

Working Paper

On Reconciliation of Traditional Water Quality Models and Activated Sludge Models

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ABSTRACT

Models of the oxidation of organic material developed for river water quality management and for biological wastewater treatment differ widely in state variables and process descriptions due to their development history, environmental conditions and the objectives of the two approaches. The IAWPRC/IAWQ Activated Sludge Model No. 1 (ASM-1) resulted from a coordinated effort of a dedicated specialist group at the mid 1980s and thus free of the inconsistencies inherent in ambient water quality models such as QUAL2E developed in the course of the past three decades. The reconciliation of the ASM-1 and QUAL2E attempted in the present work may help in developing integrated pollution abatement strategies considering treatment and riverine processes in a unified way. It is shown that, after some modifications, a model similar to ASM-1 can be successfully applied to riverine conditions. It is also demonstrated that simple first-order kinetics models (such as the Streeter-Phelps and extended Streeter-Phelps ones) can be derived from the ASM-1 and QUAL2E as their asymptotic forms under the assumption that "fast" variables attain their long-term equilibrium levels. Models of ASM-1 type should, therefore, be applied when there are abrupt temporal or spatial changes in the system, otherwise simpler models adequately reflect the behavior of the oxidation system. Finally, an international effort to develop a standardized and improved river water quality model following the procedure of ASM-1 looks more than desirable.

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ON RECONCILIATION OF TRADITIONAL WATER QUALITY MODELS AND ACTIVATED SLUDGE MODELS

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1. INTRODUCTION

Bacterial decomposition of organic material is one of the major environmental processes by which by-products of organic life are recycled to the pool of mineral components. This process is the basis of natural self-purification of rivers and lakes, and it is also used in waste treatment processes to remove organic pollution from wastewater. Models of bacterial decomposition have thus been developed in two major environmental engineering fields - ambient water quality management ("nature conservation" models) and wastewater treatment (technological processes models).

From the water quality management point of view, however, waste processing in the treatment plant is but one of the stages in the pathway of waste disposal. The treated effluent is usually discharged into a river or other natural waters, where bacterial waste stabilization continues. From the point of view of efficient emission control it is necessary to take into account both stages together. In principle, one can conceive a methodology which would allow consideration of wastewater treatment units and the receiving waters as one controllable entity; exploiting synergies of the combined system to increase the robustness, sustainability, efficiency and reduce costs of the control policies. For instance, some portion of the waste could be treated at the plant while the other portion will be designated for effective self-purification in the river.

Unfortunately, due to large differences in the two types of models, at present it is impossible to reconcile the two modelling approaches in one integrated methodology. To illustrate this point, let us take the state-of-the-art technology model, Activated Sludge Model No. 1 (ASM-1, Henze et al, 1987), and the widely used river water quality model supported by the US EPA, QUAL2E (Brown and Barnwell, 1987). Despite the fact that both models describe roughly the same set of biochemical processes, the models differ significantly from each other both in state variables, in the representation of reactions and in parameters. This prevents taking an integrated approach to the plant-river system (in fact, the linkage of the two models would face serious difficulties). While it is clear that river models can not be employed for

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handling treatment processes, the opposite statement is not true. Thus the question to be addressed is, whether after some modifications, an activated sludge model could not be applied for riverine conditions. Only a few attempts are known in this respect (Rinaldi et al., 1979; Koncsos et al., 1994). A systematic comparison of the two approaches to water quality modelling also has not been performed. This work tries to fill this gap.

The structure of the paper is as follows. First, the development history of the modelling approaches is compared. Second, the model structures of QUAL2E and ASM-1 is analyzed with respect to state variables, processes and parameters. The application of a "technological" model similar to the ASM-1 to a river follows. It is shown that in the riverine situation, ASM-1 can exhibit a behavior similar to simpler models of Streeter-Phelps type. Building on this illustration, a more general picture of the relationship between simple river water quality models (like extended Streeter-Phelps) and their more complex counterparts - QUAL2E and ASM-1 - is discussed in the next section. It is shown that simpler models could be derived from more complex ones under certain conditions as their asymptotic or reduced form. The discussion concludes with implications for the practical use of more complex models versus simpler ones.

2. DEVELOPMENT HISTORY

One of the major reasons for the difference in model structure of traditional water quality and treatment plant models lies in the history of model development. The conventional water quality models (the roots of which go back to the Streeter-Phelps model - cf. Steeter and Phelps, 1925), such as the US EPA models QUAL2 and WASP5 (Ambrose e.a., 1993), represent results of decades long evolution. Most of them were initiated in a nature conservation department, in a university or a consulting company. They were later "enhanced", "expanded" and "improved" while retaining the original variables and processes. This development lead to a model structure which could be best compared to a multilayer sandwich. The "bread" is the basic model serving as a foundation for later consecutive upgrades. For instance, the state variables of QUAL2E can be sorted out into three groups reflecting three distinct stages of model development:

Group 1 (which we may call as phenomenological level).

The traditional Streeter-Phelps state variables: dissolved oxygen (DO) and biological oxygen demand (BOD).

Group 2 (called as biochemical level).

Extended Streeter-Phelps model variables: ammonia (NH_3), nitrate (NO_3), nitrite (NO_2), sediment oxygen demand (SOD).

Group 3 ("ecological level").

Algae model variables: organic nitrogen, organic phosphorus, dissolved phosphorus, algae biomass as chlorophyll-a.

The three groups represent three different concepts of modelling water quality. Streeter-Phelps is a purely phenomenological model, where BOD is not the concentration of a chemical substance but the result of a bioassay test (total oxygen demand of organic material in river water). The models of the next layer (extended Streeter-Phelps and other similar models) have a typical chemical kinetic structure, where a group of first-order reactions represent in a cumulative way the complex chain of processes related to electron transfer in aerobic conditions. Finally, the algae model is of the ecosystem dynamics type which accounts for non-linear growth and decay of phytoplankton and nutrient cycling.

The combination of models of different levels of detail in QUAL2E (and in other models) is done more or less mechanically due to incremental procedure of their development: the older "working and reliable" core models ("bread") were left operational while the model acquired additional state variables and new process descriptions ("butter"). Therefore, these models contain inconsistencies due to lack of uniform underlying concept which in its turn leads to problems with substance mass balances. For example, carbonaceous BOD, being a measure of total bioavailable organic carbon, does not include the organic material in algae biomass. Hydrolysis of particulate organic matter is essentially one process, but the rates of hydrolysis of organic nitrogen and organic phosphorus are different in QUAL2E.

Another drawback of QUAL2E and similar models is the lack of a clear operational definition of the water quality parameters involved in the model. For example, it is known that there are many forms of organic nitrogen present in natural waters. The QUAL2E documentation refers to it as "organic nitrogen" and does not specify further whether it is total organic nitrogen, Kjeldahl nitrogen, particulate, dissolved, bioavailable or other. Stemming from the above features, the usage of conversion factors can not be excluded to communicate among state variables such as DO, chlorophyll-a and nutrient fractions having different units and to keep mass balance as much as possible.

By the contrary, the ASM-1 (Henze e.a., 1987) was developed as a standard model on the basis of experiences gained with a large number of activated sludge models earlier. It contains a precise specification of the variables and utilizes the relatively stable composition of municipal wastewaters. Remarkably, the ASM-1 development effort started by discussing and adopting strict operational definitions for all the state variables and substances included in the model (Grau e.a., 1987). Moreover, it was developed in "one piece" by a coordinated effort of professionals sharing this unified conceptual basis. The variables and processes are distinctly specified and material balances are closed by design. Measurement methods of variables and parameters were also considered. For "non-measurable" components such as bacteria biomass the assumption was made that their range can be obtained through the application of the model to various cases.

In ambient water quality modelling similar standardization efforts have not been carried out so far. The present work can be considered as one of the first steps in this direction (in Germany there are plans to develop a national QUAL type of model). In future, an international effort to develop a unified receiving quality model following the ASM-1 procedure looks more than desired.

3. MODEL STRUCTURE

3.1 State variables

Before one can attempt the comparison of the two different types of models and the consideration of an integrated approach to the entire wastewater-receiving water system, it is necessary to systematize the model state variables. Carbon, nitrogen and phosphorus are the major biogenic elements whose cycle defines the dynamic properties of the majority of freshwater ecosystems as well as that of activated sludge processes. Most water quality models and activated sludge models contain various organic and inorganic forms of carbon, nitrogen and phosphorus as state variables. Table 1 summarizes, after some modifications, the principal state variables of both models (ASM-1 and QUAL2E) contributing to the cycles of the three biogenic elements, so the relationship of the model structures is clear. The table cells are colored according to whether the variable is present in one model, the other or both (see note for Table 1). In addition the schematical representation of the ASM-1 and QUAL2E models components interaction is given in Figure 1.

Analysis of the Table 1 and Figure 1 leads to the observation that more state variables are present in the treatment plant models than in the traditional water quality models. First, in the activated sludge model (ASM-1), as contrasted to QUAL2E, the oxidation agents (heterotrophic and autotrophic bacteria) are accounted for, and second, particulate and dissolved organic matter are considered separately. The additional state variables (bacteria and particulate organic material) are included in ASM-1 because they strongly influence concentration profiles in the activated sludge reactor, especially electron acceptor concentrations (Henze e.a., 1987). Processes in the activated sludge reactors are essentially non-stationary and non-uniform. Major concentration changes occur within the span of tens of meters (tank dimensions) and hours (retention time); the processes are intensified by artificially maintained high concentration of the oxidation agent (bacteria). Stabilization of organic material under such conditions consists of two distinct phases: the primary particulate substrate is removed via hydrolysis and production of a dissolved substrate and then oxygen is depleted due to biomass growth on the dissolved (secondary) substrate. In the aeration tanks, these processes may or may not be separated both in time and space. In natural waterbodies, the spatial and temporal scales are much larger (unless smaller streams with artificial aeration are considered), and the processes usually occur simultaneously and in the same place. Due to relative spatial uniformity and long duration, it is usually possible for the riverine conditions to consider all "fast" variables (including the concentrations levels of the agents and intermediary reaction products) as having reached equilibrium "stabilized" levels. Therefore, models with

fewer state variables ("lumped" models, such as the Streeter-Phelps BOD-DO model) can be used successfully to describe the riverine situation (cf Section 4).

Table 1. Principal state variables of QUAL2E and ASM-1

Note for tables:

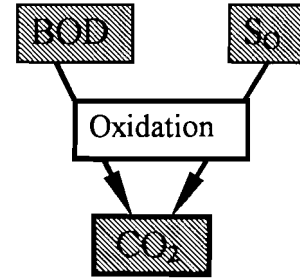
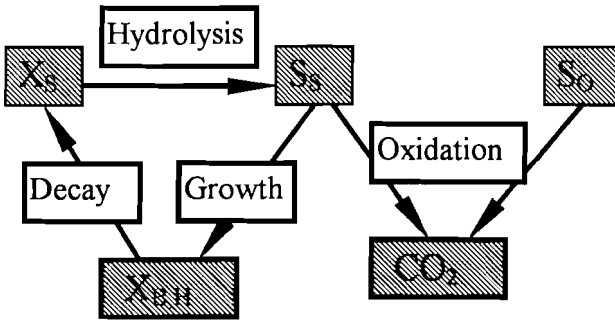
	processes and variables specific for QUAL2E
	processes and variables specific for ASM-1
	processes and variables present in both models

Symbol	Description	Units
S_O	Dissolved oxygen (principal electron acceptor)	mg/l of COD (negative)
S_S	Soluble bioavailable organic matter (principal substrate)	mg/l of COD
X_S	Particulate bioavailable organic matter	mg/l of COD
BOD	Bioassay test of bioavailable carbonaceous organic matter (principal substrate)	mg/l of dissolved oxygen
X_{BA}	autotrophic biomass	mg/l of COD
X_{BH}	heterotrophic biomass (principal electron transfer agent)	mg/l of COD
X_{BP}	algae biomass	mg/l of Chlorophyll "A"
X_{ND}	particulate organic nitrogen (bioavailable)	mg/l of N
S_{ND}	dissolved organic nitrogen (bioavailable)	mg/l of N
S_{NO3}	nitrate nitrogen	mg/l of N
S_{NH}	ammonia nitrogen	mg/l of N
S_{NO2}	nitrite nitrogen	mg/l of N
S_{PO}	dissolved inorganic reactive phosphorus	mg/l of P
X_{PD}	bioavailable particulate organic phosphorus	mg/l of P

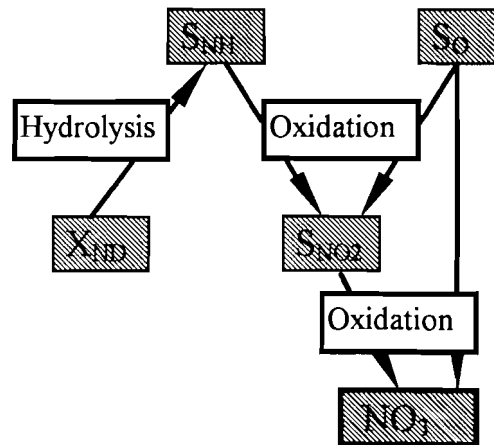
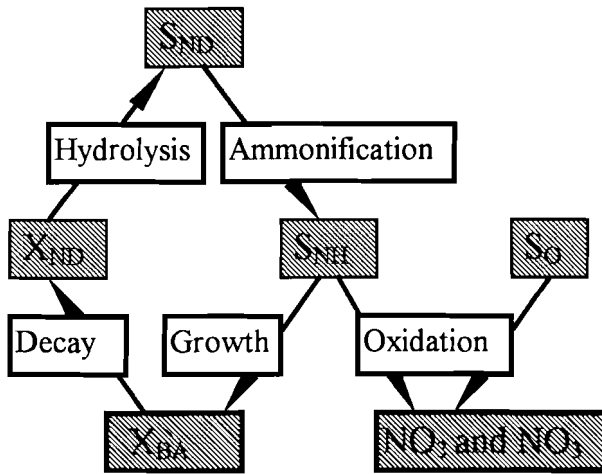
Figure 1. Major processes in QUAL2E and ASM-1.

Activated sludge model

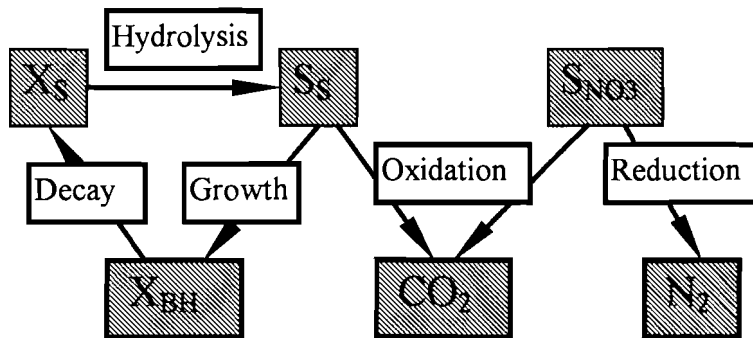
River water quality model



AEROBIC UTILIZATION OF CARBONACEOUS SUBSTRATE



AEROBIC UTILIZATION OF NITROGENOUS SUBSTRATE



NOT PRESENT

ANOXIC UTILIZATION OF CARBONACEOUS SUBSTRATE

On the other hand, ASM-1 does not consider phosphorus and nitrogen as limiting factors for biomass growth. The reason is the high concentration of all biogenic elements in the waste water and the products of its decomposition, so that such limitation would occur only rarely. Moreover, ASM-1 does not consider algae for obvious reasons. It does not incorporate phosphorus either. The second extended version of the ASM model now before completion is more comprehensive in this respect and incorporates phosphorus fractions as state variables. However, the focus is evidently P removal under well designed technological conditions atypical for natural riverine systems.

Of the three major biogenic elements, the carbon and nitrogen cycles in most cases have stronger influence on the organic material oxidation process than phosphorus. Excess phosphorus can cause intensive algae growth (eutrophication) with further influence on dissolved oxygen balance, but this topic has been thoroughly discussed elsewhere (see e.g. Thomann and Mueller, 1987). The decomposition process of algae-produced organic material does not differ substantially from that of organic material of other origin and the same process models can still be used. Thus, subsequently we will restrict our analysis to carbon and nitrogen transformations and their comparison as handled by the two model families.

3.2 Processes

The process descriptions summary (see also Figure 1) are shown in Tables 2-4 in the format used in the original report on ASM-1 (Henze e.a., 1987). The tables are arranged with respect to the major biogenic elements cycles specific both for natural waters and for treatment plants, carbon, nitrogen, and phosphorus (see also Koncsos, 1994). The cells are colored in a way similar to the Table 1. Each column in the Tables 2-4 corresponds to an ordinary differential equation for a state variable listed in the column heading. The right-hand side of the equation is the sum of products of expressions in the columns and coefficients in the same row. Thus, for example, the equation for the BOD (first column in the Table 2) will read:

$$\frac{d}{dt} \text{BOD} = (-1) \cdot (k_1 \cdot \text{BOD}) \quad (1)$$

That is, from the column titled BOD one has to take all non-empty cells and sum them, multiplying by the expressions in the "Coefficients" row. In this case, there is one non-empty cell in the first line which reads "-1" (the first multiplier), and the coefficient reads "k₁ BOD", so the product gives the right-hand side of the equation.

Table 2. Carbon cycle in QUAL2E and IAWQ models.

Process\Variable	BOD	S _s	X _s	X _{BH}	X _{BA}	S _O	Coefficient
BOD oxidation	-1					-1	k ₁ BOD
Hydrolysis		1	-1				k _h f _h X _S /(K _X +X _S /X _{BH})
Aerobic growth of heterotrophs		-1/Y _H		1		-(1-Y _H)/Y _H	μ _H f _s f _{OH} X _{BH}
Anoxic growth of heterotrophs		-1/Y _H		1			η _E μ _H f _{OH} ⁻¹ f _s f _{NO} X _{BH}
Aerobic growth of autotrophs					1	(4.57-Y _A)/Y _A	μ _A f _{NH} f _{OA} X _{BA}
Decay of heterotrophs			1-f _p	-1			b _H X _{BH}
Decay of autotrophs			1-f _p		-1		b _A X _{BA}
Algae decay						-1/α ₁	α ₁ ρX _{BP}
Algae growth						1/α ₁	α ₁ μ _P X _{BP}

Table 3. Nitrogen cycle in QUAL2E and ASM-1 models.

Process\Variable	X _{ND}	S _{ND}	S _{NO3}	S _{NO2}	S _{NH}	S _O	X _{BP}	Coefficient
Hydrolysis (combined with ammonification)	-1				-1			β ₃ X _{ND}
Hydrolysis (dissolving)	-1	1						k _h f _h X _{ND} /(K _X +X _S /X _{BH})
Ammonification		-1			1			k _a S _{ND} X _{BH}
Ammonia oxidation			1		1	-α ₅		β ₁ S _{NH}
Nitrite oxidation			1	-1		-α ₆		β ₂ S _{NO2}
Aerobic growth of autotrophs			1/Y _A		-i _{XB} ⁻ 1/Y _A	see Tab.2		μ _A f _{NH} f _{OA} X _{BA}
Aerobic growth of heterotrophs					-i _{XB}	see Tab.2		μ _H f _s f _{OH} X _{BH}
Anoxic growth of heterotrophs			-(1-Y _H)/ (2.86Y _H)		-i _{XB}			η _E μ _H f _{OH} ⁻¹ f _s f _{NO} X _{BH}
Decay of heterotrophs	i _{XB} ⁻ -f _p i _{XP}							b _H X _{BH}
Decay of autotrophs	i _{XB} ⁻ -f _p i _{XP}							b _A X _{BA}
Algae decay	α ₁					-α ₄	-1	ρX _{BP}
Algae growth			-(1-F)α ₁		-Fα ₁		1	μ _P X _{BP}

Table 4. Phosphorus cycle in QUAL2E model.

Process\Variable	X_{PD}	S_{PO}	S_O	X_{BP}	Coefficient
Hydrolysis	-1	1			$\beta_4 X_{PD}$
Algae decay	α_2		$-\alpha_4$	-1	ρX_{BP}
Algae growth		$-\alpha_2$	α_3	1	$\mu_P X_{BP}$

The summary of the process description comparisons is given in the Table 5.

Table 5. Process descriptions in ASM-1 and QUAL2E.

Subject	ASM-1	QUAL2E
Carbonaceous Substrate	ASM divides carbonaceous substrate into readily available (which is assumed dissolved) and less readily available (which is assumed particulate). The particulate substrate has to be acted upon by an active agent (heterotrophic bacteria) to be made available. The process rate depends on the amount of bacteria present.	Carbonaceous substrate is presented in a "lumped" way (both dissolved and particulate) as a BOD bioassay test result.
Nitrogenous Substrate	Essentially the same representation (particulate and dissolved, with the transition rate dependent on the agent concentration). In addition, an ammonification phase is introduced during which nitrogenous bioavailable substrate (intermediate product) is converted to ammonia (primary nitrogenous substrate) by heterotrophs.	Nitrogenous substrate is represented as particulate organic nitrogen (not bioavailable) and ammonia (readily bioavailable for electron transfer). Conversion (hydrolysis) rate is introduced as a parameter subject to calibration.
Electron Acceptor	Both dissolved oxygen and nitrate are considered as electron acceptors.	Only dissolved oxygen can act as electron acceptor
Oxidation Agent	Two types of agents are considered, autotrophic and heterotrophic bacteria. The heterotrophic bacteria use nitrate and dissolved oxygen as electron acceptors and carbonaceous organic matter as substrate. Autotrophs use only dissolved oxygen as an electron acceptor and only ammonia as substrate.	No direct representation of oxidation agent is provided by the model.
Biogenic Elements Cycle	Only carbon and nitrogen cycles are modelled (they are the most essential for the operation of activated sludge process, phosphorus is abundant and cannot affect biomass growth; see also the text).	Carbon, nitrogen and phosphorus cycles are included since all of them play important role in freshwater ecosystems.

Table 5. Process descriptions in ASM-1 and QUAL2E (continued).

Subject	ASM-1	QUAL2E
Limiting factors	Electron acceptors and substrate availability are the limiting factors. Biogenic elements are abundant and do not limit biomass growth. Ammonia nitrogen is considered as biogenic element (ammonia consumption is modeled), but no ammonia limitation is introduced.	Substrate limitation and biogenic elements limitation are considered. No electron acceptor limitation is taken into account since substrate concentrations are low and acceptor is assumed to be available. Nutrient limitation is considered, since biogenic elements can be scarce.

From Table 5 it follows that the process descriptions in ASM-1 and QUAL2E strongly vary in detail. Since ASM-1 contains more processes, it also contains more parameters (12 rate coefficients in ASM-1 versus 4 in QUAL2E taken without phosphorus cycle). In principle the larger number of parameters in ASM-1 entail more difficulties during model calibration. The authors of ASM-1 reason, however, that since the composition of municipal wastewater is relatively stable, most parameters would remain constant (Henze et al, 1987). Of course local differences are inevitable. Furthermore, industrial contributions, variations in retention time and dilution rate in the sewerage system will also influence the strength and composition of wastewater flowing to the plant. Therefore, both models need to be calibrated (and validated) to data prior to application. In this respect it can be noted that though the overall number of coefficients in ASM-1 is large, only some of them critically influence model behavior and need case-dependent calibration. The model is not sensitive to changes in other parameters and they can be selected from the default range. If we would apply a model of the ASM-1 type to the riverine conditions, the sensitive parameters also would need to be calibrated. Since they depend, among other things, on external and morphological, hydraulic etc. conditions which are different in treatment plant and in natural waters, the range from which they are selected can change from that recommended for wastewater processes modelling (cf. Section 4).

4. APPLICATION OF ACTIVATED SLUDGE MODEL TO SIMULATE RIVER WATER QUALITY

In view of the desirability of developing integrated emission control strategies which consider artificial treatment and natural self purification on common grounds, it seems logical and attractive to try to link the two different types of models or even more to take a model similar to the ASM-1 as a basis for such an approach. However, due to specifics of receiving waters, the model cannot be literally taken "as is". Modifications are certainly needed to reflect differences in processes, factors, rates, compositions and concentration/biomass levels. One such modification is nutrient limitation of bacterial growth since concentration of nutrients in the river water can become quite low. However, principal differences lie in the spatial-temporal scale (days and tens of kilometers instead of hours and tens of meters).

To find out the consequences of change in temporal and spatial scale, ASM-1 was tested in a "riverine" situation on a hypothetical stretch about 50 km long with no additional emissions along the watercourse. Concentrations of 10 mg/l oxygen equivalent of particulate organic material and of 5 mg/l of particulate organic nitrogen were assumed at the upstream end, and oxidation was facilitated by heterotrophic bacteria (initial concentration varied between 1 and 10 mg/l). Additional dissolved oxygen input due to natural reaeration was modeled as a first-order transfer process with a rate of 2 l/day (coefficient K_5 in Eq. (3)). Numeric analysis was made with the help of interactive river water quality modelling system "DESERT" developed in the Water Resources Project of IIASA (Ivanov et al, 1995). Variants of profiles of the state variables are shown in Figures 2-4.

As the objective is the comparison and reconciliation of the two modelling approaches, it is necessary to recall that larger temporal and spatial scales of the riverine situation have important bearing on the behavior of the system. Under certain conditions some processes can behave "fast" in relation to others and can be therefore treated as "stable", i.e. at equilibrium. The dynamics of such a system is essentially controlled by "slow" processes and variables. In the activated sludge model all intermediate substances in principle can play the role of "fast" variables, which leave particulate organic carbon and nitrogen (primary substrate) and dissolved oxygen and nitrate (final electron acceptors) as controlling "slow" variables. In many cases it is possible to formulate a model containing only "slow" variables whose behavior would be similar to that of the original model under asymptotical conditions. This procedure (called model reduction) is widely applied in many areas of physics and mathematics. A long history of successful application of "lumped" models of organic material oxidation in rivers suggests that such full reduction of river water quality models is indeed possible. A note should be made, however, that the reduction leads to loss of accuracy of the model. Depending on the parameter values and on travel time certain state variables (for instance, bacteria biomass) may not reach equilibrium level in considered river stretches (Koncsos e.a., 1994).

Technically, the derivation of the fully lumped, or "reduced" model with 3 parameters is based on the assumption that "fast" variables quickly attain their respective equilibrium levels. (see Appendix 1 for more details). The following model is the result of full reduction:

$$\frac{d}{dt} X_S = - K_1 X_S, \quad (1)$$

$$\frac{d}{dt} X_{ND} = - K_2 X_{ND}, \quad (2)$$

$$\frac{d}{dt} S_O = - K_3 X_S - K_4 X_{ND} + K_5 (S_O^* - S_O), \quad (3)$$

where $K_1 - K_4$ are coefficients defined in Appendix 1,

K_5 is reaeration coefficient (characterizing the physical process of dissolved oxygen diffusion into the waterbody).

This reduced 3-parameter model is equivalent to extended Streeter-Phelps model with BOD divided into two parts, CBOD and NBOD (roughly corresponding to particulate organic carbon and organic nitrogen in the ASM-1). Such reduction implies that organic matter hydrolysis is a relatively slow process, and transformation of dissolved components is relatively fast. This is, of course, an approximation, because consequent oxidation of dissolved nitrogen components requires a certain amount of time (so-called "nitrogen lag"), which is not considered in extended Streeter-Phelps model. Both ASM-1 and QUAL2 do account for the lag between substrate utilization and oxygen consumption, the first by introducing the autotrophic bacteria growth process and the second by representing sequential oxidation of nitrogen species $\text{NH}_3 - \text{NO}_2 - \text{NO}_3$, each stage with its specific first-order decay rate. In addition, ASM-1 introduces the time lag between hydrolysis and oxidation of organic carbon. QUAL2E, however, does not provide for the carbon-related lags since it models organic carbon oxidation as a one-step first order process, having inherited this description from the earlier models of Streeter and Phelps (cf. Introduction).

For QUAL2E, if $\beta_3 \ll \beta_1, \beta_2$ (Table 3), i.e. when the nitrogen oxidation is fast with respect to hydrolysis, intermediate nitrogen components NH_3 and NO_2 can be considered "fast" variables and an asymptotic model of the form (1)-(3) can be derived from QUAL2E in a way similar to previous calculation (in the case of QUAL2E, the phosphorus cycle does not influence the organic decomposition process and the model used for comparison resembles an earlier versions of the same model, QUAL1). Therefore, both QUAL2E and ASM-1 can be approximated by extended Streeter-Phelps model under suitable conditions. The accuracy of the simplified model in each particular case depends on the relationship between the process rates of hydrolysis and oxidation.

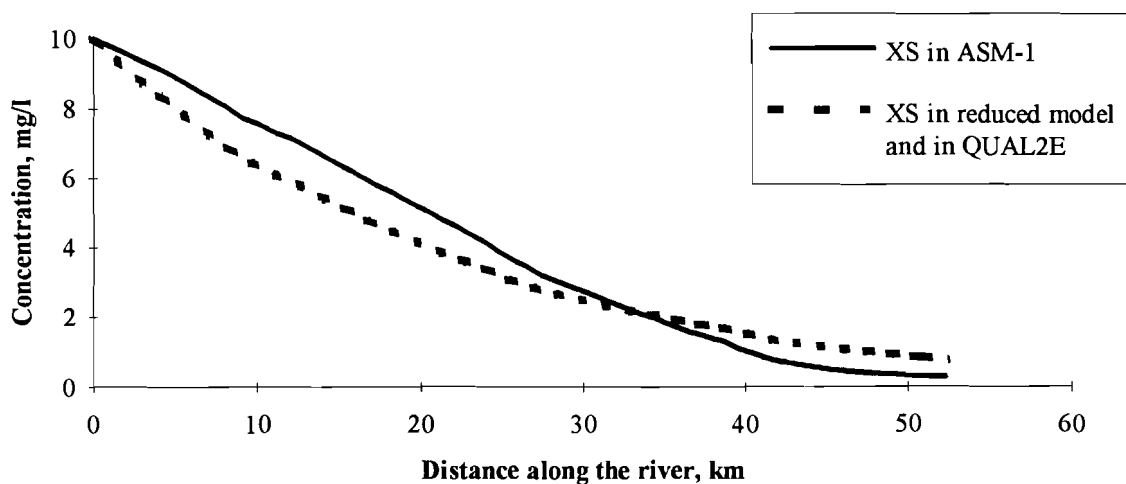


Figure 2. Simulated particulate organic material profiles for ASM-1 with original set of parameters, QUAL2E and reduced model.

Thus, three models of organic decomposition were tested numerically: QUAL2E without phosphorus cycle, ASM-1 using parameters recommended in the IAWPRC report (Henze et al, 1987), and the extended Streeter-Phelps model with parameters selected as shown in Appendix 1 to simulate asymptotic behavior of both of more complex models. The parameters of QUAL2E which correspond to coefficients $K_1 - K_5$ were selected in accordance the respective values of the reduced model, and the rest of the parameters were taken from a list of default values in Brown and Barnwell (1987). Several simulations were made with different initial substance concentrations upstream of the stretch. Subsequently, initial bacteria concentration X_{BH} was selected to get the best accordance for particulate substrate X_S between ASM-1 and the other two models. Resulting concentration profiles for the three models are shown in the Figures 2-5. Particulate substrate is governed by the same equation in QUAL2E and in Streeter-Phelps model, so there are only two profiles in Figure 2.

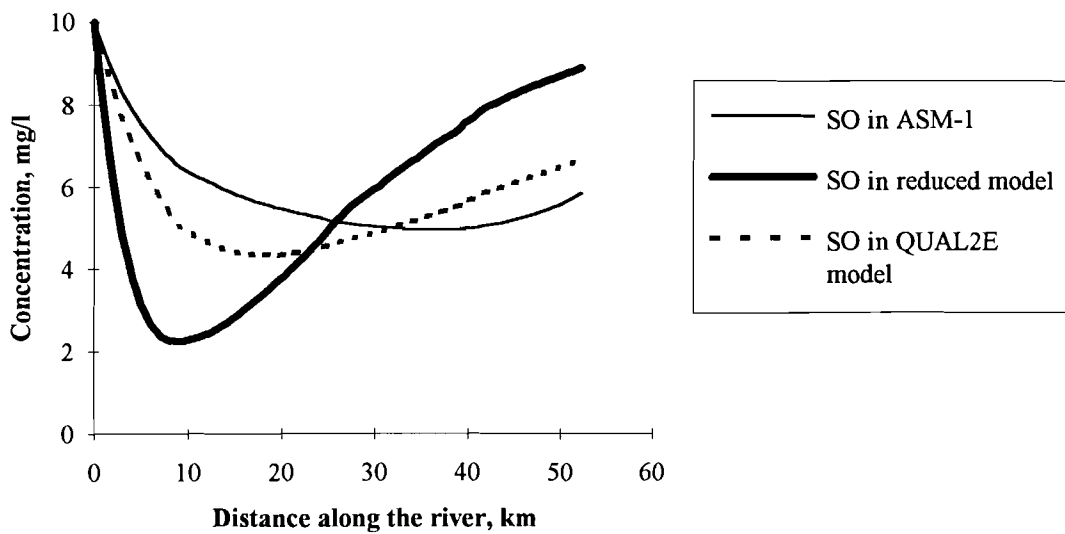


Figure 3. Simulated dissolved oxygen longitudinal profiles for ASM-1, QUAL2E and reduced model.

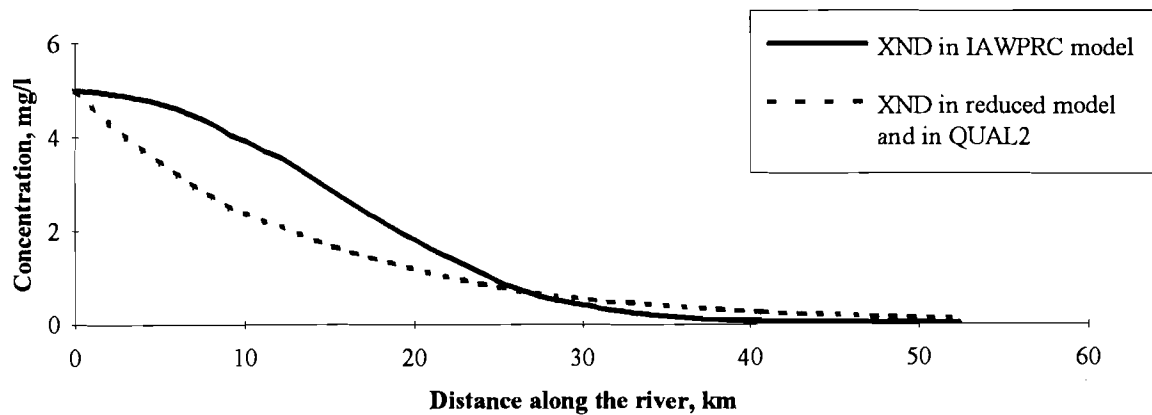


Figure 4. Simulated organic nitrogen longitudinal profiles for ASM-1, QUAL2E and reduced model.

Even while initial data were selected so that the two models perform as closely as possible in terms of the primary substrate, nitrate and dissolved oxygen profiles still differ significantly from each other. Other simulations show that depending on initial bacteria concentrations results are quite different across all concerned parameters. Taken directly, these results could suggest that the two model approaches are unreconcilable: either the ASM-1 cannot be applied to river situation, or Streeter-Phelps model is structurally not suitable to model water quality processes. From practice we know the latter statement is wrong. As to the former, more detailed analysis shows reason for such behavior.

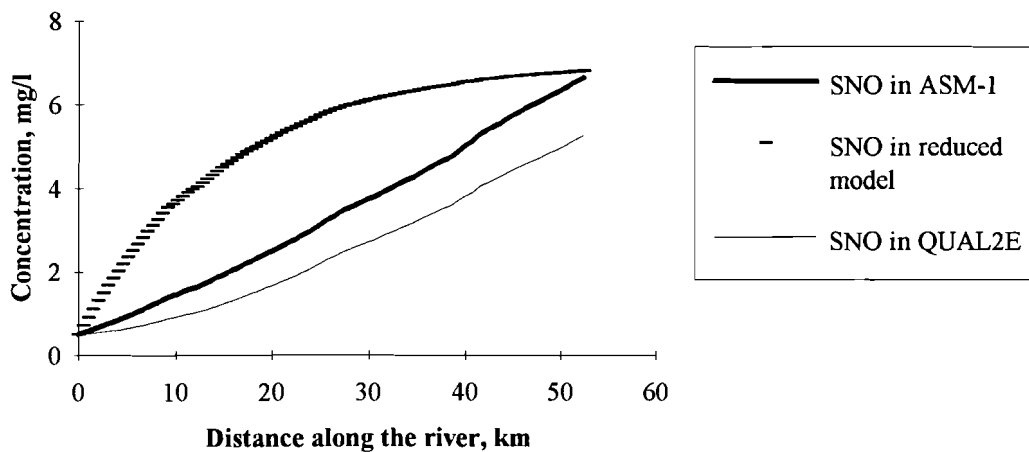


Figure 5. Simulated nitrate longitudinal profiles for ASM-1, QUAL2E and reduced model.

Several additional series of simulations with ASM-1 were performed. These numerical experiments showed that the dissolved substrate (dissolved organic material, dissolved organic nitrogen and ammonia) can virtually always be treated as “fast” variables due to the structure of the system equations. Bacterial biomass, however, was far from equilibrium, actually exhibiting exponential growth. If the same range of parameters were transferred without change from the activated sludge process model to the river water quality model, the models of Streeter-Phelps type would very rarely match the observed data at all, both for the substrate profiles and for the electron acceptor. Moreover, the biomass of bacteria would be much higher than it is actually observed in practice. One harmonizing explanation could be that the parameter values controlling bacteria growth have to be modified for the river conditions. Bacteria growth in the ASM model is controlled by the availability of substrate via the Michaelis-Menten relationship. However, in a riverine environment substrate is a relatively “fast” variable and quickly attains the equilibrium level. In this new “partial equilibrium” situation the control over the bacteria biomass is passed to the amount of particulate organic material available for hydrolysis.

As mentioned earlier, in the activated sludge process substantial changes in concentration of substrate and electron acceptor occur within time span of several hours (retention time of the tank) and spatial scale of tens of meters (the size of the aeration tank). These changes occur due to the intensive decomposition processes involving electron transfer. High agent concentration needed for these high process rates is maintained artificially by pumping

activated sludge from the secondary clarifier back to the tank. In this way, the bacteria concentration as well as the relative concentration of bacterial biomass with respect to particulate organics is held artificially at high level. It can be supposed that the hydrolysis efficiency per unit of bacterial biomass (expressed as k_h parameter in the ASM-1) would be lower in this case as contrasted to the riverine conditions, where the ratio of biomass per food is lower and overall bacteria concentration is small. Maximum bacteria biomass which can be fed per unit weight of organics (reversely proportional to K_X parameter in the ASM-1) should, however, be smaller in the riverine situation because the food had already been partially converted to harder digestible materials in contrast to fresh wastewater in the aeration basin. Of course, actual process rates have to be established individually in each case against field measurements but the general tendency most likely will be the same.

Larger spatial and temporal scale of process occurrence could also have important implications on the possible parameter ranges. For instance, it is easy to demonstrate that in a situation of prolonged growth on the same substrate (which is typical for a river), in order for bacteria to be able to act on the substrate at all, the hydrolysis rate should be larger than at least the bacteria mortality rate divided by the heterotrophic yield coefficient; even more so to ensure stable growth of the bacterial population (Appendix 2). Otherwise, the dissolved organic material production rate (hydrolysis) would be too low to provide bacteria with enough substrate to grow quickly enough to compensate for dieoff. In actual figures this requirement leads to maximal hydrolysis rates of 4-10 1/day, larger than that recommended in the IAWPRC report, 2.2 1/day. Since we observe in most rivers bacterial growth on a substrate actually present in river water, it is likely that this is the situation in riverine environment. To match rates of substrate decomposition observed in practice, the K_X parameter has to be set to a higher value than recommended for the activated sludge model (0.15). If we set the organic material/bacterial biomass ratio to a realistic value of 5, then setting $K_X = 10$ and $k_h = 8$ 1/day would result in the organic removal rate of 0.2 1/day, within the range of typical values for a river. This modification of parameters is consistent with the above mentioned tendencies regarding the concentration of bacteria and composition of food in a river. We can conclude that in order to adjust ASM-1 parameters for a river situation, the suggested ranges of the two hydrolysis parameters K_X and k_h should be changed according to the above notes.

Several series of simulations with the modified hydrolysis parameters ($K_X = 10$, $k_h = 8$ 1/day) were performed with the same conditions as before. Since the bacterial growth was controlled by the hydrolysis process, the results were not strongly influenced by the initial bacterial concentration. Bacterial biomass demonstrated typical "fast variable" behavior in these series profile, quickly attaining an equilibrium level and maintaining this level steadily through the rest of the profile.

The substrate profiles for two of these series are shown in the Figure 6 together with the substrate profile for reduced model and for QUAL2E. Dissolved oxygen and bacterial biomass are plotted in Figures 7 and 8, respectively. Figures 9 and 10 display longitudinal profiles for organic nitrogen and nitrate.

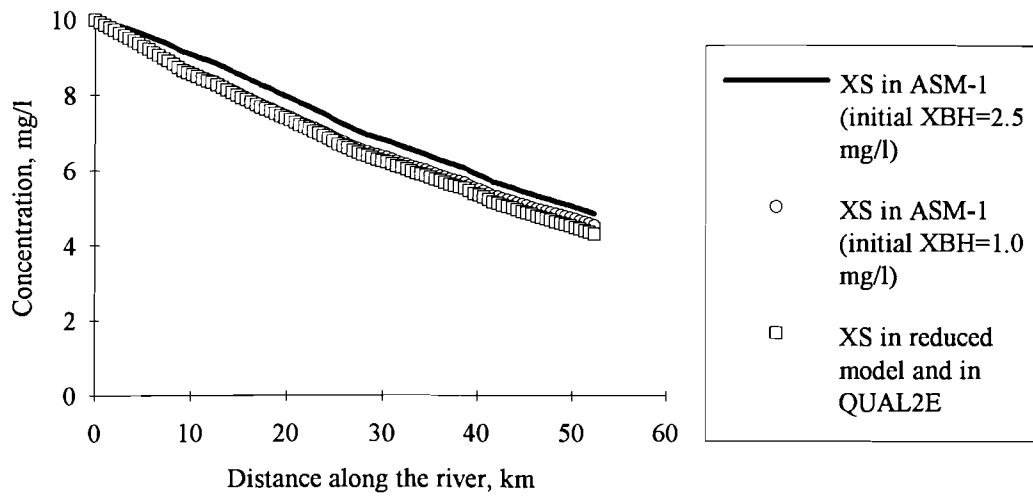


Figure 6. Simulated substrate longitudinal profiles for ASM-1 with modified parameters, QUAL2E and reduced model.

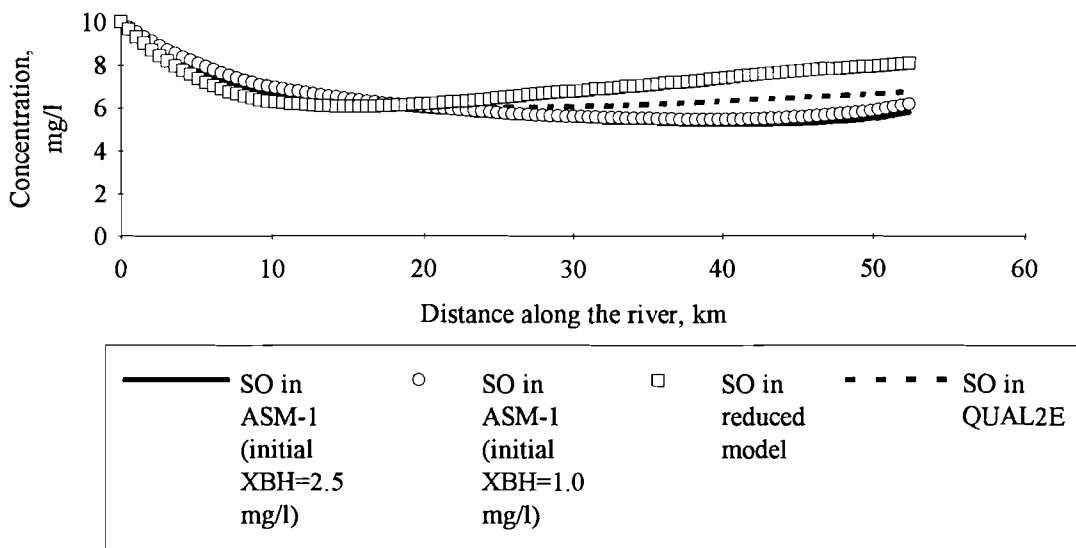


Figure 7. Simulated dissolved oxygen longitudinal profiles for ASM-1 with modified parameters, QUAL2E and reduced model.

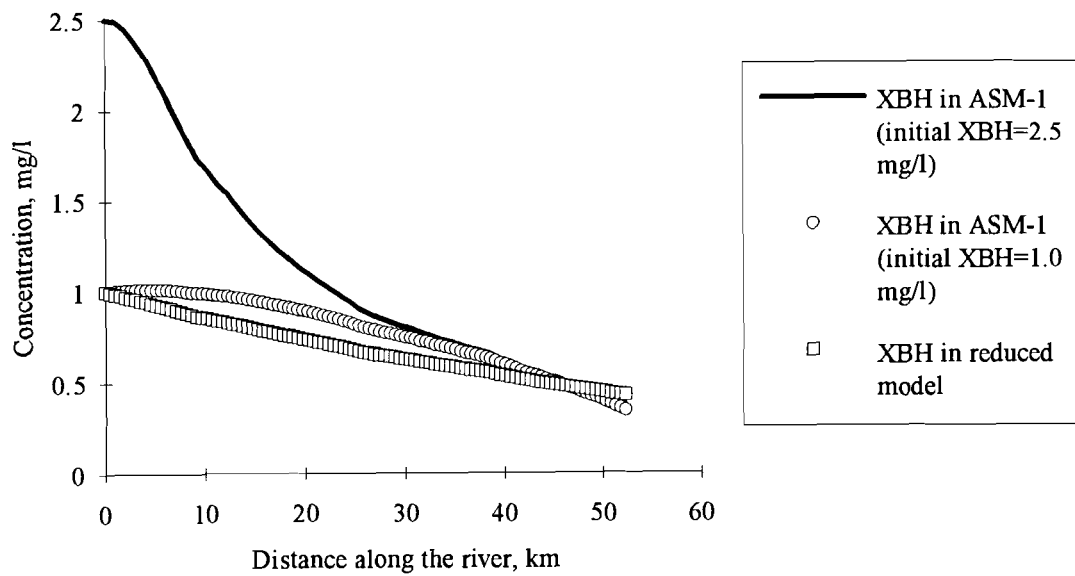


Figure 8. Simulated heterotrophic bacterial biomass longitudinal profiles for ASM-1 and reduced model (not present in QUAL2E).

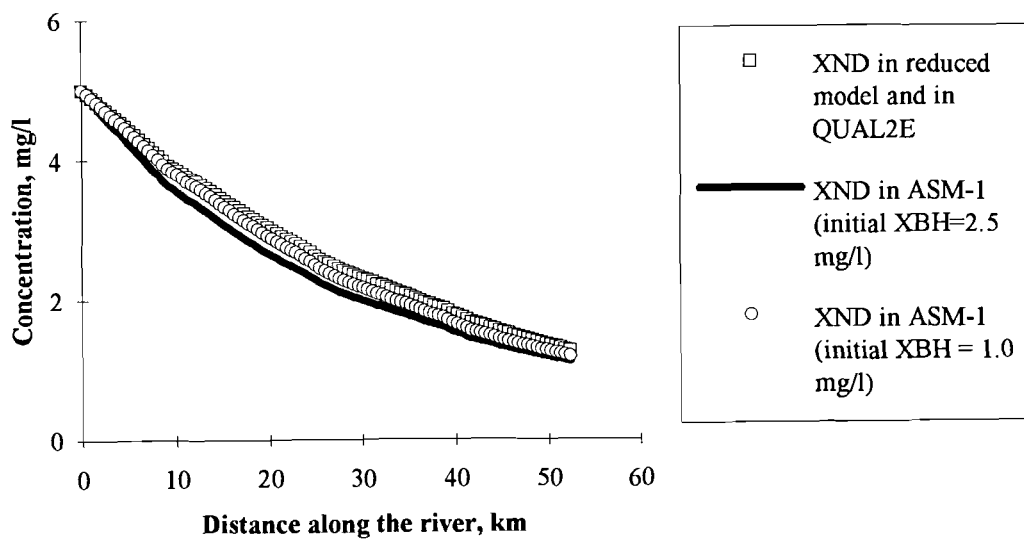


Figure 9. Simulated organic nitrogen longitudinal profiles for ASM-1, QUAL2E and reduced model.

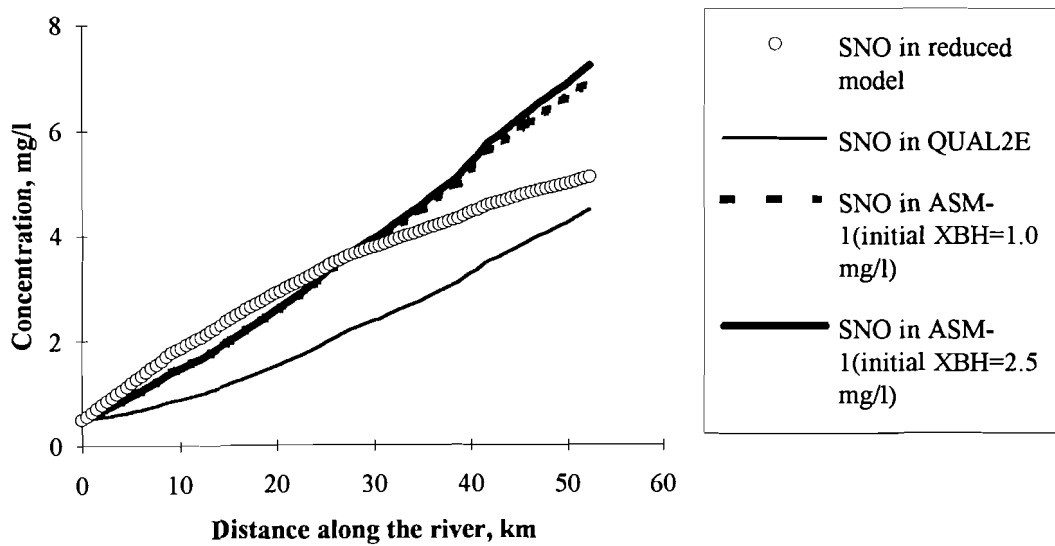


Figure 10. Simulated nitrate longitudinal profiles for ASM-1 with modified parameters, QUAL2E and reduced model.

As one can see from Figures 6-10, the reduced model (extended Streeter-Phelps) can accurately reproduce the behavior of more complex models in asymptotical case, i.e. the case of spatial and temporal uniformity of driving forces (e.g. no emissions). When there are abrupt concentration changes (instream emissions or temporal changes of upstream boundary conditions), the situation may change.

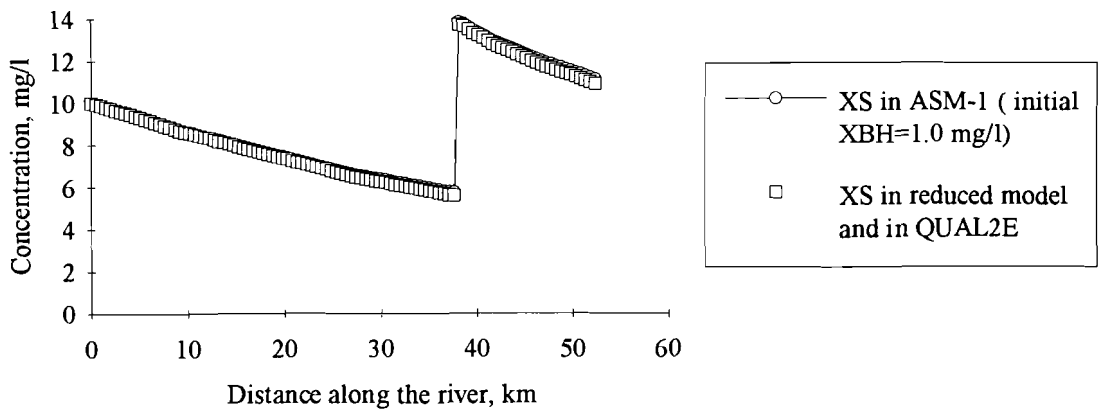


Figure 11. Simulated particulate organics longitudinal profiles for ASM-1 with modified parameters, QUAL2E and reduced model.

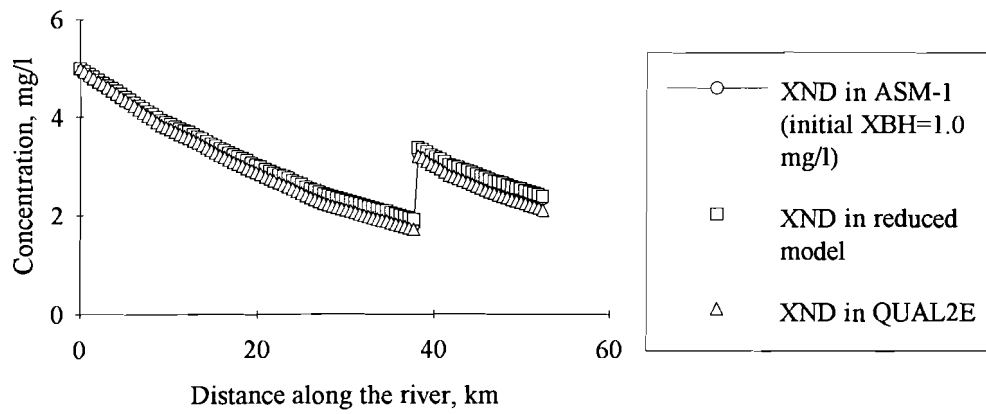


Figure 12. Simulated organic nitrogen longitudinal profiles for ASM-1, QUAL2E and reduced model.

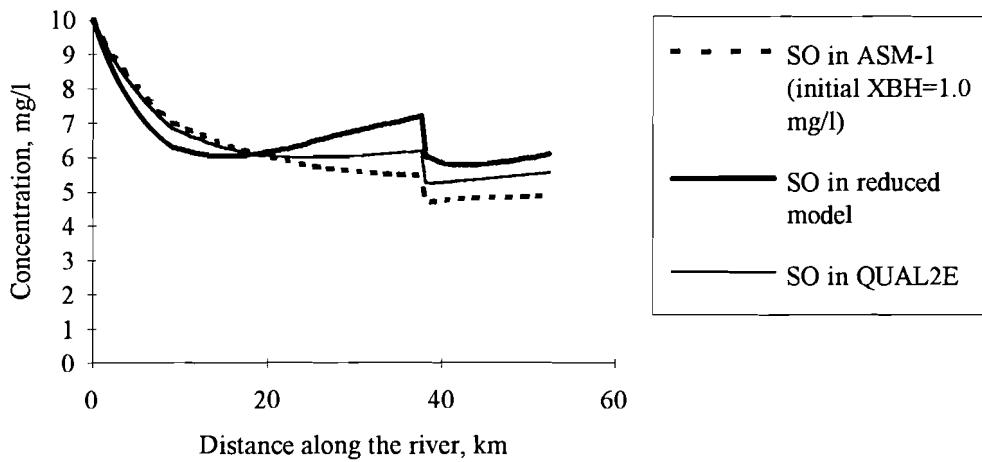


Figure 13. Simulated dissolved oxygen longitudinal profiles for ASM-1 with modified parameters, QUAL2E and reduced model.

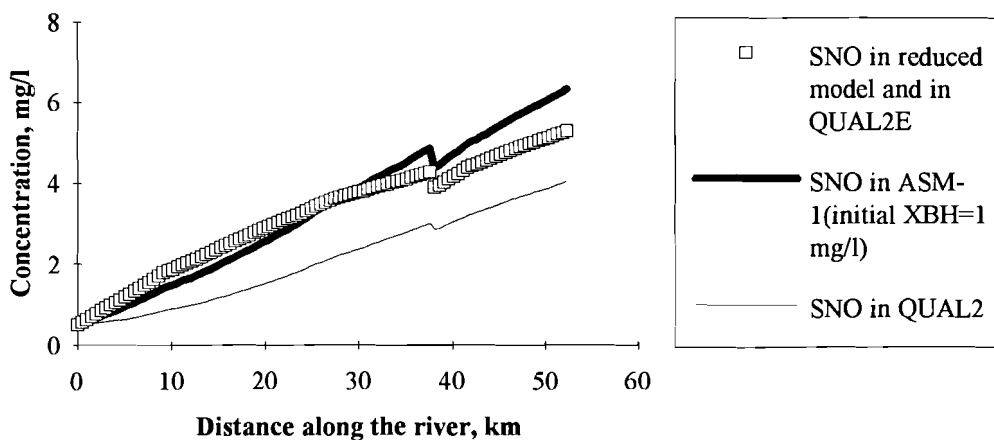


Figure 14. Simulated nitrate longitudinal profiles for ASM-1 modified parameters, QUAL2E and reduced model.

In subsequent simulations shown on Figures 11-14, a relatively large emission was introduced to the stretch of the river, causing abrupt changes of the instream concentrations. As a result, the overall accuracy of reduced model representing more complex models behavior was significantly lower. However, the substrate profiles (Figures 11 and 12) were reproduced much better than electron acceptor profiles (Figures 13 and 14). This is in harmony with the well-known observation from the practice of modelling activated sludge treatment plants (Henze et al, 1987) that for accurate simulation of acceptor profiles the oxidation agent (bacteria) is needed as a state variable of the model. Therefore in situations with sudden (spatial or temporal) changes, like the modelling of accidents, spills, the impact of floods etc., use of more complex model will be preferred to simplified ones such as Streeter-Phelps.

5 DISCUSSION

As is shown in the Figures 11-14, the reduced model (Streeter-Phelps) differs from the original model (ASM-1) when confronted with a non-uniform instream or upstream conditions (emissions or temporal changes). In practice the situations when emissions and other factors cause drastic changes in concentrations may occur in channels, small rivers, or in upper sections of a larger river, where sewage discharge may constitute a significant portion of streamflow and travel time is small (for instance, sections of Upper Ruhr; Koncsos e.a., 1994). In such river conditions application of ASM-1 and its modifications could improve the accuracy of model prediction. For lowland rivers (like the Ohio River for which the Streeter-Phelps model was originally applied) such situation would not be typical. The Figure 13 shows a deviation of dissolved oxygen concentration of 1-2 mg/l. Depending on the situation, the deviation may be even more significant and has to be considered in the model selection procedure.

Another example of possible use of ASM-1 for rivers is the sediment processes model. The river sediment in many cases have a significant influence on a surface water quality through sediment oxygen demand and release of substances like phosphorus, methane, and hydrogen sulfide. Up to now, our understanding of the river sediment processes is relatively poor, and most of the models are semi-empirical in nature (cf. Di Toro et al, 1990). Since organic material and biomass concentration in sediment is high, one may expect to apply ASM-1 type of approach to this case in the form close to the original formulation.

If the situation requires application of a more complex model, data availability and calibration could become an issue. As the calibration is considered, sensitivity tests would indicate the most important parameters which should be calibrated against data, and the rest of the parameters could be selected from the default range. When data is scarce and error corrupted, Monte-Carlo based procedures such as Hornberger-Spear-Young (HSY) methodology (Hornberger and Spear, 1984; Masliev and Somlyódy, 1994; Koncsos e.a., 1994) could be used for the model calibration. It should be mentioned that the HSY type methods allow not only parameter estimation against error corrupted data, but to a certain extent account for uncertain model structure.

With the model as complex as ASM-1 not only data scarcity but also measurability of certain parameters (for instance, X_{BH}) can be a problem. In most cases the bacteria biomass concentration is not known. To circumvent the problem, the model itself can be used to estimate bacteria biomass under certain assumptions (Koncsos e.a., 1994). Using the ASM-1, the outcome of a BOD test can be predicted if the initial concentrations of X_S , X_{BH} , S_S are known and nitrification does not occur. If we assume that $S_S=0$ or that S_S comprises a known portion of X_S , then we have two unknown parameters (initial X_S and X_{BH}). To find the unknowns we have two known quantities - COD (total organic material) and BOD which equals total oxygen consumption during the test. Optimization procedures like least-squares method can be used to solve the inverse problem at hand.

6 CONCLUSIONS

- During the evolutionary development of traditional water quality models in the course of the past three decades or so, state variables and processes were not introduced in a systematic, coordinated way. As a result, there are a number of incongruities. The IAWPRC/IAWQ activated sludge model, on the contrary, were developed in a single coordinated effort at the mid 1980s in a conceptually harmonized framework. It seems useful to reconcile these two model approaches - their state variables, rates, and process descriptions for the aim of integrating emission control strategies based on the unified description of treatment technological processes and "self-purification" in natural receiving waters. An international standardization effort similar to the development of ASM-1 looks more than desired for ambient water quality models.
- Test simulations show that a model similar to ASM-1 can simulate water quality in rivers. Due to differences in spatial and temporal scale, concentration ranges, and environmental conditions, some changes must be introduced into the model. They include the introduction of nutrient limitation and modification of rate coefficients controlling hydrolysis.
- In riverine situations, several state variables of the modified ASM-1 have properties of "fast" variables (in the sense of system control engineering). The systems dynamics is controlled by particulate organic material and electron acceptor (dissolved oxygen or nitrate). The other variables quickly attain "quasi-equilibrium" level. Assuming quasi-equilibrium, the ASM-1 can be reduced to a phenomenological model similar to Streeter-Phelps.
- Models of "reduced" type (Streeter-Phelps and its extensions) will be most appropriate when there are no abrupt changes in environmental conditions, loads, hydraulics etc. so that "fast" variables are able to attain their quasi-equilibrium levels. Such situations are likely to occur in the lower sections of rivers, in large rivers, reservoirs etc. In the spatially inhomogenous waterbodies or when rapid temporal changes take place (small rivers,

channels, large emissions), the performance of models of ASM-1 type is expected to be better than that of "reduced" models. Another possible area of application of the complex models such as ASM-1 is the simulation of the processes in the river sediment, where concentration ranges are closer to that occurring during wastewater treatment.

- Selection of simple versus more complex models should be based on environmental conditions, admissible model inaccuracy, data availability, and computational resources. Non-measurable parameters such as bacteria biomass could be estimated using the measured concentrations and the model itself. This inverse problem can be solved using conventional optimization methods. When data is scarce and error corrupted, probabilistic methods for parameter estimation such as Hornberger-Spear-Young should be used to account for uncertainty in data. For simple models these techniques allow also to take into account inadequate model structure at a price of more uncertain prediction.

LIST OF NOTATIONS

State variables

S_O - dissolved oxygen, mg/l

S_S - soluble bioavailable organic matter, mg/l of COD

X_S - particulate bioavailable organic matter, mg/l of COD

BOD - bioassay test of bioavailable carbonaceous organic matter, mg/l of dissolved oxygen

X_{BA} - autotrophic biomass mg/l of COD

X_{BH} - heterotrophic biomass, mg/l of COD

X_{BP} - algae biomass, mg/l of dry biomass

X_{ND} - particulate bioavailable organic nitrogen, mg/l of N

S_{ND} - dissolved bioavailable organic nitrogen, mg/l of N

S_{NO_3} - nitrate nitrogen, mg/l of N

S_{NH} - ammonia nitrogen, mg/l of N

S_{NO_2} - nitrite nitrogen, mg/l of N

S_{PO} - dissolved inorganic reactive phosphorus, mg/l of P

X_{PD} - bioavailable particulate organic phosphorus, mg/l of P

Stoichiometry

K_X - parameter of hydrolysis limitation by bacterial biomass (dimensionless)

Y_H - heterotrophic yield (dimensionless)

Y_A = autotrophic yield (dimensionless)

f_P - part of biomass which is particulate, dimensionless

i_{XB} - part of biomass which is nitrogen, dimensionless

i_{XP} - part of dead biomass which is nitrogen, dimensionless

α_1 - part of algae which is nitrogen, dimensionless

α_2 - part of algae which is phosphorus, dimensionless

α_3 - rate of oxygen production per unit of algal photosynthesis, mgO / mg dry biomass

α_4 - rate of oxygen uptake per unit of algae respired, mgO / mg dry biomass

α_5 - rate of oxygen uptake per unit of ammonia nitrogen oxidation, mgO / mg N

Half saturation constants

K_{OH} - oxygen half saturation concentration for heterotrophic growth, mg/l

K_{OA} - oxygen half saturation concentration for autotrophic growth, mg/l

K_{NH} - ammonia half saturation concentration for autotrophic growth, mg/l

K_S - substrate half saturation for heterotrophic growth, mg/l

K_{NO} - nitrate half saturation for heterotrophic growth in anoxic conditions, mg/l

Rates

μ_H - maximal growth rate of heterotrophic bacteria, 1/day

μ_A - maximal growth rate of autotrophic bacteria, 1/day

b_H - mortality rate of heterotrophic bacteria, 1/day

b_A - mortality rate of autotrophic bacteria, 1/day

k_h - maximal hydrolysis rate, 1/day

k_a - maximal ammonification rate, 1/day/(mg/l)

K_5 - reaeration rate, 1/day

k_1 - BOD decay rate, 1/day

μ_P - growth rate of algae, 1/day

ρ - algae respiration rate, 1/day

β_1 - rate of oxidation of ammonia nitrogen, 1/day

β_2 - rate of oxidation of nitrite nitrogen, 1/day

β_3 - rate of organic nitrogen hydrolysis, 1/day

External conditions

S_O^* - saturation oxygen level, mg/l

Factors

η_g - correction factor for growth under anoxic conditions

η_h - correction factor for hydrolysis under anoxic conditions

f_{OH} - factor for oxygen limitation of heterotrophic growth:

$$f_{OH} = S_O / (S_O + K_{OH})$$

f_{OA} - factor for oxygen limitation of autotrophic growth:

$$f_{OA} = S_O / (S_O + K_{OA})$$

f_{NH} - factor for ammonia limitation:

$$f_{NH} = S_{NH} / (S_{NH} + K_{NH})$$

f_S - factor for substrate limitation of heterotrophic growth:

$$f_S = S_S / (S_S + K_S)$$

f_{NO} - factor for nitrate limitation for heterotrophic growth in anoxic conditions:

$$f_{NO} = S_{NO} / (S_{NO} + K_{NO})$$

f_h - factor for hydrolysis:

$$f_h = f_{OH} + \eta_h f_{NO} f_{OH}^{-1}$$

F - fraction of algae ammonia uptake

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APPENDIX 1. DERIVATION OF THE "REDUCED" QUASI-EQUILIBRIUM WATER QUALITY MODEL

In order to derive the "reduced" model, let us suppose that bacteria and dissolved substrate quickly attain equilibrium level. According to general principles of dynamic systems, levels of quasi-equilibrium are attained at points where the time derivative of the respective variable is close or equal to zero.

Let us denote X_{BH}^* as the equilibrium level of heterotrophic bacteria concentration and S_s^* as the equilibrium level for the dissolved substrate. For heterotrophic bacteria we have the governing equation

$$\frac{d}{dt} X_{BH} = \mu_H \frac{S_s}{K_s + S_s} f_H X_{BH} - b_H X_{BH}; \quad (1)$$

therefore, the equilibrium condition

$$\mu_H \frac{S_s^*}{K_s + S_s^*} f_H X_{BH}^* - b_H X_{BH}^* = 0, \quad (2)$$

i.e., the processes of the growth and decay of bacteria are compensated by each other. For the dissolved substrate, similarly, the equilibrium condition is

$$-\frac{1}{Y_H} \mu_H \frac{S_s^*}{K_s + S_s^*} f_H X_{BH}^* + k_h f_h \frac{X_s}{K_x + \frac{X_s}{X_{BH}^*}} = 0, \quad (3)$$

i.e., substrate release from hydrolysis has to be offset by heterotrophic uptake. Substituting the first term in (3) (bacterial uptake) using (2), we obtain

$$-\frac{1}{Y_H} b_H + k_h f_h \frac{X_s}{K_x X_{BH}^* + X_s} = 0 \quad (4)$$

from which it follows that the bacterial biomass at equilibrium is equal to

$$X_{BH}^* = \frac{X_s}{K_x} \left(\frac{k_h f_h Y_H}{b_H} - 1 \right) \quad (5)$$

Note that in order for X_{BH}^* to be positive, the term in parenthesis in the Eq. (5) has to be positive, which means that certain conditions on the relationship between model parameters should hold. It is easy to prove (Appendix 2) that if the opposite is true (and X_{BH}^* is negative), bacteria concentration is limited by the initial concentration of substrate at all times. Effectively it means the exponential dieoff of bacteria due to the inability to break down particulate organics fast enough to provide themselves with dissolved substrate. This is unlikely to be observed in natural waters, usually abundant with bacteria. Therefore, the aforementioned conditions are satisfied in all practically interested cases.

Let us denote this key parameter as α :

$$\alpha = \frac{k_h f_h Y_H}{b_H} \quad (6)$$

It is a positive dimensionless number (see above), most likely in the range of 0.5-5. Assume for estimations $\alpha=1$. Together with parameter K_X it defines ratio of bacterial biomass to particulate organic material:

$$\frac{X_{BH}^*}{X_S} = \frac{\alpha}{K_X} \quad (7)$$

Since this ratio is of the order of 0.1-0.2, the K_X parameter for a typical riverine situation is most likely in the region of 5-10 (depending on the actual parameter values).

In a similar way we can derive the equilibrium level for autotrophic bacteria:

$$X_{BH}^* = \frac{\alpha b_H \left(\frac{X_{ND}}{Y_H} + i_{XB} X_S \right)}{K_X b_A \left(i_{XB} + \frac{1}{Y_A} \right)} \quad (8)$$

The equations for the "slow" or "controlling" state variables can be obtained by substituting the fast variables in the governing equation with their respective equilibrium levels. If we neglect the contribution of the autotrophic bacterial biomass to the particulate organics mass balance (in practice, a safe enough assumption), then the equation for particulate organic material takes a familiar form of exponential decay, like in a Streeter-Phelps model:

$$\frac{d}{dt} X_S = -K_1 X_S \quad (9)$$

where the rate K_1 is linear with respect to the α value:

$$K_1 = \frac{\alpha b_H}{K_X} \left(\frac{1}{Y_H} - (1 - f_p) \right) \quad (10)$$

For particulate organic nitrogen, a similar equation is correct:

$$\frac{d}{dt} X_{ND} = - K_2 X_{ND}, \quad (11)$$

if we neglect the organic nitrogen contribution from the heterotrophic bacteria decay (again, in riverine situation, a viable assumption). The first-order decay rate K_2 is proportional to α :

$$K_2 = \frac{\alpha b_H}{K_X Y_H} \left(\frac{\frac{1}{Y_A} + f_p i_{XP}}{\frac{1}{Y_A} + i_{XB}} \right) \quad (12)$$

The dissolved oxygen equation would then read similar to the extended Streeter-Phelps model:

$$\frac{d}{dt} S_O = - K_3 X_S - K_4 X_{ND}, \quad (13)$$

where the rates K_3 and K_4 are defined as follows:

$$K_3 = \frac{\alpha b_H}{K_X} \left(\frac{1 - Y_H}{Y_H} \frac{f_O}{f_H} + \frac{4.57 - Y_A}{Y_A} \frac{i_{XB}}{\frac{1}{Y_A} + i_{XB}} \right) \quad (14)$$

$$K_4 = \frac{\alpha b_H}{K_X} \left(\frac{1}{Y_H} \frac{4.57 - Y_A}{Y_A} \frac{1}{\frac{1}{Y_A} + i_{XB}} \right) \quad (15)$$

Similar linear differential equation can be derived for nitrate nitrogen. If the omitted terms would be taken into account, the reduced model will still be linear, but the equation for X_S and X_{ND} will contain both X_S and X_{ND} in the right-hand sides.

APPENDIX 2. INEQUALITY IMPOSED ON THE HYDROLYSIS COEFFICIENTS IN QUASI-EQUILIBRIUM CONDITIONS

Let us sum the two governing equations, that for heterotrophic bacteria X_{BH} and for dissolved substrate S_S multiplied by heterotrophic yield Y_H . The term with bacterial growth will cancel out. For the combined variable $X_{BH} + S_S Y_H$ we will have the following differential equation:

$$\begin{aligned} \frac{d}{dt}(X_{BH} + S_S Y_H) &= Y_H k_h \frac{X_S}{K_X + \frac{X_S}{X_{BH}}} f_h - b_H X_{BH} = \\ &= \left(\frac{Y_H k_h f_h}{b_H} \frac{X_S}{K_X X_{BH} + X_S} - 1 \right) X_{BH} b_H \end{aligned} \quad (16)$$

Since X_{BH} is positive (being a concentration), the following inequalities hold:

$$\frac{X_S}{K_X X_{BH} + X_S} < 1 \quad (17)$$

and

$$Y_H k_h f_h \frac{X_S}{K_X X_{BH} + X_S} < Y_H k_h f_h. \quad (18)$$

Therefore, if $Y_H k_h f_h < b_H$, then the right-hand side of the Eq. (16) is always negative and the combined variable $X_{BH} + S_S Y_H$ is monotonically decreasing, asymptotically reaching zero. In this case there is no bacteria growth; rather, it is a case of bacteria dieoff caused by inability of heterotrophs to break down particulate organics fast enough to provide themselves with dissolved substrate.