Driven by economic, ecological and community considerations, waste(water) treatment plants (WWTP’s) are increasingly transformed into water resource recovery facilities (WRRF’s). Next to the long recognized and successfully recovered resources, water and energy, attention is growing to extract more value products from waste(waters), in particular nutrients. Although today many processes for nutrient recovery have been proposed and applied to varying degrees, challenges remain in improving their operational performance, decreasing the economic costs and recovering the nutrients as marketable products with added value for the agricultural sector. Moreover, finding the appropriate combination of technologie(s) for a particular waste flow and the optimal process conditions for the overall treatment train prior to decision-making is a key concern.

Mathematical models have become very important tools for technology design, optimizing performance and process troubleshooting as they are both time and cost efficient. Although a number of models of WWTP’s have been developed and applied extensively, these state-of-the-art models are limited by omission of key fundamental physicochemical processes, which play a major role in WRRF’s. Moreover, to date no general models for nutrient recovery systems based on adequate solution speciation and reaction dynamics are available and implemented. Consequently, models to adequately put together a treatment train of unit processes and their operating conditions to maximize resource recovery and fertilizer quality are missing.
The reported research aimed at developing general integrated biological-physicochemical three-phase process models for the best available resource recovery systems based on in-depth solution speciation and reaction kinetics. The developed models are to be applied not only as a tool for process optimization of single nutrient recovery systems, but also for determination of optimal unit process combinations. In this way resource recovery from a particular waste stream can be maximized and energy and chemical requirements minimized. As such, the proposed nutrient recovery model (NRM) library can provide a refined framework which can direct thinking prior to decision-making (design, control/operation strategies, research).

Four key unit processes were selected for modelling: anaerobic digestion (NRM-AD), P-precipitation/crystallization (NRM-Prec), NH₃-stripping (NRM-Strip), air scrubbing (NRM-Scrub), as well as four ancillary units: chemical dosing (NRM-Chem), heat exchanger (NRM-heat), storage tank (NRM-Store) and settler (NRM-Settle). Each dynamic mathematical model is built using: i) the definition of a chemical speciation model using geochemical modelling software (PhreeqC/MinteqC), ii) the description of a physicochemical and biochemical transformation model tailored to the models developed in the first step, and iii) the selection of a reactor mass balance model to describe the (time-dependent) process conditions. To facilitate numerical solution, a generic mechanism for calling PhreeqC outputs from the Modelica-coded transformation models using the WEST-Tornado software kernel has been developed.

Simulation results show good agreement with experimental results under steady state conditions. However, outputs were very sensitive to the influent ionic composition through its direct effect on pH. For optimization of process performance and sustainability, a more detailed influent characterization than is common for WRRF’s today is recommended. Such data are currently being collected under dynamic conditions at full-scale in order to further calibrate/validate the NRM kinetics.