

INTRODUCTION

Effective utilisation wastewater treatment plant (WWTP) mathematical models requires that they are well calibrated. However, difficulties (with important parameters not identified and uncertainties in interpretation of model output results) can be experienced in model calibration, especially due to (i) the intricate relationships of model output variables with model input factors, resulting in non-linearity, and (ii) the limitations experienced in procuring and reconciling data required for determination of the model input factors.

OBJECTIVE:

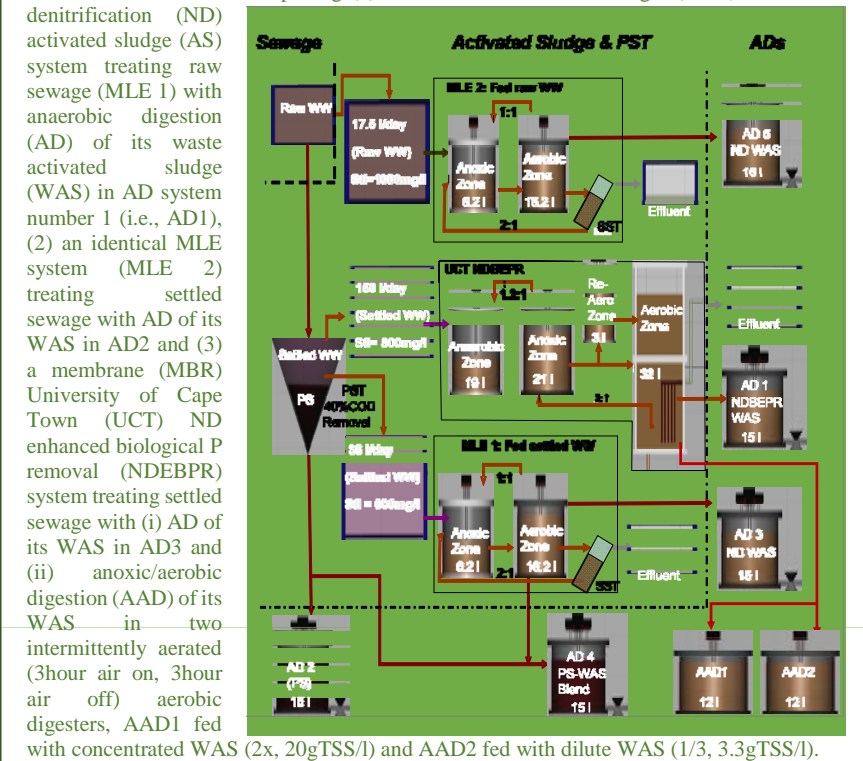
To apply the BIOMATH protocol (Vanrolleghem *et al.*, 2003) in providing a guidance towards calibration of a plant-wide model that includes phosphorus. The three phase (aqueous-gas-solid) University of Cape Town plant wide (UCT-PW) model (Ikumi *et al.*, 2013) that was calibrated against the experimental layout described below is used as a case study for this calibration procedure.



How do we ensure that observations in experimental set up below can be accurately predicted in similar systems, using UCT PWM?

EXPERIMENTAL SET-UP

The experimental layout of Ikumi (2011) is used in this study. It replicates at laboratory scale three WWTP schemes, comprising (1) a Modified Ludzack – Ettinger (MLE) nitrification–denitrification (ND) activated sludge (AS) system treating raw sewage (MLE 1) with anaerobic digestion (AD) of its waste activated sludge (WAS) in AD system number 1 (i.e., AD1),



UCT PLANTWIDE MODEL DESCRIPTION

Speciation Subroutine (In background of both sub models): Comprises algebraic equations for the "instantaneous" dissociation or association reactions of relevant weak acid species

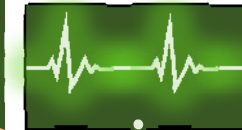
ASM2-3P Sub model:

Bioprocesses mediated by OHO, ANO and PAO organism groups as for ASM2 (Henze *et al.*, 1995).
Inter-phase transfer processes (i.e. gas evolution and mineral precipitation).

ADM-3P Kinetic Processes:

Bioprocesses mediated by the four recognised AD organism groups as is done in IWA ADM1 (Batstone *et al.*, 2002).
Inter-phase transfer Processes (i.e. gas evolution and mineral precipitation).

For their compatibility, the ASM2-3P and ADM3P models have the same comprehensive set of model components (supermodel approach, Volcke *et al.*, 2006)



MODEL PERFORMANCE CHECK

1. AS systems using ASM2-3P:

- When high NO₃ recycled to Un-aerated zone
- * Un-aerated zone gets anoxic.
- * No PAO growth (hence no polyphosphate (PP) stored)
- * Ortho-Phosphates (OP) used as OHO growth nutrients.

When very low NO₃ recycled to Un-aerated zone

- * Un-aerated zone gets anaerobic.
- * If high P and VFA is available, PAO growth (hence PP storage, using OP, Mg²⁺, Ca²⁺ and K⁺) occurs.
- * The OP also used for biomass (both OHO and PAO) growth nutrients.

2. Anoxic - Aerobic Digesters (AADs) using ASM2-3P:

- * Low VFA in WAS and no "anaerobic" period. - PAOs cant grow, but undergo endogenous respiration, but releasing stored PP faster than their death rate.
- * Ammonia gets low due to nitrification, hence struvite doesn't precipitate (newberryite and bieberite become the common P precipitants).

3. Anaerobic Digesters Using ADM3P:

- * Release of organically bound N, with BPO hydrolysis, causes increased alkalinity and pH.
- * Initial release of PP with VFA uptake and PHA storage causes increased alkalinity.
- * PAOs die faster than their Endogenous respiration rate due to no alternating aerobic condition, releasing their PHA and any remaining stored PP.
- * Slower release of organically bound P (as H₃PO₄) does not influence change in total alkalinity
- * Rapid release of PP and associated Mg²⁺ and the slow release of biomass N and P generate high concentrations of P, NH₄⁺ and Mg²⁺ species in the AD liquor, which promotes struvite precipitation.
- * This struvite precipitation decreases the total alkalinity, increases CO₂ partial pressure and decreases AD pH.

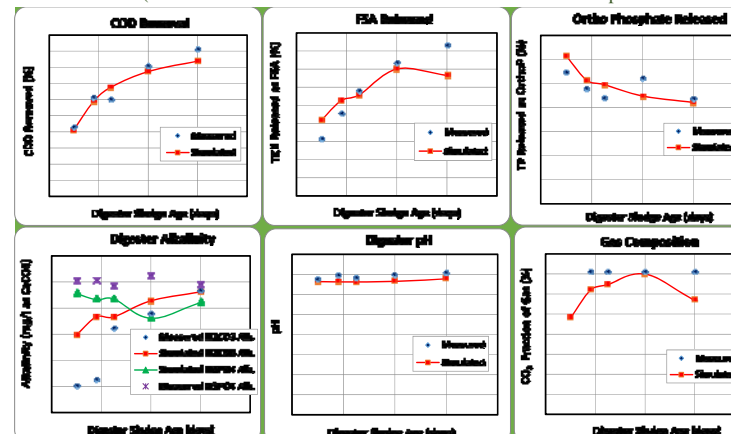
MODEL EVALUATION PROCESS

Model Verification: To initiate the evaluation of the UCT-PW model (Ikumi *et al.*, 2013), the systematic method proposed by Hauduc *et al.* (2010) was applied to verify that material (COD, C, H, O, N, P, Mg, K and Ca) balances were achieved in the determination of all stoichiometric processes.

Parameter Values: The initial values for suitable kinetic and stoichiometric parameters as obtained experimentally or from literature were entered, and given the typical value range, determined according to the methods proposed by Brun *et al.* (2002).

Sensitivity Analysis: The parameters were subsequently evaluated using two different methods of global sensitivity analysis: (1) Standardised Regression Coefficients (SRC) and (2) Morris Screening. The results obtained using these methods are used to identify important parameters (prioritisation of those with greatest effects), non-influential parameters (those that can be 'fixed' at any value within their range without effecting outputs) and interacting parameters (Neumann, 2012).

Model Calibration and Validation: Non-influential parameters were set at their default values and random samples were drawn from the remaining subset of parameters. For the sampled parameter sets simulations were conducted and predicted model outputs were compared with observed outputs. During this calibration phase, a consistent set of parameter values was used to simulate all experimental systems/ periods, and detailed explanations of observed discrepancies (if any) were reported by Ikumi (2011). The figures show a comparison between the data measured and simulated by the three phase AD dynamic model for the AD fed with NDBEPR WAS (i.e. the AD effluent from UCT NDBEPR linked to AD in a plant wide setting).



CLOSURE

The BIOMATH protocol was applied for the calibration of the UCT-PW model, for promotion of its widespread utilisation in a reproducible way. However, it is noted that the effective calibration of this model requires a further step - from modelling the laboratory scale systems (under controlled and completely mixed environments) to assessment of model predictions for full-scale wastewater treatment plant systems, interlinked to plant-wide configurations. This prospective work may be of particular interest to the IWA group on benchmarking of control strategies for WWTPs who are including P into an extended BSM model.

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