THE MODELING OF A LARGE INDUSTRIAL WASTEWATER TREATMENT PLANT

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ABSTRACT

The ASM3 model in the GPS-X wastewater treatment plant simulator was used to model a wastewater treatment plant that treats waste from a chemical production plant. The wastewater plant uses a step-feed activated sludge process for biological treatment and circular sloping bottom clarifiers for secondary clarification. The composition of the influent waste stream was highly variable during the study period and this posed special challenges for influent characterization. Despite the elevated wastewater temperatures encountered at the plant (> 26 ^{o}C), the default Arrhenius expression and its coefficients were found to be applicable for modeling the temperature dependence of the ASM3 kinetic parameters. The autotrophic growth rate was found to be generally low in the plant possibly due to inhibitory substances in the influent. In the plant, denitrification was observed in the aeration basins and ASM3 was modified to handle aerobic denitrification. The sludge settling characteristics varied and this required dynamic calibration of the settling model parameters. The calibrated model was used to conduct a number of simulation studies designed to improve the understanding of the plant and to assess the impact of loading changes (e.g. increased organic loading) and operational changes (e.g. changes in step-feed strategy).

KEYWORDS

Industrial wastewater, chemical industry wastewater, modeling, simulation, ASM3, activated sludge.

INTRODUCTION

The application of the currently published activated sludge models (e.g. ASM1 and ASM3) to the modeling of plants treating domestic wastewater has been well documented. Despite this, the application of these models to the simulation of facilities treating industrial waste has been less common. The simulation of industrial activated sludge plants poses special challenges due to the highly variable nature of the wastewater and the extreme operating conditions often encountered (Bury et al., 2002).

This paper describes the application of the ASM3 model to the modeling and simulation of a large industrial wastewater treatment plant. Details on the ASM3 model are provided by Henze et al. (2000). The plant modeled in this study is Eastman Chemical's Kingsport, Tennessee wastewater treatment plant (WWTP) which is a step-feed activated sludge plant with conventional secondary clarification. The aerobic reactor system consists of four parallel trains and each train has three aeration basins in series. The influent flow to the aerobic reactor system is divided equally among the trains. The plant also has equalization and diversion tanks to manage the loading to the activated sludge system and belt filter-presses for dewatering of the waste activated sludge (WAS). The plant treats waste from a plant that manufactures chemicals, plastics, and synthetic fibers. The wastewater is highly variable in both flow and composition and is mainly comprised of short-chained alcohols and acids. The Kingsport wastewater treatment plant has been described in detail by Churn et al. (1990).

The calibrated plant model was used to conduct a number of simulation studies to assess the impact of organic and nutrient loading changes, operational changes, and events such as toxic spills. The main objective of the project was to demonstrate how process modeling and simulation can be applied in the industrial wastewater treatment field.

METHODOLOGY

The modeling study was conducted using GPS-X, which is a steady-state and dynamic wastewater treatment plant simulator. GPS-X can model a wide variety of wastewater treatment unit operations and processes including attached growth and fixed film biological reactors and solids separation systems such as clarifiers and membrane filters. The simulator has a graphical user interface which allows users to connect process objects together to create a plant layout. Process objects are graphical representations of unit operations and processes. Users can decide which wastewater constituents are considered in the plant layout (for example whether phosphorus is considered) and select which models are used to describe the influent and each process object.

The biological models in GPS-X are based on the International Water Association (IWA – formerly IAWQ) family of activated sludge models (Henze et al., 2000), which are all included in GPS-X. The simulator can predict the effects of biological growth processes and solids separation on conventional water quality parameters including carbonaceous biochemical oxygen demand ($cBOD_5$), chemical oxygen demand (COD), total Kjeldhal nitrogen (TKN), total suspended solids (TSS), ammonia nitrogen, nitrate/nitrite nitrogen, and soluble phosphorus.

The modeling study was conducted in a series of stages to make the work more manageable and to ensure successful completion of the project. The project included four major phases: project initiation, data analysis, model setup and calibration, and plant analysis.

The project initiation phase involved the fundamental project planning and established a roadmap for the project. At this stage, additional data requirements were identified and Eastman personnel collected additional COD, total organic carbon (TOC), $cBOD_5$, TSS, and volatile suspended solids (VSS) data which assisted in the characterization of the influent and effluent wastewater.

In the data analysis phase a historical review was conducted to summarize the operation of the Kingsport WWTP during 2002. The results of this analysis served as the basis for the model setup and calibration work.

The main goal of the model setup and calibration phase was to develop a model that accurately predicted plant performance given the 2002 plant operating data. The plant layout was constructed in GPS-X based on the plant schematics and operating data and included all of the important unit operations and processes in the plant. Simplifications were made where possible to reduce the complexity of the layout. These included removing the neutralization tanks and grit basins and combining the four final clarifiers into one unit with an equivalent surface area.

The plant model was calibrated to the dynamic data from the calibration period by characterizing the influent and by adjusting certain key ASM3 kinetic parameters. The calibrated model was then verified using additional dynamic data from 2002. As will be discussed later in the RESULTS Section, the calibration procedure revealed that the plant receives a highly variable waste stream and this required special consideration to ensure that the model accurately represented plant behavior.

In the plant analysis phase the calibrated GPS-X simulation model was used as a basis for a number of "what-if" scenarios. These scenarios were created based on discussions with Eastman. The "what-if" analysis showed how the plant model can be used, for example, to select the best sludge retention time (SRT) for the plant, estimate the COD loading capacity of the plant, and assess the impact of step-feed changes.

RESULTS

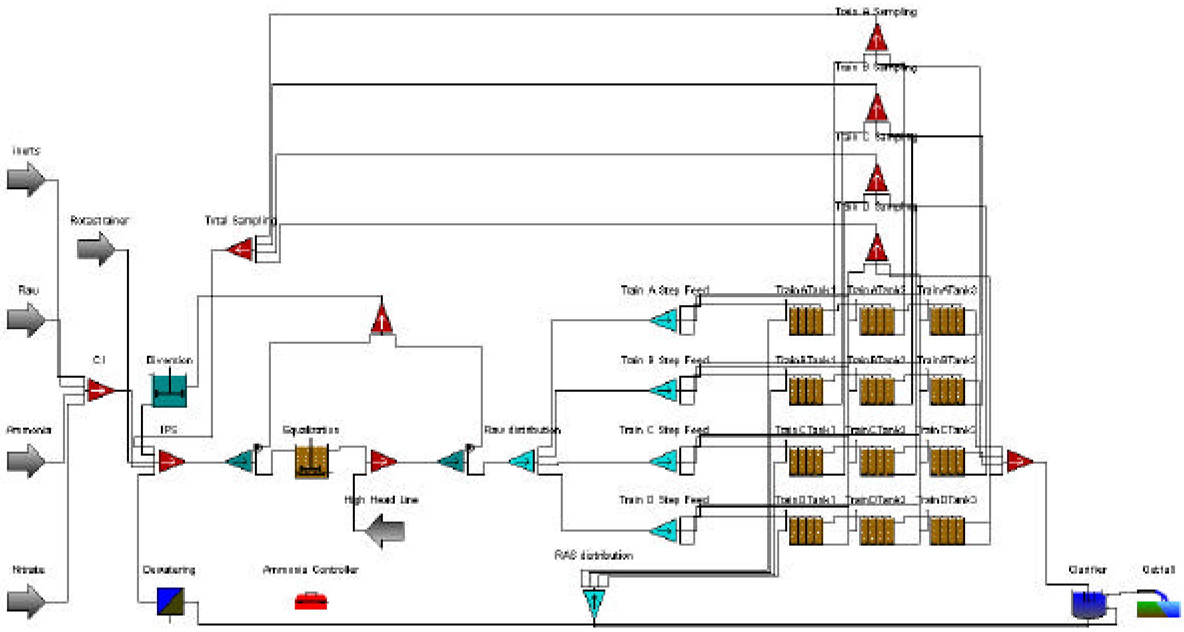
Layout Description

The GPS-X layout which represents the Kingsport WWTP is shown in Figure 1. The GPS-X layout includes the following influent streams: raw waste, ammonia, ammonium nitrate, rotastrainer solids, inert solids, and a high head line. Each waste stream has been modeled separately to facilitate the characterization of the raw waste stream.

The combined interceptor (CI) receives the raw waste stream, the inert solids stream, and the ammonia stream. The influent pumping station (IPS) receives the CI flow, the rotastrainer solids flow, the pumped flow from the diversion system, the filtrate from the belt-filter presses, the ammonium nitrate stream, and the sampling flows from the aeration basins. The plant continuously samples mixed liquor from the aeration basins and this contributes a considerable amount of solids to the waste stream leaving the influent pumping station.

After the IPS, the waste stream flows to the equalization tank. A reactive tank model (CSTR object) has been used for the equalization tank to account for possible COD removal due to denitrification. An ammonia controller was used to control the flow rate of the ammonia stream so that the model matches the measured ammonia concentrations in the equalization tank. This approach was required because no information was available on the daily amounts of ammonia added before the influent pumping station. The high head line, which contains a considerable amount of ammonia, joins the main wastewater flow after the equalization tank. Flow can be diverted before the equalization tank and after the high head line to the diversion tank. Flow is pumped from the diversion tank back to the influent pumping station.

Figure 1 – GPS-X Plant Layout



The equalization tank effluent flows to the aerobic reactor system. Splitters are used to handle the step-feed distribution to each aerobic reactor train. The layout has been configured with a separate reactor object for each aeration basin. This is required because sampling flows are pumped from each basin and because during certain times of the year the aeration trains have different step-feed distributions.

The overflows from the four aerobic reactor trains are combined and fed to the clarification system. The four final clarifiers, which are circular with sloping bottoms, are represented by one large clarifier in the layout. This is done to simplify the layout and because data are only available for the combined recycle activated sludge (RAS) and WAS streams from the four clarifiers. The clarifier model in GPS-X was modified to allow pumping of the RAS and the WAS from different levels as is done in the plant. The WAS is pumped to the belt-filter presses, which are represented by one dewatering object, and the filtrate from the presses is returned to the IPS.

The ASM3 biological model was selected for the biological processes because it includes storage of readily available substrate, which is an important process to capture for plants treating wastewaters with high amounts of soluble substrate like the Kingsport WWTP. In addition, a modified version of the model, in TOC terms, is available in the literature and could be implemented in GPS-X if desired at a later date. This is significant as the plant measures the influent TOC online but not the COD.

Model Setup and Calibration

Eastman provided data for the Kingsport plant for the period from January 1, 2002 to November 12, 2002. These data were augmented by additional data from a spot sampling exercise and some estimated values provided by Eastman. The model was calibrated using data from the first 60 days of 2002 and verified using the remaining 2002 operating data. Because the influent composition and sludge settleability varied considerably throughout 2002, constant influent coefficients and model parameter values could not be used.

Influent characterization is one of the most important steps in the calibration of wastewater treatment plant models. It involves determining the stoichiometry of the influent streams so that the available water quality measurements (e.g. total COD) can be partitioned into the state variables used in the biological model. Past experience has shown that once the influent is properly characterized, the kinetic and stoichiometric parameters in the biological model often require minimal adjustment.

The characterization of the influent waste streams in this study was particularly challenging because these streams are highly variable and online flow and composition measurements were not available for all streams. It became apparent during initial attempts at model calibration that using a constant influent characterization would not allow for prediction of all operating periods in 2002.

Approximately 80% of the raw waste stream is comprised of low molecular weight acids (e.g. acetic, butyric, and propionic) and alcohols (methanol, ethanol, and isopropanol). The remaining 20% is made up of a variety of organic chemicals depending on the particular product being manufactured at the chemical plant. In addition, inert organic solids and inert inorganic solids are added periodically to the plant in the rotastrainer solids and inert solids streams.

The stoichiometric parameters for the influent waste streams were initially estimated during the data analysis phase and were further refined during the calibration. COD and TSS balances were written around the IPS and the equalization tank to help capture the varying nature of the influent waste streams. Based on the influent characterization work, it was determined that the plant receives a relatively constant amount of soluble COD throughout the year but a highly variable amount of particulate COD.

The calibration of the ASM3 model involved the adjustment of key kinetic parameters as necessary to match the measured plant data. As a starting point for model calibration, the default kinetic and stoichiometric parameters used in the ASM3 model were taken from a calibration of ASM3 done by Koch et al. (2000). Given the calibrated raw waste stream stoichiometry and the calibrated composition of the solids streams, certain kinetic parameters were then further adjusted to improve the agreement with the plant measurements.

The average wastewater temperature in the aeration basins was measured in the plant and varied between 26 ^{o}C (January) and 37 ^{o}C (July and August). The measured temperatures were used in the GPS-X layout as the ASM3 model uses the Arrhenius equation to model the temperature dependence of its kinetic parameters. Although the temperatures encountered in the plant were outside the recommended temperature range for ASM3 (8 ^{o}C to 23 ^{o}C), the default ASM3 temperature coefficients were found to be applicable to the modeling of the Kingsport plant.

Important model calibration steps included the following:

- Adjustment of the maximum heterotrophic growth rate and the aerobic heterotrophic endogenous respiration rate parameters to match the measured TSS concentrations in the aeration basins.
- Adjustment of the maximum autotrophic growth rate to match the measured ammonia concentrations in the aeration basins. The low values required for this parameter (0.4 d^{-1} to 0.6 d^{-1}) suggest that nitrification is always inhibited to some extent in the plant as more than enough nitrogen is added to meet the nutrient requirements of the biomass.
- Modification of ASM3 to handle denitrification occurring in the aeration basins. After discussions with plant staff, it was confirmed that some denitrification does occur in the aeration basins (especially in the third basin of each train), as well as in the equalization tank.
- Calibration of the final clarifier model to match the measured effluent TSS, WAS TSS, and RAS TSS measurements. The sludge settling characteristics at the plant were found to vary considerably throughout the year due to variable polymer dosing prior to the clarifiers and this required the use of the dynamic parameter estimation tool in GPS-X.
- Calibration of the empirical belt-filter press model.

Following the calibration steps outlined above, good agreement was obtained between the measured and simulated values for all the important model variables. The reliability of the calibration was tested using the remaining plant data available for 2002.

The simulation results for the TSS concentration of the combined overflow from the four final aeration basins are shown in Figure 2 while the results for the effluent TSS concentration are shown in Figure 3. These plots are for the entire 2002 operating period considered (January 1, 2002 to November 12, 2002). For a more detailed discussion of the calibration results see Schraa et al. (2004). Based on the calibration results the project team concluded that the model could adequately predict plant performance and was suitable for analyzing plant operation and performing “what-if” simulations.

Figure 2 – Simulation Results for TSS Conc. of Combined Overflow from Four Final Aeration Basins

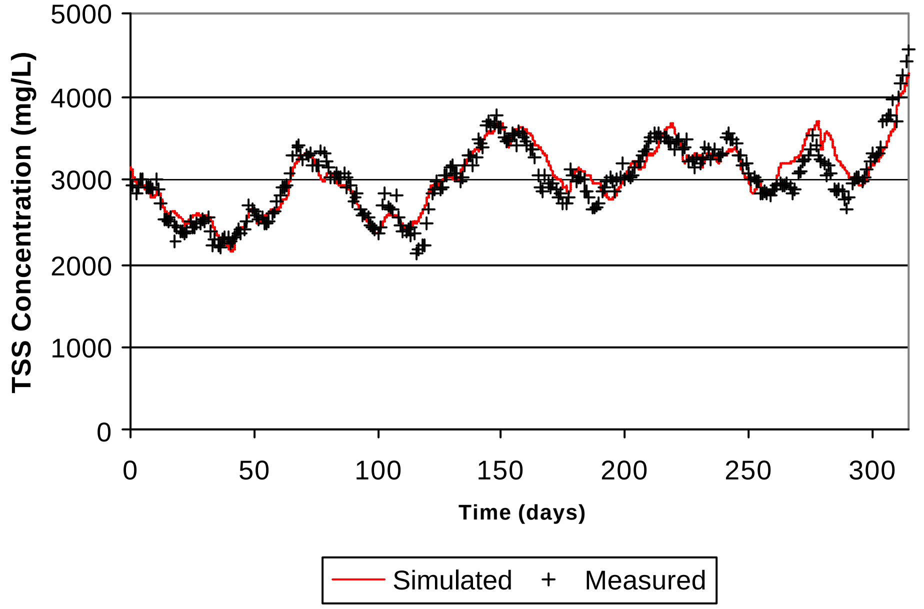
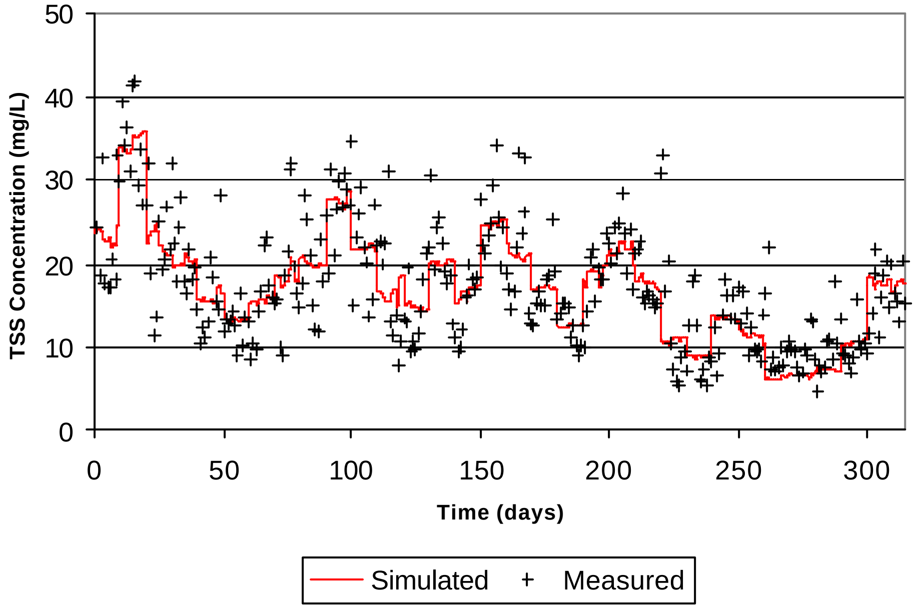


Figure 3 – Simulation Results for Effluent TSS Concentration



Plant Analysis

The calibrated Kingsport plant layout was used to run a number of "what-if" simulations that were of interest to plant staff. Some of the studies conducted included:

- Analysis of the impact of changes in plant SRT
- Analysis of the impact of changes in plant COD loading
- Analysis of the impact of changes in plant ammonia loading
- Simulation of a toxic spill that inhibits bacterial growth
- Analysis of the impact of changes in step-feed strategy

The results of the influent COD and step-feed analyses are presented here. See Schraa et al. (2004) for the results of the SRT analysis.

A base case set of operating and loading conditions was developed for the "what-if" scenarios to provide a common basis for the simulations. Eastman requested that the following operational settings be used:

- Wastewater temperature = 35 ^{o}C
- SRT = 15 days
- Step-feed flow split of 50/30/20 (on a percentage basis) to basins 1, 2, and 3 respectively for each train
- Dissolved oxygen (DO) concentration targets in the basins are 3 mg/L in basins 1 and 2, and 1.6 mg/L in basin 3 for each train
- RAS return ratio (RAS to aerobic reactor system influent flow ratio) = 0.25
- No diversion of influent waste stream

In addition, influent data and model parameter values were required to establish the base case. The period from March 2, 2002 to March 27, 2002 was chosen as the base case period for this purpose. This period was chosen because the influent streams were fairly stable in terms of flow and composition. Averages were calculated for all the influent data and the model parameters across this period and these values were used to establish the base case for the "what-if" scenarios.

GPS-X has a sensitivity analysis tool that allows the user to conduct both steady-state and dynamic sensitivity studies to determine the impact of changes in model variables and parameters. To study the impact of the influent COD loading on plant performance, the GPS-X analyze tool was used to conduct a steady-state sensitivity analysis. The analyze tool was configured to calculate the steady-state of the plant at successive raw waste stream COD values ranging from 700 mg/L to 2,500 mg/L in intervals of 100 mg/L while maintaining a constant SRT of 15 days and a constant influent flow rate.

Figure 4 shows a plot of the effluent $cBOD_5$ concentration during the influent COD sensitivity analysis. The model predicts that plant can still meet its effluent $cBOD_5$ limit (18 mg/L) when the raw waste influent COD is increased to 2,500 mg/L. Although not shown, the model indicates that solids loading to the clarifiers will be increased substantially when the influent COD is increased to 2,500 mg/L.

Figure 4 – COD Sensitivity Analysis Results for Effluent $cBOD_5$ Concentration

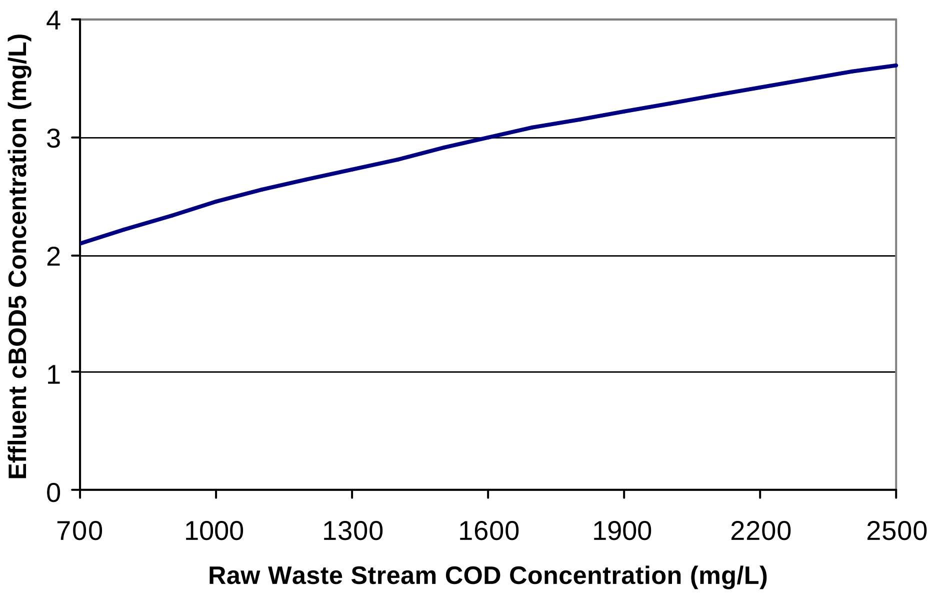


Figure 5 shows a plot of the effluent nitrogen concentrations (total nitrogen, ammonia nitrogen, and nitrate nitrogen) during the influent COD sensitivity analysis. The model predicts that the plant removes more total nitrogen at higher influent COD values due to increased denitrification.

Although not shown here, the model also predicts the impact of influent COD on the air flow required and the mass of sludge produced. By adding their operating and sludge disposal costs to the model, plant staff can use the model to determine the cost impacts of an increased organic loading.

A step-feed scenario was created that allowed plant staff to study the impact of changes in the step-feed ratios used in the plant at a constant SRT. In this scenario the simulation is started at steady-state with all four trains operating in plug-flow mode (i.e. 100% of flow to tank 1). The plant is allowed to run in this configuration for 45 days and then the step-feed distribution to all trains is changed and the simulation is run for another 45 days. This process is repeated over a range of step-feed distributions ranging from complete plug-flow to having no raw wastewater flow to tank 1. Table 1 shows the step-feed ratios used during the simulations. The 45 day period between the step-feed changes is used to allow the plant to reach steady-state between changes.

A plot of the TSS concentration of the combined overflow from the four final aeration basins is shown in Figure 6. As expected, the solids loading to the clarifiers drops as more flow is diverted to the second tank instead of the first tank. Although not shown here, this analysis can be used by plant staff to select a step-feed strategy that minimizes the loading on the clarifiers while maintaining an acceptable level of treatment. The step-feed analysis was repeated for the case of poor settling in the clarifiers.

Figure 5 – COD Sensitivity Analysis Results for Effluent Nitrogen Concentrations

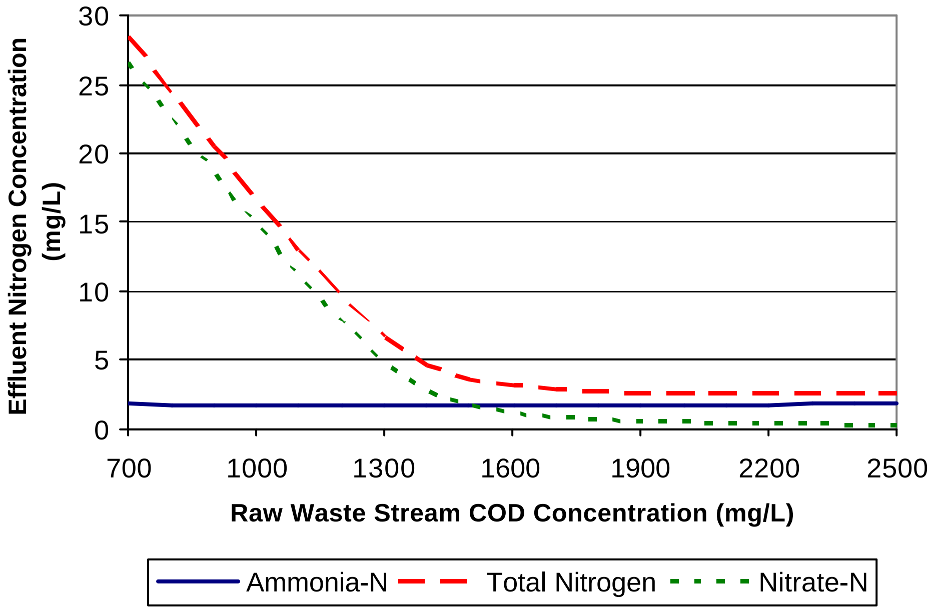
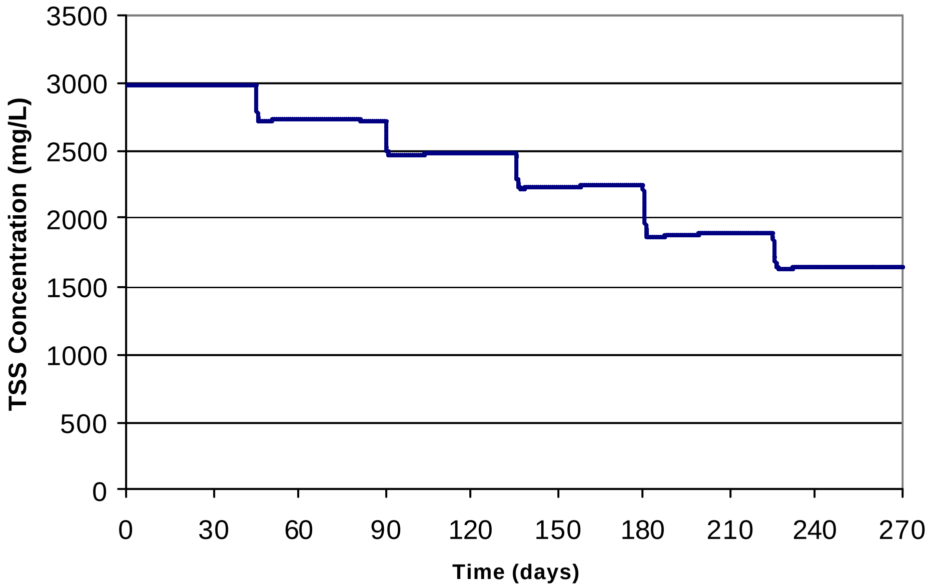


Table 1 – Step-Feed Ratio Data Used in Step-Feed Analysis Scenario

Simulation Period	Step-Feed Ratio (%)		
	Tank 1	Tank 2	Tank 3
0 to 44 days	100	0	0
45 to 89 days	70	20	10
90 to 134 days	50	30	20
135 to 179 days	30	50	20
180 to 224 days	10	70	20
225 to 269 days	0	80	20

Figure 6 – Step-Feed Sensitivity Analysis Results for TSS Conc. of Combined Overflow from Four Final Aeration Basins



DISCUSSION

This study has demonstrated that the ASM3 model is applicable to the modeling of wastewater treatment plants treating chemical industry wastewater but that special considerations are required. Some of the important issues that may require consideration when modeling industrial wastewater treatment processes are discussed below:

- The influent streams are often highly variable in composition and depend on the production schedule at the manufacturing plant. As a result, the influent stoichiometry may be variable. Separating combined waste streams into simpler individual waste streams can help simplify the analysis. Mass balances can be useful in characterizing the influent waste streams.
- It can be difficult to obtain the necessary data to complete a modeling study. Plants normally measure TOC but not COD, BOD, or TSS and may not measure all waste streams. Most wastewater models are written in terms of COD. It will often be necessary to ask the plant to conduct additional sampling to determine key ratios such as COD:TOC and VSS:TSS. Mass balances can help in estimating missing information.
- Industrial wastes can be nutrient limited and industrial WWTPs often add nitrogen and phosphorus for biomass growth. In the Kingsport plant the waste ammonia and nitrate added is in excess of the nitrogen requirements of the biomass. Phosphoric acid additions provide the phosphorus required by the biomass.
- Problems with secondary sludge settleability are common in industrial WWTPs (possibly due to nutrient limitations and inhibitory influents) and settling aides such as polymer may be used. As a

result, the settling characteristics of the sludge can vary considerably over time and this presents problems when calibrating the settling and dewatering models. Time-varying calibration of the parameters can be used if necessary.

- Inhibitory substances may be found in the influent which inhibit biomass growth (especially for autotrophs). This may require special attention to the growth rates used.
- The model may predict higher nitrate levels than measured in the plant due to denitrification occurring in aerated tanks as a result of oxygen diffusion limitations in the floc cores and tanks that are not ideally mixed. Modifications to the biological model may be required to capture this behavior.
- Due to the high organic loading rates encountered, industrial WWTPs typically operate at elevated temperatures relative to municipal wastewater. The default Arrhenius temperature coefficients found in ASM3 may not be applicable to all situations although they appeared to be satisfactory for the Kingsport model.
- It can be difficult to simulate oxygen transfer initially and using DO controllers in the model to match measured DO concentrations can be helpful. This approach eliminates the confounding effects on kinetic parameter estimation caused by DO levels that are different from those measured in the plant (Bury et al., 2002).

The Kingsport study also demonstrated that a calibrated simulation model can be a useful analysis tool for industrial wastewater treatment plants. Plant staff can learn about their plant without having to experiment with the plant and risk plant upset.

CONCLUSIONS

The ASM3 model was used to model a wastewater treatment plant treating waste from a chemical production plant. It was found that the model could accurately predict plant performance after certain issues specific to industrial wastewater treatment were addressed. The calibrated model was used to study the performance of the plant. Some general conclusions about modeling industrial wastewater treatment processes were developed that may be applicable in other modeling projects and these are listed below:

- Industrial wastewaters are highly variable in composition and the influent stoichiometry may vary.
- Mass balances may be useful in characterizing influent waste streams in the absence of necessary measurements.
- The ASM3 model can be applicable outside the recommended temperature range of 8 ^{o}C to 23 ^{o}C.
- Nitrification can be inhibited in industrial WWTPs due to inhibitory substances in the influent. Some level of inhibition may always be present and the autotrophic growth rate may be lower than for municipal wastewater.
- Denitrification may occur in aerated tanks. Aerobic denitrification can be added to ASM3 if necessary.

- Changing sludge settling characteristics in a layered settling model can be handled by using a dynamic parameter estimation algorithm.

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