A plant wide aqueous phase chemistry model describing pH variations and ion speciation/pairing in wastewater treatment process models - DTU Orbit (08/11/2017)

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There is a growing interest within the Wastewater Treatment Plant (WWTP) modelling community to correctly describe physico-chemical processes after many years of mainly focusing on biokinetics (Batstone et al., 2012). Indeed, future modelling needs, such as a plant-wide phosphorus (P) description, require a major, but unavoidable, additional degree of complexity when representing cationic/anionic behaviour in Activated Sludge (AS)/Anaerobic Digestion (AD) systems (Ikumi et al., 2014). In this paper, a plant-wide aqueous phase chemistry module describing pH variations plus ion speciation/pairing is presented and interfaced with industry standard models. The module involves extensive consideration of non-ideality by including ion activities instead of molar concentrations and complex ion pairing. The general equilibria are formulated as a set of Differential Algebraic Equations (DAEs) instead of Ordinary Differential Equations (ODEs) in order to reduce the overall stiffness of the system, thereby enhancing simulation speed. Additionally, a multi-dimensional version of the Newton-Raphson algorithm is applied to handle the existing multiple algebraic inter-dependencies (Solon et al., 2015). Simulation results show pH predictions when describing Biological Nutrient Removal (BNR) by the activated sludge models (ASM) 1, 2d and 3 (Henze et al., 2000) comparing the performance of a nitrogen removal (WWTP1) and a combined nitrogen and phosphorus removal (WWTP2) treatment plant configuration under different anaerobic/anoxic/aerobic conditions (Flores-Alsina et al., 2012). The same framework is implemented in the Benchmark Simulation Model No. 2 (BSM2) version of the Anaerobic Digestion Model No. 1 (ADM1) (WWTP3) (Batstone et al., 2002; Rosen et al., 2006) as well, predicting pH values at different cationic/anionic loads. In this way, the general applicability/flexibility of the proposed approach is demonstrated by implementing the aqueous phase chemistry module in some of the most frequently used WWTP process simulation models. Finally, it is shown how traditional wastewater modelling studies can be complemented with a rigorous description of aqueous phase and ion chemistry (pH, speciation, complexation).

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