Modelling Water Quality Management

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Abstract

In the paper a system of assumptions for the model of pollutant distribution in the river is given as well as two basic versions of such a model are presented (a simplified dynamic model and static model).

Problems of water quality control are formulated as optimization problems which depend on various models of pollutant distribution. Because of the assumed form of quality functionals and of interaction structure of models the problems can be solved with the aid of multilevel optimization techniques.

1. Simplified water quality models

The typical model which describes both transport and dilution processes as well as biochemical reactions affecting the pollutants in river water has the following form:

\[
\frac{\partial c}{\partial t} = \frac{\partial}{\partial x} \left( E \frac{\partial c}{\partial x} \right) - \frac{\partial}{\partial x} \left( \frac{Q}{A} c \right) + f(c) + \sum_{k} S_k
\]

\[c(0,t) = c_0(t)\]

where: \(c\) – pollutant concentration, \(E\) – longitudinal dispersion coefficient, \(Q\) – flow, \(A\) – cross-sectional area, \(S_k\) – sum of sinks and sources of pollutant, \(f(c)\) – function describing chemical and biochemical processes

Above equation is an one-dimensional dynamical model of pollutant concentration changes in a given river segment, in which only longitudinal diffusion is reflected.

In many water quality management problems there exist a large number of parameters and variables, connected with the number of considered pollutant indices and with size of rivers.

Usually one defines water quality state in a given region comprising a main river with its affluent taking into account several sorts of pollutants. It results in increasing dimensionality of partial differential equations. In practice this causes great computational difficulties in solving the model equations and in estimating their parameters.

In order to obtain the model better fitted to reality and more suitable for solving water quality management problems we assume that the model variables can be constant:

- in certain time-periods of considered time horizon,
- on certain river segments.

The problems of water quality management which are presented in the paper are fully adequate to the considered version of pollutant distribution and are formulated as optimization problems.

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1.1 The water quality models in steady-state conditions

Static models are used in the steady-state case, when the pollutant discharge rate is constant in a given time period and, in consequence, pollutant concentration in this time period, as measured in a fixed river site, does not vary. In this case we make the following assumptions:

A1) The influence of longitudinal dispersion is relatively small and may be neglected,
A2) A river can be divided into a set of \( N \) various length segments. The segments division points are situated into:
  - the pollutant discharge points,
  - inlets and outlets of the river,
  - the stations of water intake,
  - points in which hydraulic parameters of the river may change,
  - points in which the parameters of self-purification process may change.
A3) Biochemical reactions are of the first type,
A4) Both superficial flow and ground waters are considered to be pollutant sources and to be distributed down each section,
A5) For the \( i \)-th segment, \( i=1, \ldots, N \) both cross-sectional areas and first-order reaction coefficient are constant,
A6) All the quantities which are assumed to be time-independent (constant) are time-means values.

Under assumptions A1) - A6), the model describing pollutant distribution into the \( i \)-th river segment has the following form:

\[
\frac{dc_i}{dx} = \left( \frac{c_i}{Q_i} \frac{dQ_i}{dx} + \frac{A_i}{Q_i} k_i c_i + \frac{S_i}{Q_i} \frac{dQ_i}{dx} \right) \quad (2a)
\]

where:
- \( S_i \) – concentration of pollutants from superficial flow or ground water,
- \( x_0 \) – initial point of the \( i \)-th segment,
- \( x_f \) – final point of the \( i \)-th segment,
- \( L_i \) – length of the \( i \)-th segment,
- \( N \) – number of segment.

The boundary conditions for the \( i \)-th segment are given by the following water balance equation:

\[
Q_i(x_0)c_i(x_0) = Q_{i+1}(x_{f_{i+1}})c_{i+1}(x_{f_{i+1}}) + c_i(x_0) \quad (2b)
\]

where: \( \xi \) – waste load discharged at the initial points

The model is completed with the equation:

\[
x_{0i} = x_{f_{i-1}} \quad (2c)
\]

The equations (2a) – (2c) describe static pollutant decay model. The distributed pollutants sources can be essential in situations when the influence of agricultural pollutants cannot be neglected.

The equation (2b) expresses the initial conditions for the \( i \)-th segment. It follows from the Eq. (2b) that the pollutant concentration trajectory is discontinuous at the partition points.
It follows from equations (2a) - (2c) that the model of pollutant distribution in the whole river can be decomposed into $N$ submodels describing pollutant decay in particular river segments.

1.2 The simplified dynamical water quality model

To formulated a simplified dynamical model of pollutant decay in river, besides of the assumption A1) we assume that:

B1) Each particular section of river can be divided (down stream) into segments having homogeneous and constant hydraulic conditions, and the decay of pollutant concentration is uniform and non-varying in this segment. This means, that temporal values of parameters and variables not vary along length of this segment. In particular segment they are approximately uniform and can be represented by unique values.

B2) Assuming the waste substance to be completely mixed, each segment can be treated as a continuous chemical reactor. This means that while river network section can be treated as a system of the $N$ interconnected, ideally mixed reactors describing pollutant decay in particular network segments.

B3) Each segment is characterized by its length, width and slope. The length of each segment is chosen in such a manner that the change of intensity of the pollutant flow in this segment can be neglected.

B4) The following model parameters: cross-sectional area, first-order biochemical reaction coefficient and average volume of the segment are constant in the whole time horizon.

B5) There exist only point-type waste discharges, which are continuously discharged into river.

B6) The segment division points are situated into:

- pollutant discharge points,
- inlets and outlets of the river,
- water intakes,
- the points in which hydraulic and self-purification parameters may change.

Such a division allows to treat the river and its affluents as a system consisting of $N$ interconnected subsystems. Assumptions (B1)-(B2) give rise to the space-wise lumping and as result, the dynamics of pollutant decay may be described by a system of ordinary differential equations. From the above assumptions follows, that it is possible to determine the length of segments in such a manner that time delays in input variables can be neglected. In consequence, the whole river network can be treated as a system of the $N$ interconnected, ideally mixed reactors describing pollutant decay in particular segments.

Under assumptions B1) - B6), the dynamical model describing pollutant distribution in the $i$-th river segment has the following form:

$$ \frac{v_i}{dt} \sum_{j \neq i} Q_{j} c_{j} - Q_{i} c_{i} - k_{i} c_{i} + z_{i} $$

$$ c_{i}(t_0) = c_{i0} \quad t \in [t_0, T] \quad i = 1 \quad N $$

where: $v_i$ – the average volume of water load, $v_i = A_i \cdot L_i$, $Q_i$ – flow in $i$-th segment, $c_i$ – pollutant concentration in $i$-th segment, $z_i$ – waste load discharged at $i$-th segment, $T$ – time horizon

The equation of interactions between segments is:
\( W_{ei} = \sum_{j \neq i} L_{ij} Q_{ij} \) \hspace{1cm} (3b)

where: \( W_{ei} \) – input to the \( i \)-th segment which is outflows from adjacent segments, \( L \) – zero-one matrix, reflecting the structure of interaction between segments.

The dynamical model can be applied to the problems of water quality protection in river network as well as to the rivers with reservoirs. In this model distributed waste sources are not reflected.

2. The water quality control problems in steady-state conditions

The static model (2a) - (2c) can be used for two purposes: a) as simulation model for analyzing the influence of certain parameters on the model variables and b) in water quality control problem. In case a) we must make additional assumptions concerning flow and pollutants from superficial flow or ground water.

In case b) we can formulate the following problems:

Problem 1

Assuming, that quantities of the waste load discharged at the \( i \)-th point and distributed waste load are decision variables of the model and locations of the waste discharge points are not known, it is necessary to find both expected quantities of waste loads and location of the waste discharge points, which ensure desirable quality of the river water. The problem can be formulated as follows.

Find such values of decision variables \( S \) and \( \xi \) minimizing the performance functional:

\[
\min_{S, \xi} \left\{ J = \sum_{i=1}^{N} \left( \frac{1}{2} \int_{x_0}^{x_f} \| c_i(x) - \tilde{c}_i \|^2 dx + \kappa_i(S, \xi) \right) \right\} \tag{4}
\]

subject to equations (2a) - (2c).

In this problem the number of waste discharge points is known, but their locations i.e. the values of \( x_0 \) are not known.

As it result from the equation (2a) - (2c), one can decompose the model of pollutant distribution in the whole river into a set of \( N \) submodels describing changes of pollutant concentrations in the particular river segment. The submodels are interconnected with the aid of mass balance equations in the partition points. Because of this, above problem can be solved by means of two-level methods of trajectory decomposition.

As result one obtains the following two-level structure:

First-level task: (local problems)

For given values \( x_0 \) and \( \xi \) for each segment \([x_0, x_f]\), one solve the following local problem:

\[
\min_{\xi_i, S_i} J_i(S_i, \xi_i) = \frac{1}{2} \int_{x_0}^{x_f} \| c_i(x) - \tilde{c}_i \|^2 dx + \kappa_i(S_i) \tag{5}
\]

subject to equation (2a) – (2c).
Here, $S_i$, i.e. distributed waste load, is treated as a control variable, whereas $c_i$, i.e. pollutant concentration in the $i$-th segment, occurs as state variable.

**The second level problem**

The task of the coordinator level is to predict the quantities of waste loads $\xi_i$ discharged at partition points and to find location of these points (i.e. to find values of $x_0$).

Values of these variables are determined according to the following algorithm:

\[
\begin{align*}
(x_0)_{i+1} &= (x_0)_{i+1} - k \cdot \delta x_0_{i+1} \\
(\xi)_{i+1} &= (\xi)_{i+1} - k \cdot \delta \xi_{i+1}
\end{align*}
\]  

\[
\delta x_0_{i+1} = -\frac{n_i}{Q(x_{f,i})} \cdot \psi_i(x_{f,i}) \cdot c_i(x_{f,i}) - H_i|_{x=x_{f,i}} + H_{i+1}|_{x=x_0_{i+1}}
\]  

\[
\delta \xi_{i+1} = -\frac{Q_{i+1}(x_0_{i+1})}{Q(x_{f,i})} \cdot \psi_i(x_{f,i})
\]

where:

\[
H_i = -J(c_i, S_i) - \psi_i \left( \frac{n_i}{Q} c_i - \frac{A_i}{Q} k c_i + \frac{u_i}{Q} S_i \right)
\]

\[
v_i = \frac{dQ}{dx}
\]

$H_i(\cdot, \cdot)$ - Hamiltonian for the $i$-th problem

$\psi_i$ - conjugate variable related to the state equation

$H_i|_{x=x_{f,i}}$, $H_{i+1}|_{x=x_0_{i+1}}$ - means that Hamiltonian values are calculated for $x=x_{f,i}$ and $x=x_0_{i+1}$

According to the presented model, each segment is considered independently of the others on the first level of control structure. On the other hand, it is the task of the second level to find such values of the variables $\xi_i$ and $x_0$ that allow to meet all the requirements concerning water quality along the whole length of the river.

In the case, when the location of waste discharge points is known, the problem can be simplified and has the following form:

**Problem 2**

Assuming, that the locations of the waste discharge points are known (i.e. $x_0 = x_{f,i}$, $x_i = x_{j}$ are given) one wants to determine such values of the waste load $\xi_i$ discharged at the $i$-th point and distributed waste loads $S_i$ which ensure desirable quality of river water.

It results in the following problem:

\[
J(S, \xi_c, x) = \sum_{i=1}^{N} \left( \frac{1}{2} \int_{x_{f,i}}^{x_{f,i+1}} [c_i(x) - c]^2 + \int_{x_{f,i}}^{x_{f,i+1}} dx + \xi_i(S_i, \xi_i) \right)
\]  

$s \in [x_{j-1}, x_j]$
subject to equations (2a) - (2c)

where:  \( x_{i-1}, x_i \) - initial and final points of the \( i \)-th segments,  \( x_1, x_N \) - initial and final points of the whole river.

Because in this problem we deal with a fixed partition of the river into a set of sections and since locations of the partition points are known, one can apply modified trajectory decomposition method, based on the augmented Lagrange functionals which are associated with interconnection equation (2b). As result one obtains the following two-level structure:

**First-level problem:**
For given values of the multipliers \( \pi \) and values of waste discharge \( \xi \) one solve \( N \) independent local problems related to particular segment \([x_{i-1}, x_i], i=1,\ldots,N\)

\[
\min_{S_i} L_i(S_i, \xi_i, \pi, \rho)
\]  \hspace{1cm} (8a)

where:

\[
L_i(S_i, \xi_i, \pi, \rho) = J_i(S_i, \xi_i) + \pi_i \left( \frac{Q_i(x_i)}{Q_{i+1}(x_i)} \xi_i(x_i) + \frac{1}{Q_{i+1}(x_i)} \xi_{i+1}(x_i) \right) + \frac{1}{2} \left[ \frac{Q_i(x_i)}{Q_{i+1}(x_i)} \xi_i(x_i) + \frac{1}{Q_{i+1}(x_i)} \xi_{i+1}(x_i) \right]^2
\]  \hspace{1cm} (8b)

The task of the lower level is to find - for each segment - optimal values of control variable \( S_i \) and corresponding to it values of state variable \( \xi_i \).

Overall optimal solution one obtain as a result of coordination of local solutions corresponding to particular river sections. Multipliers \( \pi \) and the quantities \( \xi \) of waste loads discharged at partition points are treated as coordination variables and are determined as solutions of the following second-level problem:

**Second-level problem**

\[
\max_{\pi} \min_{\xi} L_d(\rho, \pi, \xi)
\]

where:  \( L_d(\cdot, \cdot, \cdot) \) - dual functional

\[
L_d(\rho, \pi, \xi) = \sum_{i=1}^{N} L_i(\rho, \pi, \xi)
\]  \hspace{1cm} (9a)

\[
L_d(\rho, \pi, \xi) = \min_{(S_i, \xi_i) \in B_i} L_i(S_i, \xi_i, \pi, \rho)
\]  \hspace{1cm} (9b)

\[
B_i = \{(S_i, \xi_i) : \text{such that Eq.(2a) is satisfied}\}
\]  \hspace{1cm} (9c)

If the dual functional is differentiable the coordination variables can be obtained according to the following algorithm:
\[
\zeta^{l+1}_{i+1}(x_i) = c^l_{i+1}(x_i) - \frac{Q}{Q_{i+1}} c^l_i(x_i) \tag{10a}
\]
\[
\zeta^{l+1}_j = -\frac{\partial f_j}{\partial x_i} - \rho \left( \frac{Q}{Q_{i+1}} c^l_j(x_i) + \frac{1}{Q_{i+1}} \zeta^l_{i+1}(x_i) - c^l_{i+1}(x_i) \right) \tag{10b}
\]

Iteration (10a)-(10b) result from stationarity conditions for dual functional.

In above structure the control variables i.e. distributed waste loads and point waste loads are calculated on two different levels. Calculation of the values of loads \( S \) connected with agricultural pollutants is executed for each segment of river independently, whereas the values of waste discharges \( \xi \) are calculated on the coordination level.

3. Dynamical model of water quality control problem

Assume, that there exist waste treatment plants with a given capacities \( \nu_k \) and efficiencies \( \eta_k \). Then the load of waste discharged to the river after treatment has form: \( k=1,\ldots,K \)

\[
z_k = \left( 1 - \eta_k \right) \tilde{c}_k
\]

In this case one can formulate the following constraints:

\[
\eta_k - \tilde{c}_k(t) \leq \nu_k \tag{11b}
\]

\[
c_z(t) \leq \bar{c}
\]

Problem 3

This problem concerns determining the optimal waste discharge policy for existing waste treatment plants, which ensures a desirable quality of the river water, and can be formulated as follows:

\[
\min_{z} \left\{ J(z) = \sum_{i=1}^{N} f_i(z_i) \right\}
\]

subject to constraints (3a), (3b), (11b) – (11c)

As follows from the equations Problem 3 can be decomposed into \( N \) interconnected subproblems. Each of these subproblems concern determining, such waste discharge policy, which ensures proper level of waste quality in the particular segments of the river network.

As a consequence, one can solve this problem using mixed method of coordination which is based on application of the augmented Lagrange functional associated with the interconnection Eq. (3b). One obtains the following two-level structure:

First level local problems

For fixed values of \( \pi, W \), and for each segments of river network:

\[
\min_{z_i} \left\{ \bar{L}_i(z_i, x_i, \pi, W, \rho) \right\} \tag{12a}
\]

subject to constraints (3a), (11b)-(11c)
where:

\[
\tilde{E}(z_i, \bar{c}_i, W_e, \pi, \rho) = J_i(z_i) \int_{t_i}^{T} \left[ \pi_i, W_{ei} - \left( Q_i c_i \sum_j L_{ij} \pi_j \right) + \frac{1}{2} \rho || W_{ei} \|^2 + \frac{1}{2} \rho || Q_i c_i \|^2 - \rho \left( Q_i c_i \sum_j L_{ij} \pi_{ej} \right) \right] dt
\]

(12b)

\[\pi - \text{Lagrange multiplier associated with the interaction equation (3b)}\]

\[\rho - \text{the penalty coefficient}\]

For fixed values of \(\pi\) and \(W_e\), we obtain for each segment the optimal quantities of waste load discharged to the i-th segment and the values of state variables.

The global solution for the river network is obtained as a result of coordination of the local problems by means of the multipliers \(\pi\) and inflows \(W_e\).

The second-level task is to find the saddle point of the proper dual functional:

\[
\max_{\pi} \min_{W_e} \tilde{E}(\rho, \pi, W_e)
\]

(13a)

where: \(\tilde{E}(\cdots)\) - dual functional associated with the problem

\[
\tilde{E}(\rho, \pi, W_e) = \min_{(z_i, \bar{c}_j) \in A} \tilde{E}(z_i, \bar{c}_i, W_e, \pi, \rho)
\]

(13b)

\[A_i = \{ (z_i, \bar{c}_i) \mid \text{such that constraints (3a), (11b)-(11d) are fulfilled} \}\]

(13c)

\[
\tilde{E}(\rho, \pi, W_e) = \sum_{i=1}^{N} \tilde{E}_i(\rho, \pi, W_e)
\]

(13d)

5. Conclusion

In the static model distributed pollutants sources are reflected what can be essential in situations when the influence of agricultural pollutants cannot be neglected. In the case, when the locations of waste discharge points are unknown the task of coordination level is to predict the quantities of waste loads discharged at partition points and to find location of these points. The values of control variables are determined on two various levels – the point-type waste loads (connected with industrial and urban sources) are determined on the upper level and the distributed waste loads (connected with agricultural pollutants) are determined independently for each river segment.

The dynamical model can be applied to the problems of water quality protection in river network as well as to the river with reservoirs. In this model distributed waste sources are not reflectd. The structure of interconnections between particular segments results in possibility of application of mixed coordination method to calculate optimal temporal values of waste loads.
Bibliography


