Summary

This PhD research aimed at the optimisation and the smooth operation of anaerobic digestion and wastewater treatment. The research objectives were threefold. The first one is to implement and validate anaerobic digestion models as tools to pursue the above aim. Second, anaerobic digestion models should be integrated in plant-wide modelling. The third research objective is to develop, automate, apply and validate on-line titrimetric monitoring of anaerobic digestion and wastewater treatment processes.

A general review defined the links among modelling, monitoring and different data categories in an optimisation scheme for design and operation of anaerobic digestion. The review also guides the data collection activity that is dependent on anaerobic reactor types and wastewater characteristics. Therefore, it leads to a better definition of the anaerobic model and the monitoring system.

In achievement of the first objective, the IWA ADM1 model is implemented in the WEST simulation platform where different reactor configurations can be easily defined. For a successful standard ADM1 implementation, key updates were necessary to the model compared to the descriptions in the IWA ADM1 model report. Simpler modelling approaches for anaerobic digestion are introduced by the Siegrist (1995 version) and the AM2 models. A general procedure for pH calculation was developed to improve the simulation speed when using simple DE solvers. The general procedure can be applied with any model and was extended to calculate cation concentrations and to implement a Titrimetric Analyser Simulator, TAS, in WEST. The ADM1 implementation was validated using three different simulators: WEST, AQUASIM and SIMULINK. In one of the first world-wide endeavours, the ADM1 was validated with an experiment with very rapid dynamics. Excellent agreement between the measurements and simulation results from the three implementations was achieved. A conceptual approach was developed to achieve a detailed characterisation of the wastewater according the ADM1 state vector without laborious measurements of the influent wastewater. An update to the model was introduced to describe the effect of hydrodynamics on the solids retention and to make the modelling of highrate reactors simple and possible. The ADM1 was also extended to study and simulate the effect of irreversible toxicity on the anaerobic digestion process. A complete pathway for cyanide degradation and a procedure to model acclimatisation of the anaerobic digestion process to toxicants were developed. The model extension was validated using 3 lab-scale Upflow Anaerobic Sludge Bed (UASB) reactors with three different feedings of cyanide. Although the model was calibrated with data from only one reactor, agreement between measurements and simulation results was achieved in the three reactors. The AM2 control model implementation was validated for anaerobic digestion of vinasses. A general protocol was designed to use the Optimal Experimental Design (OED) procedure to set up

the monitoring system and the sensor network at an anaerobic digestion plant. The protocol was validated using a virtual case study that implements ADM1 as data generator and AM2 as the control model. The OED application showed the value of on-line monitoring of pH, alkalinity, VFA and biogas measurements.

In achievement of the second objective, a flexible approach of using model transformers is presented for integration of anaerobic digestion models in a plant-wide model. The approach is illustrated by connecting the Siegrist (1995 version) anaerobic digestion model with the standard Activated Sludge Model (ASM1). The example extends the standard benchmark model of activated sludge systems by a thickener, an anaerobic digestion unit and a centrifuge to simulate the practice of sludge treatment and drying. Overflows from the thickener and the centrifuge are recycled to the activated sludge plant inlet. The transformers allow flexibility to connect other flows than sludge to the digester and the digester to other post-treatment processes. The expected digester output and the impact of the recycled flows on the activated sludge plant were correctly simulated. The same designed plant was then applied to compare two interfacing methods to connect ASM1 and ADM1. The first method (CBIM) is designed to interface two models according their Petersen matrix definitions. The second method (MCN) was specifically developed to connect ASM1 and ADM1. This work is the first systematic application of the (CBIM) method and to present the results of both methods. Both methods have the same plant-wide output, i.e. effluent water quality, produced biogas and produced sludge. However, the CBIM method provides flexibility that helps in a better simulation of the digester dynamics in allowing better parameter estimation, control design and implementation of advanced treatment processes, e.g. for highrate nitrogen removal.

In achievement of the third objective, monitoring equipment and titrimetric applications were first reviewed. Three titrimetric analysers that were used throughout this research are described. Two of them were developed in previous research but were not commercially available. A third one was developed in parallel to and with support of this research and is now commercially available for on-line implementation methods. The titrimetric methods are reviewed and classified according their mathematical interpretation. The Buffer Capacity Software (BCS) was developed for robust off- and on-line determination of unknown buffer mixtures without human input or interaction. An automatic initialisation procedure has been developed as an extension to the Buffer capacity Optimal Model Builder (BOMB) software sensor. The initialisation procedure automatically determines from a titration curve which buffers are in the titrated sample and estimates lower and upper bounds of their concentrations. This information is required to run the BOMB optimisation. The extension has been integrated as a software layer around BOMB and the

result is BCS. The Titrimetric Analyser Simulator (TAS) is used to test the BCS's reliability to measure buffer systems in an anaerobic digester that is operated under strong dynamics and with very fast transitions between different buffer combinations. The BCS has been tested and is now working with off- and on-line titrimetric analysers. BCS was applied in three different case studies of titrimetric monitoring and compared with other titrimetric and standard methods. The three titrimetric analysers described in this research were also tested via these applications. In the first case study the BCS was applied for titrimetric monitoring of digester overload conditions, measuring bicarbonate, VFA and lactate. In the second case study, the BCS and titrimetric methods were challenged by complicating factors. An experiment was performed at an industrial scale digester in the presence of external doses of di- and tri-protic cations (calcium and iron ions). Also a complex mixture of buffer components was dosed to the anaerobic digester effluent. Titration was performed on-line using the titrimetric on-line analyzer AnaSense®. On-line measurements of VFA, bicarbonate, ammonia, phosphorus and lactic acid were compared with standard measurements. Results from the second case study were highly influenced by buffer interferences and precipitation dynamics. However, the results correlated nicely with the standard measurements and are suitable for control applications. The approximate titrimetric methods were robust in determining the bicarbonate and VFA concentrations. In the third case study, the BCS was tested for the titrimetric monitoring of highrate nitrogen removal processes that are used to treat digester liquors, i.e. using combined SHARON-Anammox processes. The BCS accurately measured total ammonia and total nitrite, both variables that are useful for process control. Also, from the same titration experiment the BCS measured phosphorus that is considered toxic to the Anammox biomass.

Finally, the three objectives of this research are achieved to large extent and, therefore, the developed tools can support future research and applications to optimise anaerobic digestion and wastewater treatment systems.