Establishment and calibration of consensus process model for nitrous oxide dynamics in water quality engineering

Research on biological nitrogen removal (BNR) in wastewater treatment plants (WWTP) has historically focused on achieving good effluent quality, with more recent attention to energy savings and carbon dioxide (CO2) foot-prints. Novel processes and operating conditions are being implemented that enhance cost and energy efficiency in BNR, while maintaining effluent quality. Now, increasing attention is placed on direct emissions of nitrous oxide (N2O) as by-product of BNR. N2O is a greenhouse gas (GHG) with a high warming potential and also an ozone depleting chemical compound. Several N2O production pathways have been identified from pure culture studies, while mechanisms are still being unravelled. Heterotrophic bacteria (HB) and ammonium oxidizing bacteria (AOB) are well known to produce N2O. However, the effect of environmental factors on N2O production is not yet well understood. Current process modelling efforts aim to reproduce experimental data with mathematical equations, structuring our understanding of the system. Various mechanistic models with different structures describing N2O production have been proposed, but no consensus exists between researchers. Hence, the existing plant-wide GHG models still lack a complete biological process model that can be integrated in a methodology that assesses N2O emissions and their impact on overall plant performance. A mathematical model structure that describes N2O production during biological nitrogen removal is proposed. Two autotrophic and one heterotrophic biological pathways are coupled with abiotic processes. The model stoichiometry and process rates synthesize a comprehensive literature review on the metabolism of microbes involved in nitrogen removal. The proposed model can describe all relevant NO and N2O production pathways with fewer parameters than present in other proposed models. A novel experimental design based on the developed model and on extant respirometric techniques is introduced. Monitoring dissolved oxygen and N2O allowed the isolation of individual processes and the estimation of parameters associated to oxygen consumption (endogenous activity, nitrite and ammonium oxidation) and N2O production (NN, ND and HD pathway contributions). To estimate parameters of the N2O model a rigorous procedure is presented as a case study. The calibrated model predicts the NO and N2O dynamics at varying ammonium, nitrite and dissolved oxygen levels in two independent systems: (a) an AOB-enriched biomass and (b) activated sludge (AS) mixed liquor biomass. A total of ten (a) and seventeen (b) parameters are identified with high accuracy (coefficients of variation < 25%). The critical validation of the model response and the estimated parameter values represent a novel and rigorous tool for N2O modelling studies. For the first time, uncertainty associated with parameter estimation from N2O models is reported, this procedure is recommended to be included with best-fit simulations. Additionally, modelling electron competition in heterotrophic processes is explored via an analogy to current intensity through resistors in electric circuits. While further model validation is required, this approach captured the electron competition during denitrification for four different carbon sources. Overall, a combination of modelling and experimental efforts to study N2O dynamics was successfully implemented. Results represent a step forward in the development of consensus process model for N2O emissions in WQE processes.