# Wastewater treatment modelling in practice: a collaborative discussion of the state of the art

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## ABSTRACT

Three consulting teams conducted independent modelling projects for three different wastewater treatment plants ranging in size from approximately 113,800 $m^3$/d (30 mgd) to 530,000 $m^3$/d (140 mgd), in different parts of the world (USA and Finland). The plants have different treatment objectives ranging from nitrification and partial denitrification (nitrate plus nitrite $<8.7$ mg/L) to enhanced nutrient removal (total nitrogen $<3$ mg/L, total phosphorus $<0.3$ mg/L). Commonly-used models were applied in the case studies, including ASM3 (using the GPS-X simulator), New General (using GPS-X), Dold (using BioWin), and a variation of the Dold model methanol degradation capabilities (NGmeth within GPS-X). The authors compare and contrast the modelling approaches taken, including calibration and validation approaches, sensitivity analyses, and the application of results to full-scale studies, designs and operations. Despite several differences between the approaches, there are many similarities which are discussed in light of the IWA draft uniform protocol for activated sludge modelling. The authors also discuss current modelling limitations and offer suggestions to improve the state of the art.

**Key words** | calibration, full-scale, modelling, nitrogen removal, solids balance, wastewater treatment

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## INTRODUCTION

It is standard practice for engineers to use models in the design of wastewater treatment facilities; however, several models are available to use, and several approaches can be taken in model calibration and design optimisation. The draft IWA uniform protocol for activated sludge modelling (Gillot *et al.* 2007) discusses several published guidelines: STOWA

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(Hulsbeek *et al.* 2002; Roeleveld & van Loosdrecht 2002), BIOMATH (Vanrolleghem *et al.* 2003), WERF (Melcer *et al.* 2004), and HSG (Langergraber *et al.* 2004). This paper comments on the guidelines in reference to three case studies conducted by three independent consulting teams.

## CASE STUDY: DENVER, COLORADO (USA)

The Metro Wastewater Reclamation District first began using models in 2001, though regulatory changes have driven the implementation of new facilities, and the need to sharpen the accuracy of existing models. The District's Robert W. Hite Treatment Facility has a current annual average flowrate of 530,000 $m^3$/d (140 mgd) or 1.8 million population equivalents (p.e.). Discharge limits include monthly average ammonia concentrations that vary by month, and a seven-day average nitrate (plus nitrite) concentration of 8.7 mgN/L. Through 2,018, the District plans implement over $1 billion in capital projects. A central component for success is the calibrated, whole-plant model that can be used by the entire team for planning, design and operation.

### Materials and methods

Consultants, planners and operators worked together to calibrate a dynamic model of the existing facility, including all liquid and biosolids processes using GPS-X (Hydromantis). In June and October 2007, the District conducted intensive sampling campaigns to characterize diurnal flow and load patterns, COD fractions, the maximum specific growth rate for autotrophs ($\mu max_a$), and several other parameters. Based on high food-to-microorganism rate testing (Melcer *et al.* 2004), a $\mu max_a$ of 0.85 $d^{-1}$ was used in the model, with a autotrophic decay rate of 0.17 $d^{-1}$ and Arrhenius value on the growth rate of 1.072. A few other changes were made to the GPS-X defaults including an increase in the anoxic growth rate from 0.37 to 0.7 to calibrate the full-scale denitrification. In the New General model, this factor is used to account for the observed behaviour that the maximum rate of substrate utilization is lower under anoxic than aerobic conditions (if the value is 1.0, heterotrophs will utilize substrate at the same rate under anoxic and aerobic conditions). The District repeated the sampling campaigns two more times for model validation purposes and these results were not yet available for publication. The models used for each process are summarized in Table 1.

The calibrated model is being used by District staff for plant operations, and it was also used to design future facilities that include a Centrate and Return Activated Sludge Re-aeration Basin (CaRRB). Because pH and alkalinity were important design parameters, a parallel BioWin (Envirosim) model was developed for the secondary treatment process. BioWin contains a sophisticated pH module that includes gas phase modelling, inhibition, and

**Table 1** | Whole-plant model of the Robert W. Hite Treatment Facility (Denver, CO USA)

| Unit process | Physical model | Process model |
|---|---|---|
| Primary settling (North) | 1 circular unit, 10 layers | Simple 1-D (Takács *et al.* 1991) |
| Primary settling (South) | 1 circular unit, 10 layers | Simple 1-D (Takács *et al.* 1991) |
| Air activated sludge system (North) | 8 CSTRs in series | New general |
| High purity oxygen system (South) | 3 CSTRs in series | New general |
| Secondary settling (North) | 1 circular unit | Simple 1-D (Takács *et al.* 1991) |
| Secondary settling (South) | 1 circular unit | Simple 1-D (Takács *et al.* 1991) |
| Dissolved air floatation | 1 unit, 10 layers | Simple 1-D floatation |
| Gravity thickening | 1 unit, 10 layers | Simple 1-D (Takács *et al.* 1991) |
| Acid-phase digestion | 1 CSTR | GPS-X basic model |
| Methane-phase digestion | 1 CSTR | GPS-X basic model |
| Sludge and centrate holding tanks | 4 units, CSTR | none |
| Centrifuges | Dewatering | Constant capture |

precipitation reactions for struvite, calcium phosphates, and iron and aluminium hydroxides and phosphates. Plant alkalinity data were entered into the BioWin model, which had $\mu max_a$ set-points of 0.85 $d^{-1}$ within the aeration basin and CaRRB. The BioWin model predicted when alkalinity became depleted, and when the lower pH limited nitrification within CaRRB. The results were transferred to the GPS-X model by adjusting the $\mu max_a$ (in the GPS-X CaRRB only) to 0.6 $d^{-1}$, the value that resulted in the same CaRRB effluent ammonia concentration for both models. Another important finding from the pH modelling was that the percent of the RAS flow to CaRRB could be raised from 30 to 50 percent to completely nitrify the centrate. The RAS flow will therefore be an important control parameter for operations staff.

## Results and discussion

### Calibration and solids balance

Although October is a transitional period in plant operation, the model predicted the rise in MLSS concentration and the diurnal effluent nitrate (plus nitrite) concentration reasonably well (Figure 1). The District is currently using the model to evaluate 'what if' scenarios at the plant and to predict effluent quality on a monthly basis.

### Sensitivity analysis

The model of the future facilities was used to optimize the size of both the anaerobic and anoxic zones, and to evaluate the risk of nitrifier washout at different design SRTs. This approach is common (Takács *et al.* 2007); however, a tiered loading approach was also taken, in which the design maximum month conditions were run through the model, with peak week and peak day conditions simulated in the middle of the month. The approach is often called a "birthday cake" or "wedding cake" analysis since the influent loads increase and decrease with time in the shape of a tiered cake. The analysis was repeated using several SRT values, and the average, peak and minimum effluent ammonia concentrations were plotted as a function of SRT (Figure 2), which enabled the team to select a design value that weighed capital costs against the risk of nitrifier washout.

## CASE STUDY: ESPOO, FINLAND

The Suomenoja WWTP (City of Espoo, Finland) is a single-sludge denitrification-nitrification (DN) plant designed for 250,000 p.e. (110 000 $m^3$/d, 29 MGD). The severe climate in the region and the ever-increasing loads of COD and nitrogen, which currently exceed the original design values, make operating the plant particularly challenging. The main operating goals are i) to keep the MLSS concentration as low as possible to prevent sludge washout, ii) to ensure sufficient nitrification, and iii) to minimize the use of chemicals. The whole-plant solids balance and the operation of the DN-process were analysed by dynamic modelling and simulation.

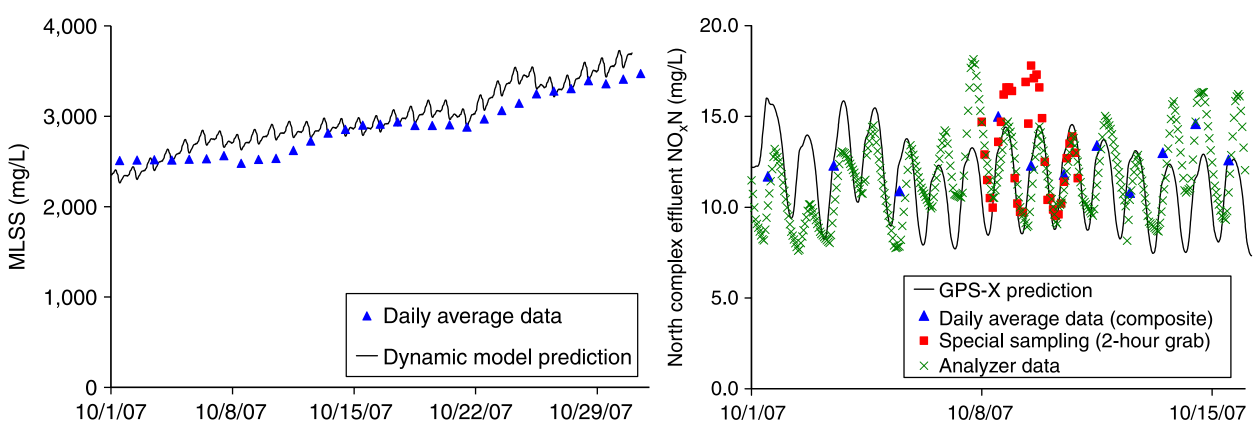


**Figure 1** | Calibration results–MLSS concentration (left), and effluent $NO_xN$ (right).

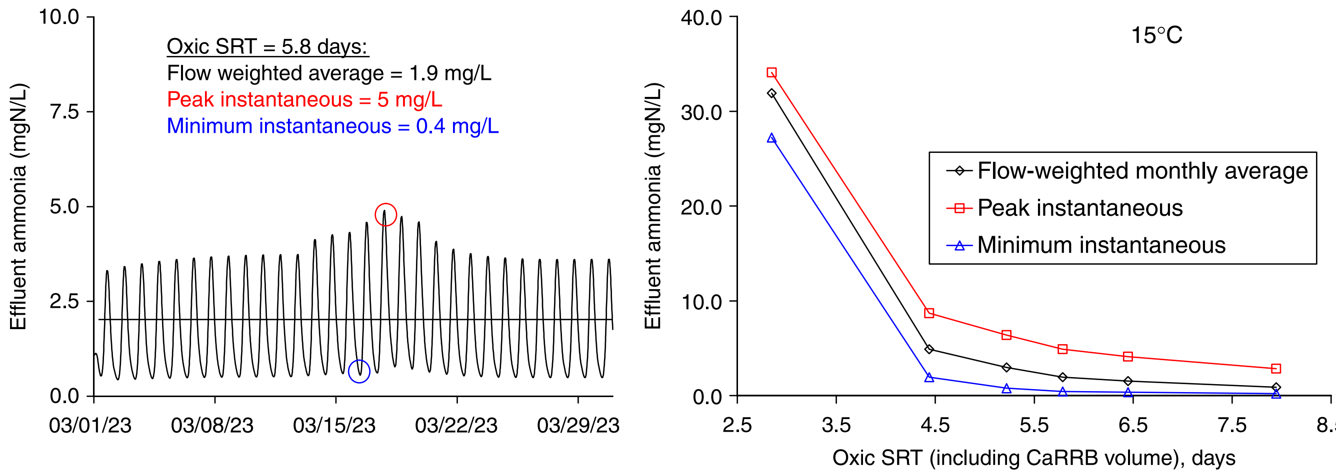


**Figure 2** | Selecting a design SRT using a 'wedding cake' analysis (left) and plotting the peak, average and minimum effluent ammonia concentrations for several SRTs (right).

## Materials and methods

Similar to the Denver approach, special sampling campaigns were conducted to collect dynamic model inputs. Plant data for three separate periods were used for balance calculations, calibration and validation, respectively. Balances of flowrates, iron, phosphorus, and nitrogen were calculated for the whole plant, the water process, the biological process, and the sludge treatment process. The assumptions for each unit process are presented in Table 2. The solids balance was analysed with a whole-plant model. To reduce calculation time and to account for the specific structure of the secondary settling tanks, nitrogen removal was analysed with a submodel that included only the activated sludge process and secondary settling.

The model was calibrated following the protocol described by Hulsbeek *et al.* (2002). After adjusting the model structure, wastewater characterisation, and WAS rate, the calibration was fine-tuned with the following model parameters: $i_{N,XI}$; $b_{A,O}$; $b_{A,NO}$; $K_{NH,A}$; $\eta_{NO}$; and $K_{O2}$, Parameters were adjusted according to engineering judgement without using numerical fitting methods.

## Results and discussion

### Calibration and validation

Primary settling and sludge thickening were the most difficult unit processes to calibrate. Simultaneous calibration of the quality of biosolids treatment sidestream and primary effluent was especially challenging, since the used settling model assumes that all particulate COD fractions ($X_I$, $X_S$, $X_{STO}$) settle at the same speed, contrary

**Table 2** | Solutions for modelling the unit processes at Espoo Suomenoja wastewater treatment plant

| Unit process | Physical model | Process model |
|---|---|---|
| Pre-aeration | CSTR | ASM3 (Gujer *et al.* 1999) |
| Primary settling | 1 rectangular basin, 8 layers | Simple 1-D (Takács *et al.* 1991) + ASM3 |
| Activated sludge | Plug-flow (1 CSTR per compartment) | ASM3 |
| Secondary settling | 1 rectangular unit, 10 layers | Simple 1-D + ASM3 |
| Thickening | 1 round unit, 5 layers | Simple 1-D |
| Anaerobic digestion | 1 CSTR | GPS-X basic model |
| Equalisation | 1 CSTR | none |
| Dewatering | Dewatering | Constant capture |

to practical observations. The number of layers in the primary settler model, settling rates in the primary settler and in the thickener and the ratio of $S_S/X_S$ in the plant influent were used as calibration parameters. Thus, the ratio of total substrate to inert particulate material $[(X_S + S_S)/X_I]$ was calibrated acceptably, which was important for proper simulation of sludge production. For simulation of nitrogen removal with a submodel of the biological process, a specifically determined characterisation for primary effluent was used. For winter conditions, the fractionation of the wastewater COD had to be recalibrated (Hulsbeek *et al.* 2002; Gillot *et al.* 2007). The model calibration and validation results are shown on Figure 3.

## Solids balance

The objective of the solids balance simulations was to establish relationships between the operating parameters of sludge treatment, plant-internal loadings, and MLSS concentration. The model showed that insufficient thickening and digestion capacity and the overflow from the storage tank situated before the centrifuges were the main causes of problems with solids balance control. In the simulations, internal TSS and COD loads could be reduced from 60% to less than 10% of the total load treated by minimizing overflows from the storage tank and by reducing the hydraulic loading on the thickener.

## Nitrogen removal

Nitrogen removal simulations enabled more efficient use of methanol. Sludge recycling rates and the selection of the methanol feed point were found to have a significant effect on the methanol dose required to achieve 70% nitrogen removal. The simulated concentrations of readily biodegradable COD (state variable $S_S$ in ASM3) carried over from the last anoxic reactor to the first aerobic reactor are plotted in Figure 4, on the left. The respective cumulative amounts of $S_S$, given as equivalent amounts of methanol, are plotted on the right. Both plots are given for two sets of operational settings, namely: i) total recirculation ratio, in terms of (return sludge flow + internal recirculation flow)/influent flow, 430%; methanol feed to second anoxic compartment and ii) total recirculation ratio 230%; methanol feed to first anoxic compartment. By reducing the total sludge circulation flow to the required minimum and by not dosing methanol to the last anoxic reactor (in this case the second reactor, which is current practice at the plant), the wastage of methanol could be cut by 30% which could mean annual savings of 30,000 to 50,000 euro. Optimal settings were determined by steady-state simulations, and the results were checked with dynamic simulations. Dynamic simulations resulted in significantly smaller differences between the tested scenarios than did steady-state simulations, which stresses the importance of not relying on steady-state simulations alone when optimizing plant operation.

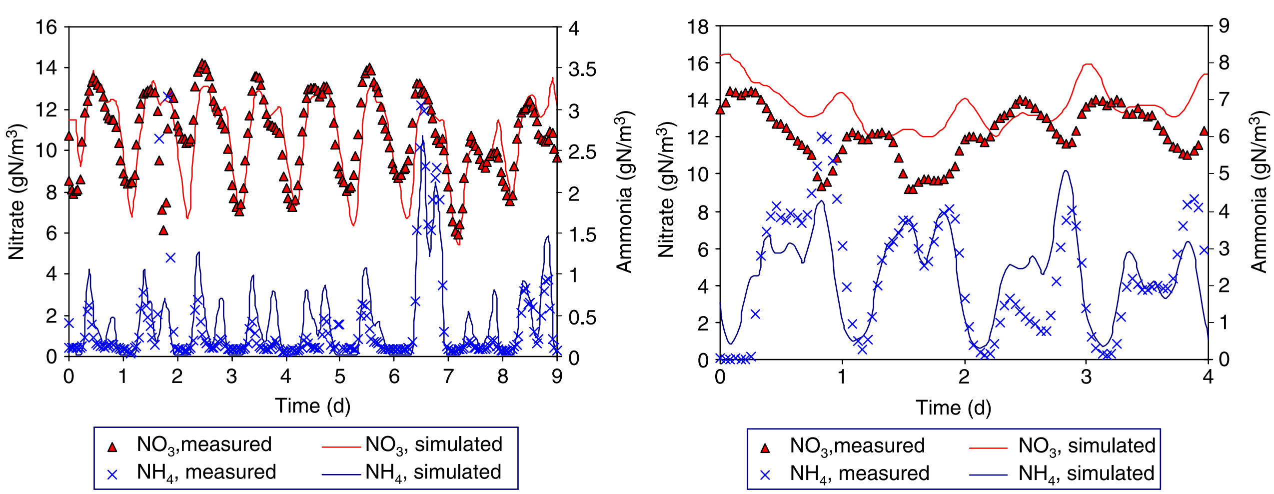


**Figure 3** | Simulated and measured ammonium and nitrate nitrogen at the end of aeration line for model calibration (left, T = +19°C) and validation (right, T = +9°C).

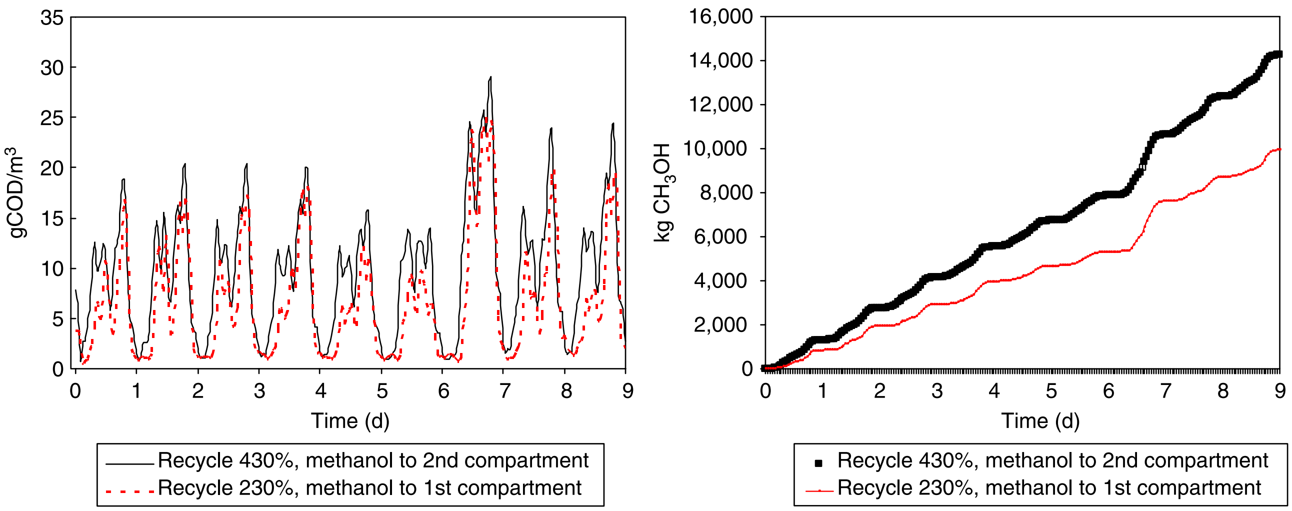


**Figure 4** | Readily biodegradable COD ($S_S$) at the end of anoxic phase (gCOD/m$^3$, left), i.e. carried over to aerobic phase and thus of no use for denitrification, and the respective cumulative amounts of $S_S$ (methanol equivalent, right) with two sets of operational settings. Total nitrogen removal rate 70% and T = +10°C in both cases.

## CASE STUDY: UPPER MARLBORO, MARYLAND (USA)

The 113,800 m$^3$/d (30 mgd), or 250,000 p.e. Western Branch Wastewater Treatment Plant, owned and operated by the Washington Suburban Sanitary Commission (WSSC), includes three separate activated sludge systems in series: a high rate activated sludge (HRAS) system, a nitrification activated sludge (NAS) system, and a denitrification activated sludge (DNAS) system. As the plant is scheduled to begin achieving year-round enhanced nutrient removal (ENR)-level performance (TN $<$ 3.0 and TP $<$ 0.3 mg/L), three ENR alternatives were evaluated. Alternative 1A is the existing process configuration. Alternative 1B is similar to 1A and employs a pre-anoxic zone in the NAS system with an HRAS bypass line for carbon addition to conserve methanol. Alternative 2 combines the NAS and DNAS systems into a single system and also incorporates a pre-anoxic zone with HRAS bypass carbon feed.

### Materials and methods

Development of the process model followed a stepwise approach presented by Frank (2007) and is similar to the previous two approaches in that dynamic data was collected. Two intensive sampling programs during different modes of WWTP operation rendered datasets for model calibration (14 days) and verification (7 days). Most of the calibration efforts involved iteratively adjusting the raw wastewater COD states. The New General model has a number of updated default parameters in recent literature so the updated values were used initially in place of the GPS-X defaults. It is recommended that these parameters be changed to reflect the most recent research (Copp 1993; Melcer *et al.* 2004).

A new approach for modelling methanol degradation with independent methylotrophic and heterotrophic biomasses was employed as proposed by Takács *et al.* (2007) using kinetics according to Dold *et al.* (2007) by incorporating a new library (methlib) and a new biological model (NGmeth) into GPS-X. The NGmeth model is essentially the New General model (Barker & Dold 1997) with capability for modelling methanol degradation. The new process rates replicate anoxic growth of methylotrophs on methanol, decay of methylotrophs, and aerobic growth of heterotrophs on methanol. A summary of the models used in the Western Branch WWTP layout is presented in Table 3.

### Results and discussion

#### Calibration and validation

Although the composite variable raw wastewater (RWW) characteristics were generally typical of municipal wastewater, the model calibration could not be achieved using

**Table 3** | Whole-plant model of the Western Branch WWTP (Upper Marlboro, MD USA)

| Unit process | Physical model | Process model |
|---|---|---|
| HRAS bioreactors | 1 CSTR | NGmeth |
| HRAS clarifiers | 1 rectangular unit, 10 layers | Simple 1-D (Takács *et al.* 1991) |
| NAS bioreactors | 2 CSTRs in series | NGmeth |
| NAS clarifiers | 1 rectangular unit, 10 layers | Simple 1-D (Takács *et al.* 1991) |
| DNAS bioreactors | 1 CSTR | NGmeth |
| Chemical phosphorus removal | Inline chemical dosage | OP Half-Saturation Rate Limiting (Hydromantis) |
| Nitrogen stripping channels | 5 CSTRs in series | NGmeth |
| DNAS clarifiers | 1 circular unit, 10 layers | Simple 1-D (Takács *et al.* 1991) |
| Tertiary filtration | Sand filter | Continuously backwashing constant solids removal |
| Dissolved air flotation thickening | Dewatering | Constant capture |
| Centrifuges | Dewatering | Constant capture |

typical municipal wastewater stoichiometric relationships – a significantly greater fraction of particulate inert COD was required. Without this adjustment, aerobic nutrient uptake due to biomass assimilation was significantly greater than indicated by the HRAS and NAS clarifier effluent concentrations. To resolve this issue, the rates of hydrolysis were adjusted by slowing the aerobic rate and increasing the anaerobic rate. With these adjustments in place, the model was better able to predict the nutrient demand in each sludge system and the measured plant behaviour as a whole.

It was also found that the rate equation used in the New General model to predict the hydrolysis of particulate organic nitrogen was deficient. In the GPS-X default model, soluble organic nitrogen is predicted to be produced only under aerobic conditions, even though particulate organic carbonaceous material is hydrolyzed with and without oxygen. The sampling data indicated that the measured ammonia concentration exiting the DNAS bioreactor is greater than the ammonia entering that basin. This means that there is a net production of ammonia, but the default GPS-X model could not predict this. To account for this behaviour, the predicted nitrogen hydrolysis rate was tied directly to the hydrolysis of particulate carbonaceous material irrespective of the presence of oxygen. Figure 5 illustrates the calibration of two locations in the WWTP model (DNAS bioreactor mixed liquor and NAS clarifier effluent nutrients).

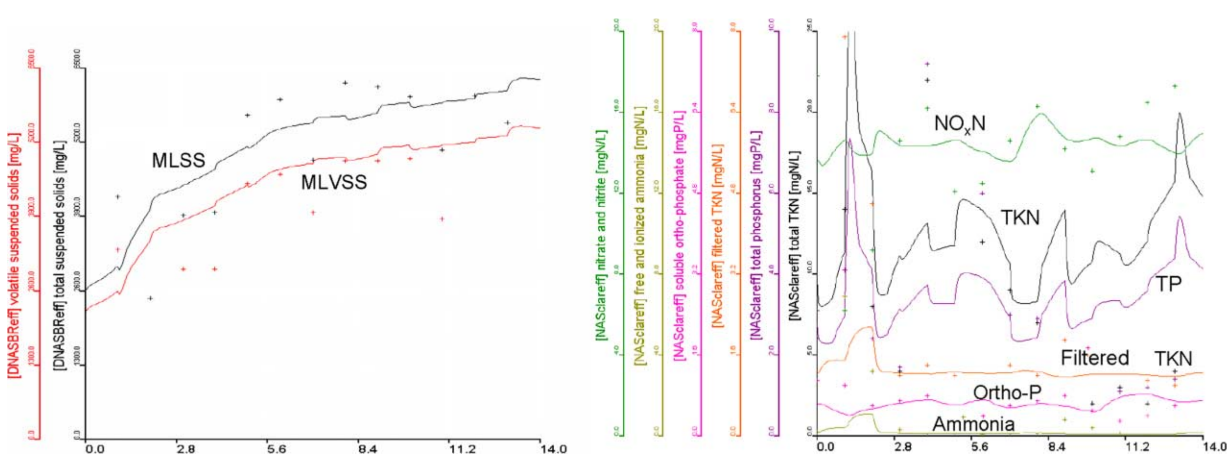


**Figure 5** | Illustration of calibration for DNAS bioreactor MLSS and MLVSS (left) and NAS clarifier effluent nutrients (right).

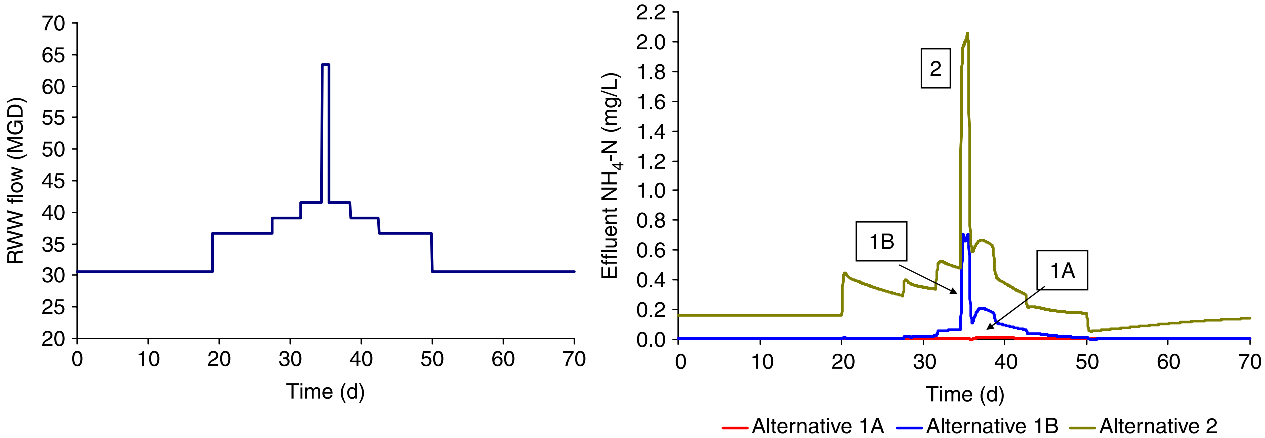


**Figure 6** | Basis of dynamic simulations for raw wastewater flow (left), and dynamic model response of ammonia for alternatives 1A, 1B, and 2 (right).

### Steady-state and dynamic modelling

Annual average and maximum 30-day conditions were evaluated on a steady-state basis at the minimum design temperature of 12°C. Higher intensity loadings were evaluated on a dynamic basis by stepping up the RWW flow and loadings the respective maximum loading condition and duration, and then stepping them back down in the reverse order ("wedding" or "birthday cake" analysis). Graphical illustrations of the dynamic RWW flow and the model's response, relative to effluent ammonia concentration are provided in Figure 6, showing that the combined NAS/DNAS system (Alt 2) results in the highest effluent ammonia. This observation seemed peculiar at first, having the longest aerobic SRT (excluding HRAS) of the three alternatives. Investigation showed that the longer SRT, working in tandem with lengthy anoxic conditions, reduced the overall ammonia removal performance when compared to the three-sludge alternatives (1A and 1B). This occurs because about one-half of the total NAS/DNAS system SRT is exposed to anoxic conditions, allowing organic nitrogen to resolubilise into ammonia.

## CONCLUSIONS

While there are several differences in the modelling approaches described in this paper, three common factors were essential to the success of the projects: (1) additional sampling to define dynamic model inputs and influent fractions, (2) careful planning, and (3) effective and frequent communication among all team members. It is especially essential for large or complicated plants, that plant personnel be closely involved. Schematics of the plant should be referenced in order to avoid misunderstandings in terminology or sample locations. Operators and laboratory technicians need to be involved, since they can help determine if data and model outputs are within typical ranges.

### Influent characterization

In each case study, influent characterization was very important, since wastewater composition is site-specific, and not necessarily consistent throughout the year. The modeller may have to "re-calibrate" the model to take into account seasonal discharges, as opposed to "validating" the model (although the modeller should not adjust kinetic parameters after the initial calibration). For two of the case studies, it was necessary to considerably increase the fraction of particulate inert COD from the default values, so it is important to measure as many of the COD fractions as possible (Melcer *et al.* 2004).

### Whole-plant modelling

The preferred modelling approach is to use a whole-plant model, including all liquid and biosolids processes; however, there are always exceptions. Examples include the Denver project, where a parallel model of one of the secondary treatment facilities was used to investigate issues related to pH. For the Western Branch project, a parallel model for one of the HRAS trains was used to approximate the spatial distribution of oxygen uptake when compartmentalized into multiple zones in series for aeration system retrofit considerations. Both parallel models allowed analysis of specific parameters that could not be addressed in the whole-plant model. There are always challenges in balancing project budgets with model complexity, but the Espoo example also demonstrated that parallel modelling can be a good solution to slow simulation time.

## Dynamic versus Steady-State modelling

Each study revealed differences in steady state and dynamic simulation results, especially at the low values of SRT as shown in the Denver project, so it is best to include dynamic checks in all modelling efforts. Project budgets can limit the amount of additional sampling that can be done, so the modeller should keep a database of other projects and develop typical diurnal curves. The modeller should always state their dynamic influent assumptions, and compare steady state model output with dynamic results.

## Calibration and validation

### Sampling

The biggest difference between the three case studies was the method of calibration and the length of time allocated for sampling. The Denver project involved three 14-day sampling efforts, and the dynamic calibration and validation focussed on the 30-day periods surrounding the sampling events. The Espoo work used a 9-day dataset for dynamic model calibration, a 3-day period for dynamic validation, and 3 months of operating data for the solids balance. The Upper Marlboro study included a 14-day sampling period for calibration, and a 7-day period for validation. While budgets always influence the scope of a project, team members must weigh the risk associated with reducing sampling (and modelling) efforts with the goals of the project.

### Hydrolysis rate, anoxic growth, and other parameters

The case studies also took different approaches in fine-tuning model parameters. The Upper Marlboro calibration required a reduction in the aerobic hydrolysis rate to limit the nutrient demand in the plant's HRAS and NAS sections. The reduction was the key to matching the effluent ammonia and soluble phosphate concentrations in each section of the model. On the other hand, the Denver model was calibrated without any adjustment to the hydrolysis rate, but with an increase in the anoxic growth factor. In the Espoo work, the model was unable to match the nitrification and denitrification rates with default kinetic parameters, probably because of very well-adapted autotrophic biomass and floc-internal denitrification. The solution was to lower the autotrophic decay rates and to increase the anoxic reduction factor and DO saturation constant for heterotrophs.

## Current limitations

The cases studied identified some important model limitations. In the Espoo plant modelling, the most difficult process to calibrate was the primary settling because clarifier models assume equal settling velocities for all particular COD fractions. Using a biological model in conjunction with a settling model complicates calibration efforts, but is often necessary. But perhaps the biggest limitation is the lack of a standard modelling approach among consultants, although progress is being made (Gillot *et al.* 2007; Copp *et al.* 2008).

## The value of modelling

The case studies presented here serve to demonstrate how models can significantly improve the evaluation, design and operation of wastewater treatment facilities. The Denver model was used to develop a cost-efficient design for the new facilities, and is now being used to optimize operation during construction. The Espoo modelling work also helped optimize plant operation, and an important finding was to not dose carbon to the last anoxic compartment in order to avoid unnecessary carryover of RBCOD to the aerobic reactors. Also, because methylotrophs are very temperature-sensitive (Dold *et al.* 2007), it was concluded that the yearly average nitrogen removal rate target of 70% could be more cost-effectively met by running the plant at 80% nitrogen removal in the summer and 60% nitrogen removal in winter. Finally, models play a critical role at facilities with low discharge limits such as the Western Branch WWTP in Upper Marlboro, Maryland, where ENR limits include 3 mg/L TN and 0.3 mg/L TP. Modeling showed that maintaining the existing three-sludge system provides for the most robust nutrient removal process with the least sensitivity to nitrifier washout and the lowest effluent TN of the alternatives evaluated.

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