## **Benchmark Simulation Model No.1**

**Modelling and Control Case Study** 



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Ramesh Saagi, PhD student Lund University, Sweden 2/26/2014

# Benchmark Simulation Model No. 1 (BSM1) – Modelling and Control Case Study

#### **Overview**

This report on Benchmark Simulation Model No. 1 (BSM1) is submitted as a part of the self-study course for the completion of PhD degree at IEA, Lund University. Benchmark simulation models (BSM1, BSM1\_LT, BSM2) consist of predefined plant layout, process models, sensor and actuator models, influent characteristics and evaluation criteria. They are developed with an objective to evaluate control strategies in wastewater treatment plants (wwtp) (Jeppsson et al., 2013).

The BSM1 plant layout (Fig. 1) includes the activated sludge system and the secondary clarifier. Sensor and control handles for the biological aeration system and settling tanks are available in the toolbox. Influent data for different weather conditions (constant, dry weather, storm weather, rain) is available for a 1-week evaluation period. Evaluation criteria based on effluent quality and operational costs are implemented.

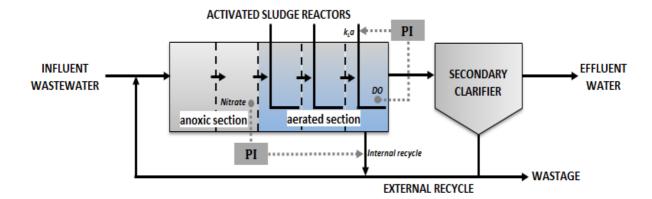


Figure 1: BSM1 plant layout with default controls

Two case studies are performed on the existing BSM1:

- 1. Implementation of Activated Sludge Model No. 3 (ASM3) in BSM1;
- 2. Implementation of a feedback controller for step-feed inflow distribution.

### 1. ASM3 implementation in BSM1

#### Introduction

Activated Sludge Models: The International Water Association (IWA) has developed activated sludge models that are used to describe biological processes taking place in a wastewater treatment plant. Different activated sludge models namely ASM1, ASM2, ASM2d and ASM3 are currently available

(The IWA Task Group on Mathematical Modelling for Design and Operation of Biological Wastewater Treatment, 2000).

ASM1: Activated Sludge Model No. 1 (ASM1) contains model description for the removal of organic matter and nitrogen. Chemical oxygen demand (COD) is used as a measure of organic matter. It can accept either oxygen or nitrate as the electron acceptor. The model is the first attempt at standardization of activated sludge models that were earlier being developed at various research institutes.

ASM2: Activated Sludge Model No. 2 (ASM2) is an extension to ASM1 and includes the description of biological phosphorous removal processes as well. The biomass is modelled to have internally stored components such as poly- $\beta$ -hydroxyalkanoate and polyphosphate (poly-P). The ASM2 model also overcomes some of the limitations of ASM1 model.

ASM2d: The capabilities of ASM2 are further extended by adding the denitrifying activity of Phosphorous accumulating organisms (PAO) to allow for a better description of the dynamics of phosphate and nitrate. It can also model chemical precipitation of phosphates.

ASM3: Based on the experiences of using earlier models, Activated Sludge Model No. 3 was developed. It is similar to ASM1 in terms of its ability to describe the biological removal of organic matter and nitrogen. ASM3 recognizes and incorporates storage polymers in the heterotrophic activated sludge conversion. Also, the death regeneration hypothesis in ASM1 is replaced with endogenous respiration and decay rates are electron acceptor dependant.

Existing BSM1 uses ASM1 as the underlying model for the biological processes. The aim of this exercise is to develop the BSM1 system where the biological reactions are modelled based on ASM3. This new implementation (BSM1\_ASM3\_v2) is ring tested with the existing ASM3 implementation in BSM1 (BSM1\_ASM3\_v1).

#### Methods

Matlab/Simulink is used for the implementation of BSM1. The underlying activated sludge models are implemented as S-functions in Matlab. In order to modify the BSM1 to use ASM3 for the biological process modelling, the following changes in the existing code are made:

- 1. Init files: Update the stoichiometric and kinetic parameters according to ASM3 parameters used in BSM1\_ASM3\_v1;
- 2. Influent data: Influent data is modified according to the state variables available in ASM3;
- 3. Biological process model: Replace the ASM1 s-function with that of ASM3;
- 4. Other models: Update the delay and settler model to reflect the new state variables. Update the performance evaluation script according to new state variables.

#### Differences in ASM3 implementations (BSM1\_ASM3\_v1 and BSM1\_ASM3\_v2)

Only the 13 state variables present in the ASM3 model are used in the new implementation. No additional dummy state variables are used. A constant temperature of 20 °C is assumed and the kinetic parameter values at 20 °C are used. In BSM1\_ASM3\_v1, apart from the 13 state variables, it contains state variables for temperature and five dummy states.

The stoichiometric parameters for all the reactions are computed in the init file and the resulting matrix [12\*13] is used as an input argument for the ASM3 S-function. The parameter matrix has to

be converted into an array [156] to be used as an input argument for the S-function. The values from the input argument are read into a matrix [12\*13] within the S-function. The complete S-function is provided in Appendix 3.

BSM1\_ASM3\_v1 has a 10-layer reactive settler model with temperature correction. BSM1\_ASM3\_v2 also has a 10-layer settler model but does not have a reactive settler model and temperature correction. In the current implementation, two sets of for loops were used to define the soluble and particulate state variable derivatives instead of defining all the derivatives individually. Appendix4 provides the S-function for the implementation.

The results of the new implementation are ring tested with the existing one. Only open loop implementations for the steady state and dynamic conditions are available in BSM1\_ASM3\_v1. Hence, ring testing only for the open loop models was done.

#### **Results and discussion**

The average effluent concentrations and loads for both the implementations matched in both steady state and dynamic conditions. The results for the aggregated values (EQI, sludge production etc) also matched well. Any differences beyond the 8th digit and with a negligible relative error are not considered.

Errors were found in both the earlier and the current implementations. Most of the errors were in the performance evaluation and state initialization scripts. In terms of the S-function implementations, it is the ring testing of the settler model that took longer than that of the ASM3 model. This is mainly because of the relatively higher complexity of settler model. Hence, it is more prone to coding errors. The reactive and temperature models of the earlier settler were turned off during ring testing.

The ring testing has identified errors in the earlier implementation and the necessary changes are made. Below is the list of all the errors and the corrections made to them.

Table 1: List of corrections made in BSM1\_ASM3\_v1

Variable	Previous	Updated	Comments			
Influent	15°C/*dynamic	20°C	In the current implementation,			
temperature			temperature has no effect of kinetic			
			parameters. Hence the temperature in the previous version was changed only for the purpose of ring testing.			
Influent quality			Effluent flow vector was incorrectly used to			
index (perf_plant)	Qevec	Qinvec	calculate the influent quality.			
SNKjin (perf_plant)	iN_SI*inpart(:,2);	iN_SI*inpart(:,1);	Incorrect state variables used to compute			
	in_SS*inpart(:,3)	in_SS*inpart(:,2)	input Kjeldahl nitrogen.			
SNKje (perf_plant)	settlerpart(:,23);	settlerpart(:,22);	Incorrect state variables used to compute			
	settlerpart(:,24);	settlerpart(:,23);	input Kjeldahl nitrogen.			
	settlerpart(:,32)	settlerpart(:,30)				
SNOe (perf_plant)			Incorrect state variable used to compute			
	settlerpart(:,27)	settlerpart(:,29)	effluent SNO.			

BOD5 (perf_plant)			BOD5 computation includes XTSS as well as XBA, XBH and XSTO. This results in using TSS twice. XBA was defined twice.
CODin, CODe (perf_plant)			COD computation included TSS as well as XBA, XBH, XSTO. This results in using TSS twice, which is incorrect.
XI_5 (stateset)	settlerinit(m,127)	settlerinit(m,137)	Incorrect state variable used to compute the initial state for settler model.
XO5_1 (stateset)			State variable defined twice in the stateset file.

The final ring testing results of the consolidated influent and effluent quality indices are presented below. Complete results from perf\_plant script are available in Appendix 1 and Appendix 2. The steady state indices are perfectly in agreement. The dry weather influent indices are in agreement but the effluent indices have minor differences in the 3rd and 4th decimal places.

Table 2: Results of ring testing ASM3 implementation in BSM1

Index	ASM3_v1		ASM3_v2		
muex	Steady state	Dry influent	Steady state	Dry influent	
Influent quality index (original)	38734.8904	38733.8545	38734.8904	38733.8545	
Influent quality index (updated)	47041.8067	47040.0126	47041.8067	47040.0126	
Effluent quality index (original)	7047.2933	7036.3134	7047.2933	7036.3128	
Effluent quality index (updated)	4672.659	4957.9417	4672.659	4957.9413	
Operational cost index (original)	22603.0211	22541.4411	22603.0211	22541.4412	
Operational cost index (updated)	15741.6151	15680.0351	15741.6151	15680.0352	

## 2. Implementation of a feedback controller for step feed influent distribution

#### Introduction

Step-feed is one of the many available process configurations available for activated sludge systems used in biological wastewater treatment. Figure 2 describes the process configuration. As the name suggests, the influent is distributed to different compartments of the biological reactor. Return sludge is pumped to the beginning of the activated sludge tank. Each compartment generally comprises of an anoxic zone for predenitrification and an aeration zone. Many plants in Sweden and across the world employ step feed configuration to efficiently address nitrogen removal from wastewater (Åmand, 2008).

The step-feed configuration provides the following benefits:

- 1. No internal recirculation is needed as the biodegradable substrate for predenitrification is available through the fresh influent wastewater in each compartment. This reduces operational costs.
- 2. As the influent wastewater is distributed across the compartments, the return sludge in the first compartment is less diluted and hence has higher MLSS. A gradient of MLSS develops

- along the compartments. The average MLSS achieved is higher than that achieved without step feed of the influent. This means higher SRT for the same biological reactor volume.
- 3. Higher MLSS in the activated sludge system do not lead to clarifier overloading as the MLSS in the last compartments is lower.
- 4. The effect of toxic influents can be reduced due to higher level of dilution with return sludge.
- 5. Also, the flexible operation provides the possibility to avoid washout of solids during wet weather conditions by varying the step feed distribution.

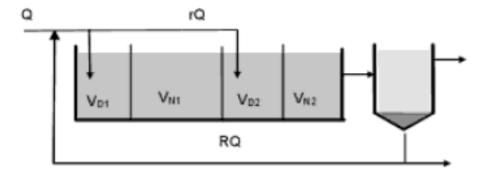


Figure 2: Step feed process configuration

Flow distribution control: Step ratio (r) is used to determine the ratio of influent distributed across different compartments in a reactor. For the above figure, step ratio is defined as the fraction of influent sent to the second anoxic tank. For a fixed volume of the reactor, feeding more inflow to the first compartment (low step ratio) and passing it through all the compartments provides better nitrification as the influent ammonia now has a higher retention time. On the other hand, a higher fraction of inflow into the later compartments (high step ratio) will provide the necessary biodegradable substrate that is required for the denitrification of nitrate formed in the first aerobic zone. Hence, a step-feed configuration with low step ratio will lead to better nitrification whereas that with a high step ratio will lead to better denitrification.

It should be noted that the step feed configuration has an intrinsic problem (Olsson et al., 2005). In situations with high fractions to the initial compartments will lead to better nitrification but the nitrate so produced cannot be denitrified efficiently in the later compartments. Similarly, when the inflow fraction is high to the later part of the reactor aiming to improve denitrification. The amount of nitrate present can be limited due to lack of internal recirculation and less nitrification in the earlier compartments. Hence, it is essential to develop proper limits for the control strategy so that it does not worsen the situation.

#### **Methods**

Simulation platform: A modified BSM1 plant configuration is used to study the impact of the control strategy. The modified BSM1 plant has the following configuration. It consists of two compartments, each with an anoxic and aerobic zone. Additionally, the final compartment is an aerobic zone with oxygen control. The volumes of the anoxic and aerobic tanks remain the same as in the original BSM1 model. Also the oxygen controllers in both BSM1 and step-feed implementations are the same. The controller for internal recirculation is now replaced with that for step ratio.

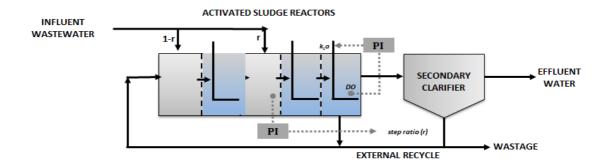


Figure 3: Modified BSM1 step-feed plant layout

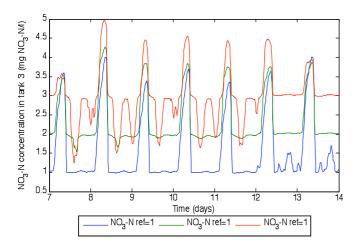
Control strategy: The control strategy is based on the nitrate concentration in the 2<sup>nd</sup> anoxic tank (tank 3). A nitrate sensor in tank 3 determines the nitrate concentration in the anoxic tank. The error between the measured value and nitrate setpoint provides the step ratio for the influent. A PI controller is used. An offset step ratio of 0.5 is used for the situation when there is no error. If the error is positive (measurement > setpoint), this indicates that denitrification is the limiting process. Hence step ratio is increased to provide more inflow to the second anoxic tank. On the other hand, if the error is negative (measurement < set point), there is little nitrate in the second anoxic tank. This is due to limited nitrification happening in the first aeration reactor. Hence, the control strategy will decrease the step ratio allowing more influent to pass through the beginning of the activated sludge system. The control strategy is similar to the one suggested by Olsson et al. (2005) except that the former tries to arrive at an upper limit based on maintaining a constant F/M ratio in both the compartments while the limit value in the current study is set based on simulation results.

It should be understood that it may be difficult to completely control the nitrate concentration in the anoxic tank based on the step ratio. In a step feed process, a control strategy aiming at reducing effluent nitrate concentration will increase the effluent ammonia concentration and vice versa. Hence, the current control strategy is limited to a maximum step ratio of 0.8. Any further increase will decrease the effluent ammonia quality drastically as the residence time for nitrifying bacteria decreases.

#### **Results and discussions**

#### Identification of the correct set point

The control strategy tries to maintain the nitrate concentration in the  $2^{nd}$  anoxic tank as long as the step ratio does not exceed 0.8. A very high set point will lead to high nitrate concentrations in the effluent. Having a setpoint that is very low will lead to insufficient nitrification in the system. The control strategy is evaluated at different set points of 1 mg  $NO_3$ -N/I, 2 mg  $NO_3$ -N/I and 3 mg  $NO_3$ -N/I in the second anoxic tank. Below are the nitrate profiles in reactor three with different set points.



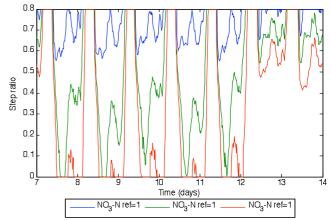


Figure 4a: Nitrate concentration in second anoxic tank for different nitrate set points.

The figures indicate that as the set point increases the controllability decreases and also the variation in step ratio increases. At a setpoint of SNO=1, the controller was able to achieve the set point during most of the week except when the inflow nitrate concentration exceeds SNO=1. In such cases, although the controller tries to increase the step ratio, it does not reduce the nitrate concentration. At higher setpoints, the controller fails to either drop or increase the nitrate concentration to meet the reference value. A look at the step ratio for these setpoints reveals that the controller attempts to vary the step ratio but that does not have much impact on the nitrate levels. A set point of SNO=1 is chosen based on the above results. The PI controller is tuned manually. Kp=-5 and Ti=200 are chosen to achieve the above results.

#### **Evaluation of process configuration and control strategy**

Table 3: Comparison of quality and cost indices for BSM1, BSM1 step-feed, BSM1 step-feed with control.

Process	IQ	EQ	OCI		Effluent SNH
closed loop BSM1	52081.4	6146.478	16351.54	12.58403	2.203075
step-feed (fixed step ratio-0.5)	52081.4	5942.554	15953.99	13.10961	1.710975
step-feed with control	52081.4	6246.547	15845.27	12.80522	2.285363

The above table indicates that the control situation has the lowest operational cost and also the poorest effluent quality. It can be seen that the differences in quality and costs are very small in all cases. It might be surprising that the costs are same in all three cases considering that the step feed configuration does not need recirculation. The lack of recirculation has resulted in a slight decrease in costs but also in the step-feed situation the costs for aeration has increased compensating the reduction in pumping costs. Hence, the net costs did not get greatly affected. The increase in aeration costs is due to the increased requirement for nitrification in the last aerobic tank at high step ratios. High step ratios lead to higher ammonia loads in the last aerobic tanks and as a consequence high aeration requirement to nitrify the ammonia load. It can be said that the step-feed

configuration with a fixed step feed ratio has the best performance as it has the best effluent quality at a lower cost.

#### **Conclusions**

The studied control strategy was able to limit the nitrate concentration in the second anoxic tank within the limits for major part of the operation. In certain time periods, the controller was unable to manipulate the process to achieve the setpoint. This is due to: 1) The constraints on the step ratio; and, 2) Influent wastewater carbon and nitrogen loads. It can be said that the step-feed configuration did lead to some benefits in terms of operational costs and effluent quality. It should be noted that although the step-feed configuration has many benefits compared to conventional activated sludge process, it is mainly dependent on the biodegradable substrate and ammonia loads available in the influent. Step-feed configuration might be more beneficial in wastewaters with high influent carbon to nitrogen ratios as this provides sufficient biodegradable substrate for denitrification without putting much load on the nitrification. Future research can be directed at evaluating such a case study.

#### References

Jeppsson, U., Alex, J., Batstone, D.J., Benedetti, L., Comas, J., Copp, J.B., Corominas, L., Flores-Alsina, X., Gernaey, K.V., Nopens, I., Pons, M.N., Rodrígues-Roda, I., Rosen, C., Steyer, J.P., Vanrolleghem, P.A., Volcke, E.I., Vrecko, D. (2013). Benchmark simulation models, quo vadis?. *Wat. Sci. & Technol.*, 68(1): 1-15.

Henze, M., Gujer, W., Mino, T., van Loosdrecht, M. (2000). *Activated Sludge Models*. IWA Publishing, London, UK.

Åmand, L. (2008). Evaluation of the step-feed biological nutrient removal process at Kungsängen wastewater treatment plant (*Master's thesis*). *Uppsala University, Uppsala, Sweden*.

Olsson, G., Nielsen, M., Yuan, Z., Lynggaard-Jensen, A., Steyer, J.-P. (2005). *Instrumentation, Control and Automation in Wastewater Systems*. IWA Publishing, London, UK.

#### Appendix 1. Steady state results for ring testing ASM3 in BSM1

#### BSM1\_ASM3\_v1

Overall plant performance

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#### Effluent average concentrations based on load

Effluent average flow rate = 18061 m3/d
Effluent average SO conc = 3.614 mg (-COD)/I
Effluent average SI conc = 30 mg COD/I
Effluent average SS conc = 0.16706 mg COD/I
Effluent average SNH conc = 0.26945 mg N/I
Effluent average SN2 conc = 23.3232 mg N/I
Effluent average SNO conc = 14.3808 mg COD/I
Effluent average SALK conc = 3.7378 mol HCO3/I
Effluent average XI conc = 6.1788 mg COD/I
Effluent average XS conc = 0.87495 mg COD/I
Effluent average XBH conc = 6.0965 mg COD/I
Effluent average XSTO conc = 1.0444 mg COD/I
Effluent average XBA conc = 0.47563 mg COD/I
Effluent average XBA conc = 0.47563 mg COD/I
Effluent average XBA conc = 1.18319 mg TSS/m3

Effluent average Kjeldahl N conc = 1.1931 mg N/l

Effluent average total N conc = 15.5738 mg N/I (limit = 18 mg COD/I)
Effluent average total COD conc = 44.8374 mg COD/I (limit = 100 mg COD/I)
Effluent average BOD5 conc = 5.232 mg/I (limit = 10 mg/I)

#### Effluent average load

Effluent average SO load = 65.2732 kg (-COD)/day
Effluent average SI load = 541.83 kg COD/day
Effluent average SS load = 3.0173 kg COD/day
Effluent average SNH load = 4.8665 kg N/day
Effluent average SN2 load = 421.2408 kg N/day
Effluent average SNO load = 259.7308 kg N/day
Effluent average SNO load = 67.5077 kmol HCO3 /day
Effluent average XI load = 111.5957 kg COD)/day
Effluent average XS load = 15.8024 kg COD/day
Effluent average XBH load = 110.1092 kg COD/day
Effluent average XSTO load = 18.8638 kg COD/day
Effluent average XBA load = 8.5904 kg COD/day
Effluent average XBA load = 8.5904 kg COD/day
Effluent average TSS load = 213.6965 kg TSS/day

Effluent average Kjeldahl N load = 21.5483 kg N/d Effluent average total N load = 281.2791 kg N/d Effluent average total COD load = 809.8088 kg COD/d Effluent average BOD5 load = 94.4957 kg/d

#### Other effluent quality variables

Influent Quality (I.Q.) index = 38734.8904 kg poll.units/d (original BSM1 version)

Effluent Quality (E.Q.) index = 7047.2933 kg poll.units/d (original BSM1 version)

Influent Quality (I.Q.) index = 47041.8067 kg poll.units/d (updated BSM1 version)

Effluent Quality (E.Q.) index = 4672.659 kg poll.units/d (updated BSM1 version)

Average sludge production for disposal per day = 2169.569 kg SS/dAverage sludge production released into effluent per day = 213.6965 kg SS/d

Total average sludge production per day = 2383.2655 kg SS/d

Average aeration energy per day = 8548.416 kWh/d (original BSM1 version) Average aeration energy per day = 4265.6 kWh/d (updated BSM1 version)

#### BSM1\_ASM3\_v2

Overall plant performance

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Effluent average concentrations based on load

Effluent average flow rate = 18061 m3/d Effluent average SO conc = 3.614 mg (-COD)/l Effluent average SI conc = 30 mg COD/l Effluent average SS conc = 0.16706 mg COD/l

Effluent average SNH conc = 0.26945 mg N/I (limit = 4 mg N/I)

Effluent average SN2 conc = 23.3232 mg N/I
Effluent average SNO conc = 14.3808 mg N/I
Effluent average SALK conc = 3.7378 mol HCO3/m3
Effluent average XI conc = 6.1788 mg COD/I
Effluent average XS conc = 0.87495 mg COD/I
Effluent average XBH conc = 6.0965 mg COD/I
Effluent average XSTO conc = 1.0444 mg COD/I
Effluent average XBA conc = 0.47563 mg COD/I

Effluent average TSS conc = 11.8319 mg SS/l (limit = 30 mg SS/l)

Effluent average Kjeldahl N conc = 1.1931 mg N/l

Effluent average total N conc = 15.5738 mg N/I (limit = 18 mg COD/I)
Effluent average total COD conc = 44.8374 mg COD/I (limit = 100 mg COD/I)
Effluent average BOD5 conc = 5.232 mg/I (limit = 10 mg/I)

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Average sludge production for disposal per day = 2169.569 kg SS/dAverage sludge production released into effluent per day = 213.6965 kg SS/d

Total average sludge production per day = 2383.2655 kg SS/d

Average aeration energy per day = 8548.416 kWh/d (original BSM1 version) Average aeration energy per day = 4265.6 kWh/d (updated BSM1 version) Average pumping energy per day (for Qintr, Qr and Qw) = 2966.76 kWh/d (original BSM1 version)

Average pumping energy per day (for Qintr, Qr and Qw) = 388.17 kWh/d (based on BSM2 principles)

Average mixing energy per day = 240 kWh/d (based on BSM2 principles)

Total added carbon volume = 0 m3 Average added carbon flow rate = 0 m3/d Total added carbon mass = 0 kg COD Average added carbon mass per day = 0 kg COD/d

#### **Operational Cost Index**

Sludge production cost index = 10847.8451 (using weight 5 for BSM1) Aeration energy cost index = 8548.416 (original BSM1 version)

Updated aeration energy cost index = 4265.6 (updated BSM1 version) Pumping energy cost index = 2966.76 (original BSM1 version)

Updated pumping energy cost index = 388.17 (based on BSM2 principles) Carbon source addition cost index = 0

Mixing energy cost index = 240 (based on BSM2 principles)
Total Operational Cost Index (OCI) = 22603.0211 (original BSM1 version)
Updated Total Operational Cost Index (OCI) = 15741.6151 (using new aeraration and pumping costs)

#### Effluent violations

95% percentile for effluent SNH (Ammonia95) = 0.26945 g N/m3 95% percentile for effluent TN (TN95) = 15.5738 g N/m3 95% percentile for effluent TSS (TSS95) = 11.8319 g SS/m3 Average pumping energy per day (for Qintr, Qr and Qw) = 2966.76 kWh/d (c version)

Average pumping energy per day (for Qintr, Qr and Qw) = 388.17 kWh/d (ba principles)

Average mixing energy per day = 240 kWh/d (based on BSM2 principles)

Total added carbon volume = 0 m3 Average added carbon flow rate = 0 m3/d Total added carbon mass = 0 kg COD Average added carbon mass per day = 0 kg COD/d

#### Operational Cost Index

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Aeration energy cost index = 8548.416 (original BSM1 version)
Updated aeration energy cost index = 4265.6 (updated BSM1 version)
Pumping energy cost index = 2966.76 (original BSM1 version)
Updated pumping energy cost index = 388.17 (based on BSM2 principles)
Carbon source addition cost index = 0
Mixing energy cost index = 240 (based on BSM2 principles)
Total Operational Cost Index (OCI) = 22603.0211 (original BSM1 version)
Updated Total Operational Cost Index (OCI) = 15741.6151 (using new aerara pumping costs)

Sludge production cost index = 10847.8451 (using weight 5 for BSM1)

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#### Appendix 2. Dynamic results for ring testing ASM3 in BSM1 with Dryinfluent

BSM1\_ASM3\_v1

Overall plant performance during time 7 to 14 days

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Effluent average concentrations based on load

Effluent average flow rate = 18061.3305 m3/d

Effluent average SO conc = 3.1666 mg (-COD)/l

Effluent average SI conc = 30 mg COD/I

Effluent average SS conc = 0.1704 mg COD/I

Effluent average SNH conc = 0.9931 mg N/I

Effluent average SN2 conc = 23.485 mg N/I

Effluent average SNO conc = 13.493 mg COD/I

Effluent average SALK conc = 3.8537 mol HCO3/l

Effluent average XI conc = 6.4506 mg COD/I

Effluent average XS conc = 0.91867 mg COD/I

Effluent average XBH conc = 6.3505 mg COD/I

Effluent average XSTO conc = 1.1022 mg COD/l

Effluent average XBA conc = 0.48741 mg COD/I

Effluent average TSS conc = 12.3424 mg TSS/m3

Effluent average Kjeldahl N conc = 1.9426 mg N/l

Effluent average total N conc = 15.4356 mg N/I (limit = 18 mg COD/I)

Effluent average total COD conc = 45.4798 mg COD/I (limit = 100 mg COD/I)

Effluent average BOD5 conc = 5.4561 mg/l (limit = 10 mg/l)

Effluent average load

-----

Effluent average SO load = 57.1933 kg (-COD)/day

Effluent average SI load = 541.84 kg COD/day

Effluent average SS load = 3.0776 kg COD/day

Effluent average SNH load = 17.9367 kg N/day

Effluent average SN2 load = 424.171 kg N/day

Effluent average SNO load = 243.7009 kg N/day

Effluent average SALK load = 69.6027 kmol HCO3 /day

Effluent average XI load = 116.5062 kg COD)/day

Effluent average XS load = 16.5924 kg COD/day

Effluent average XBH load = 114.6985 kg COD/day

Effluent average XSTO load = 19.9073 kg COD/day

Effluent average XBA load = 8.8033 kg COD/day

Effluent average TSS load = 222.92 kg TSS/day

Effluent average Kjeldahl N load = 35.0864 kg N/d Effluent average total N load = 278.7873 kg N/d

Effluent average total COD load = 821.4253 kg COD/d

Effluent average BOD5 load = 98.5442 kg/d

Other effluent quality variables

-----

Influent Quality (I.Q.) index = 38733.8545 kg poll.units/d (original BSM1 version) Effluent Quality (E.Q.) index = 7036.3134 kg poll.units/d (original BSM1 version) Influent Quality (I.Q.) index = 47040.0126 kg poll.units/d (updated BSM1 version)

Effluent Quality (E.Q.) index = 4957.9417 kg poll.units/d (updated BSM1 version)

Sludge production for disposal = 15100.7712 kg SS

Average sludge production for disposal per day = 2157.253 kg SS/d

Sludge production released into effluent = 1560.4397 kg SS

BSM1\_ASM3\_v2

Overall plant performance during time 7 to 14 days

\*\*\*\*\*\*\*\*\*\*\*\*\*\*

Effluent average concentrations based on load

.....

Effluent average flow rate = 18061.3305 m3/d Effluent average SO conc = 3.1666 mg (-COD)/I

Effluent average SI conc = 30 mg COD/I

Effluent average SS conc = 0.1704 mg COD/I

Effluent average SNH conc = 0.9931 mg N/I (limit = 4 mg N/I)

Effluent average SN2 conc = 23.485 mg N/I

Effluent average SNO conc = 13.493 mg N/I

Effluent average SALK conc = 3.8537 mol HCO3/m3

Effluent average XI conc = 6.4506 mg COD/I

Effluent average XS conc = 0.91867 mg COD/l

Efficient average XBU average COD/

Effluent average XBH conc = 6.3505 mg COD/l

Effluent average XSTO conc = 1.1022 mg COD/I

Effluent average XBA conc = 0.48741 mg COD/l

Effluent average TSS conc = 12.3424 mg SS/I (limit = 30 mg SS/I)

Effluent average Kjeldahl N conc = 1.9426 mg N/l

Effluent average total N conc = 15.4356 mg N/l (limit = 18 mg COD/l)

Effluent average total COD conc = 45.4798 mg COD/l  $\,$  (limit = 100 mg COE  $\,$ 

Effluent average BOD5 conc = 5.4561 mg/l (limit = 10 mg/l)

Effluent average load

-----

Effluent average SO load = 57.1933 kg (-COD)/day

Effluent average SI load = 541.8399 kg COD/day

Effluent average SS load = 3.0776 kg COD/day

Effluent average SNH load = 17.9367 kg N/day

Effluent average SN2 load = 424.171 kg N/day

Effluent average SNO load = 243.7009 kg N/day

Effluent average SALK load = 69.6027 kmol HCO3/day

Effluent average XI load = 116.5061 kg COD/day

Effluent average XS load = 16.5924 kg COD/day

Effluent average XBH load = 114.6985 kg COD/day

Effluent average XSTO load = 19.9073 kg COD/day

Effluent average XBA load = 8.8033 kg COD/day

Effluent average TSS load = 222.92 kg SS/day

Effluent average Kjeldahl N load = 35.0864 kg N/d

Effluent average total N load = 278.7873 kg N/d

Effluent average total COD load = 821.4253 kg COD/d

Effluent average BOD5 load = 98.5442 kg/d

Other effluent quality variables

-----

Influent Quality (I.Q.) index = 38733.8545 kg poll.units/d (original BSM1 v Effluent Quality (E.Q.) index = 7036.3128 kg poll.units/d (original BSM1 v Influent Quality (I.Q.) index = 47040.0126 kg poll.units/d (updated BSM1 v Influent Quality (I.Q.) index = 47040.0126 kg poll.units/d (updated BSM1 v Influent Quality (I.Q.) index = 47040.0126 kg poll.units/d (updated BSM1 v Influent Quality (I.Q.) index = 47040.0126 kg poll.units/d (updated BSM1 v Influent Quality (I.Q.) index = 47040.0126 kg poll.units/d (updated BSM1 v Influent Quality (I.Q.) index = 47040.0126 kg poll.units/d (updated BSM1 v Influent Quality (I.Q.) index = 47040.0126 kg poll.units/d (updated BSM1 v Influent Quality (I.Q.) index = 47040.0126 kg poll.units/d (updated BSM1 v Influent Quality (I.Q.) index = 47040.0126 kg poll.units/d (updated BSM1 v Influent Quality (I.Q.) index = 47040.0126 kg poll.units/d (updated BSM1 v Influent Quality (I.Q.) index = 47040.0126 kg poll.units/d (updated BSM1 v Influent Quality (I.Q.) index = 47040.0126 kg poll.units/d (updated BSM1 v Influent Quality (I.Q.) index = 47040.0126 kg poll.units/d (updated BSM1 v Influent Quality (I.Q.) index = 47040.0126 kg poll.units/d (updated BSM1 v Influent Quality (I.Q.) index = 47040.0126 kg poll.units/d (updated BSM1 v Influent Quality (I.Q.) index = 47040.0126 kg poll.units/d (updated BSM1 v Influent Quality (I.Q.) index = 47040.0126 kg poll.units/d (updated BSM1 v Influent Quality (I.Q.) index = 47040.0126 kg poll.units/d (updated BSM1 v Influent Quality (I.Q.) index = 47040.0126 kg poll.units/d (updated BSM1 v Influent Quality (I.Q.) index = 47040.0126 kg poll.units/d (updated BSM1 v Influent Quality (I.Q.) index = 47040.0126 kg poll.units/d (updated BSM1 v Influent Quality (I.Q.) index = 47040.0126 kg poll.units/d (updated BSM1 v Influent Quality (I.Q.) index = 47040.0126 kg poll.units/d (updated BSM1 v Influent Quality (I.Q.) index = 47040.0126 kg poll.units/d (updated BSM1 v Influent Quality (I.Q.) index = 47040.012

Effluent Quality (E.Q.) index = 4957.9413 kg poll.units/d (updated BSM1 v

Sludge production for disposal = 15100.7712 kg SS

Average sludge production for disposal per day = 2157.253 kg SS/d

Sludge production released into effluent = 1560.4397 kg SS

Average sludge production released into effluent per day = 222.92 kg SS/d Total sludge production = 16661.211 kg SS

Total average sludge production per day = 2380.173 kg SS/d

Total aeration energy = 59838.912 kWh (original BSM1 version)

Average aeration energy per day = 8548.416 kWh/d (original BSM1 version)

Total aeration energy = 29859.2 kWh (updated BSM1 version)

Average aeration energy per day = 4265.6 kWh/d (updated BSM1 version)

Total pumping energy (for Qintr, Qr and Qw) = 20767.32 kWh (original BSM1 version)

Average pumping energy per day (for Qintr, Qr and Qw) = 2966.76 kWh/d (original BSM1 version)

Total pumping energy (for Qintr, Qr and Qw) = 2717.19 kWh (based on BSM2 principles)

Average pumping energy per day (for Qintr, Qr and Qw) = 388.17 kWh/d (based on BSM2 principles)

Total mixing energy = 1680 kWh (based on BSM2 principles)

Average mixing energy per day = 240 kWh/d (based on BSM2 principles)

Total added carbon volume = 0 m3

Average added carbon flow rate = 0 m3/d

Total added carbon mass = 0 kg COD

Average added carbon mass per day = 0 kg COD/d

#### Operational Cost Index

-----

Aeration energy cost index = 8548.416 (original BSM1 version)

Updated aeration energy cost index = 4265.6 (updated BSM1 version)

Pumping energy cost index = 2966.76 (original BSM1 version)

Updated pumping energy cost index = 388.17 (based on BSM2 principles)

Carbon source addition cost index = 0

Mixing energy cost index = 240 (based on BSM2 principles)

Total Operational Cost Index (OCI) = 22541.4412 (original BSM1 version)

Updated Total Operational Cost Index (OCI) = 15680.0352 (using new aeraration

Sludge production cost index = 10786.2652 (using weight 5 for BSM1)

#### Effluent violations

and pumping costs)

95% percentile for effluent SNH (Ammonia95) = 3.5628 g N/m3 95% percentile for effluent TN (TN95) = 18.6351 g N/m3 95% percentile for effluent TSS (TSS95) = 15.0024 g SS/m3

The maximum effluent total nitrogen level (18 mg N/I) was violated during 0.66667 days, i.e. 9.5238% of the operating time. The limit was violated at 3 different occasions.

The maximum effluent ammonia nitrogen level (4 mg N/I) was violated during 0.14583 days, i.e. 2.0833% of the operating time. The limit was violated at 2 different occasions.

Average sludge production released into effluent per day = 222.92 kg SS/ $^{\circ}$  Total sludge production = 16661.211 kg SS Total average sludge production per day = 2380.173 kg SS/ $^{\circ}$ 

Total aeration energy = 59838.912 kWh (original BSM1 version)

Average aeration energy per day = 8548.416 kWh/d (original BSM1 versic

Total aeration energy = 29859.2 kWh (updated BSM1 version)

Average aeration energy per day = 4265.6 kWh/d (updated BSM1 version)

Total pumping energy (for Qintr, Qr and Qw) = 20767.32 kWh (original BS

Average pumping energy per day (for Qintr, Qr and Qw) = 2966.76 kWh/c

Total pumping energy (for Qintr, Qr and Qw) = 2717.19 kWh (based on BS Average pumping energy per day (for Qintr, Qr and Qw) = 388.17 kWh/d principles)

Total mixing energy = 1680 kWh (based on BSM2 principles)

Average mixing energy per day = 240 kWh/d (based on BSM2 principles)

Total added carbon volume = 0 m3

Average added carbon flow rate = 0 m3/d

Total added carbon mass = 0 kg COD

Average added carbon mass per day = 0 kg COD/d

#### Operational Cost Index

-----

Aeration energy cost index = 8548.416 (original BSM1 version)

Updated aeration energy cost index = 4265.6 (updated BSM1 version)

Pumping energy cost index = 2966.76 (original BSM1 version)

Updated pumping energy cost index = 388.17 (based on BSM2 principles)

Carbon source addition cost index = 0

Mixing energy cost index = 240 (based on BSM2 principles)

Total Operational Cost Index (OCI) = 22541.4412 (original BSM1 version)

Updated Total Operational Cost Index (OCI) = 15680.0352 (using new aera

Sludge production cost index = 10786.2652 (using weight 5 for BSM1)

#### Effluent violations

costs)

95% percentile for effluent SNH (Ammonia95) = 3.5628 g N/m3 95% percentile for effluent TN (TN95) = 18.6351 g N/m3 95% percentile for effluent TSS (TSS95) = 15.0024 g SS/m3

The maximum effluent total nitrogen level (18 mg N/I) was violated during 0.66667 days, i.e. 9.5238% of the operating time. The limit was violated at 3 different occasions.

The maximum effluent ammonia nitrogen level (4 mg N/I) was violated during 0.14583 days, i.e. 2.0833% of the operating time. The limit was violated at 2 different occasions.

#### Appendix 3. S-function for ASM3 implementation in BSM1

```
* ASM3 is a C-file S-function for IAWO AS Model No 3.
* /
#define S FUNCTION NAME asm3 ramesh
#include "simstruc.h"
#include <math.h>
#define XINIT ssGetArg(S,0) /* Initial state values */
#define KINETIC ssGetArg(S,4)
                           /* Kinetic Coefficients */
* mdlInitializeSizes - initialize the sizes array
static void mdlInitializeSizes(SimStruct *S)
{
   ssSetNumContStates( S, 13); /*13 number of continuous states
   ssSetNumDiscStates( S, 0); /* number of discrete states
   ssSetNumInputs(          S, 15);  /* number of inputs
   ssSetNumOutputs( S, 14); /* number of outputs
   ssSetDirectFeedThrough(S, 1);
                                /* direct feedthrough flag
   ssSetNumSampleTimes( S, 1);
                                /* number of sample times
   ssSetNumSFcnParams( S, 5);
                                /* number of input arguments
   ssSetNumRWork( S, 0);
                                /* number of real work vector elements
                    s, 0);
                                /* number of integer work vector
   ssSetNumIWork(
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 < 13; i++) {</pre>
  x0[i] = mxGetPr(XINIT)[i];
}
* mdlOutputs - compute the outputs
static void mdlOutputs(double *y, double *x, double *u, SimStruct *S, int
tid)
{
 int i;
  for (i = 0; i < 13; i++)
    y[i] = x[i];
  y[13]=u[13];
}
* 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)
{
double kh, kx, ksto, nnox, ko2, knox, ks, kxsto, muh, knh4, kalk, bho2,
bhnox, bstoo2, bstonox, mua, kanh4, kao2, kaalk, bao2, banox;
double stoich[12][13];
double proc[12];
double reac[13];
double vol, SO sat;
double xtemp[1\overline{3}];
int i;
int j;
for (i=0;i<12;i++)</pre>
 for (j=0; j<13; j++)</pre>
  stoich[i][j]=mxGetPr(PAR)[i+(j*12)];
```

```
}
kh=mxGetPr(KINETIC)[0];
kx=mxGetPr(KINETIC)[1];
ksto=mxGetPr(KINETIC)[2];
nnox=mxGetPr(KINETIC)[3];
ko2=mxGetPr(KINETIC)[4];
knox=mxGetPr(KINETIC)[5];
ks=mxGetPr(KINETIC)[6];
kxsto=mxGetPr(KINETIC)[7];
muh=mxGetPr(KINETIC)[8];
knh4=mxGetPr(KINETIC)[9];
kalk=mxGetPr(KINETIC)[10];
bho2=mxGetPr(KINETIC)[11];
bhnox=mxGetPr(KINETIC)[12];
bstoo2=mxGetPr(KINETIC)[13];
bstonox=mxGetPr(KINETIC)[14];
mua=mxGetPr(KINETIC)[15];
kanh4=mxGetPr(KINETIC)[16];
kao2=mxGetPr(KINETIC)[17];
kaalk=mxGetPr(KINETIC)[18];
bao2=mxGetPr(KINETIC)[19];
banox=mxGetPr(KINETIC)[20];
vol = mxGetPr(V)[0];
SO sat = mxGetPr(SOSAT)[0];
for (i = 0; i < 13; i++)
   if (x[i] < 0.0)
     xtemp[i] = 0.0;
   else
     xtemp[i] = x[i];
proc[0] = kh*((xtemp[8]/xtemp[9])/(kx+(xtemp[8]/xtemp[9])))*xtemp[9];
Hydrolysis */
proc[1] = ksto*(xtemp[0]/(ko2+xtemp[0]))*(xtemp[2]/(ks+xtemp[2]))*xtemp[9];
/* Aerobic storage of Xsto */
proc[2] =
ksto*nnox*(ko2/(ko2+xtemp[0]))*(xtemp[5]/(knox+xtemp[5]))*(xtemp[2]/(ks+xtemp[5]))
mp[2]))*xtemp[9]; /*Anoxic storage of Xsto*/
proc[3] =
muh*(xtemp[0]/(ko2+xtemp[0]))*(xtemp[3]/(knh4+xtemp[3]))*(xtemp[6]/(kalk+xtemp[3]))
emp[6]))*((xtemp[10]/xtemp[9])/(kxsto+(xtemp[10]/xtemp[9])))*xtemp[9];
/*Aerobic Growth */
proc[4] =
muh*nnox*(ko2/(ko2+xtemp[0]))*(xtemp[5]/(knox+xtemp[5]))*(xtemp[3]/(knh4+xtemp[5]))
emp[3]))*(xtemp[6]/(kalk+xtemp[6]))*((xtemp[10]/xtemp[9])/(kxsto+(xtemp[10]
/xtemp[9])))*xtemp[9]; /*Anoxic Growth, Denitrification */
proc[5] = bho2*(xtemp[0]/(ko2+xtemp[0]))*xtemp[9]; /*Aerobic endogenous
respiration */
proc[6] = bhnox*(ko2/(ko2+xtemp[0]))*(xtemp[5]/(knox+xtemp[5]))*xtemp[9];
/*Anoxic endogenous respiration */
proc[7] = bstoo2*(xtemp[0]/(ko2+xtemp[0]))*xtemp[10]; /*Aerobic respiration
of Xsto*/
proc[8] =
bstonox*(ko2/(ko2+xtemp[0]))*(xtemp[5]/(knox+xtemp[5]))*xtemp[10]; /*Anoxic
respiration of storage */
```

```
proc[9] =
mua*(xtemp[0]/(kao2+xtemp[0]))*(xtemp[3]/(kanh4+xtemp[3]))*(xtemp[6]/(kaalk)
+xtemp[6]))*xtemp[11]; /* Aerobic growth of nitrifiers */
proc[10] = bao2*(xtemp[0]/(kao2+xtemp[0]))*xtemp[11]; /*Aerobic endogenous
respiration of autotrophs*/
proc[11] =
banox*(kao2/(kao2+xtemp[0]))*(xtemp[5]/(knox+xtemp[5]))*xtemp[11]; /*Anoxic
endogenous respiration of nitrifiers, Assume Ka, nox = Knox */
for (j=0; j<13; j++)</pre>
  {
  reac[j]=0;
   for (i=0; i<12; i++)</pre>
    reac[j]=reac[j] + proc[i]*stoich[i][j];
    }
  }
if (u[14] < 0.0)
 dx[0] = 0.0;
else
  dx[0] = (1.0/vol)*(u[13]*(u[0]-x[0]))+reac[0]+u[14]*(SO sat-x[0]); /* DO
concentration change, aeration input as Kla */
for (j=1; j<13; j++)</pre>
 {
   dx[j]=1.0/vol*(u[13]*(u[j]-x[j]))+reac[j];
 * 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? */
                           /* MEX-file interface mechanism */
#include "simulink.c"
#else
                           /* Code generation registration function */
#include "cg sfun.h"
#endif
```

## Appendix 4. S-function for a 10-layer non reactive settler implementation with ASM3 state variables – BSM1

```
* SETTLER1D is a C-file S-function for defining a 10 layer settler model.
* can simulate 0, 1 or 10 layers for the solubles by using MODELTYPE
 * Copyright: Ulf Jeppsson, IEA, Lund University, Lund, Sweden
#define S FUNCTION NAME settlerasm3
#include "simstruc.h"
#include <math.h>
#define XINIT ssGetArg(S,0)
#define PAR ssGetArg(S,1)
#define DIM ssGetArg(S,2)
#define LAYER ssGetArg(S,3)
 * mdlInitializeSizes - initialize the sizes array
static void mdlInitializeSizes(SimStruct *S)
    ssSetNumContStates( S, 130); /* number of continuous states
                         S, 0); /* number of discrete states
   ssSetNumDiscStates(
                         S, 16); /* number of inputs
   ssSetNumInputs(
                         S, 159); /* number of outputs
   ssSetNumOutputs(
   ssSetDirectFeedThrough(S, 1); /* direct feedthrough flag
   ssSetNumSampleTimes( S, 1);
                                   /* number of sample times
   ssSetNumSFcnParams(
                         s, 4);
                                   /* number of input arguments
                                   /* number of real work vector elements
   ssSetNumRWork(
                         s, 0);
   ssSetNumIWork(
                         s, 0);
                                   /* number of integer work vector
elements*/
                         S, 0); /* number of pointer work vector
   ssSetNumPWork(
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 < 130; i++) {
   x0[i] = mxGetPr(XINIT)[i];
}
* mdlOutputs - compute the outputs
static void mdlOutputs(double *y, double *x, double *u, SimStruct *S, int
  int i;
    /* underflow */
    y[0]=x[9]; /* SO */
y[1]=x[19]; /* SI */
     y[2]=x[29]; /* SS */
     y[3]=x[39]; /* SNH */
     y[4] = x[49]; /* SN2 */
     y[5] = x[59]; /* SNO */
     y[6]=x[69]; /* Salk */
     y[7]=x[79]; /* XI */
     y[8]=x[89]; /* XS */
     y[9]=x[99]; /* XH */
     y[10] = x[109]; /* XSTO */
     y[11] = x[119]; /* XA */
     y[12] = x[129]; /* XTSS */
     y[13]=u[14]; /* Q_r */
     y[14]=u[15]; /* Q_w */
     /* effluent */
     y[15]=x[0];
     y[16] = x[10];
     y[17] = x[20];
     y[18]=x[30];
     y[19] = x[40];
     y[20] = x[50];
     y[21] = x[60];
     y[22] = x[70];
     y[23]=x[80];
     y[24] = x[90];
     y[25] = x[100];
     y[26] = x[110];
     y[27] = x[120];
     y[28]=u[13]-u[14]-u[15]; /* Q e */
     for (i = 0; i < 130; i++) {
         y[i+29] = x[i];
  }
```

```
* 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)
{
double v0 max, v0, r h, r p, f ns, X t, area, h, feedlayer, volume;
double Q_f, Q_e, Q_u, v_up, v_dn, v_in, eps;
int i,j;
double vs[10];
double Js[11];
double Jstemp[10];
double Jflow[11];
double xtemp[130];
v0 max = mxGetPr(PAR)[0];
v0 = mxGetPr(PAR)[1];
r_h = mxGetPr(PAR)[2];
r_p = mxGetPr(PAR)[3];
f_ns = mxGetPr(PAR)[4];
X t = mxGetPr(PAR)[5];
area = mxGetPr(DIM)[0];
h = mxGetPr(DIM)[1]/mxGetPr(LAYER)[1];
feedlayer = mxGetPr(LAYER)[0];
volume = area*mxGetPr(DIM)[1];
eps = 0.01;
v in = u[13]/area;
Q f = u[13];
Q u = u[14] + u[15];
Q = u[13] - Q u;
v up = Q e/area;
v dn = Q_u/area;
for (i = 0; i < 130; i++) {</pre>
   if (x[i] < 0.0)
     xtemp[i] = 0.0;
   else
     xtemp[i] = x[i];
}
for (i = 0; i < 10; i++) {</pre>
   vs[i] = v0*(exp(-r h*(xtemp[120+i]-f ns*u[12]))-exp(-r p*(xtemp[120+i]-f ns*u[12]))
f ns*u[12])));
   if (vs[i] > v0 max)
      vs[i] = v0 max;
   else if (vs[i] < 0)
     vs[i] = 0;
}
```

```
for (i = 0; i < 10; i++) {
   Jstemp[i] = vs[i]*xtemp[120+i];
for (i = 0; i < 11; i++) {
   if (i < (feedlayer-eps))</pre>
      Jflow[i] = v up*xtemp[120+i];
   else
      Jflow[i] = v dn*xtemp[120+i-1];
}
Js[0] = 0;
Js[10] = 0;
for (i = 0; i < 9; i++) {
   if ((i < (feedlayer-1-eps)) \&\& (xtemp[120+i+1] <= X t))
      Js[i+1] = Jstemp[i];
   else if (Jstemp[i] < Jstemp[i+1])</pre>
      Js[i+1] = Jstemp[i];
   else
      Js[i+1] = Jstemp[i+1];
}
/* soluble components SO, SI, SS, SNH, SN2, SNO, SALK */
for (j=0; j<7; j++)
  for (i = 0; i < 10; i++)
   {
     if (i < (feedlayer-1-eps))</pre>
         dx[i+10*j] = (-v up*xtemp[i+10*j]+v up*xtemp[i+1+10*j])/h;
     else if (i > (feedlayer-eps))
         dx[i+10*j] = (v dn*xtemp[i-1+10*j]-v dn*xtemp[i+10*j])/h;
     else
         dx[i+10*j] = (v in*u[j]-v up*xtemp[i+10*j]-v dn*xtemp[i+10*j])/h;
   }
}
/* particulate components XI, XS, XA, XSTO, XB, XTSS */
for (j=7;j<13;j++)</pre>
     dx[10*j] = ((xtemp[10*j]/xtemp[120])*(-Jflow[0]-
Js[1]) + (xtemp[1+10*j]/xtemp[121])*Jflow[1])/h;
 for (i = 1; i < 10; i++)</pre>
    if (i < (feedlayer-1-eps))</pre>
        dx[i+10*j] = ((xtemp[i+10*j]/xtemp[i+120])*(-Jflow[i]-
Js[i+1]) + (xtemp[i-1+10*j]/xtemp[i-1+10*j]
1+120])*Js[i]+(xtemp[i+1+10*j]/xtemp[i+1+120])*Jflow[i+1])/h;
    else if (i > (feedlayer-eps))
        dx[i+10*j] = ((xtemp[i+10*j]/xtemp[i+120])*(-Jflow[i+1]-
Js[i+1]) + (xtemp[i-1+10*j]/xtemp[i-1+120]) * (Jflow[i]+Js[i]))/h;
      dx[i+10*j] = (v in*u[j]+(xtemp[i+10*j]/xtemp[i+120])*(-Jflow[i]-
Jflow[i+1]-Js[i+1])+(xtemp[i-1+10*j]/xtemp[i-1+120])*Js[i])/h;
  }
}
/*
```