FACT SHEET

Liquid Stream Fundamentals: Whole Plant Modeling

Whole plant modelling has become an increasingly more accessible and popular tool to help engineers and operators understand, design, and optimize the complex interconnected pieces of water resource recovery facilities. It allows the user to simulate multiple scenarios in a speedy, low-cost and low-risk environment to evaluate alternatives, identify necessary improvements, develop design parameters, and evaluate potential operational modifications. The simulations can also be useful for transferring process knowledge between stakeholders.

What is Whole Plant Modeling?

Whole plant modeling, in wastewater treatment, is the mathematical simulation or representation of the many interacting processes and recycle streams that make up a Water Resource Recovery Facility (WWRF) (Figure 1). Wastewater process models use multiple mathematical equations together to describe various unit processes across a WRRF (i.e. primaries, bioreactors, clarifiers, aeration system, thickeners, digesters, disinfection, filters, etc.). The various models represent the biological, chemical, and physical reactions that occur at a WRRF. Modeling is a valuable resource that can help assess the performance of existing or proposed WRRFs under different loading or operational scenarios to meet various effluent quality standards. Thus, whole plant models are employed as decision-making tools to guide a facility with operational modifications and where to invest in capital improvements (Figure 1).

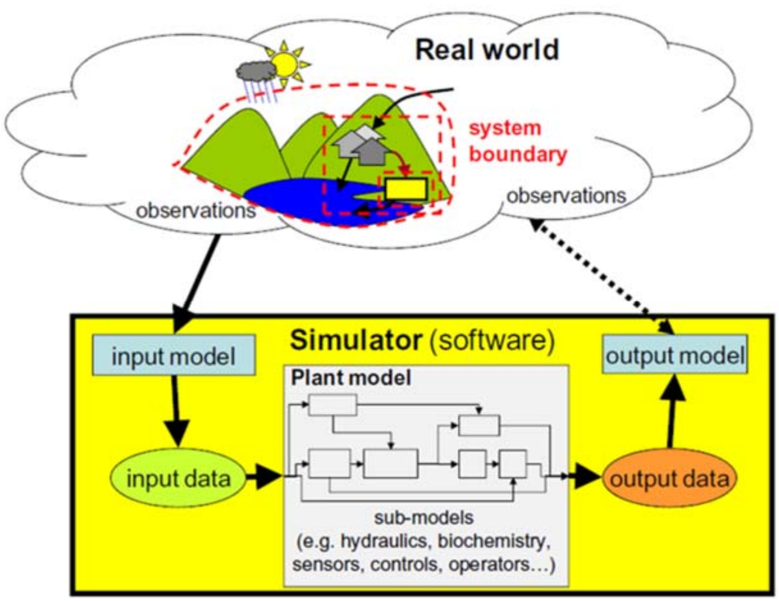

Figure 1 – Connection between real world observation and a plant model (Guidelines for Using Activated Sludge Models, Figure 2.2)

Modeling individual process units began over 100 years ago with bacterial generation models which over many iterations evolved into the formal Activated Sludge Model 1 in 1987. Process modeling has become increasingly relevant in the wastewater industry over the past several decades. The computer revolution – including the personal computer, has allowed for more accurate and complex models (i.e. dynamic sludge settling in a clarifier, biofilm systems, phosphorus precipitation, anaerobic digestion, detailed air supply and distribution systems, power generation, etc). Moreover, the development of various process simulators, or commercially available software packages, has allowed users to conduct model simulations in a user-friendly interface. The graphical user interface of the simulators allows users to construct models of WRRFs, using a schematic that shows how process units are interconnected (Figure 2). Each unit process model may be made up of several sub-models, which describe different facets of the unit process operation and performance. For example, an activated sludge basin may include a kinetic model to describe biokinetic reactions, an air supply and distribution model, and oxygen transfer model to describe the mass transfer of oxygen to the activated sludge.

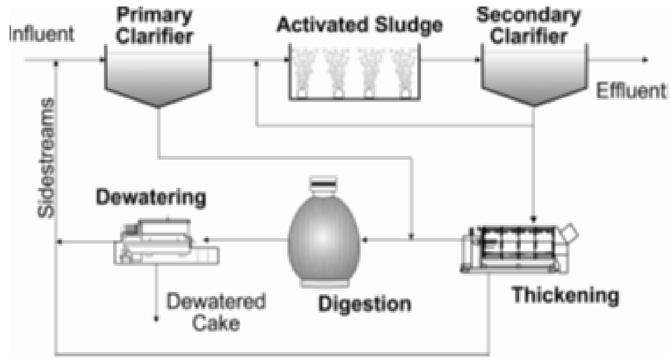

Figure 2 - Example model flow schematic showing process flow linkages between unit processes.

(An Introduction to Process Modeling for Designers Manual of Practice No. 31, Figure 2.2)

Whole plant process simulations can be static or dynamic. Static or steady-state simulations analyze averaged process performance over an extended period of time. They are useful for design and capacity evaluation purposes. Dynamic simulations use time-varying inputs to predict the performance of the system during transient operational conditions. They can predict a range of pollutant concentrations in the effluent stream over the course of a day, week, season, or even a year according to the objectives and availability of data. Dynamic simulations provide the capability for users to evaluate the performance impact of discrete increased (or decreased) loading periods, such as the impact of a wet-weather event.

Commercial Simulators

Although there are general-purpose science and engineering simulators available, whole plant modeling is usually performed using wastewater specific software packages such as the examples listed below. The benefits of using commercial software include an easy to use graphical interface, predetermined data input structures, default process models with default parameters (which result from extensive data gathered from the whole world), and the ability to simulate steady-state and dynamically. The packages differ in the specific process units provided, sub-model options (pH, metal salts, temperature, energy etc.) and the output data options.

- BioWin (EnviroSim)
- GPS-X™ (Hydromantis)
- SIMBA# (InCTRL)
- STOAT (WRc)
- SUMO© (Dynamita)
- WEST (MIKE powered by DHI)

Uses of Whole Plant Models

To meet today's effluent standards, most WRRFs utilize many unit processes along their treatment train, with recycle streams that return from one location to another. The utilization of a whole plant model is necessary to make sense of such complex interconnected systems in a way that is not possible with simple calculations or rules of thumb. Simulators also provide a speedy, low-cost and low-risk environment to experiment with facility operation. Some of the many uses of whole plant models are listed below.

Design	• **Calculating system requirements such as size, aeration, and chemical additions of a new or upgraded system** • **Quantifying the risk of not meeting performance targets at various design conditions**
Evaluate	• **Determining the ability of an existing treatment system to achieve stricter treatment goals under existing or through a process change** • **Estimating increased biological growth requirements of a new waste stream that could impact sludge production**
Optimize	• **Developing new control strategies using dynamic simulations that minimize energy consumption, operational costs, and/or effluent nutrient loads.** • **Comparing multiple scenarios or alternatives to find the most optimal solution and aid in decision making**
Communicate	• **Training engineers and plant operators to understand the dynamic behavior and process interactions of their wastewater treatment plant.** • **Providing insight or validation of current operational strategies for all stake-holders** • **Facilitating the research of new and developing technologies. For example, models can be used to help interpret and understand pilot test data, and then this information can be used to design a full-scale system**

Table 1— Benefits and Uses of Whole Plant Models

Modeling Protocol

As with any study, it is imperative that protocol is defined and followed in a modeling study. The International Water Association (IWA) Good Modeling Practice (GMP) Task group analyzed the similarities and differences in previously published protocols and developed the GMP unified protocol.

Deviating from the protocol, such as using poor quality data for calibration or skipping calibration and validation altogether, can be considered engineering negligence, and can result in designs that fail to meet effluent criteria. A successful modeling study assumes frequent communication between modelers and stakeholders during each stage.

GMP Unified Protocol Steps	Deliverables
Project Definition	A document that defines agreement on the technical conditions and budget
Data Collection and Reconciliation	Reconciled (checked for quality and consistency) data sets used for subsequent steps of the modeling project and identified deviations from the original project definition
Plant Model Set-up	Plant model and descriptive document; identified deviations from the original project definition and demonstrates solid understanding of how the facility is currently run
Calibration and Validation	A verified model that includes calibrated and validated parameters and can represent the plant and descriptive document; identified deviations from the original project definition
Simulation and Result Interpretation	The final version of the plant model(s) and a final report including model interpretation

Table 2 – Outline of the Good Modeling Practice Unified Protocol

Importance of Data Quality for Calibration

The accuracy of any model is highly dependent on the quality of the data used to develop the model. A typical colloquialism of whole plant modelers is "Garbage in means garbage out". The accuracy of the model inputs will directly affect the accuracy of the results it produces, and the modelers confidence in those results. Thus, care should be taken when developing and obtaining model input data to ensure the predicted results are representative and justified for use in making design or operational decisions. It is necessary to analyze the available influent, operational, and performance data to determine historical trends, relationships between parameters, and the presence of outliers. In addition, for steady-state modeling, routine, non-continuous operations like sludge wasting and solids dewatering need to be converted to a continuous basis by calculating 7-day or 30-day moving averages. Historical data should be collected for a representative period of time; three years of data helps to ensure that seasonal variations can be understood and addressed as necessary.

The main source of existing or historical data is the routine information collected at the plant daily. This may include SCADA data files, tabulations of analytical results, and manual meter readings. The wastewater parameters that are most commonly measured (and required for process modeling) include the following:

- **Flow**
- **COD**
- **BOD_5**
- **TSS (MLSS)**
- **VSS (MLVSS)**
- **TKN**
- **Ammonia-N**
- **Nitrate-N**
- **Nitrite-N**
- **Total Phosphorus**
- **Ortho-P**
- **Alkalinity**
- **Temperature**
- **pH**
- **DO**

In developing the process model, the determination of the influent wastewater ratios (i.e. COD/BOD5, BOD5/TP, BOD5/N, soluble/particulate) is particularly important to ensure reliable model results. While influent characterization is one of the most important data pieces in modeling, it is also common that the most valuable data (such as soluble versus particulate portions) is not routinely measured at WRRFs. If adequate data is lacking to appropriately characterize the influent, 'missing' data should be gathered using a specially created sampling program.

Whatever the purpose of the model is, it is likely that some additional sampling and analysis will be needed. Special sampling programs should result in 10-20 data points over 2-4 times the facility's normal sludge age for reasonable statistical analysis. Daily 24-hour flow-weighted composite samples of the influent, primary effluent, secondary effluent is ideal. For most dynamic sampling campaigns, at least 2 days of dynamic sampling every 1-2 hours during "typical" days is required. If weekend impacts are important to the question being asked, the campaign may need to include weekend sampling. Additional operational monitoring may also be needed such as measuring mass flows of solids or nutrients at recycle streams or at other points within the facility.

The results of special sampling should be compared and reconciled with the larger historical database to ensure its representativeness (i.e. comparison of ratios to typical wastewater composition).

A powerful way to identify systematic errors in the data (where entire data sets might be off, perhaps due to a poorly calibrated sensor) is to perform flow balances and mass balances on inert components. There are several areas of the plant that can always ensure a closed mass balance, such as the solids in and out of a clarifier, or solids thickening or dewatering. If a mass-balance error is detected, it should be rectified before using the data in the model.

The overarching goal of calibration and validation is to improve reliability and reproducibility of simulation results while identifying the conditions within which the predictions are robust. Calibration is an iterative process of adjusting input parameters until simulation results match an observed set of data within an acceptable error. The calibrated model is then validated with a separate set of data to ensure the use of the calibrated model with the level of confidence required to meet the modelling objectives. The calibration effort can be stopped when a defined variance (typically 10-15%, or otherwise established by project stakeholders) in the MLSS concentration as a percent or variance in effluent concentration in milligrams per liter has been met.

Limits of Whole Plant Modeling

Despite their usefulness, it is important to understand the limitations of model accuracy. For example, current simulators cannot currently predict:

- the settling characteristics (such as the SVI or settling rate) of activated sludge
- microbiological inhibition
- degraded performance due to incomplete mixing
- polymer consumption
- performance at lower substrate, nutrient, or oxygen concentrations

As discussed in the previous section, no model will be better than the data with which it was calibrated. These limits are examples of quantifiable uncertainty, that is, sub-models that are known to be uncertain, and the degree of uncertainty can be reduced by further study.

There is also irreducible uncertainty - uncertainty that cannot be reduced by any degree of study. For example, no amount of study would be able to quantify future flows and loads beyond a certain point. Even the best calibrated model has a level of uncertainty associated with many aspects of it. Although models will never match reality. reality they are a great tool for sensitivity analysis and identification of the most important parameters that impact "good treatment performance. The models will always produce 'an' answer, as process models used in wastewater are considerably "over-parameterized", meaning that there are too many parameters than can be adjusted to fit a set of data. It's up to the user to determine if that answer is realistic and valid. A model cannot replace a well-trained Operator or Process Engineer. Users must apply their own safety factors and good judgment in determining how close to the wire to push the plant based on modeling predictions.

Future of Whole Plant Modeling

The need for whole plant models will increase as financial limits, land use limits, and stricter effluent limits for recognized and new pollutants continue to drive innovation and affordable high level decision-making. In addition, climate change may result in extreme weather events, previously unknown to a given facility. The development and verification of models is ongoing as is the improvement in computational capacity. Some current research areas are listed below (adapted from Guidelines for Using Activated Sludge Models Table 2.2).

- Biokinetics of very low nutrient concentrations
- Oxygen transfer with variable alpha factors
- Computational fluid dynamic models in clarifiers
- Hydrolysis kinetics
- Diffuser and membrane fouling
- Floc formation/morphology regarding foaming/bulking
- Sulfur chemistry & biology
- Nitrous oxide green house has emissions
- Fate & treatment of microconstituents
- Biofilm & granular sludge

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Acknowledgments

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