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Modelling River Water Quality for System-Wide Benchmark Simulation Models

Ramesh Saagi

Division of Industrial Electrical Engineering and Automation
Faculty of Engineering, Lund University

MODELLING RIVER WATER QUALITY
FOR
SYSTEM-WIDE BENCHMARK SIMULATION MODEL

Ramesh Saagi
Lund University, Sweden

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Abstract

System-wide evaluation of urban wastewater systems (UWS) has been increasingly recognized as a necessary step to optimize the operation of sewer and wastewater treatment plants in order to achieve improved river water quality. Modelling and optimization of control strategies on an UWS level are one of the ways to improve river water quality in an effective manner using existing infrastructure or in tandem with planned expansions. Benchmark simulation models (BSMs) are being widely used for process and control modelling in wastewater treatment plants. A spatial expansion of the plant-wide BSM2 is envisioned to make it suitable to study integrated control strategies. The BSM2 will be integrated with the catchment, sewer system and river quality models. In this context, the report aims at the selection of river quality model used for the system-wide BSM. It describes briefly various river water quality models available and delves into details of two commonly used river quality models (Duflow and River Water Quality Model No. 1 (RWQM1)). Finally, RWQM1 is chosen, some simplifications are made and implemented in MatLab. This will further be integrated with BSM2 and its sewer and catchment extension.

1. Introduction

Urban wastewater infrastructures, like sewers and wastewater treatment plants (WWTPs), are generally operated and optimized individually in spite of the similarity in objectives of both systems. One of the common goals of these systems is the reduction of any harmful impacts of discharges on receiving waters. Different indirect measures like overflow reduction for combined sewer overflows (CSOs) and high effluent quality for WWTPs are used to achieve this objective. These criteria do not take into consideration the interactions between the sewer and WWTP. Hence, individual operations can lead to sub-optimal achievement of the objective. In this regard, it is necessary to understand the interactions and also evaluate various holistic approaches to achieve system-wide objectives. Integrated modelling of urban wastewater system (UWS) has evolved as a major modelling tool to perform evaluation of these systems with an objective to improve receiving water quality. Various modelling tools and approaches are currently available (Rauch et al., 2002).

One such tool that is currently under development is the system-wide extension of the Benchmark Simulation Model No. 2 (BSM2). BSMs are simulation tools for benchmarking of wastewater treatment plant control strategies (Gernaey et al., 2014). Initially, this toolbox focused only on the activated sludge line (BSM1, BSM1_LT). It was further extended and a plant–wide BSM, which also includes pretreatment and sludge handling, was developed (BSM2). Currently, BSM2 is being improved to enhance the description of plant-wide models and also to include other subsystems of the UWS (Jeppsson et al., 2013). Looking outside the fence of WWTPs to include the sewer system and river in the evaluation of control strategies is driven by the need for integrated evaluation.

In this regard, BSM2 has been extended spatially to include the sewer and catchment network. The upstream sewer is now linked to the WWTP and control operations for the extended system are demonstrated (Saagi et al., 2014). The next logical step is to include the river water quality model and link it to the sewer plus WWTP extended BSM.

2. Objective

The objective of this article is to identify a suitable river water quality model for the system-wide BSM.

The following characteristics are identified as necessary features for the river quality model to be used in the system-wide BSM.

1. Ability to describe dynamics of dissolved oxygen, organic matter and nutrients (nitrogen and phosphorous) under the influence of wastewater discharges from WWTP and sewer system.

2. Ease of information exchange with existing activated sludge models for WWTPs.

3. Mass conservation of COD as well as individual elements especially C, N and P.

3. State of the art

The origin of river water quality models began in 1925 when Streeter and Phelps (1925) described the dissolved oxygen (DO) changes observed in a river due to discharge of organic matter. It is a simple model that describes the processes that affect oxygen concentration in a river. The model can describe the DO sag curve generally occurring in rivers due to discharge of organic matter. The next major improvement in river water quality models was the USEPA QUAL family of models. QUAL2E is developed after a series of modifications to QUAL-1 and QUAL-11 models (Brown and Barnwell, 1987). It includes various processes that effect the concentration of oxygen, organic matter and nutrients. It describes interactions between nitrogen, phosphorous, dissolved oxygen and also algae. The model has been further developed and QUAL2K is the latest version in use (Chapra et al., 2008). QUAL2K has improved conversion processes like biological oxygen demand (BOD) speciation, anoxia, sediment-water interactions, bottom algae and pathogens in comparison to QUAL2E. Water quality analysis simulation program (WASP) also developed by USEPA is another commonly used model for river quality modelling (Di Toro et al., 1983). Unlike other models, WASP is a platform that provides a choice between different kinds of modelling options for flow (1D, 2D etc.) and biochemical conversions (linear, nonlinear kinetics). It allows a compartmental approach giving users a great degree of flexibility. WASP7 is the latest in a series of WASP models (Wool et al., 2001). It includes eutrophication module, organic chemical module and a mercury model. Additional models like hydrodynamic flow models and sediment models can also be linked to it. The Duflow water quality model developed by Lijklema (1996) is one of the models currently being used in UWS analysis. It is available in commercial softwares like WEST and SIMBA. Another model that is currently available is the River Water Quality Model No. 1 (RWQM1) (Reichert et al., 2001a). This model is the result of an IWA task group set up to identify the missing gaps in river quality models and to build a river model that can be linked to the activated sludge family of models. Duflow and RWQM1 are two commonly used models for different integrated UWS evaluation studies (e.g. Reichert et al., 2001a; Langeveld et al., 2013) and hence described in more detail below.

3.1. Duflow river quality model

Duflow is a simulation engine that consists of modules to simulate the hydraulics and biochemical processes taking place in a river (Stowa/MX Systems, 2004). The quality model developed at Wageningen University is aimed at simulating dissolved oxygen, organic matter and ammonia dynamics in a river. The model described below is based on the current implementation of the Duflow quality model in WEST.

State variables

Major state variables included in the model are dissolved oxygen (DO), organic substrate (divided into different components) and ammonium (NH_4) (Table 1).

Organic substrate is described by chemical oxygen demand (COD) and biological oxygen demand (BOD). Measured BOD and COD values can be used to define the organic substrate state variables for the model. BOD is fractionated into BODfast and BODslow. A fraction of the remaining COD (COD-BOD) is also available as BODslow. BODfast is divided into state variables BOD1 (readily biodegradable fraction) and BOD1p (particulate fraction). Similarly BODslow is also divided into BOD2 and BOD2p state variables. Hence organic substrate is represented by four state variables namely BOD1, BOD1p, BOD2 and BOD2p (Figure 1). Additionally, a temporary sediment oxygen demand is described to model the effect of delayed oxygen consumption due to wastewater discharges into a river.

Table 1: List of state variables for the Duflow river quality model

Definition	Notation
Oxygen	O_2
Soluble fast biodegrabale substrate	BOD1
Particulate fast biodegradable substrate	BOD1p
Soluble slowly biodegradable substrate	BOD2
Particulate slowly biodegradable substrate	BOD2p
Ammonium nitrogen	NH4
Temporary sediment oxygen demand	BODs

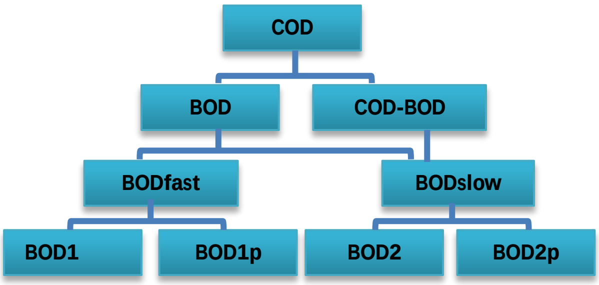

Figure 1: Classification of state variables for the Duflow river quality model in WEST

Biological processes

1. Oxidation of organic substrate: Organic substrate is oxidized in the presence of oxygen. It is the major contributor for oxygen depletion in the river. The rate of oxidation depletion depends linearly on the availability of substrate. The dependence on oxygen is described by Monod kinetics. Biomass is not considered as a state variable. It is assumed that sufficient biomass is always present and oxidation is not limited by the availability of biomass. Oxidation processes are described both in the bulk water phase and the sediment phase.

1.1. Bulk water phase: All BOD state variables are oxidized in the bulk water phase. The rate of oxidation varies between BODfast (BOD1, BOD1p) and BODslow (BOD2, BOD2p) state variables with BODfast decay rate being higher than that of BODslow.

1.2. Sediment phase: Two oxygen consuming processes are modelled in the sediment phase.

1.2a. Continuous oxygen demand due to sediment organic substrate: A constant sediment oxygen demand (SOD) is assumed to be present in the sediment layer. The rate of oxidation depends on the depth of the bulk water phase in the river. The deeper the sediment layer, the lesser is the oxygen available for oxidation and hence lesser oxidation.

1.2b. Oxidation of temporary sediment oxygen demand (BODs): BODs arises due to settling of particulate organic substrate (BOD1p, BOD2p) from combined sewer overflows (CSO) and wastewater treatment plant (WWTP) discharges into the river. It is considered as a state variable. BODs is only affected by biological transformation and does not undergo any transport. As in the case of SOD, oxidation of BODs is also influenced by the depth of bulk water phase in a similar manner.

2. Nitrification: Nitrification of ammonia occurs in the presence of oxygen. The rate of nitrification is linearly related to ammonia concentration in the river. The effect of oxygen is modelled using a Monod term. The process takes place at a slower rate than organic substrate consumption. Biomass is not considered as a state variable and is non-limiting to the process rate.

3. Photosynthesis: Macrophytes can have a strong influence on the oxygen concentration in the river. Oxygen production due to photosynthesis is influenced by the intensity of solar radiation and the concentration of macrophytes in the system. The macrophyte biomass is not considered as a state variable. It is supplied externally either as a constant value or as a time series.

4. Respiration of macrophytes: Respiration of macrophytes is modelled as a continuous process that is dependent only on the amount of macrophyte biomass. It is assumed that sufficient oxygen is always available for respiration. Respiration affects the oxygen state variable as the process leads to consumption of oxygen. The macrophyte concentration used here is the same as that supplied to the photosynthesis process.

Physical processes

5. Reaeration: Surface reaeration is modelled as a diffusion process by which oxygen from the atmosphere reaches the water phase. It is dependent on the temperature (which in turn determines the saturation oxygen concentration) and the oxygen concentration in the river.

6. Sedimentation: Particulate substrate state variables in the bulk water phase (BOD1p, BOD2p) undergo sedimentation. These state variables are deposited in the sediment layer as BODs. The rate of sedimentation differs for both the state variables with BOD2p settling at a faster rate than BOD1p.

7. Diffusion: Diffusion of BOD1, BOD2 and NH4 state variables from the sediment to bulk water phase is also included in the model. This can be considered as the resuspension of organics and ammonia in the bulk water phase. In the current WEST implementation diffusion processes are not simulated although available in the model data base.

Table 2 provides a list of parameters used in the model and also the external variables. The parameters here are described at reference temperature and temperature correction factors have to be used for other temperatures.

Table 2: List of parameters and external variables for the Duflow river quality model

	Parameters	
Parameter	Unit	Description
K_{d1}	1/d	Decay rate BOD1
K_{d2}	1/d	Decay rate BOD2
K_{BODs}	1/d	Decay rate BODs
V_{s1}	m/d	Sedimentation rate BOD1p
V_{s2}	m/d	Sedimentation rate BOD2p
K_{O2}	gO_2/m^3	Saturation coefficient for BOD decay on oxygen
K_{nit}	1/d	Nitrification rate
K_{NO2}	gO_2/m^3	Saturation coefficient for nitrification on oxygen
K_{SO2}	gO_2/m^3	Saturation coefficient for SOD decay on oxygen
ProdM	$(gO_2/g\ M)\ /(W/m^2)/d$	Oxygen production macrophyte biomass
ResM	$(gO_2/g\ M)\ /d$	Oxygen respiration macrophyte biomass
SBOD1	$g/m^2/d$	Diffusion rate BOD1
SBOD2	$g/m^2/d$	Diffusion rate BOD2
SNH4	$gN/m^2/d$	Diffusion rate SNH4
SOD	$g/m^2/day$	Sediment oxygen demand
K_La	1/d	Reaeration coefficient
	External Variables (Time series)	
I	W/m^2	Radiation at water surface (per hour)
M	g/m^2	Macrophyte biomass

A stoichiometric matrix including the process equations is presented in Table 3.

Table 3: Stoichiometric matrix for the Duflow river quality model as implemented in WEST

State variables	O_2	BOD1	BOD1p	BOD2	BOD2p	NH4	BODs	Rate
	g/m3	gBOD/m3	gBOD/m3	gBOD/m3	gBOD/m3	gN/m3	gBOD/m3	
Biological Process								
1a. Oxidation of BOD1	-1	-1						k_{d1} * BOD1*O_2/(K_{O2}+O_2)
1b. Oxidation of BOD2	-1			-1				k_{d2} *BOD2* O_2/(K_{O2}+ O_2)
2a. Oxidation of BOD1p	-1		-1					k_{d1}* BOD1p* O_2 (K_{O2}+ O_2)
2b. Oxidation of BOD2p	-1				-1			k_{d2} *BOD2p* O_2 (K_{O2}+ O_2)
3a. Sediment oxidation-continuous	-1							k_{dSOD} *(SOD/Z)* O_2 (K_{so2}+ O_2)
3b. Sediment oxidation-temporary	-1						-1	k_{dBODs} *(BODs/Z)* O_2 (K_{so2}+ O_2)
4a. Photosynthesis of algae	1							k_{prodM} *I*M/Z
4b. Respiration of algae	-1							k_{prodM} *M/Z
5. Nitrification	-4.57					-1		k_{nit} *NH4* O_2 (K_{NO2}+ O_2)
Physical processes								
6a. Sedimentation of BOD1p			-1				1	V_{s1}*BOD1p
6a. Sedimentation of BOD1p					-1		1	V_{s2}*BOD2p
7. Aeration	1							K_La*(CS- O_2)
8a. Diffusion of BOD1		1						SBOD1/Z
8b. Diffusion of BOD2				1				SBOD2/Z
8c. Diffusion of NH4						1		SNH4/Z

In the process rate equations, state variables are denoted in black, parameters in red and source/sink components in blue. DO is modelled as "–"BOD and hence the stoichiometric coefficients are unity for all processes except for oxygen in nitrification process. 4.57 is the gO_2/gNH_4-N oxidized.

3.2. River Water Quality Model No. 1

The IWA Task Group on River Water Quality Modelling was set up to develop a river water quality model that could be used together with IWA activated sludge models currently in use. The task group identified some limitations in the existing models and developed the RWQM1. The major features of this model in comparison to earlier models are:

1. Biomass population as state variable: Earlier river models either assumed that biomass is always available or used a constant biomass concentration to calculate dynamics of DO and nutrients. RWQM1 includes biomass state variables and also modelled their influence on other state variables.

2. Elemental composition of different state variables is considered as the starting point and COD conversions are made based on these fractions.

3. Conservation of elemental masses and COD. It is ensured that the stoichiometric coefficients used for different state variables in the model lead to conservation of not only COD but also elemental masses for carbon (C), hydrogen (H), oxygen (O), nitrogen (N) and phosphorous (P).

The complete version of RWQM1 consists of 24 state variables and 23 processes. Some of these 23 processes are further divided leading to a total of 30 processes. Reichert et al. (2001a) presents different simplifications of the model and proposes methods to choose the right kind of model for different purposes.

State variables

State variables involved in RWQM1 can be broadly classified into organic matter, biomass, nutrients (nitrogen and phosphorous) and oxygen (Table 4). Some additional state variables that are used in chemical equilibria modelling are also included. All state variables for organic material are described in terms of their elemental mass fractions ($\alpha_C\alpha_H\alpha_O\alpha_N\alpha_P$) of C, H, O, N and P, respectively. Additionally, it is possible to add any new element using the mass fraction α_X where X represents the new element or a combination of elements other than C, H, N, O and P. This makes it possible to use the mass fractions as model parameters and calculate stoichiometric coefficients accordingly so that mass balances of elements remain closed during the conversion processes. Below is a brief description of different state variables.

Table 4: List of state variables used in RWQM1

Definition	Notation
Dissolved organic substrate	SS
Inert dissolved organic substrate	SI
Ammonium	SNH4
Ammonia	SNH3
Nitrite	SNO2
Nitrate	SNO3
Part of inorganic dissolved phosphorous	SHPO4
Part of inorganic dissolved phosphorous	SH2PO4
Dissolved oxygen	SO2
Sum of dissolved CO_2 and H_2CO_3	SCO2
Bicarbonate	SHCO3
Dissolved carbonate	SCO3
Hydrogen ions	SH
Hydroxyl ions	SOH
Dissolved calcium ions	SCa
Heterotrophic organisms	XH
Organisms oxidizing ammonia to nitrite	XN1
Organisms oxidizing nitrite to nitrate	XN2
Algae and macrophytes	XALG
Consumers	XCON
Particulate organic material	XS
Inert particulate organic material	XI
Phosphate adsorbed to particles	XP
Particulate inorganic material	XII

1. Organic matter: State variables that represent organic substrate include SS, SI, XS, XI and XII. SS represents the dissolved organic substrate that is readily available for biodegradation. SI is the inert dissolved organic substance. It is assumed that it does not undergo any biotransformation. XS is the particulate organic substance that is available for biodegradation only after hydrolysis. Particulate inerts are divided into XI (inert particulate organics) and XII (particulate inorganic material). While XI is produced but never consumed, XII is neither produced nor consumer in the processes modelled.

2. Biomass: Different biomass state variables available in the model are XH (heterotrophic organisms), XN1, XN2 (nitrifiers), XALG (algae and macrophytes), XCON (consumers-higher order organisms). Heterotrophs (XH) grow aerobically as well as anoxically. XN1 are nitrifiers that oxidize ammonia to nitrite and XN2 oxidize nitrite to nitrate. XALG includes algae and macrophytes that use photosynthesis for energy production. XCON are consumers that feed on algae, bacteria and particulate organics.

3. Nitrogen: Nitrogen state variables are SNH4 (ammonium), SNH3 (ammonia), SNO2 (nitrite), SNO3 (nitrate) and SN2 (elemental nitrogen). SNH3 is only involved in the equilibrium reactions between SNH4 and SNH3.

4. Phosphorous: Phosphorous state variables used in the model are SHPO4, SH2PO4 (inorganic dissolved phosphorous) and XP (adsorbed phosphorous). Distribution of inorganic dissolved phosphorous into SHPO and SH2PO4 depends on the pH.

5. Oxygen: Dissolved oxygen is modelled as SO2.

Other state variables included are SCO2 (dissolved carbon dioxide and H2CO3), SHCO3 (bicarbonate), SCO3 (carbonate), SH (hydrogen ions), SOH (hydroxyl ions) and SCa (dissolved calcium ions). These state variables are mainly used in pH calculations. SHCO3, SH, SH20 and SN2 are used in order to make sure that the elemental mass balances are preserved.

Processes

1. Aerobic growth of heterotrophs: Heterotrophic organisms (XH) consume dissolved organic substrate, oxygen and nutrients for growth. If ammonia concentration reaches very low levels, nitrate uptake takes place instead of ammonia uptake.

2. Aerobic endogeneous respiration: Biomass undergoes respiration. It is an oxygen consuming process. Endogeneous respiration is modelled for different biomass state variables (XH, XN1, XN2, XALG, XCON).

3. Anoxic growth of heterotrophs: Under anoxic conditions, denitrification is modelled as a two step process that converts nitrate to molecular nitrogen with nitrite as the intermediate. Nitrate and nitrite are used as the electron acceptors, respectively.

4. Anoxic endogeneous respiration of heterotrophs: In the absence of oxygen, heterotrophic biomass can undergo respiration in a one-step process where nitrate is converted to molecular nitrogen.

5. Growth of nitrifiers: Autotrophic organisms that oxidize ammonia to nitrate are modelled as two different organisms (XN1, XN2). Growth of XN1 leads to oxidation of ammonia to nitrite and that of XN2 leads to oxidation of nitrite to nitrate.

6. Growth of algae: Algae growth occurs in the presence of sunlight. Depending on the nitrogen source, it is modelled as two processes (with ammonia/nitrate as nutrient sources).

7. Growth of consumers: Consumers are higher order organisms. They depend on algae, particulate organic matter and bacteria for growth.

8. Death of algae/consumers: Algae and consumers are converted into slowly biodegradable particulates and inert organic matter.

9. Hydrolysis: Conversion of slowly biodegradable particulates to dissolved substrate is catalyzed by heterotrophs.

10. Phosphate processes: Adsorption of phosphate to particulate matter and release of bound phosphate as inorganic dissolved phosphorous are modelled in two different processes.

11. Chemical equilibria: Chemical equilibria is modelled between 1) CO_2, HCO_3^- , 2) HCO_3^- and CO_3^{2-}, 3) H_20, H^+ and OH^-, 4) NH_4 and NH_3, 5) $H_2PO_4^-$ and HPO_4^{2-}, and 6) Ca^{2+}, CO_3^{2-} and $CaCO_3$.

The Gujer matrix for the complete qualitative RWQM1 is described in Table 5 (Reichert et al., 2001b). "+" sign indicates a positive coefficient, "-" sign indicates a negative coefficient and "?" sign indicates a stoichiometric coefficient that is dependent on the composition of organic substances and process involved.

Table 5: Qualitative stoichiometric matrix for RWQM1 (Reichert et al., 2001b)

Component →	i	(1)	(2)	(3)	(4)	(5)	(6)	(7)	(8)	(9)	(10)	(11)	(12)	(13)	(14)	(15)	(16)	(17)	(18)	(19)	(20)	(21)	(22)	(23)	(24)
j	Process ↓	S_S	S_I	S_{NH4}	S_{NH3}	S_{NO2}	S_{NO3}	S_{HPO4}	S_{H2PO4}	S_{O2}	S_{CO2}	S_{HCO3}	S_{CO3}	S_H	S_{OH}	S_{Ca}	X_H	X_{N1}	X_{N2}	X_{ALG}	X_{CON}	X_S	X_I	X_P	X_{II}
(1a)	Aerobic Growth of Heterotrophs with NH4	-		?				?		-	+			?			1								
(1b)	Aerobic Growth of Heterotrophs with NO3	-					-	?		-	+			?			1								
(2)	Aerobic Resp. of Het.			+				+		-	+			-			-1						+		
(3a)	Anoxic Growth of Heterotrophs with NO3	-				+	-	?			+			?			1								
(3b)	Anoxic Growth of Heterotrophs with NO2	-				-		?			+			?			1								
(4)	Anoxic Resp. of Het.			+			-	+			+			-			-1						+		
(5)	Growth of 1st-stage Nitrifiers			-		+		-		-	-			+				1							
(6)	Aerobic Respiration of 1st-stage Nitrifiers			+				+		-	+			-				-1					+		
(7)	Growth of 2nd-stage Nitrifiers					-	+	-		-	-			-					1						
(8)	Aerobic Respiration of 2nd-stage Nitrifiers			+				+		-	+			-					-1				+		
(9a)	Growth of Algae with NH4			-				-		+	-			-						1					
(9b)	Growth of Algae with NO3						-	-		+	-			-						1					
(10)	Aerobic Resp. of Algae			+				+		-	+			-						-1			+		
(11)	Death of Algae			(+)				(+)		(+)	?			?						-1		+	+		
(12a)	Growth of Cons. on XALG			(+)				(+)		-	?			?						-	1	+			
(12b)	Growth of Cons. on XS			(+)				(+)		-	?			?							1	-			
(12c)	Growth of Cons. on XH			(+)				(+)		-	?			?			-				1				
(12d)	Growth of Cons. on XN1			(+)				(+)		-	?			?				-			1				
(12e)	Growth of Cons. on XN2			(+)				(+)		-	?			?					-		1				
(13)	Aerobic Resp. of Cons.			+				+		-	+			-							-1		+		
(14)	Death of Consumers			(+)				(+)		(+)	?			?							-1	+	+		
(15)	Hydrolysis	+		(+)				(+)		(+)	?			?								-1			
(16)	Eq. CO2 <-> HCO3										-1	1		+											
(17)	Eq. HCO3 <-> CO3											-1	1	+											
(18)	Eq. H2O <-> H + OH													1	1										
(19)	Eq. NH4 <-> NH3			-1	1									+											
(20)	Eq. H2PO4 <-> HPO4							1	-1					+											
(21)	Eq. Ca <-> CO3												+			1									
(22)	Ads. of Phosphate							-1																1	
(23)	Des. of Phosphate							1																-1	

4. Simplified RWQM1 for system-wide BSM

Considering the objectives in choosing the river water quality model for a system-wide BSM, it is decided that a simplified version of RWQM1 will be implemented in the benchmark model. The following simplifications are made to RWQM1.

1. pH calculations are omitted. Hence the chemical equilibria state variables (SCO2, SCO3, SOH, SH2PO4, SCa) used exclusively for pH calculations are also removed.

2. XII is not included as it does not participate in any transformation process. Particulate inorganic inerts (XII) are combined with XI (particulate organics inerts). This will not have any adverse effects as XI is only produced during some processes but never consumed.

3. Consumers are not involved in the model. Hence the XCON state variable and the process involving consumers (growth, respiration and death) are removed.

The simplified version now contains 18 state variables and 17 processes. Elemental composition of various organics is assumed to be as shown in Table 6. These assumptions are based on the mass fractions used in Reichert et al. (2001a).

Table 6: Mass fractions of C, H, N, O and P for organic matter state variables used in the simplified RWQM1

	SS	SI	X_H	X_N1	X_N2	X_ALG	X_S	X_I	Units
Carbon	0.570	0.610	0.520	0.520	0.520	0.360	0.570	0.610	gC/gOM
Hydrogen	0.080	0.070	0.080	0.080	0.080	0.070	0.080	0.070	gH/gOM
Oxygen	0.280	0.280	0.250	0.250	0.250	0.500	0.280	0.280	gO/gOM
Nitrogen	0.060	0.030	0.120	0.120	0.120	0.060	0.060	0.030	gN/gOM
Phosphorous	0.010	0.010	0.030	0.030	0.030	0.010	0.010	0.010	gP/gOM

The processes and state variables involved are already described above (Section 3.2) for RWQM1. Stoichiometric coefficients are calculated according to the formulae defined in Reichert et al. (2001b) to ensure that elemental and COD balances are met. Stoichiometric (Table 7) and kinetic parameters (Table 8) are mentioned below. The stoichiometric matrix is available in Appendix 1.

Table 7: Stoichiometric parameters for the simplified RWQM1

Notation	Description	Value	Unit
$Y_{H,aer}$	Yield for aerobic heterotrophc growth	0.60	gXH/gSS
$Y_{H,anox,NO3}$	Yield for anoxic heterotrophc growth with nitrate	0.50	gXH/gSS
$Y_{H,anox,NO2}$	Yield for anoxic heterotrophc growth with nitrite	0.30	gXH/gSS
$f_{I,BAC}$	Inert fraction of respired bacteria (autotrophs & heterotrophs)	0.20	gXI/gXH;XN1;XN2
Y_{N1}	Yield for growth of 1st stage nitrifiers	0.13	gXN1/gNH4-N
Y_{N2}	Yield for growth of 2nd stage nitrifiers	0.03	gXN2/gNO2-N
$f_{I,ALG}$	Fraction of particulate organic matter that becomes inert during algae death	0.20	gXI/gXALG
$Y_{ALG,death}$	Yield for death of algae	0.62	g(XS+XI)/gXALG
Y_{HYD}	Yield for hydrolysis	1.00	gSS/gXS

Table 8: Kinetic parameters for the simplified RWQM1

Notation	Description	Value	Unit
kgro,alg	Maximum specific growth rate for algae	2	1/d
kgro,haer	Maximum aerobic specific growth rate of heterotrophs	2	1/d
kgro,hanox	Maximum anoxic specific growth rate of heterotrophs	1.6	1/d
kgro,n1	Maximum specific growth rate of 1st stage nitrifiers	0.8	1/d
kgro,n2	Maximum specific growth rate of 2nd stage nitrifiers	1.1	1/d
khyd	Hydrolysis rate constant	3	1/d
kdeath,alg	Specific death rate for algae	0.1	1/d
kresp,n1	Maximum specific respiration rate of 1st stage nitrifiers	0.05	1/d
kresp,alg	Maximum specific respiration rate of algae	0.1	1/d
kresp,haer	Maximum aerobic specific respiration rate of heterotrophs	0.2	1/d
kresp,hanox	Maximum anoxic specific respiration rate of heterotrophs	0.1	1/d
Khpo4,hanox	Saturation coefficient for anoxic growth of heterotrophs on phosphate	0.02	gP/m3
Khpo4,n1	Saturation coefficient for growth of 1st stage nitrifiers on phosphate	0.02	gP/m3
Khpo4,n2	Saturation coefficient for growth of 2nd stage nitrifiers on phosphate	0.02	gP/m3
Kn,alg	Saturation coefficient for growth of algae on nitrogen	0.1	gN/m3
Knh4,alg	Saturation coefficient for growth of algae on ammonia	0.1	gN/m3
Kn,haer	Saturation coefficient for aerobic growth of heterotrophs on nitrogen	0.2	gN/m3
Knh4,n1	Saturation coefficient for growth of 1st stage nitrifiers on ammonia	0.5	gN/m3
Kno3,hanox	Saturation coefficient for anoxic growth of heterotrophs on nitrate	0.5	gN/m3

Table 8: Kinetic parameters for the simplified RWQM1 (continued)

Notation	Description	Value	Unit
Kno2,hanox	Saturation coefficient for anoxic growth of heterotrophs on nitrite	0.2	gN/m3
Kno2,n2	Saturation coefficient for growth of 2nd stage nitrifiers on nitrite	0.5	gN/m3
Ko2,alg	Inhibition coefficient for endogenous respiration of algae	0.2	gO/m3
Ko2,haer	Inhibition coefficient for aerobic endogenous respiration of heterotrophs	0.2	gO/m3
Ko2,n1	Inhibition coefficient for aerobic endogenous respiration of 1st stage nitrifiers	0.5	gO/m3
Ko2,n2	Inhibition coefficient for aerobic endogenous respiration of 2nd stage nitrifiers	0.5	gO/m3
Ks,haer	Saturation coefficient for aerobic growth of heterotrophs on dissolved organic substrate	2	gCOD/m3
Ks,hanox	Saturation coefficient for anoxic growth of heterotrophs on dissolved organic substrate	2	gCOD/m3
KI	Saturation coefficient for growth of algae on light	500	W/m2
βalg	Temperature correction factor for algae growth rate	0.046	1/C
βh	Temperature correction factor for heterotrophic growth rate	0.07	1/C
βhyd	Temperature correction factor for hydrolysis	0.07	1/C
βn1	Temperature correction factor for 1st stage nitrifier growth rate	0.098	1/C
βn2	Temperature correction factor for 2nd stage nitrifier growth rate	0.069	1/C
kads	1st order rate for phosphorous adsorption	0.5	1/d
kdes	1st order rate for phosphorous desorption	0.3	1/d

Hydraulic model: RWQM1 describes only the transformation processes involved in the river system. The hydraulic system is modelled as a series of varying volume tanks. Each of the tanks in series represents a river stretch. It is assumed that the river stretches are trapezoid in shape. Flow rate is determined by using Manning's formula for open channel flows (Eq. 1).

$$Q = \frac{k}{n}.A.R_h^{\frac{2}{3}}S^{\frac{1}{2}}$$

Eq. 1

where A is the cross sectional area of the river stretch (m^2), R_h is the hydraulic radius (m) and S is the horizontal slope of the river stretch. n is the dimensionless Manning's roughness coefficient and k is used here for conversion of units. Flow rate Q is expressed in m^3/d. The river stretch is assumed to be a trapezoid shape with bottom width (Wb (m)), bank slope (z) and length (L (m)). The river depth is h (m) for a given volume V (m^3). Equations 1-5 are used to represent Q in terms of known parameters (Wb, z, L, n, S) and the state variable V.

$$A = V/L$$

Eq. 2

$$P = W_b + 2.(1 + zb)^2.h$$

Eq. 3

$$R_h = A/P$$

Eq. 4

$$h = -\frac{W_b}{2z} + \sqrt{\frac{W_b}{4z^2} + \frac{V}{Lz}}$$

Eq. 5

Volume of the stretch for each time step is obtained using the differential equation (Eq. 6), which is a volume balance across the stretch.

$\frac{dV}{dt} = Qin - Q$	**Eq. 6**

For each of the state variables in the transformation model, the change in concentration (*C_i*) is represented using a mass balance for the component *i* (Eq. 7).

$\frac{dC_i}{dt} = \frac{Qin}{V}\ (C_{in}, i - C_i) + r_i$	**Eq. 7**

The number of such stretches required to represent a river can be determined using a calibration procedure.

5. Conclusions

Modelling of the river subsystem is an important aspect to understand the impact of sewer and WWTP discharges into the river and to study various scenarios for improving the river quality. Modelling of river quality has undergone major changes. River quality modelling is currently being employed to study integrated operation and management of UWS. In order to evaluate control strategies on an UWS scale, a modified version of RWQM1 is implemented as an extension to BSM2. In the future, the tool can be used to perform river quality evaluation under various operational and management scenarios.

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Appendix 1: Stoichiometric matrix for simplified RWQM1

Table 9: Stoichiometric matrix for the simplified RWQM1s implemented in system-wide benchmark simulation model

Component ®	I	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18
j	Process ¯	SS	SI	SNH4	SNO2	SNO3	SHPO4	SO2	SHCO3	SH	XH	XN1	XN2	XALG	XS	XI	XP	SH2O	SN2
		gCOD	gCOD	gN	gN	gN	gP	gO	gC	gH	gCOD	gCOD	gCOD	gCOD	gCOD	gCOD	gP	moles H20	gN
1	Aer. Growth XH (SNH4)	-1.85344		-0.01242			-0.00828	-0.85344	0.267137	0.022614	1							-0.00396	
2	Aer. Growth XH (SNO3)	-1.85344				-0.01242	-0.00828	-0.79664	0.267137	0.020839	1							-0.00485	
3	Aer. Resp. XH			0.070822			0.017395	-0.76788	0.247257	0.016668	-1					0.232116		-0.00853	
4	Anox. Growth XH (SNO3)	-2.22413			1.071111	-1.07111	-0.00621		0.385174	0.031697	1							-0.00695	
5	Anox. Growth XH (SNO2)	-3.70688			-1.62871		0.002071		0.857323	-0.04476	1							0.044608	1.678412
6	Anox. Resp. XH			0.070822		-0.26876	0.017395		0.247257	-0.00253	-1					0.232116		0.001065	0.268759
7	Growth XN1			-4.77883	4.704284		-0.01864	-15.129	-0.32305	0.649242		1						0.34698	
8	Aer. Resp. XN1			0.070822			0.017395	-0.76788	0.247257	0.016668		-1				0.232116		-0.00853	
9	Growth XN2				-20.7083	20.63373	-0.01864	-22.3258	-0.32305	-0.03345			1					0.005635	
10	Aer. Resp. XN2			0.070822			0.017395	-0.76788	0.247257	0.016668			-1			0.232116		-0.00853	
11	Growth XALG (SNH4)			-0.06451			-0.01075	1	-0.38708	-0.02834				1				0.002056	
12	Growth XALG (SNO3)					-0.06451	-0.01075	1.294916	-0.38708	-0.03756				1				-0.00255	
13	Aer. Resp. XALG			0.058062			0.008602	-0.59827	0.255901	0.017733				-1		0.401731		0.002144	
14	Death XALG			0.028515			0.004086	0.203717	0.001763	-0.00163				-1	0.954644	0.249073		0.008234	
15	Hydrolysis	1													-1				
16	Adsorption of phosphate						-1										1		
17	Desorption of phosphate						1										-1		

Appendix 2: Matlab code for simplified RWQM1

```
/*
 *simplified RWQM1 model with varying volumes
 *copyright: Ramesh Saagi, Lund University, Sweden
 */

#define S_FUNCTION_NAME RWQM1s

#include "simstruc.h"
#include <math.h>

#define XINIT   ssGetArg(S,0)    /* Initial value for volume of the river
stretch */
#define DIM ssGetArg(S,1)        /* Dimensions of the river */
#define STOICH  ssGetArg(S,2)    /* Stoichiometric values matrix for RWQM1s */
#define KINETIC ssGetArg(S,3)    /* Kinetic Coefficients */

/*
 * mdlInitializeSizes - initialize the sizes array
 */
static void mdlInitializeSizes(SimStruct *S)
{
    ssSetNumContStates(    S, 19)    /* number of continuous states; 18+vol   */
    ssSetNumDiscStates(    S, 0);    /* number of discrete states             */
    ssSetNumInputs(        S, 22);   /* number of inputs (states+Q+T+kla+I)   */
    ssSetNumOutputs(       S, 22);   /* number of outputs(states+Qout+T+kla+I)*/
    ssSetDirectFeedThrough(S, 1);    /* direct feedthrough flag               */
    ssSetNumSampleTimes(   S, 1);    /* number of sample times                */
    ssSetNumSFcnParams(    S, 4);    /* number of input arguments             */
    ssSetNumRWork(         S, 0);    /* number of real work vector elements   */
    ssSetNumIWork(         S, 0);    /* number of integer work vector elements*/
    ssSetNumPWork(         S, 0);    /* number of pointer work vector elements*/
}

/*
 * mdlInitializeSampleTimes - initialize the sample times array
 */
static void mdlInitializeSampleTimes(SimStruct *S)
{
    ssSetSampleTime(S, 0, CONTINUOUS_SAMPLE_TIME);
    ssSetOffsetTime(S, 0, 0.0);
}

/*
 * mdlInitializeConditions - initialize the states
 */

static void mdlInitializeConditions(double *x0, SimStruct *S)
{
    int i;

for (i = 0; i < 19; i++) {
   x0[i] = mxGetPr(XINIT)[i];
}
}

/*
 * mdlOutputs - compute the outputs
 */
```

```
static void mdlOutputs(double *y, double *x, double *u, SimStruct *S, int tid)
{
    double Across, h, n, zh,Wb,zb,L, P, Rh;
    int i;
    n = mxGetPr(DIM)[0]; /*Manning's coefficient*/
    zh = mxGetPr(DIM)[1]; /* Slope along the horizontal length of the river */
    Wb = mxGetPr(DIM)[2]; /* Bottom width of the river stretch */
    zb = mxGetPr(DIM)[3]; /* Slope along the river bank represented as
horizontal distance/vertical distance */
    L = mxGetPr(DIM)[4]; /* Length of the river stretch */

    Across = x[18]/L;   /* Cross sectional area of the river stretch assuming
that it is same across the stretch  (Vol/length)*/
    h = -Wb/(2*zb)+pow((Wb*Wb/(4*zb*zb)+x[0]/(L*zb)),0.5); /* Water level for
the river stretch */
    P = Wb+2*pow((1+zb*zb),0.5)*h; /* Wetted perimeter . Trapezoidal shape
assumed */
    Rh = Across/P; /* Hydraulic radius */

        for (i = 0; i < 18; i++)
    {
     y[i] = x[i];
    }

    y[18] = (1*Across*pow(Rh,(2/3))*pow(zh,0.5)/n)*60*60*24; /*Outflow =
k*A*Rh^(2/3)*zh^(1/2)/n and conversion to m3/day; k=1 m^(1/3)/s conversion for
units  */
    y[19] =  u[19]; /*x[i]; /* Volume of the stretch filled with water */
    y[20] = u[20]; /*h; /* Water level for the river stretch */
    y[21] = u[21]; /*Across; /* Cross sectional area of the river stretch
assuming that it is same across the stretch  (Vol/length)*/
}

/*
 * mdlUpdate - perform action at major integration time step
 */

static void mdlUpdate(double *x, double *u, SimStruct *S, int tid)
{
}

/*
 * mdlDerivatives - compute the derivatives
 */

static void mdlDerivatives(double *dx, double *x, double *u, SimStruct *S, int
tid)
{

    int i, j;
    double stoich[18][18], proc[18], reac[18], xtemp[19];
    double k_groalg, k_grohaer, k_grohanox, k_gron1, k_gron2, k_hyd, k_deathalg,
           k_respalg, k_resphaer, k_resphanox, k_respn1, k_respn2,
           K_hpo4alg, K_hpo4haer, K_hpo4hanox, K_hpo4n1, K_hpo4n2, K_nalg,
           K_nh4alg, K_nhaer, K_nh4n1, K_no3hanox, K_no2hanox, K_no2n2, K_o2alg,
           K_o2haer, K_o2n1, K_o2n2, K_shaer, K_shanox, KI, balg, bh, bhyd, bn1,
           bn2, k_ads,k_des, so2_sat,T,T0,kla,kla_corr;
    double Across, h, n, zh,Wb,zb,L, P, Rh, Qout, vel;
```

```
    /* Stoichiometric coefficients */
    for(i=0;i<18;i++)
        {
          for(j=0;j<18;j++)
            {
                stoich[i][j]=mxGetPr(STOICH)[i+(j*18)];
            }
        }
    /*Kinetic parameters*/

    k_groalg=mxGetPr(KINETIC)[0];
    k_grohaer=mxGetPr(KINETIC)[1];
    k_grohanox=mxGetPr(KINETIC)[2];
    k_gron1=mxGetPr(KINETIC)[3];
    k_gron2=mxGetPr(KINETIC)[4];
    k_hyd=mxGetPr(KINETIC)[5];
    k_deathalg=mxGetPr(KINETIC)[6];
    k_respalg=mxGetPr(KINETIC)[7];
    k_resphaer=mxGetPr(KINETIC)[8];
    k_resphanox=mxGetPr(KINETIC)[9];
    k_respn1=mxGetPr(KINETIC)[10];
    k_respn2=mxGetPr(KINETIC)[11];
    K_hpo4alg=mxGetPr(KINETIC)[12];
    K_hpo4haer=mxGetPr(KINETIC)[13];
    K_hpo4hanox=mxGetPr(KINETIC)[14];
    K_hpo4n1=mxGetPr(KINETIC)[15];
    K_hpo4n2=mxGetPr(KINETIC)[16];
    K_nalg=mxGetPr(KINETIC)[17];
    K_nh4alg=mxGetPr(KINETIC)[18];
    K_nhaer=mxGetPr(KINETIC)[19];
    K_nh4n1=mxGetPr(KINETIC)[20];
    K_no3hanox=mxGetPr(KINETIC)[21];
    K_no2hanox=mxGetPr(KINETIC)[22];
    K_no2n2=mxGetPr(KINETIC)[23];
    K_o2alg=mxGetPr(KINETIC)[24];
    K_o2haer=mxGetPr(KINETIC)[25];
    K_o2n1=mxGetPr(KINETIC)[26];
    K_o2n2=mxGetPr(KINETIC)[27];
    K_shaer=mxGetPr(KINETIC)[28];
    K_shanox=mxGetPr(KINETIC)[29];
    KI=mxGetPr(KINETIC)[30];
    balg=mxGetPr(KINETIC)[31];
    bh=mxGetPr(KINETIC)[32];
    bhyd=mxGetPr(KINETIC)[33];
    bn1=mxGetPr(KINETIC)[34];
    bn2=mxGetPr(KINETIC)[35];
    k_ads=mxGetPr(KINETIC)[36];
    k_des=mxGetPr(KINETIC)[37];
    kla_corr = mxGetPr(KINETIC)[38];

    T0 = 20;
    T = u[19];

    so2_sat=  14.65-0.41*T + 0.00799*pow(T,2)-0.0000778*pow(T,3); /*Elmore and
Hayes (1960), Used in WEST 2014 */
    kla= kla_corr*3.9*pow((vel/86400),0.5)*pow(h,-0.67)*pow(1.024,T-T0);/*Kla =
3.9*U^(1/2)/H^(3/2), a correction factor is added to simulate artificial
reaeration */
    if (kla>=0)
```

```
        kla = kla;
    else
        kla = 0;

    /* conversion of any negative state variable values to zeros */
    for (i = 0; i < 19; i++)
        {
        if (x[i] < 0.0)
            xtemp[i] = 0.0;
        else
            xtemp[i] = x[i];
        }

    /* Process rate for each process */

    proc[0] = k_grohaer*exp(bh*(T-T0))*(xtemp[0]/(K_shaer+xtemp[0]))*(xtemp[6]/(K_o2haer+xtemp[6]))*(xtemp[2]/(K_nhaer+xtemp[2]))*(xtemp[5]/(K_hpo4haer+xtemp[5]))*xtemp[9];
    proc[1] = k_grohaer*exp(bh*(T-T0))*(xtemp[0]/(K_shaer+xtemp[0]))*(xtemp[6]/(K_o2haer+xtemp[6]))*(K_nhaer/(K_nhaer+xtemp[2]))*(xtemp[4]/(K_nhaer+xtemp[4]))*(xtemp[5]/(K_hpo4haer+xtemp[5]))*xtemp[9];
    proc[2] = k_resphaer*exp(bh*(T-T0))*(xtemp[6]/(K_o2haer+xtemp[6]))*xtemp[9];
    proc[3] = k_grohanox*exp(bh*(T-T0))*(xtemp[0]/(K_shanox+xtemp[0]))*(K_o2haer/(K_o2haer+xtemp[6]))*(xtemp[4]/(K_no3hanox+xtemp[4]))*(xtemp[5]/(K_hpo4hanox+xtemp[5]))*xtemp[9];
    proc[4] = k_grohanox*exp(bh*(T-T0))*(xtemp[0]/(K_shanox+xtemp[0]))*(K_o2haer/(K_o2haer+xtemp[6]))*(xtemp[3]/(K_no2hanox+xtemp[3]))*(xtemp[5]/(K_hpo4hanox+xtemp[5]))*xtemp[9];
    proc[5] = k_resphanox*exp(bh*(T-T0))*(K_o2haer/(K_o2haer+xtemp[6]))*(xtemp[4]/(K_no3hanox+xtemp[4]))*xtemp[9];
    proc[6] = k_gron1*exp(bn1*(T-T0))*(xtemp[6]/(K_o2n1+xtemp[6]))*(xtemp[2]/(K_nh4n1+xtemp[2]))*(xtemp[5]/(K_hpo4n1+xtemp[5]))*xtemp[10];
    proc[7] = k_respn1*exp(bn1*(T-T0))*(xtemp[6]/(K_o2n1+xtemp[6]))*xtemp[10];
    proc[8] = k_gron2*exp(bn2*(T-T0))*(xtemp[6]/(K_o2n2+xtemp[6]))*(xtemp[3]/(K_no2n2+xtemp[3]))*(xtemp[5]/(K_hpo4n2+xtemp[5]))*xtemp[11];
    proc[9] = k_respn2*exp(bn2*(T-T0))*(xtemp[6]/(K_o2n2+xtemp[6]))*xtemp[11];
    proc[10] = k_groalg*exp(balg*(T-T0))*((xtemp[2]+xtemp[4])/(K_nalg+xtemp[2]+xtemp[4]))*(xtemp[2]/(K_nh4alg+xtemp[2]))*(xtemp[5]/(K_hpo4alg+xtemp[5]))*(u[22]/(u[22]+KI))*xtemp[12];
    proc[11] = k_groalg*exp(balg*(T-T0))*((xtemp[2]+xtemp[4])/(K_nalg+xtemp[2]+xtemp[4]))*(K_nh4alg/(K_nh4alg+xtemp[2]))*(xtemp[5]/(K_hpo4alg+xtemp[5]))*(u[22]/(u[22]+KI))*xtemp[12];
    proc[12]= k_respalg*exp(balg*(T-T0))*(xtemp[6]/(K_o2alg+xtemp[6]))*xtemp[12];
    proc[13] = k_deathalg*exp(balg*(T-T0))*xtemp[12];
    proc[14] = k_hyd*exp(bhyd*(T-T0))*xtemp[13];
    proc[15] = k_ads*xtemp[5];
    proc[16] = k_des*xtemp[15];
    proc[17] = kla*(so2_sat-xtemp[6]);

   /* Change in concentration of state variables due to reactions */
    for(j=0; j<18 ;j++)
  {
   reac[j]=0;
   for(i=0; i<18; i++)
    {
     reac[j]=reac[j] + proc[i]*stoich[i][j];
```

```
    }
  }

    /* Hydraulic parameters */

    n = mxGetPr(DIM)[0]; /*Manning's coefficient*/
    zh = mxGetPr(DIM)[1]; /* Slope along the horizontal length of the river */
    Wb = mxGetPr(DIM)[2]; /* Bottom width of the river stretch */
    zb = mxGetPr(DIM)[3]; /* Slope along the river bank represented as 
horizontal distance/vertical distance */
    L = mxGetPr(DIM)[4]; /* Length of the river stretch */

    Across = x[18]/L;   /* Cross sectional area of the river stretch assuming 
that it is same across the stretch  (Vol/length)*/
    h = -Wb/(2*zb)+pow((Wb*Wb/(4*zb*zb)+x[18]/(L*zb)),0.5); /* Water level for 
the river stretch */
    P = Wb+2*pow((1+zb*zb),0.5)*h; /* Wetted perimeter . Trapezoidal shape 
assumed */
    Rh = Across/P; /* Hydraulic radius */
    Qout = (1*Across*pow(Rh,(2/3))*pow(zh,0.5)/n)*60*60*24; /*Outflow = 
k*A*Rh^(2/3)*zh^(1/2)/n and conversion to m3/day; k=1 m^(1/3)/s conversion for 
units  */
    vel = Qout/Across; /* Flow velocity of the river stretch */

    for(j=1;j<18;j++)
     {
        dx[j]=((u[18]/x[18])*(u[j]-x[j]))+reac[j];
     }

    dx[18] = u[18]-Qout;
}

 /*
 * mdlTerminate - called when the simulation is terminated.
 */

static void mdlTerminate(SimStruct *S)
{
}

#ifdef  MATLAB_MEX_FILE    /* Is this file being compiled as a MEX-file? */
#include "simulink.c"      /* MEX-file interface mechanism */
#else
#include "cg_sfun.h"       /* Code generation registration function */
#endif
```