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SOME ISSUES CONCERNING THE PROBLEMS OF WATER QUALITY MODELING IN DISTRIBUTION SYSTEMS

WYBRANE PROBLEMY MODELOWANIA JAKOŚCI WODY W SIECIACH WODOCIĄGOWYCH

Abstract: Some issues concerning the most popular practical problems encountered during modeling the water quality in water distribution systems were presented. The mathematical basis of water quality modeling, commonly understood as chlorine distribution modeling, covering the governing equations, initial and boundary conditions description as well as required and necessary simplifications, were discussed. Then, the most popular computer models of water quality in distribution systems used in environmental engineering practice, such as: input-output (I/O) model, inverse chlorine decay model and forward simulation, were introduced. The modeling assumptions, model structure and limitations, advantages and disadvantages of given models were also discussed.

Keywords: water quality modeling, water distribution system, chlorine decay

Introduction (Mathematical preliminaries)

Water quality modeling in distributions systems concerns the prediction of water pollution with the use of mathematical simulation techniques. The formation of a water quality numerical model requires gathering of formulas and parameters determining the position and momentum of pollutants in the water body (ie of water supply systems) [1, 2]. But in practice, modeling of water quality encounters many practical problems caused by the complexity of the phenomenon, mutual interaction of considered effects and complication of their mathematical description. Thus, modeling of water quality may be considered a difficult task.

The governing equations for the single-phase heterogeneous mixture covers widely presented laws of mass conservation, momentum conservation and conservation of energy. The movement equations (mass and momentum conservation) after assumption of fluid density, diffusion and viscosity coefficients constancy take the form of well known Navier-Stokes equations [3].

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The process of diffusion in fluids is described by Fick's laws. The steady state diffusion is described by the first Fick's law and Fick's second law (Equation 1) is used when non-steady or continually changing state diffusion is considered [4, 5]:

$$\frac{\partial c_i}{\partial t} = D_{Mi} \nabla^2 c_i \quad (1)$$

where c_i = concentration in dimensions of studied substance [g m^{-3} , mol m^{-3}]; t = time [s]; D_{Mi} = diffusion coefficient [$\text{m}^2 \text{s}^{-1}$].

When diffusion and advection appear at the same place and time in the mixture body, the stream of pollutant may be represented by diffusion-advection equation [5-7]:

$$\frac{Dc_i}{Dt} = D_{Mi} \nabla^2 c_i \quad (2)$$

where Dc_i/Dt means material (substantive) derivative of c_i .

In some situations the concentration of pollutants may be alerted by sources or sinks of the pollutant. The chemical, biological and physical reactions may be responsible for the sink and sources appearance - in this case the diffusion-advection equation is written as:

$$\frac{Dc_i}{Dt} = D_{Mi} \nabla^2 c_i + R_i \quad (3)$$

where R_i = total source-sink term for i substance.

The total source-sink term in the diffusion-advection equation describes the three dimensional course of chemical, biological or physical reactions of i substance occurring in the mixture body - usually the combined effect of bulk and wall reactions. The processes determining the value of source-sink term in the environmental engineering may cover: disinfectants decay, water oxidization, organic matter mineralisation, photosynthesis, nitrification, gravitational separation, gain and decrement of bacteria number, adsorption, oxygen consumption and others. The intensity of source-sink factors may also expressly vary in different parts of a studied system - the transit long segments with steady value of R_i and relatively short parts of spatially varied value distribution and discharge rate, usually regarded as a point discharge sources, may be observed. Moreover, the intensity of chemical reaction course varies also in time, so time is another very important factor in the description of pollutants movement in the water body. Thus, the kinetics of processes comprises the problems of chemical, biological or physical reactions duration and their inequality in time.

Generally, the reaction kinetics for the decay process of selected substance may be written as follows:

$$\frac{dc_i}{dt} = -k_i c_i^n \quad (4)$$

where n is a power to which the concentration term is raised (usually 0÷2); k_i = reaction rate constant.

The unit of reaction rate constant depends on the global rate of reaction ie zero rate [$\text{mol dm}^{-3} \text{s}^{-1}$], first-rate [s^{-1}], second-rate [$\text{mol}^{-1} \text{dm}^3 \text{s}^{-1}$]. We may notice that for the unlimited order n the constant unit is [$\text{mol}^{1-n} \text{dm}^{3n-3} \text{s}^{-1}$]. The reaction rate constant repre-

sents variable reactions occurring in selected systems ie bulk reaction (k_b), wall reaction (k_w) and mass transfer (k_f).

We may see that to prepare the water quality model in selected system, the governing equations and their parameters along with the source-sink term to the diffusion-advection equation are required. In this case the reaction kinetics and reaction rate constants appropriate to the studied phenomenon becomes necessary.

The next steps in the water quality mathematical model development are geometrical characteristics of a selected system, information about its physical properties and finally assignment of initial and boundary conditions. Description of initial conditions required to numerical modeling of water quality is rather easy - the knowledge about the governing equations parameters in every considered point of the system at the first time step ($t = 0$) of simulation is required. Boundary conditions usually are presented as the mathematical formulas which have to be met by the governing equations of the prepared simulation on the limits of the studied system. Generally, four different types of constant or time dependant boundary conditions are used in modeling: Dirichlet, Neuman, Hankel and mixed condition. In case of modeling, the quality of water transmitted through the pipes system, the rate of chemical, biological and physical reactions occurring on the pipe wall and their influence on the water quality may be controlled by the boundary conditions, usually Neuman or mixed type. The actual knowledge of constant or time dependent source-sink term for the diffusion-advection equation is necessary. Thus, the proper description of reaction kinetics, its order and reaction rate constant (k_w) to assign the boundary conditions for pollutants transport in water is required.

The scheme of water quality computer modeling system is shown in Figure 1.

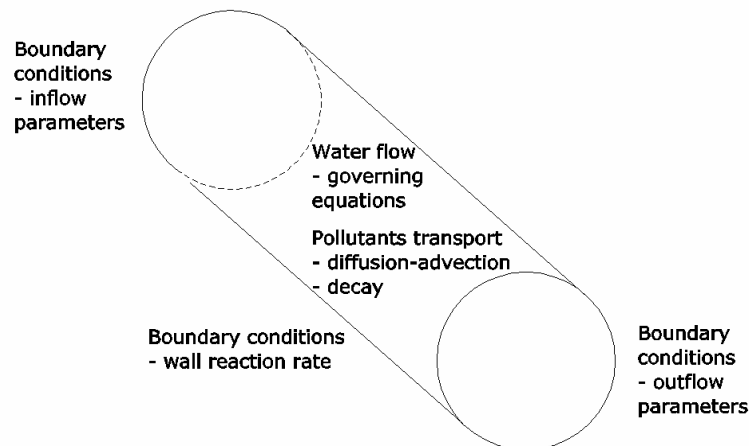


Fig. 1. Scheme of water quality computer modeling system

The presented above abbreviated bases of water quality modeling show the high complexity of the studied problem. The numerical methods (finite difference method and finite element method) for producing approximate solutions to ongoing processes are obvious and necessary.

Water quality modeling in drinking-water distribution systems

The quality of water delivered to the customers depends on its initial chemical and physical composition, the proper choice of purification technology, technical condition of water storage tanks and the pipe network as well as hydraulic conditions and exploitation manner of the water supply system.

The water quality is determined by: oxygen decay, disinfectant decay, the formation of disinfection by-products (trihalomethanes, THMs), change of color, smell and turbidity. The disinfectant content, usually residual chlorine is one of the most popular parameters certifying the quality of transported water. Maintenance of residual chlorine minimal concentration inside the whole water distribution system protects water against microorganism development and deterioration of its quality parameters.

Chlorine propagation inside the water distribution system may be studied with the use of mathematical models comprehensively describing the variable hydraulic conditions and reflecting individual factors influencing the disinfectant decay. Modeling of water quality in this case may be understood as the monitoring of water quality parameters increase or decrease.

Simulation of residual chlorine concentration in selected water supply network nodes makes gathering the knowledge about transported water quality possible and helps in considering the network segments/parts in which water quality deterioration occurs.

Chlorine added to water during the process of disinfection reacts with organic and non-organic matter. Thus, the residual chlorine decay in time, regardless of the other factors influencing its decay, is observed [8-11]. The decrease of chlorine concentration below the minimal level may cause secondary development of microorganisms. Otherwise, excessive chlorine dose added to water during disinfection process may cause formation of dangerous disinfection by-products.

The water quality models, including the most popular chlorine decay models, are based on four basic assumptions [12]:

- distribution network consisting of sources, pipes and nodes,
- fixed flow directions in pipes,
- all hydraulic parameters known,
- chlorine concentration in all outer sources known.

The algorithms used to simulate the behavior of chlorine in a water distribution system are based either on steady-state or on dynamic approaches. More accurate are the dynamic models, which simulate changes in the spatial distribution of contaminants throughout the piping system under a time dependent customer demand. The dynamic models can be classified as Eulerian- and Lagrangian-based method. Both models are based on one-dimensional flow, quasi-steady network hydraulics, instantaneous and complete nodal mixing, ideal plug flow with negligible longitudinal dispersion and a single contaminant with one or multiple sources and first order kinetic decay function that occurs at bulk flow and the pipe wall. In Eulerian-based method [13], the pipes are divided into a number of equally sized segments, and these segments move between fix points in the pipe. Lagrangian-base (event- and time-driven) methods divide the pipes into variable segments.

The models described in literature [8-10, 14, 15] are based on one dimensional advection-diffusion equation:

$$\frac{\partial c_{i,t}}{\partial t} + u_i \frac{\partial c_{i,t}}{\partial x} + D_x \frac{\partial^2 c_{i,t}}{\partial x^2} + R(c_{i,t}) = 0 \quad (5)$$

where $c_{i,t}$ = cross-sectional average chlorine concentration in pipe i as a function of distance x and time t [$\text{mg}\cdot\text{dm}^{-3}$]; u_i = flow velocity in pipe i [$\text{m}\cdot\text{s}^{-1}$]; t = time [s]; D_x = diffusion coefficient in direction x [$\text{m}^2\cdot\text{s}^{-1}$]; $R(c_{i,t})$ = the reaction rate expression/term (as a function of concentration).

The modeling research presented by Al-Omari et al [16] showed that in turbulent flow diffusional transport does not considerably affect the calculation results and may be neglected. Then, equation (5) may be written as:

$$\frac{\partial c_{i,t}}{\partial t} = -u_i \frac{\partial c_{i,t}}{\partial x} - R(c_{i,t}) \quad (6)$$

The source term in equation (6) $R(c_{i,t})$, describes the intensity of bulk and wall reactions occurring between chlorine and organic and non-organic substance. The total first-order bulk and wall reactions are usually assumed in chlorine decay modeling [17, 18]:

$$R(c_{i,t}) = -k_0 c_{i,t} \quad (7)$$

where k_0 = first-order reaction rate [d^{-1}].

The chlorine decay reaction rate in this case is proportional to the chlorine concentration in the first power.

The chlorine consumption effecting wall reactions covers the decay constant, mass transport and known relation of the pipe area to its volume [19, 20]. Then, the overall decay rate constant may be presented as [17, 18]:

$$k_0 = k_b + \frac{k_w k_f}{r_h (k_w + k_f)} \quad (8)$$

where r_h is the hydraulic radius [m].

In Table 1 the examples of different reaction rate expressions, which can also be used in numerical modeling are presented [21, 22].

The value C_L indicates that the chlorine will decay to a minimum limiting level and no further in order to insufficient organic matter.

As mentioned above, dynamic models are based on the assumption of complete and instantaneous mixing of fluids in water distribution system nodes. Concentration at a branching node equals the weighted average of the downstream concentrations of all pipes that join at that node. Thus, the chlorine concentration may be described as [22]:

$$Cnc_{j,t_j} = \frac{\sum_{i=1}^{N_{inpj}} Q_i c_{i,t} + Q_E C_E}{\sum_{i=1}^{N_{inpj}} Q_i + Q_E}, \quad j = 1, \dots, N_{jn} \quad (9)$$

where N_{inpj} = is the number of incoming pipes at node j ; N_{jn} = the total number of nodes in the network; Q_i = rate of discharge in pipe i , Q_E = the external source flow into at node j [$\text{m}^3\cdot\text{s}^{-1}$]; C_E = the external source concentration into at node j [$\text{mg}\cdot\text{dm}^{-3}$].

The greatest problem in municipal water quality modeling is collecting the necessary input data to the model, especially bulk decay (k_b) and wall demand (k_w) coefficient as well as their calibration. In modeling, practice the assumption of known k_w for all pipes,

resulting from difficulties in field research, is popular. The real values of k_w are then obtained during the calibration process.

Table 1

The examples of different reaction rate expressions

Reaction		Equation
1	First-order bulk and wall reactions	$R(c_{i,t}) = -k_{b,li}c_{i,t} - \frac{k_{w,li}k_{fi}}{r_{hi}(k_{w,li} + k_{fi})}c_{i,t}$
2	First-order bulk and zero-order wall reactions	$R(c_{i,t}) = -k_{b,li}c_{i,t} - \text{Min}\left(\frac{k_{fi}c_{i,t}}{r_{hi}}, \frac{k_{w,0i}}{r_{hi}}\right)$
3	Second-order bulk reaction with respect to chlorine only and first-order wall reaction	$R(c_{i,t}) = -k_{b,2i}c_{i,t}^2 - \frac{k_{w,li}k_{fi}}{r_{hi}(k_{w,li} + k_{fi})}c_{i,t}$
4	Second-order bulk reaction with respect to chlorine only and zero-order wall reaction	$R(c_{i,t}) = -k_{b,2i}c_{i,t}(c_{i,t} - C_L) - \frac{k_{w,0i}k_{fi}}{r_{hi}(k_{w,li} + k_{fi})}c_{i,t}$
5	Two component second-order bulk decay and first order wall reactions	$R(c_{i,t}) = -k_{b,2i}c_{i,t}(c_{i,t} - C_L) - \frac{k_{w,li}k_{fi}}{r_{hi}(k_{w,li} + k_{fi})}c_{i,t}$
6	Two component second-order bulk and zero-order wall reactions	$R(c_{i,t}) = -k_{b,2i}c_{i,t}(c_{i,t} - C_L) - \text{Min}\left(\frac{k_{w,0i}}{r_{hi}}, \frac{k_{fi}}{r_{hi}}c_{i,t}\right)$

where: r_{hi} = the hydraulic radius [m]; $k_{w,li}$ = the first order wall reaction parameter [$\text{m}\cdot\text{d}^{-1}$]; $k_{b,li}$ = the first order bulk decay parameter [d^{-1}]; k_{fi} = the mass transfer coefficient [$\text{m}\cdot\text{d}^{-1}$]; $k_{w,0i}$ = the zero-order wall reaction parameter [$\text{mg}\cdot\text{d}^{-1}\cdot\text{m}^{-2}$]; $k_{b,2i}$ = the second-order bulk decay parameter [$\text{dm}^3\cdot\text{mg}^{-1}\cdot\text{d}^{-1}$]; C_L = the limiting concentration of chlorine [$\text{mg}\cdot\text{dm}^{-3}$]

Thus, in order to obtain the reliable results the simultaneous calibration of used and calculated coefficients has to be ensured by the water quality models.

Several models that determine chlorine concentrations throughout a water distribution system have been described in literature [13, 23-25]. But the changes in water quality that take place in the network are still very difficult to study by the use of mathematical models due to the complexities arising out of varying hydraulic conditions and non-applicability of universal chlorine reaction kinetics. Nowadays, three types of numerical models are popular to calculate the changes of chlorine concentration in water distribution systems:

- input-output model I/O [26, 27],
- inverse chlorine decay model [16, 22, 25],
- forward simulation [10, 13, 28].

Input-output model and inverse model are the developed forms of the forward simulation model. The auto-calibration of unknown chlorine decay/demand coefficients is possible in these models. The calibration in the forward model is realized by trial-and-error method [10] or weighted-least-squares method based on Gauss-Newton minimization technique [22].

Input-output model (I/O) developed by Zierolf et al [26] is used to track chlorine propagation in a distribution system and to calibrate the wall demand coefficient in a system without water storage tanks. This numerical model identifies all pipes covering flow paths between upstream and downstream sampling points and determines k_w for

these pipes. Shang et al [27] enhanced the basic I/O model with particle backtrack algorithm (PBA) which made including water storage tanks and multiple water sources possible. In the I/O model using a particle backtrack algorithm, the output concentrations is modeled as a variable depending on input concentrations, network hydraulics and physical characteristics of the pipe network. Under the assumption of first-order chlorine decay reaction, the I/O model has the following form

$$C_0(T_0) = \sum_{j=1}^N \gamma_j c_{ij} (T_0 - t_j) \quad (10)$$

where: C_0 = output chlorine concentration [$\text{mg}\cdot\text{dm}^{-3}$], N = number of flow path between inputs and output, T_0 = output time [s], c_{ij} = chlorine input concentration for path j [$\text{mg}\cdot\text{dm}^{-3}$], γ_j = unitless impact coefficient of path j (sensitivity of output concentration to path input concentration).

Under the assumption of first order chlorine decay, the modeled chlorine output can be expressed explicitly in terms of only these wall demand coefficients that affect the output concentration, and therefore the sensitivity of the modeled chlorine concentration to wall demand coefficients can be calculated efficiently [27]. But uncertainty in parameter estimate depends strongly on the design of output measurement location.

The inverse chlorine decay model was developed by Islam et al [25]. In this model, chlorine decay coefficients for each pipe in the network are known, chlorine concentrations at some of the nodes are known by specification, while chlorine concentration at the source is unknown. It is desired to determine the unknown source concentration, so that the specified and the calculated concentrations match. This model, according to the number of equations and unknown variables, solves three cases:

1. evendetermined case - the number of unknown variables equals the number of governing equations,
2. overdetermined case - the number of equations is more than the number of unknowns,
3. underdetermined case - the number of the unknowns is higher than the number of available equations.

The inverse model gives accurate results for the even and the overdetermined cases for both: source concentration and chlorine decay coefficient [16], but for the underdetermined case, the results are not satisfactory in some instances.

The forward model of water quality, which tracks changes in chlorine concentration depending on time and localization, consists of the hydraulic model and elements describing chlorine transport along the pipe system. Chlorine propagation along the pipe network in this model is described by the simplified transport equation (2) and calculated numerically by Lagrangian time-driven method [29]. The predicted chlorine concentrations are depend on chlorine and reagents reactions parameters described as overall, bulk and wall. Chlorine distribution in water stream is described by first-order kinetics model. All necessary input parameters needed for this model are either an overall first-order reaction parameter or bulk reaction parameter along with the wall reaction parameters depending upon the type of reaction rate expressions, described by equations (7)-(9) presented in Table 1. The decay parameters are determined experimentally by the bottle

test, wall and overall reaction parameters are obtained by the calibration of data gathered in the field.

The forward model provides a good tool to calibrate the water quality model, it can estimate the parameters efficiently involved in overall first order, first and zero-order wall reaction kinetics [22]. This model shows good correspondence of results and measured values in fixed hydraulic conditions and for turbulent flows ($Re > 10000$). The quality of correspondence increases with the distance between nodes and the water source. The source chlorine concentration is calculated by a trial-and-error procedure. But the same trial-and-error procedure used for model calibration appears to be complicated and time-consuming.

Summary and conclusions

The changes in water quality that take place throughout the distribution system are still very difficult to simulate by mathematical models due to the complexities arising out of varying hydraulic conditions and non-applicability of universal chlorine reaction kinetics.

The first necessary required step in creation of any water quality models is a properly calibrated hydraulic model. The proper realization of the hydraulic model and its calibration determine the correct assessment of water network hydraulic conditions and changes of selected pollutants concentration inside the water distribution system. The fundamental difficulties during the hydraulic model calibration are: the proper setting of measurement points, real values of water flow and pressure measurement and assumption of maximum difference between simulated and measured values.

Varied nature of chlorine's reactivity makes it difficult to predict chlorine levels throughout a water system. Water quality models can only be reliable when the mechanisms of chlorine dissipation within the water system are properly defined. The predicted chlorine concentrations within the network are governed by reaction parameters, that is overall, bulk and wall coefficients. Bulk chlorine decay coefficient can be determined by the laboratory bottle test. But the wall demand coefficient depends on pipe characteristics such as material, age, degree of corrosion which can differ significantly in the system. Uncertainty in wall demand coefficient estimates are also caused by chlorine measurements error.

The available water quality models have many disadvantages preventing the proper assessment of water quality in the whole system of water distribution or limiting their usage only to small networks as well as simulating changes in fixed hydraulic conditions. These limitations force continuous research the aim of which is the creation of new models or upgrading the already existing ones to allow the analysis of water quality in every distribution system, in spite of its structure or hydraulic conditions.

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WYBRANE PROBLEMY MODELOWANIA JAKOŚCI WODY W SIECIACH WODOCIĄGOWYCH

Abstrakt: Przedstawiono wybrane zagadnienia dotyczące najczęściej pojawiających się problemów w modelowaniu jakości wody wodociągowej. Zaprezentowano podstawy matematyczne modelowania numerycznego jakości wody, często pojmowanego jako modelowanie rozkładu chloru, obejmujące równania stanu, warunki brzegowe i początkowe. Przedstawiono także najczęściej stosowane uproszczenia w opisie matematycznym opisywanego zjawiska. Następnie w pracy omówiono najpopularniejsze modele jakości wody stosowane w inżynierii środowiska: model wejście-wyjście (I/O), model odwrócony oraz model postępujący. Zaprezentowano także założenia modelowe, struktury omawianych modeli, ich zalety oraz wady i ograniczenia.

Słowa kluczowe: modelowanie jakości wody, sieć wodociągowa, rozkład chloru