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Optimal Sequencing in Installing Wastewater Treatment Plants[1]

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Abstract

If a set of wastewater treatment plants is to be installed in a river basin within a given time period, an interesting optimization problem is to select the best sequence in which the plants should be built. Two sequencing problems of this kind are discussed in this paper, and branch and bound algorithms are proposed for solving them. The validity of some simplifying assumptions and the effectiveness of the methods from a computational point of view are shown by analyzing the case of the Rhine river in The Federal Republic of Germany.

1. Introduction

A problem that has been extensively dealt with in the recent literature on river pollution is that of optimal design and allocation of wastewater treatment plants in a river basin. The criterion followed by most of the authors consists in minimizing the total cost of the plants that give rise to a tolerable stream quality index. The solution of this optimization problem, from now on called primary optimization problem, is represented by a set S of plants that, once installed, will entail a water quality that satisfies certain standards. The cost of such an

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optimal solution is usually so high that it takes a reasonably long time--i.e. several years--before all the plants are installed. For example, in the case of the Rhine river described in this paper the cost of the optimal solution amounts to approximately $15 billion which is about 20% of the annual budget of the Federal Government of the F.R.G.

Hence, after solving the primary optimization problem one is usually faced with the secondary optimization problem of determining the best sequence in which the plants must be built, i.e. the sequence $\{s_t\}_{t=1}^{N}$, where s_t is the set of plants activated in year t (so that $s_{t_1} \cap s_{t_2} = \emptyset$ (empty set) if $t_1 \neq t_2$ and $\bigcup_{t=1}^{N} s_t = S$) and N is the number of years within which all plants are to be installed. The economic constraint that actually generates this sequencing problem can be specified in different ways. The most realistic one seems to be the uniform distribution of the investment over the N years. In other words, if the cost of the plants we are to install within N years is C, then the amount of money C_t we are allowed to spend during the first t years ($t = 1,2,\ldots,N$) must be less than or equal to Ct/N. An interesting feature of this rule is that the decisions taken in the first t years (i.e. the set of plants that have been activated during the first t years) influence future budgets, because the money available in year (t + 1) is $C(t + 1)/N - C_t$, which is, in general, more than the average budget C/N because of past savings. This is the main characteristic that differentiates this problem from those which have been dealt with in the literature (Deininger, 1965; Revelle et al., 1969).

In order to specify the objective function for the sequencing problem we must first define a water quality index by means of which we can determine, for any subset $S_t \subset S$ of the plants installed up to the year t, the associated pollution index P_t of the river basin. The initial (year 0) and final (year N) values of the pollution index are given, since $S_0 = \emptyset$ (empty set) and $S_N = S$ for any sequence $\{s_t\}_{t=1}^{N}$. Moreover, the pollution index P_t will in most cases be a strictly decreasing function of time, since the implementation of any subset of plants will, in general, better the conditions of the river basin. Given a pollution index, there are still many options in defining the optimization criterion; two of these seem to be of particular interest in the problem under consideration and will therefore be dealt with in this paper. The first one consists in activating each year that subset s_t of plants which gives rise to the greatest improvement, i.e. to the minimum value of the pollution index P_t. This "myopic" criterion has been extensively used in the past, in particular in control problems (e.g. minimum time control) and in mathematical programming problems (e.g. steepest descent method), and usually entails less computational effort than any alternative scheme. The second criterion, certainly more rational than the myopic one, consists in determining that sequence $\{s_t\}_{t=1}^{N}$ which minimizes the sum of the pollution indices over all years ($\sum_{t=1}^{N} P_t = \min$). Because of the saving effect described above, this sequencing problem turns out to be an optimal control problem of a dynamic system and the algorithm for its solution will therefore be quite sophisticated and time-consuming.

As far as the pollution index is concerned, following Liebman (see Kneese and Bower, 1971, pp. 94-5), we use "the total oxygen deficit in the river basin", as opposed to other indices that are related to the stream standards, such as "the mileage out of standards" (Deininger, 1965) or "the maximum deviation from the stream standards" (Revelle et al., 1969). There are two a priori reasons that justify this choice. First, this index takes into account the global situation of the basin, since each point of the river gives its contribution to the total deficit; by contrast, the maximum deviation from the stream standards is a more pointwise measure. Second, Liebman's index enjoys some remarkable properties (see next section) that make it quite attractive from a conceptual point of view and permit reasonably efficient algorithms to be devised for solving the sequencing problem.

2. The Oxygen Deficit as a Pollution Index

The problem of defining a pollution index for a river basin is certainly not a new one and many suggestions can in fact be found in the literature. The formulation of such an index can be done in two steps. First we define a water quality measure and then we suitably integrate this measure over the entire river basin. The first step is without doubt the more difficult one to accomplish, since the water quality measure should take into account the composite influence of significant physical and chemical parameters and the different uses of the water. Unfortunately, the soundest proposals known to the authors are so complex and detailed that they cannot be used for solving problems of the kind considered here, since they would require the use of models far more sophisticated than those that have so far been validated. For example, the water quality index described by R.M. Brown et al. (1972) takes into account the following eleven parameters: dissolved oxygen, fecal coliforms, pH, 5-day BOD, nitrate, phosphate, temperature, turbidity, total solids, toxic elements, pesticides; and there is no model that can predict all these variables at one time. Therefore, we are forced to select so compact a measure of water quality that any standard river quality model allows the computation of this measure. Fortunately, we do not have significant alternatives in making this choice since all reasonable measures of water quality have in common only one parameter, namely the dissolved oxygen concentration.

For these reasons the pollution index we propose is the total amount of oxygen missing in the river basin with respect to the ideal conditions of fully saturated water, i.e.

$$P = \int_{L} A(x)D(x)dx \quad , \tag{1}$$

where L is the set of spatial coordinates defining the river basin and A(x) and D(x) are, respectively, the cross-sectional area and the oxygen deficit at point x. The index P is in general time-varying, but in the following only the stationary case will be dealt with; this turns out to be justified if we assume low flow conditions.

We will now prove that under suitable assumptions the pollution index P satisfies a very important property that we call "additivity property". For this, let us first define the improvement $Q(X)$ of the index P due to the presence of a set X of wastewater treatment plants, i.e. write

$$P(X) = P_0 - Q(X) \quad , \tag{2}$$

where P_0 is the initial value of the pollution index $(Q(\emptyset) = 0)$. Now "additivity" means that the improvement due to two disjoint sets of plants A and B is the sum of the two single improvements, i.e.

$$Q(A \cup B) = Q(A) + Q(B) \quad . \tag{3}$$

Thus, the pollution index (2) can be rewritten in the form

$$P(X) = P_0 - \sum_{i \varepsilon X} q_i \quad , \tag{4}$$

where q_i is the contribution of the i-th plant to the total improvement $Q(X)$. In other words, each plant contributes separately and in an additive way to the pollution index; this is indeed a very important feature because it allows us to characterize a plant with two positive numbers, namely the cost c_i and the "quality indicator" q_i. Thus, the efficiency of the i-th plant expressed in mg of oxygen per dollar can be defined as

$$\eta_i = q_i/c_i \tag{5}$$

and will be shown to play an important role in the solution of the problem.

Different proofs of eq. (4) can be given, depending upon the kind of model and upon the spatial variability of the parameters involved in it. The simplest case is that of a basin constituted by a uniform and semiinfinite $(x \geqslant 0)$ channel in which the integral of the distributed load along the river is finite, so that all significant variables describing the system go to zero for $x \to \infty$ because of self-purification. In fact, let us first assume that the river is described by the well known Streeter-Phelps model (Streeter and Phelps, 1925):

$$\frac{dB(x)}{dx} = -k_1B(x) + U(x) + \sum_i (U_i - u_i)\,\delta(x - x_i), \tag{6a}$$

$$\frac{dD(x)}{dx} = k_1B(x) - k_2D(x), \tag{6b}$$

where $B(x)$ stands for biological oxygen demand (BOD), $U(x)$ is the BOD load distributed along the river, U_i is the BOD load of the i-th plant, u_i is the amount of BOD removed by that plant, x_i is the spatial coordinate of the plant, δ is the impulse function and k_1 and k_2 are suitable constant parameters. Since eqs. (6) are linear, their solution depends linearly on the boundary conditions $B(0)$ and $D(0)$ and on the amount u_i of BOD removed by each plant. Moreover, the integral of $D(x)$ is finite since the integral of $U(x)$ is finite, so that the pollution index $P(X)$ is well defined and is a linear functional of the deficit $D(x)$. Therefore eq. (4) a priori follows, with

$$q_i = Ku_i, \tag{7}$$

since a given amount of BOD removed will have an effect on the index $P(X)$ that is independent of the location x_i of the treatment plant (i.e., K is independent of i in eq. (7)).

Let us now prove that this result holds for the case in which the river is described by a higher-order nonlinear model of the kind

$$\frac{dW(x)}{dx} = -f(W(x), D(x)) + U(x) + \sum_i (U_i - u_i)\,\delta(x - x_i), \tag{8a}$$

$$\frac{dD(x)}{dx} = \alpha^T f(W(x), D(x)) - k_2D(x), \tag{8b}$$

where $W(x)$ can be looked upon as a suitable m-th order vector describing the various stages in the degradation of the organic pollutants, f, U(x), U_i and u_i are m-th order vectors and α^T is an m-th order row vector of conversion factors. In fact, solving eq. (8a) with respect to f and substituting in eq. (8b), one obtains

$$D = \frac{1}{k_2} \left[- \alpha^T \frac{dW}{dx} - \frac{dD}{dx} + \alpha^T U + \alpha^T \sum_i (U_i - u_i) \; \delta(x - x_i) \right] ,$$

from which

$$P(X) = A\int_0^\infty D(x)dx = \frac{A}{k_2} \left[\alpha^T W(0) + D(0) - \lim_{x\to\infty} \alpha^T W(x) - \lim_{x\to\infty} D(x) \right. \tag{9}$$

$$\left. + \alpha^T \int_0^\infty U(x)dx + \alpha^T \sum_{i\varepsilon X} U_i - \alpha^T \sum_{i\varepsilon X} u_i \right]$$

follows.

If we confine ourselves to the biochemical degradation processes, the two limits in the preceding expression are zero under the assumption that the integral of U(x) is finite; the final formula for $P(X)$ is then

$$P(X) = \frac{A}{k_2} \left[\alpha^T W(0) + D(0) + \alpha^T \int_0^\infty U(x)dx + \alpha^T \sum_{i\varepsilon X} U_i - \alpha^T \sum_{i\varepsilon X} u_i \right] , \tag{10}$$

which is of kind (4) with

$$q_i = \frac{A}{k_2} \alpha^T u_i \quad .$$

The structure of model (8) is so general that it contains as particular cases all models known to the authors; therefore, the next thing we have to do is to relax the assumptions of the channel being infinite and uniform. Thus, suppose that the river is described by a linear model of the kind

$$\frac{dz(x)}{dx} = F(x)z(x) + G(x) \left[U(x) + \sum_i (U_i - u_i) \; \delta(x - x_i)\right], \tag{11}$$

where $z(x)$ is an m-th order vector, $F(x)$ and $G(x)$ are matrices of suitable order and $0 \leq x \leq L$. Since the deficit $D(x)$ is certainly one of the components (for example the last one) of the vector $z(x)$ we can, for the sake of simplicity in notation, introduce a row vector h^T such that

$$A(x)D(x) = h^T(x)z(x),$$

where

$$h^T(x) = |00 \ldots A(x)| \quad . \tag{12}$$

For example, for the Streeter-Phelps model (6) with k_1 and k_2 dependent on x, we have

$$z(x) = \begin{bmatrix} B(x) \\ D(x) \end{bmatrix}, \qquad F(x) = \begin{bmatrix} -k_1(x) & 0 \\ k_1(x) & -k_2(x) \end{bmatrix},$$

$$G(x) = \begin{bmatrix} 1 \\ 0 \end{bmatrix}, \qquad h^T(x) = \begin{bmatrix} 0 & A(x) \end{bmatrix} .$$

Integrating eq.(11) we obtain

$$z(x) = \Phi(x,0)z(o) + \int_0^x \Phi(x,\xi)G(\xi)\left[U(\xi) + \sum_i(U_i - u_i)\delta(\xi - x_i)\right]d\xi$$

$$= \Phi(x,0)z(0) + \int_0^x \Phi(x,\xi)G(\xi)U(\xi)d\xi + \sum_i \Phi(x,x_i)G(x_i)U_i -$$

$$- \sum_i \Phi(x,x_i)G(x_i)u_i \quad ,$$

where the $m \times m$ matrix $\Phi(x,\xi)$ is the well-known transition matrix of linear systems (Zadeh and Desoer, 1963). From eqs. (1) and (12) we obtain

$$P(X) = \int_0^L h^T(x)\Phi(x,0)z(0)dx + \int_0^L h^T(x) \int_0^x \Phi(x,\xi)G(\xi)U(\xi)d\xi dx$$

$$+ \sum_i \int_0^L h^T(x)\Phi(x,x_i)dxG(x_i)U_i - \sum_i \int_0^L h^T(x)\Phi(x,x_i)dxG(x_i)u_i \quad ,$$

which is of the form (4) with

$$q_i = \int_0^L h^T(x)\Phi(x,x_i)dxG(x_i)u_i \quad . \tag{13}$$

Expression (13) for the quality indicator q_i shows that even in the case in which u_i is a scalar, the coefficient q_i/u_i is, in general, dependent upon i, and this turns out to be true also for uniform but finite channels. In other words, in a uniform river two plants characterized by the same BOD removal give rise to the same improvement of the pollution index only if they are located sufficiently far upstream. This fact explains why the total biodegradable load proposed by Deininger (1965) as a pollution index for the river basin differs from Liebman's index (1), even in the simple case of a uniform finite channel described by a Streeter-Phelps model. Finally, it is worth while noticing that eq. (4) holds also for the cases in which some of the plants are located on tributaries of the main river (this result follows immediately from the linearity of the model).

In summary, we have proved that the additivity property (4) holds for linear models under very general conditions, while for nonlinear models we can say only that there is a tendency for this property to be satisfied if the river basin is approximately uniform and if the amount of biodegradable matter going out of the river basin is small enough. An example of the validity of the additivity property for a nonlinear model is given in Section 5.

3. The Myopic Sequencing Problem

As described in the introduction, a solution of the sequencing problem is given by an ordered partition of the set S of the plants into N blocks (years), i.e. by a sequence $\{s_t\}_{t=1}^{N}$ with

$$s_i \cap s_j = \emptyset \qquad \text{if } i \neq j \ ,$$

$$\bigcup_{t=1}^{N} s_t = S \ .$$

If C(*A*) is the cost of a subset *A* of the plants ($C(A) = \sum_{i \in A} c_i$) and C is the cost of all plants (C = C(*S*)), then a sequence $\{s_t\}_{t=1}^{N}$ is said to be feasible if it satisfies the following budget constraints:

$$C(s_1) \leqslant C/N \ ,$$

$$C(s_2) \leqslant C/N + (C/N - C(s_1)) \ ,$$

$$C(s_3) \leqslant C/N + (2C/N - C(s_1) - C(s_2)) \ ,$$

$$\vdots$$

$$C(s_N) \leqslant C/N + ((N-1)C/N - \sum_{i=1}^{N-1} C(s_i)) \ ;$$

or, equivalently, a sequence is feasible if

$$C(S_t) \leqslant Ct/N \ , \qquad t = 1,2,\ldots,N \ , \tag{14}$$

where

$$S_t = \bigcup_{i=1}^{t} s_i \ .$$

The myopic sequencing problem can now be formulated as follows: <u>for each year t(t = 1,2,...,N) find the subset $s_t \subset S - S_{t-1}$ such that the pollution index $P(S_t)$ is minimized while the budget constraints (14) are satisfied.</u>

This problem would in general be very difficult to solve without making use of the additivity property described in the preceding section. Using this property, the myopic optimization problem can be stated as follows: for each year t (t = 1,2,...,N) find the subset $s_t \subset S - S_{t-1}$ such that the improvement

$$Q(s_t) = \sum_{i \in s_t} q_i$$

is maximized while constraint (14) is satisfied.

Each one of these N subproblems is a simple linear integer programming problem known in the literature as the knapsack problem. Since standard algorithms are available today for the solution of this problem (see, for instance, Kolesar, 1967; Greenberg and Hegerich, 1970; Barthes, 1975) we will not go into many details here. Nevertheless, we will briefly outline a branch and bound procedure for the solution of the knapsack problem since this will serve as a basis for the description of the algorithm presented in the next section for the non-myopic case.

Before describing how a branch and bound algorithm works in general, let us first consider a simplistic but quite attractive way of attacking the problem. For this, assume that we are interested in solving the knapsack problem related to the first year, so that we can omit subscript t in the following. Thus we have a set S of n plants with given costs c_i and quality indicators q_i, and we can assume, without loss of generality, that they are ordered by decreasing values of their efficiencies $\eta_i = q_i/c_i$, i.e.

$$\eta_1 \geqslant \eta_2 \geqslant \dots \geqslant \eta_n \quad . \tag{15}$$

We can now associate a zero-one variable x_i with each plant and assume that $x_i = 0$ means that the plant is not activated, while $x_i = 1$ means that the plant is activated. Thus, the knapsack problem is described by

$$\max \sum_{i=1}^{n} q_i x_i \tag{16}$$

subject to

$$\sum_{i=1}^{n} c_i x_i \leq C/N \quad , \tag{17}$$

$$x_i = 0,1 \quad , \qquad i = 1,\ldots,n \quad , \tag{18}$$

where n is the number of plants to be built.
If we now relax constraint (18) into the new constraint

$$0 \leq x_i \leq 1 \quad , \qquad i = 1,\ldots,n \quad , \tag{19}$$

we obtain a linear programming problem the solution of which is given by

$$\bar{x}_i = 1 \quad , \qquad i = 1,\ldots,k-1 \quad , \tag{20a}$$

$$\bar{x}_k = (C/N - \sum_{i=1}^{k-1} c_i)/c_k \quad , \tag{20b}$$

$$\bar{x}_i = 0 \quad , \qquad i = k+1,\ldots,n \quad , \tag{20c}$$

where $(k - 1)$ is the highest integer number, such that

$$\sum_{i=1}^{k-1} c_i \leq C/N \quad .$$

Therefore, the integer solution

$$x_i^* = 1 \quad , \qquad i = 1,\ldots,k-1 \quad , \tag{21a}$$

$$x_i^* = 0 \quad , \qquad i = k,\ldots,n \quad , \tag{21b}$$

is a feasible solution (called <u>simplistic</u> from now on) of the knapsack problem, and its associated improvement represents a lower bound (L.B.) for the optimal solution, i.e.

$$L.B. = \sum_{i=1}^{k-1} q_i \quad , \tag{22}$$

while the solution (20) of the linear programming problem gives an upper bound (U.B.) of the optimal solution, i.e.

$$U.B. = \sum_{i=1}^{k-1} q_i + \eta_k (C/N - \sum_{i=1}^{k-1} c_i) \quad . \tag{23}$$

The computation of L.B. and U.B. given by (22) and (23) is straightforward once the plants have been ordered according to (15); the difference between U.B and L.B. gives an upper bound for how much we can improve the feasible solution (21) by further investigations. Only in the case in which (U.B. - L.B.) is sufficiently large with respect to L.B. is the application of the branch and bound algorithm described below justified from a practical point of view.

Let us now describe the main characteristics of a branch and bound search. This method is very suitable for solving combinatorial optimization problems by successively examining subsets of the set of solutions until one of the solutions located in one of the subsets is proved to be optimal. Solution classes are obtained by assigning a value of 0 or 1 to a given set of variables. This process is usually represented on a graph, called search tree, in which each node represents a particular class of solutions (see, for example, Figure 1). The terminal nodes (leaves) of a search tree represent disjoint classes of solutions: for example, in Figure 1 node $x_1 = 0$ represents all subsets of plants not containing plant 1, node $x_2 = 0$ represents all subsets of plants containing plant 1 but not containing plant 2, while the terminal node identified by $x_2 = 1$ represents all subsets containing both plants 1 and 2. A node in a search tree is said to be closed if it contains no feasible solution or if the solution class cannot be partitioned

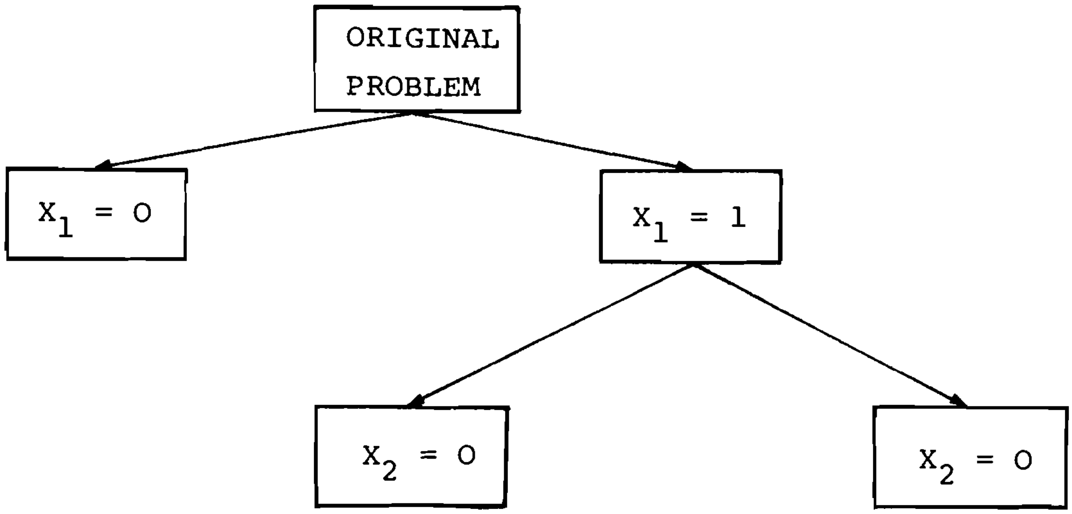

Figure 1. Example of search tree.

again (see, for example, node $x_1 = 1$ of Figure 1); or, finally, if for some reason it is known that the optimal solution is not contained in the corresponding class. By exclusion a node is called pending when it is not closed.

Now that we have introduced the convenient terminology we can describe a general branch and bound algorithm (see Barthes, 1975) for a more detailed exposition).

Algorithm

Step 0 The original problem is examined first. The whole set of solutions is assigned to the root of the search tree. At each iteration solution classes are examined as follows.

Step 1 Node Analysis

1.1. Check feasibility of the node. If the solution class contains no feasible solution, then close the node and go to step 3. Otherwise, compute a feasible solution and the corresponding lower bound for the class.

1.2. Compute an upper bound for the solution class.

Step 2 Closure of Pending Nodes

Close all pending nodes characterized by an upper bound less than or equal to the best feasible solution determined so far.

Step 3 Termination Test

If all nodes are closed, stop; otherwise go to step 4.

Step 4 Node Generation

4.1. Select the solution class corresponding to the pending node that has the highest upper bound.

4.2. Use a suitable rule to partition this class into two subclasses, i.e. decide which variable x_i has to be frozen and the first time freeze it to 1.

4.3. Close the branching node if all subclasses have been generated and go to step 1.

It is worth noticing that this algorithm is completely specified only if it is possible to compute lower and upper bounds (see points 1.1 and 1.2 of the algorithm) and if the partitioning rule of point 4.2 is given. In the case of the knapsack problem it is possible to compute an L.B. and U.B. for any solution class, as has been shown above for the set of all possible solutions (see eqs. (22) and (23)). A satisfactory partitioning rule consists in freezing the variable corresponding to $\bar{x}_k$ in (20b).

Finally it must be noted that for large scale problems the computational effort required by the algorithm may easily become prohibitive. It might therefore be convenient to replace the termination test by the following rule.

Special Rule: Stop if the difference between the highest upper bound on pending nodes and the lower bound corresponding to the best feasible solution computed so far is smaller than or equal to a given percentage of the lower bound.

This termination rule will possibly generate satisfactory suboptimal solutions within a reasonable time.

4. The Far-Sighted Sequencing Problem

We now consider the problem that consists in determining the sequence minimizing the sum of the pollution indices over the N years. The formal statement of the problem is as follows: find the sequence $\{s_t\}_{t=1}^{N}$ such that $\sum_{t=1}^{N} P(S_t)$ is minimized while the budget constraint (14) is satisfied. Since $P(S_t) = P_0 - Q(S_t)$, the minimization of $\sum_{t=1}^{N} P(S_t)$ is equivalent to the maximization of $\sum_{t=1}^{N} Q(S_t)$; thus if the additivity property (4) is fulfilled we can reformulate the problem in the following way: find the sequence $\{s_t\}_{t=1}^{N}$ such that $\sum_{t=1}^{N} \sum_{i\varepsilon S_t} q_i$ is maximized while the budget constraint (14) is satisfied.

In order to solve this problem by means of a branch and bound algorithm, it is first convenient to put it into an integer programming form. For this, let us introduce the zero-one variable x_{it} which is equal to one if plant i is built in year t, and zero otherwise. Then, taking into account that indicator q_i is weighted (N - t + 1) times in the performance index if the i-th plant is built in year t, and that for each plant i there is one and only one x_{it} equal to 1, we obtain the following linear integer programming problem:

$$\max \sum_{t=1}^{N} \sum_{i=1}^{n} (N - t + 1)\, q_i x_{it} \tag{24}$$

subject to the constraints

$$\sum_{t=1}^{N} x_{it} = 1 \quad , \qquad i = 1,\ldots,n \quad , \tag{25}$$

$$\sum_{h=1}^{t} \sum_{i=1}^{n} c_i x_{ih} \leq Ct/N \quad , \qquad t = 1,\ldots,N \quad , \tag{26}$$

$$x_{it} = 0,1 \quad , \qquad i = 1,\ldots,n \quad t = 1,\ldots,N \quad . \tag{27}$$

If we now relax the integer constraint (30) into the inequality constraints

$$0 \leq x_{it} \leq 1 \quad , \qquad i = 1,\ldots,n \quad , \quad t = 1,\ldots,N \quad , \qquad (28)$$

we obtain a linear program (24-26), (28), which is of somewhat the same structure as the one considered in the preceding section. It is easy to show that if the plants have been ordered as in (15), the solution of this linear program is given by

$$\text{Year 1} \begin{cases} \bar{x}_{i1} = 1 \,, & i = 1,\ldots,k_1 - 1 \;, \\ \bar{x}_{k_1 1} = (C/N - \sum_{i=1}^{k_1-1} c_i)/c_{k_1} \,, & \\ \bar{x}_{i1} = 0 \,, & i = k_1+1,\ldots,n \;, \end{cases} \qquad (29a)$$

$$\text{Year 2} \begin{cases} \bar{x}_{i2} = 0 \,, & i = 1,\ldots,k_1-1 \;, \\ \bar{x}_{k_1 2} = 1 - \bar{x}_{k_1 1} \,, & \\ \bar{x}_{i2} = 1 \,, & i = k_1+1,\ldots,k_2-1 \;, \\ \bar{x}_{k_2 2} = (2C/N - \sum_{i=1}^{k_2-1} c_i)/c_{k_2} \,, & \\ \bar{x}_{i2} = 0 \,, & i = k_2+1,\ldots,n \;, \end{cases} \qquad (29b)$$

.

etc.,

.

where (for $t = 1,2,\ldots,N$) k_t is defined by the conditions

$$\sum_{h=1}^{k_t-1} c_h \leq Ct/N \ , \qquad \sum_{h=1}^{k_t} c_h > Ct/N \quad .$$

The simplistic solution x^*_{it} of the integer programming problem (24-27), which is obtained from (29) by putting $x^*_{k_t t} = 0$, $x^*_{k_t,t+1} = 1$, and $x^*_{it} = \bar{x}_{it}$ in all other cases, coincides with the simplistic myopic solution (easy to check). The corresponding value of the performance (24) represents an L.B. for the optimal solution, i.e.

$$\text{L.B.} = \sum_{t=1}^{N} \sum_{i=1}^{n} (N - t + 1)\ q_i x^*_{it} \quad . \tag{30}$$

Of course, the solution of the linear program (24-26), (28) is a U.B. for the optimal solution of the sequencing problem, i.e.

$$\text{U.B.} = \sum_{t=1}^{N} \sum_{i=1}^{n} (N - t + 1)\ q_i \bar{x}_{it} \quad . \tag{31}$$

Thus if (U.B. - L.B.)/L.B. is small enough we can be satisfied with our simplistic suboptimal solution x^*_{it}; if not, we can apply the branch and bound algorithm described in the preceding section to improve the suboptimal solution, or, if possible, to get the optimal solution. The computation of an L.B. and a U.B. for each node of the searching tree can be easily carried out by solving the linear program (24-26), (28) with the x_{it} variables defining the node frozen to integer values. If $\bar{x}_{it}$ is the solution of this linear program then a feasible integer solution x^*_{it} can immediately be derived as follows. Let t_i be the maximum integer t such that $\bar{x}_{it} \neq 0$. Then for i = 1,...,n

$$x^*_{it} = 0 \qquad \text{for} \qquad t \neq t_i \ ,$$

$$x^*_{it} = 1 \qquad \text{for} \qquad t = t_i \ .$$

Thus, L.B. and U.B. can be obtained by means of (30), (31).

Finally, the partitioning rule we propose corresponds to freezing that non-integer variable $\bar{x}_{it}$ which gives the highest contribution in the upper bound (31), i.e. to select the indices (i,t) in such a way that $(N - t + 1)\ q_i \bar{x}_{it}$ is maximized.

The algorithm used for solving the case presented in the next section is somewhat different from the one just described. But we do not describe this algorithm (though it is available upon request) since this would entail too much analytical detail. The basic difference is the partitioning rule, which generates a search tree in which the analysis of each node can be carried out more quickly, since a closed form solution similar to (29) of the corresponding linear program can be used.

Finally, we must point out that these algorithms could easily become very time consuming, since the integer variables are now $N \cdot n$ instead of n as in the preceding myopic problem. Nevertheless, the advantage is that with the special termination rule based on (U.B. - L.B.)/L.B., we can easily avoid the usually very long phase of refinement necessary to get the optimal solution.

5. Application to the Rhine River

For a realistic application of the techniques described above, a section of the Rhine River in West Germany was chosen. The section extends from Mannheim-Ludwigshafen to the Dutch-German border, and is ≃ 500 km long. The major pollution sources in this section are Mannheim/Ludwigshafen with the inflow of the Neckar River, Mainz/Wiesbaden with the inflow of the Main River, Köln/Bonn, and the Ruhr district. Both a Streeter-Phelps model and an ecological model were developed for this section. The dependent variables of the ecological model are concentration N_1 of easily degradable pollutants, concentration N_2 of slowly degradable pollutants, concentration N_3 of non-degradable pollutants, bacterial mass density B, protozoan mass density P, oxygen concentration O. The model equations are

$$\dot{N}_1 = - a_{11}N_1B/(a_{12} + N_1) + a_{13} \tag{32a}$$

$$\dot{N}_2 = - a_{21}N_2B/(a_{22} + N_2 + a_{23}N_1) + a_{24} \tag{32b}$$

$$\dot{N}_3 = a_{31} \tag{32c}$$

$$\dot{B} = a_{41}N_1B/(a_{12} + N_1) + a_{42}N_2B/(a_{22} + N_2 + a_{23}N_1)$$

$$- a_{43}BP/(a_{44} + B) - a_{45}B \tag{32d}$$

$$\dot{P} = a_{51}BP/(a_{44} + B) - a_{52}P \tag{32e}$$

$$\dot{O} = a_{61}(O_s - O) - a_{62}N_1B/(a_{12} + N_1) - a_{63}N_2B/(a_{22} + N_2 + a_{23}N_1)$$

$$- a_{64}B - a_{65}BP/(a_{44} + B) - a_{66}P + a_{67}, \tag{32f}$$

where O_s and a_{ik} are parameters (which are not all independent). The model is of form (8) and has been described in detail elsewhere (Stehfest, 1973). The Streeter-Phelps model consists of the usual equations for oxygen concentration and oxygen demand and an additional equation for the non-degradable pollutants that is the same as (32c). Figures 2 and 3 show how both models fit measured data; the curves approximately describe the situation in 1971.

The optimal solution whose optimal implementation has been investigated resulted from a dynamic programming calculation. In this program the decision variables were the treatment effort in each of sixteen reaches of the river section, and the objective was to meet standards for both oxygen concentration and concentration of non-degradable pollutants at minimum cost. The details of the program are described in a forthcoming paper (Stehfest, 1976). Figure 4 shows the optimal treatment effort in all reaches, if everywhere in the section the oxygen concentration has to be > 6.5 mg/l and the concentration of non-degradable pollutant < 9 mg/l. The calculation was

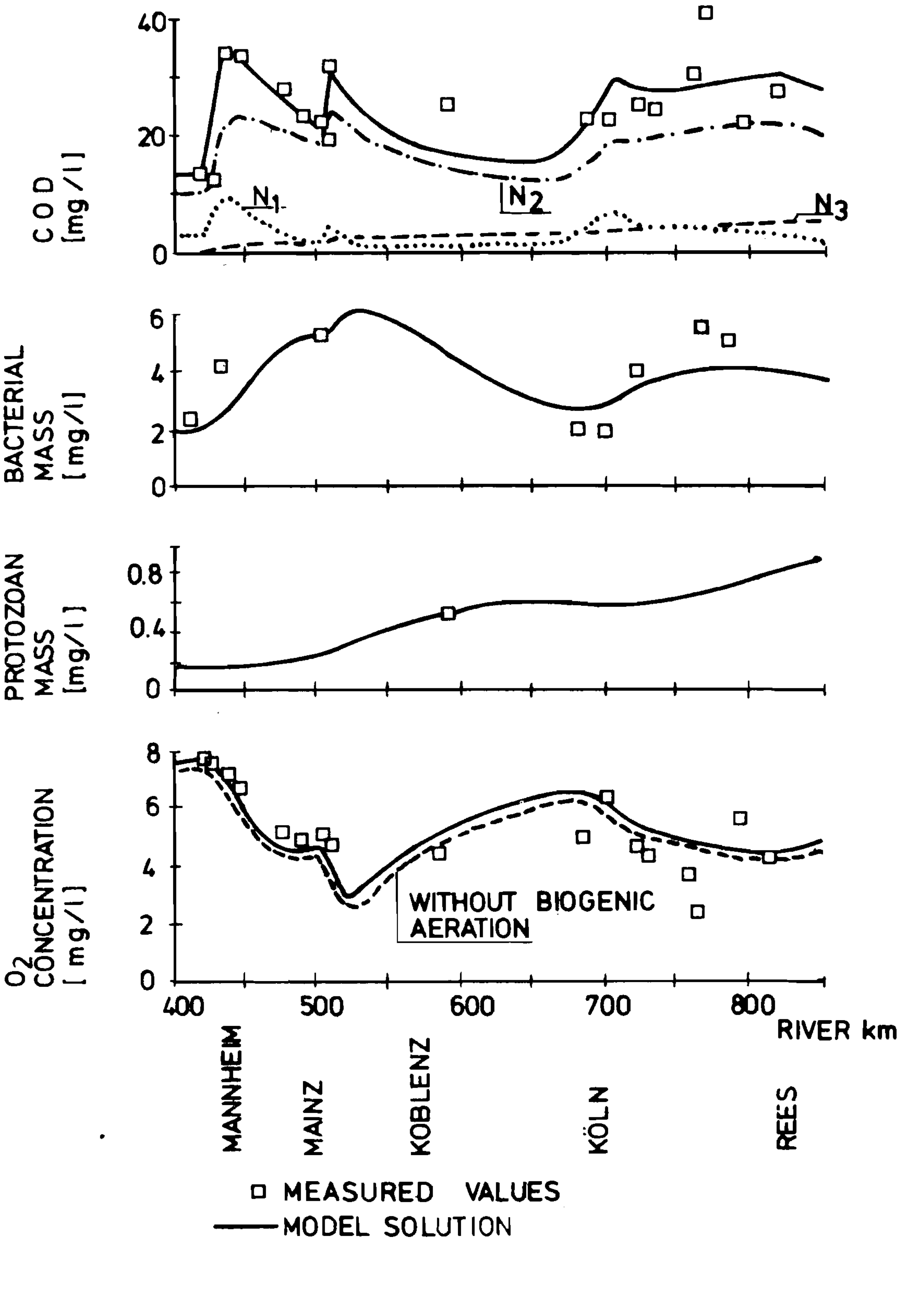

Figure 2. Comparison of measured values from the Rhine River with solution of the ecological model.

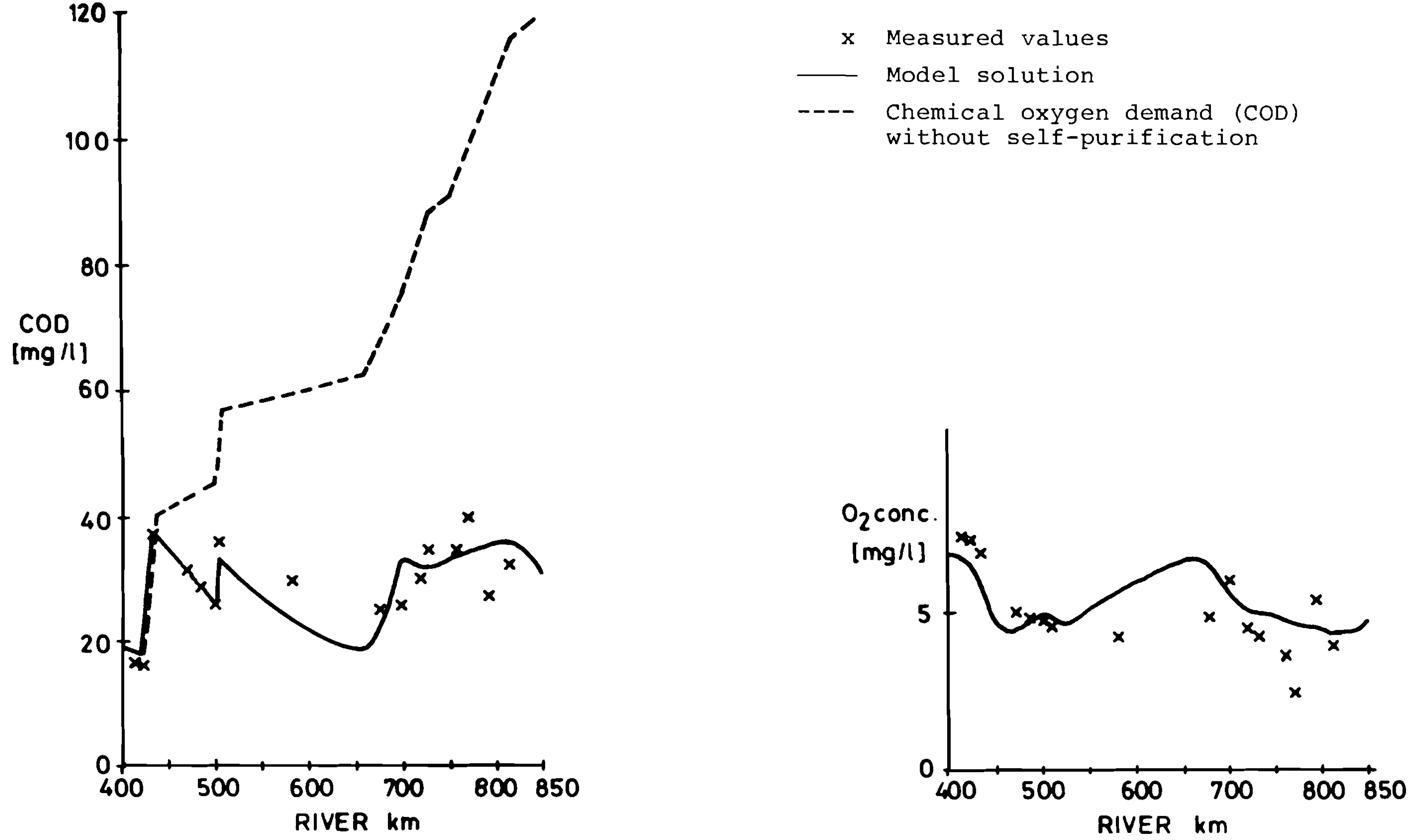

Figure 3. Comparison of measured values from the Rhine River with solution of Streeter-Phelps model.

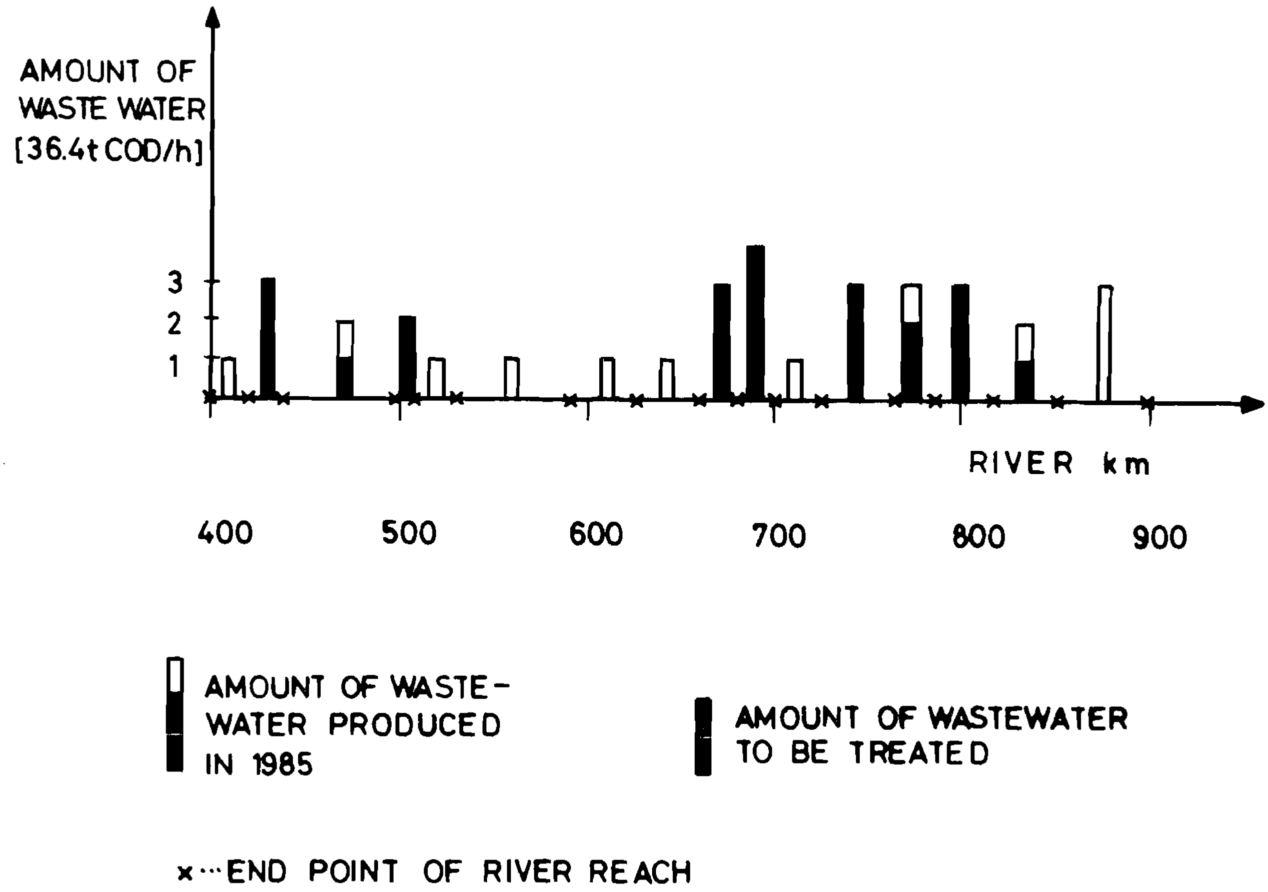

Figure 4. Optimal treatment effort along the Rhine River.

carried out for a water temperature of 20°C and mean river discharge, and the ecological model was used. The Streeter-Phelps model gave almost the same result for this combination of standards; therefore only the set of plants given in Figure 4 was used for the sequencing problem. This also allowed us to check for the effect of using different models on the optimal sequence. Each unit of waste treated, which corresponds to 36.4 tons of chemical oxygen demand per hour, was looked upon as one treatment plant. For the sequencing problem the plants in each reach were assumed to be uniformly distributed over the reach. The treatment cost per unit of waste produced was for each reach one of three distinct values. (The cost category was determined mainly by the population density in the reach.) To make these costs more realistic for the sequencing problem they were changed randomly by up to ± 25%. The costs for the 22 plants used in the sequencing problem are given in Table 1. The time within which the plants had to be installed was chosen to be five years.

Table 1: Costs and contributions to the quality improvement of treatment plants on the Rhine River (using the Streeter-Phelps model). The plants are ordered according to their location on the river.

Number	Cost [10^6 $/y]	q_i [10 t O_2]
1	19.5	2.92
2	17.2	2.93
3	21.1	2.94
4	44.6	2.99
5	25.3	2.82
6	18.6	2.76
7	28.5	2.63
8	25.7	2.61
9	27.3	2.60
10	20.4	2.59
11	22.7	2.58
12	25.9	2.57
13	17.9	2.56
14	17.7	2.43
15	28.5	2.47
16	24.6	2.45
17	21.4	2.41
18	25.9	2.35
19	28.2	2.27
20	23.2	2.19
21	19.5	2.10
22	30.6	1.73

Using the Streeter-Phelps model, the pollution index P_o before installation of any of the 22 plants was $1.04 \cdot 10^3$ t O_2; the contributions q_i (see (4)) to the improvement of this index are given in Table 1.

We will now compare the three approaches to the sequencing problem:

1. Simplistic approach, i.e. installation of plants according to their efficiency η (see 15));
2. Myopic optimization;
3. Far-sighted optimization.

The sums of the pollution indices over the installation period for the different approaches are shown in the first column of Table 2. The analogous sums can also be calculated for the

Table 2. Values of the sum of the pollution index P over the period of implementation (in 10^3 t · y).

Model Used for Optimization	Streeter-Phelps Model	Ecological Model	Ecological Model	Streeter-Phelps Model
Kind of Optimization \ $\sum_{t=1}^{N} P(S_t)$	Streeter-Phelps Model	Streeter-Phelps Model	Ecological Model	Ecological Model
Simplistic	3.401	3.440	3.070	3.168
Myopic	3.375	3.449	3.009	3.232
Overall	3.375	3.437	3.117	3.200

installation sequences that are optimal with respect to the ecological model. These values are given in column 2 of Table 2.

They are also very close to the values in the first column, mainly because the q_i's for the Streeter-Phelps model are not very different (see Table 1).

For the ecological model, the question arises whether the additivity property, which holds exactly in case of an infinite, homogeneous river, is approximately satisfied for the river section investigated. Numerical calculations showed that the q_i's depend strongly on the initial situation; i.e., a plant may have completely different effects on the pollution index depending on the year in which it is built. Only for small sub-sets χ is eq. (4) approximately fulfilled. Table 3 illustrates how the q_i values change if the conditions under which the plants are built change.

Table 3. Improvements q_i of pollution index (in 10 t O_2) by single treatment plants for different initial situations. (Crosses indicate the plants already built (initial situation).)

3.60	x	x	x	x
3.57	x	x	x	x
3.54	x	x	x	x
3.15	0.78	1.10	1.47	1.97
2.23	0.43	0.80	1.22	1.79
2.04	0.35	0.72	1.14	1.73
0.45	1.13	1.55	2.05	x
0.63	1.24	1.65	2.14	x
0.80	1.35	1.75	2.22	x
0.94	1.43	1.82	2.29	x
1.04	1.49	1.87	x	x
1.13	1.54	1.92	x	x
1.21	1.58	x	x	x
1.68	1.87	x	x	x
1.83	1.97	2.33	x	x
1.97	2.08	2.43	x	x
2.13	2.22	x	x	x
2.29	2.34	x	x	x
2.37	2.36	x	x	x
2.37	x	x	x	x
2.31	x	x	x	x
1.80	1.57	1.64	1.81	1.97

The value of the pollution index before a plant is built is $0.928 \cdot 10^3$ t O_2. Table 3 suggests that the installation sequence of all waste water treatment plants should not be decided on the basis of the q_i's calculated for the conditions at the beginning of the installation period. For the simplistic and myopic approach one can easily use q_i's that are calculated anew each year. An overall optimization that takes into account the variability of the q_i's would be far too complicated, however.

The third column of Table 2 shows the sums of the pollution indices for the different approaches to the sequencing problem using the ecological model for both optimization and pollution index. Simplistic and myopic optimizations were done with the q_i's calculated anew each year, and the overall optimization was done with the q_i's calculated for the first year. The fourth column shows the same sums for the installation sequences that are optimal with respect to the Streeter-Phelps model. The differences within the third and fourth columns are considerably greater than within the first two columns.

The computing time for 22 q_i values as well as for one step in the myopic optimization was in the order of seconds on an IBM 370/155 computer, and the storage requirement was also very moderate. The overall optimization took roughly fifteen minutes and a considerable part of the storage of that machine.

Evaluating the results of this illustrative example, which are summarized in Table 2, one can say that--considering the model uncertainties--it is sufficient to install the plants in the order given by their relative efficiency η ("simplistic optimization"). If, however, a nonlinear river quality model, such as (32) is felt to apply, the deviation from the additivity property may be so severe that the relative efficiencies have to be calculated anew for each year. In cases where the differences among plant costs are larger than in Table 1 and/or in which the ratio n/N is smaller, the differences among the three optimization approaches may become much more pronounced than in Table 2; instead of the simplistic approach, it may then be worth using a branch and bound algorithm for myopic or overall optimization.

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