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# WasteWater - a Library for Modeling and Simulation of Wastewater Treatment Plants in Modelica

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# *WasteWater* a Library for Modelling and Simulation of Wastewater Treatment Plants in Modelica

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## Abstract

The Modelica application library *WasteWater* containing three Activated Sludge Models of different complexity with the essential components of municipal wastewater treatment plants is presented. Component models are got due to the physical and biochemical modelling of activated sludge basins and secondary clarifiers. The library is verified for different operational situations by a benchmark simulation study. Simulation results of an example real-world wastewater treatment plant are shown.

**Keywords** mathematical models, simulation, object-oriented modelling, wastewater treatment

## 1 Introduction

From the point of view of a sustainable management of water and its quality, multidisciplinary teams are currently working to model, to simulate, and to optimize the design and the operation of wastewater treatment plants (WWTPs) with the global goal to reduce the pollution of the environment (receiving water) as well as the operational costs. Among other things this is due to national and international regulations, e.g. the Council Directives concerning urban wastewater treatment (91/271/EEC and 98/15/EEC) of European Commission. Nowadays large efforts are undertaken to extend the consideration of wastewater treatment to a plant wide scope, including such processes as sludge dewatering, waste sludge disposal, energy transformation by bio gas production, etc. Even including the whole or main part of the sewer system is subject of investigations.

To achieve the goals mentioned above a better understanding of microbiological behavior is needed, and its effects on wastewater control and management processes must be evaluated. That's why a number of mathematical models were developed in the past, e.g. [5, 6]. Most models are used for simulation purposes. Sometimes they are used in connection with simple control algorithms. This is also reflected in the simulation tools available.

Because of the growing effort in establishing computer models of large, complex, and heterogeneous physical systems, e.g. [8, 9, 11], an object-oriented approach has been chosen. The advantages are the suitability for multi-domain modelling, the usage of general equations of physical phenomena, the re-usability of model components, and a hierarchical model structure. The main goal consists in establishing object-oriented system models and furthermore in utilization of the automatically generated, efficient simulation code suitable both for simulation, and later on for control and optimization purposes.

Therefore the *WasteWater* library for Modelica was created that contains widely used and international accepted **A**ctivated **S**ludge **M**odels (ASM) and models for secondary clarifier describing the processes at wastewater treatment plants (WWTP) according to its physical laws with different mathematical complexity. Currently three Activated Sludge Models which are the ASM1, ASM2d and ASM3 [6] and five secondary clarifier models for each ASM are included within the library *WasteWater*. The most important parts at a WWTP are the biological part (activated sludge basin) and the secondary clarifier (settler). Components belonging to these parts are modelled for each ASM.

The verification of the approach is performed with the benchmark plant proposed by the COST benchmark study, [1]. The results published there could exactly be reproduced. Following the library *WasteWater* has been successfully applied to a real-world wastewater treatment plant.

## 2 Process and Models

Municipal wastewater treatment consists of two stages (a biological and a secondary clarification) and removes carbon, nitrogen, and phosphorus from the wastewater. Mechanical pre-treatment takes place prior these stages. There are activated sludge tanks of different properties. Nitrification takes place in an aerated section where ammonium-nitrogen ($NH_4^+$-N) is converted into nitrate-nitrogen ($NO_3^-$-N) by special bacteria under consumption of dissolved oxygen and denitrification takes place without dissolved oxygen and removes the nitrate-nitrogen. Both processes use the carbon compounds in the wastewater as energy source. Biological phosphorus removal occurs under absence of both dissolved oxygen and $NO_3^-$-N e.g. anaerobic conditions. In the secondary settler the activated sludge is separated from the cleaned water by gravity and is returned to the biological stage.

Several models exist that describe the processes taking place in the biological part of a wastewater treatment plant and a few models describing the settling process of the activated sludge within the secondary clarifier. Mostly used and accepted are models from the ASM model family [6] by the International Water Association (IWA) and layer sedimentation models. Therefore the **A**ctivated **S**ludge **M**odel No. **1** [5], the ASM2d, and the ASM3 as biological process models and the secondary settling tank models by Takács [13], Härtel [4], Otterpohl [10] and Krebs [7] are collected in a *WasteWater* library. Simulation results of the library where verified by the COST Benchmark plant configuration [1] that uses the ASM1 in connection with the secondary clarifier by Takács.

### 2.1 Activated Sludge Models

To model a wastewater system object-oriented it is useful to introduce the terms ‘potential variables’ and ‘flow variables’. The dissolved ($S_i$) and particulate concentrations ($X_i$) considered by an ASM are the potential variables in a WWTP model. The volume flow rate $Q$ of the wastewater is considered as the flow variable. These variables will be included into the components interfaces (see 3.1) and determine the mass flow rate between connected control volumes (basins). It is assumed that a basin is fully mixed and has a constant volume $V$. For such a basin the mass balance equations of an ASM define the model equations as follows:

$$\frac{dS_i}{dt} = (S_{i,\mathrm{in}} - S_i)\frac{Q_{\mathrm{in}}}{V} - r_i, \quad i \in \{I,S,NO,NH,ND,ALK\} \tag{1}$$

$$\frac{dS_O}{dt} = (S_{O,\mathrm{in}} - S_O)\frac{Q_{\mathrm{in}}}{V} - r_O + r_{\mathrm{air}}, \tag{2}$$

$$\frac{dX_i}{dt} = (X_{i,\mathrm{in}} - X_i)\frac{Q_{\mathrm{in}}}{V} - r_i, \quad i \in \{I,S,BH,BA,P,ND\} \tag{3}$$

The index $i$ here stands as example for the concentrations modelled in the ASM1 which are in equation (1) the different dissolved concentrations like inert organic matter ($S_\mathrm{I}$), substrate ($S_\mathrm{S}$), nitrate nitrogen ($S_\mathrm{NO}$), etc. and in equation (3) the particulate concentrations which are among others the heterotrophic ($X_\mathrm{BH}$) and autotrophic ($X_\mathrm{BA}$) biomass. Variables subscripted by index ‘in’, e.g. $S_{i,\mathrm{in}}$, indicate concentrations carried by the flow $Q_\mathrm{in}$ entering a considered tank. Equation (2) describes the balance of the dissolved oxygen and has an additional term for the oxygen uptake (aeration $r_\mathrm{air}$) caused by the blowers. The reaction rates $r_i$ resp. $r_O$ in the balance equations (1 – 3) are given by the model matrix of the Activated Sludge Models. The ASM1 models 13 relevant concentrations (state variables) and eight processes ($p_i$), the ASM2d is the most complex model with 19 concentrations and 21 biological processes, and the ASM3 has 13 wastewater components with 12 processes. The complete description of the models and their development is available in [6].

### 2.2 Settler System Models

The settler system models that are provided basically rely on a layer theory [4, 10, 13]. Here the settler is divided into horizontal layers of different properties with mass exchange (hydraulic and sedimentation flux) between the layers. The basis on which the sedimentation flux is modelled makes the difference in the clarifier models included in the *WasteWater* library. As example the double-exponential settling velocity function (4) by [13], that is based on the solids flux concept and applicable to both hindered and flocculant settling conditions is given as follows:

$$v_{sj} = v_0\, e^{-r_h X_j^*} - v_0\, e^{-r_p X_j^*}, \quad 0 \le v_{sj} \le v_0^{'} \tag{4}$$

with $v_{sj}$ - settling velocity in layer $j$, $X_j^*$ - suspended solids concentration in layer $j$ subject to the limiting condition $X_j^* = X_j - X_\mathrm{min}$, $X_j$ - suspended solids concentration in layer $j$, $X_\mathrm{min} = f_{ns} X_\mathrm{in}$ - minimum attainable suspended solids concentration, $f_{ns}$ - non-settleable fraction, $X_\mathrm{in}$ - mixed liquor suspended solids concentration entering the settler.

A clarifier layer model contains at least of three layers. The clarifier models provided in the library are composed of ten settler layers. All layers are characterized by flux exchanges of adjacent layers caused by hydraulic and settling mass transport. The feed layer (clarifier inflow) receives the wastewater stream from the biological part of a WWTP. There is an upward directed hydraulic flow above the inflow caused by the wastewater flow and a downward directed hydraulic flow below the inflow caused by the return and waste sludge flow at the bottom of the clarifier. In all layers a sedimentation flux occurs due to the gravity that is calculated by e.g. settling velocity function (4) multiplied by the corresponding suspended solids concentration $X_j^*$.

## 3 Object-Oriented Modelling

The library *WasteWater* consists of sub-libraries for each implemented Activated Sludge Model, e.g. ASM1, ASM2d and ASM3 besides a sub-library for icons and one for wastewater units. An ASM library itself has an interfaces sub-library for partial models and connectors, sub-libraries for preclarifier and the secondary clarifier models, a sublibrary for example wastewater treatment plant models, and contains the necessary components for modelling of wastewater treatment plants.

### 3.1 Definition of Connectors

In order to built up an Activated Sludge Model component library the first step is to define the component interfaces. The proper definition of the interfaces is an essential part because the connectors determine the independent parts of a complex model. After definition of the connectors, library components can be developed and tested independently. The main connector of an ASM library within *WasteWater* is that one between the different basins of a WWTP and consists of the flow and potential variables described in section 2.1. For example, this reads in Modelica modelling language for the ASM1 as follows:

```
connector WWFlowASM1
  package WWU = WasteWaterUnits;
  flow WWU.VolumeFlowRate Q;
  WWU.MassConcentration Si;
  WWU.MassConcentration Ss;
  ...
  WWU.Alkalinity Salk;
end WWFlowASM1;
```

Within the sub-libraries of the several secondary clarifier models different interfaces to connect and interchange information between adjacent layers are provided.

### 3.2 ASM Library Components

In this section an overview over the components inside an ASM sub-library of *WasteWater* shall be given. An ASM library consists of components describing the processes taking place in the biological stage of a WWTP (e.g. *Nitri*, *Deni*), a blower, flow mixer, flow divider, measurement devices (concentration sensors), a source and sinks for the wastewater stream, and a sub-library *SecClar* containing the clarifier models which each having classes that describe the sedimentation processes in the different secondary clarifiers.

First of all the ASM parameters and equations (process rates, reactions and derivatives of the states) and the connector information that are needed in different model classes are defined in a `partial` model which gives this information to the components. In extracts the partial model for the ASM1 reads as follows:

```
partial model ASM1Base
  package WWU = WasteWaterUnits;
  parameter Real mu_h=4.0;
  ...
  WWU.MassConcentration Si,...;
  Real p1...p8 "process rates";
  Real r1...r13 "reactions";
  Real inputSi,inputSo,...;
  Real inputXi,inputXp,...;
  Real r_air;
  equation
    p1 = ...;
    r1 = ...;
    // derivatives
    ...
    der(Xp) = inputXp + r7;
    der(So) = inputSo + r8 + r_air;
    ...
  // Outputs
  Out.Q + In.Q = 0;
  Out.Si = Si;
  ...
end ASM1Base;
```

Following components are available for each ASM:

*Deni*: It inherits graphic information and the information from the respective partial model e.g. `ASM1Base` and extends it by a specific tank volume to model a denitrification tank (`r_air = 0`).

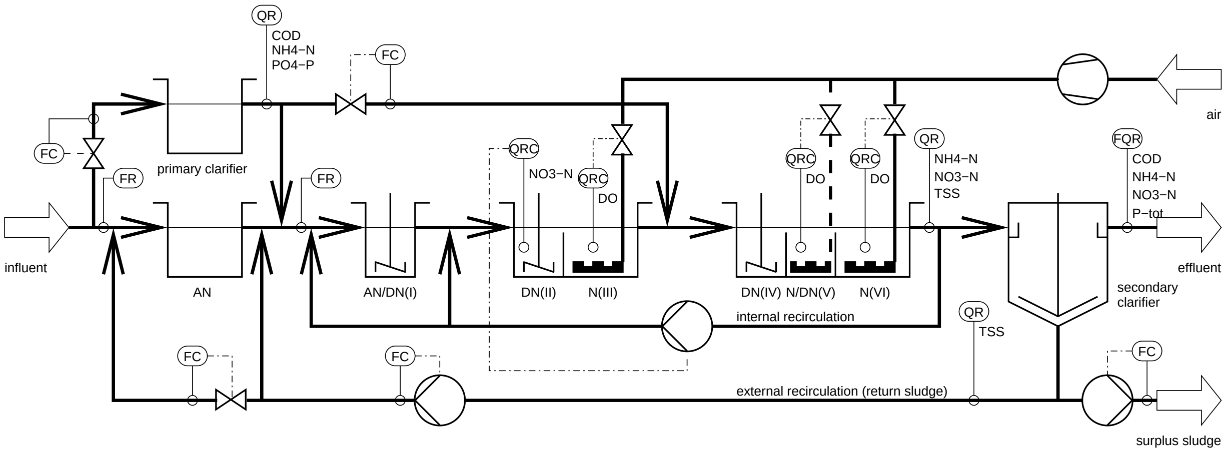

Figure 1: Simplified scheme of the example wastewater treatment plant

*Nitri*: This component is used to model a nitrification (aerated) tank of a WWTP which as well inherits graphic information and e.g. `ASM1Base` and is extended by the tank volume and aeration system dependent parameters.

```
model Nitri
 extends Icons.nitri;
 extends Interfaces.ASM1Base;
 import SI = Modelica.SIunits;
 parameter SI.Volume V "tank volume";
 //aeration system parameters
 parameter Real alpha=0.7;
 ...
 Interfaces.AirFlow AirIn;
 equation
   r_air = ...*AirIn.Q_air*...;
   // Volume dependent dilution
   inputSi = (In.Si - Si)*In.Q/V;
   inputXi = (In.Xi - Xi)*In.Q/V;
   ...
end Nitri;
```

*SecClarModTakacs*: Is a prepared component which describes a ten-layer secondary clarifier model based on Takács [13] using the sub-library *SecClar.Takacs*.

*Blower*: The blower can be used to model an air flow between a minimal ($Q_{\min}$) and a maximal ($Q_{\max}$) blower capacity as input to the nitrification tank based on a control signal.

*Pump*: This component models a wastewater pump. It generates a wastewater flow between $Q_{\min}$ and $Q_{\max}$ that is controlled by an external control signal.

*Mixer*: There are two components available which mix two respectively three different flows of wastewater of different amount and different concentration. The output is a single mixed wastewater stream.

*Divider*: These two elements divide one flow of wastewater into two separate flows of same concentration either by known flows or externally controlled by a signal.

*OxygenSensor*: The concentration of oxygen in a tank or a wastewater stream is measured and transformed into an output signal $y(t)$ that can be further processed. Similar sensors for the concentration COD, nitrate-nitrogen ($S_{\mathrm{NO}}$), ammonia-nitrogen ($S_{\mathrm{NH}}$), and others are provided.

*WWSource*: Provides all ASM data at the influent of a WWTP. The dimension depends on the used ASM. The information can also be read from a file.

*EffluentSink*: Is the receiving water at the effluent of a wastewater treatment plant and terminates a WWTP model. A similar component is the *SludgeSink*.

## 4 Example of use

For verification and validation purposes of the *WasteWater* library's components first of all the COST benchmark plant layout was used. The results published in [1] could exactly be reproduced using ASM1 components of *WasteWater*. But this is not discussed in more detail here.

Following the library *WasteWater* is applied to a real-world WWTP. The plant is situated in Jena, Germany, and has a size of 145,000 population equivalents. A model of this plant is available in each *ASM_.Examples* sub-library as complex plant example. The configuration of this WWTP is shown in Figure 1. The continuous flow WWTP is a cascade type denitrification with

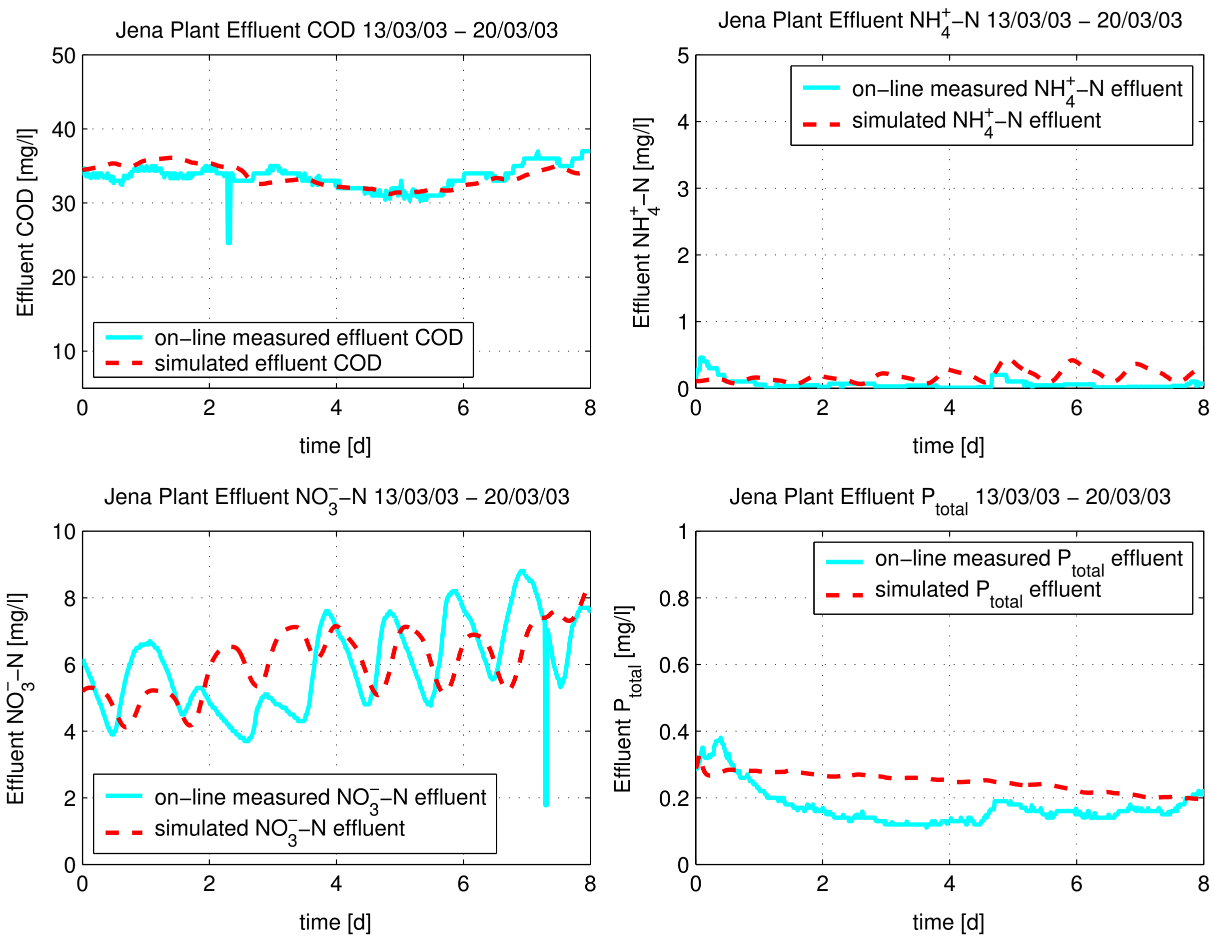

Figure 2: Simulated and on-line measured effluent values for the calibrated ASM2d WWTP example model

pre-clarification, biological and chemical phosphorus removal, and secondary settling. The plant is designed for a mean dry weather inflow of 28,500 m$^3$/d. The total volume of all activated sludge tanks is approx. 24,000 m$^3$, of which 14,000 m$^3$ can be aerated. There are two flow feedbacks, one internal recirculation from the last biological tank, and a return sludge flow from the bottom of the secondary settler, see Figure 1. An additional outflow, the surplus (waste) sludge flow, occurs at the bottom of the settler. The effluent of the WWTP is discharged to the receiving water and is located at the settlers surface.

On-line measurements are available for the influent flow rate and concentrations (chemical oxygen demand (COD)), ammonia-nitrogen, and phosphate), internal and external recycle flow rates and total suspended solids (TSS) concentrations, dissolved oxygen in the aerated tanks, effluent quality (COD, ammonia- and nitrate-nitrogen, and phosphate) as well as phosphate, ammonia- and nitrate-nitrogen at the outflow of the cascade.

The software package DYMOLA [2] is used to implement the *WasteWater* library and to perform the example simulation scenarios. A simulation diagram can be established by drag and drop of the several components of the *WasteWater* library and linking the elements together via the connectors. A system of differential-algebraic equations (DAE), in the described plant configuration using the ASM2d, with 3081 unknowns and equations and 252 state variables is established automatically by DYMOLA. The DASSL integration procedure implemented in DYMOLA is used to solve the DAE system.

Simulating real wastewater treatment plants normally needs a model calibration procedure, as the provided ASM set of parameters by IWA that is implemented in *WasteWater* has to be adapted and does not match all WWTPs. Many of the biological and kinetic parameters may vary in a limited range. Such a model calibration has been done for the ASM2d complex example plant using genetic algorithms.

Figure 2 shows the simulated effluent values COD, ammonia- ($NH_4^+$-N) and nitrate-nitrogen ($NO_3^-$-N), and total phosphorus of the calibrated ASM2d example model (dashed line) compared to the on-line measurements from the SCADA system (solid line). The simulation results are satisfactory so far for the precision of wastewater treatment process models. Obvious differences occur due to several assumptions and simplifications which need to be done during the validation phase. Further improvement of the results is expected by applying initial state estimation which is subject of current investigation.

## 5 Conclusion

An application library *WasteWater* for Modelica that collects the Activated Sludge Models ASM1, ASM2d, and ASM3 by the International Water Association (IWA) including several secondary clarifier models was developed. It contains essential WWTP components according to an object-oriented approach and based on physical modelling. The *WasteWater* library presented and its application to plants of several complexity show the usefulness and the advantages of an object-oriented modelling approach.

The compiled system model can be used for solving parameter and state estimation problems and especially as basis for ongoing control and optimization applications, see [3].

Future work is directed to use the automatically compiled system model (DAE system) of an calibrated WWTP model inside a model-predictive control algorithm within a decision support system in order to optimize the plant behavior. First open-loop optimization results are already available.

## 6 Acknowledgment

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