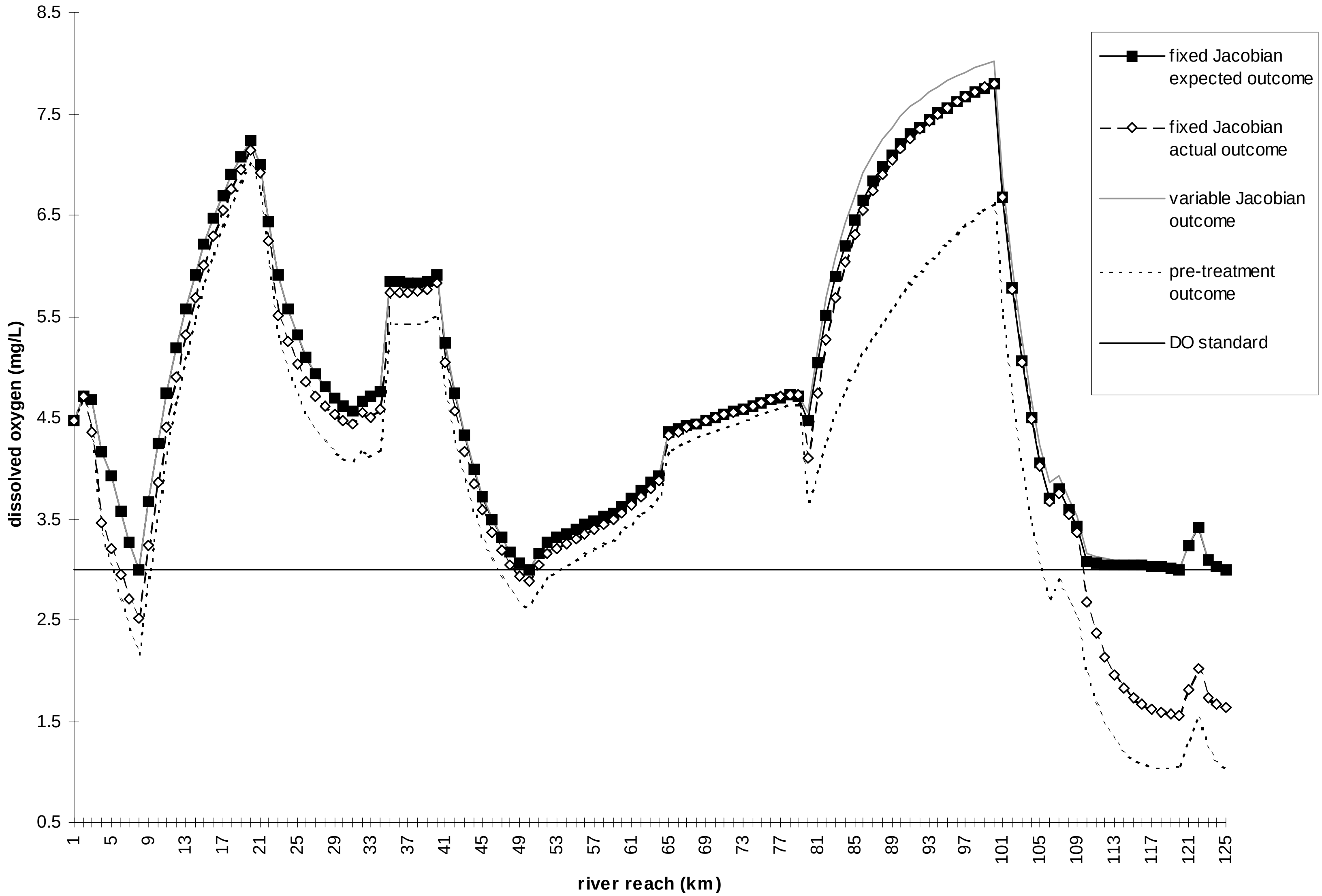


Figure 8 October Low Flow Iteration to Variable Jacobian Cost Solution (AQS = 3.0 ppm DO) : Nitra River Basin Model

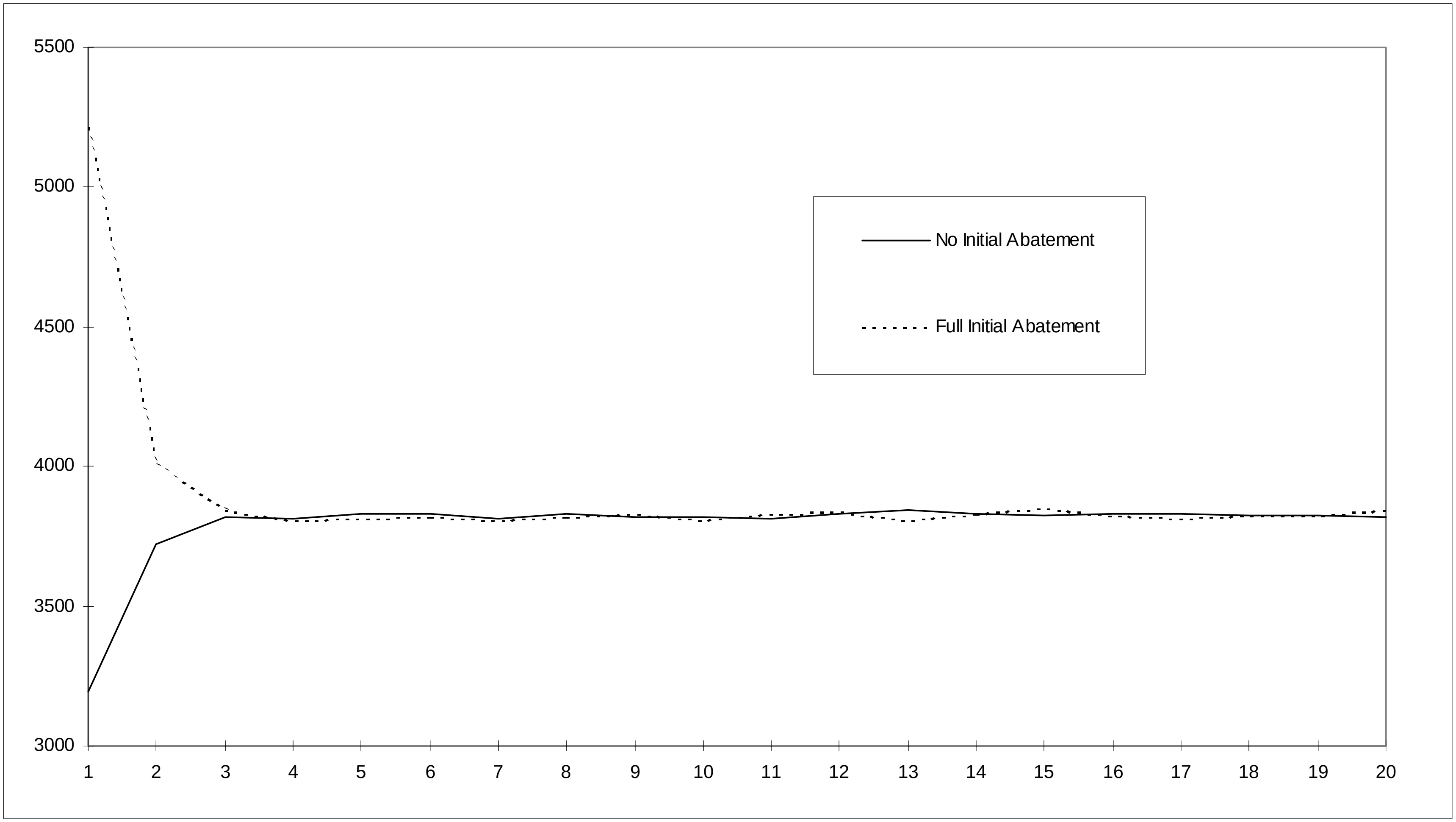


Figure 9 October Low Flow Iteration to Variable Jacobian Cost Solution (AQS = 3.0 ppm DO) : Nitra River Basin Model