

## Modelling phosphorus (P), sulfur (S) and iron (Fe) interactions for dynamic simulations of anaerobic digestion processes - DTU Orbit (09/11/2017)

### Modelling phosphorus (P), sulfur (S) and iron (Fe) interactions for dynamic simulations of anaerobic digestion processes

This paper proposes a series of extensions to functionally upgrade the IWA Anaerobic Digestion Model No. 1 (ADM1) to allow for plant-wide phosphorus (P) simulation. The close interplay between the P, sulfur (S) and iron (Fe) cycles requires a substantial (and unavoidable) increase in model complexity due to the involved three-phase physico-chemical and biological transformations. The ADM1 version, implemented in the plant-wide context provided by the Benchmark Simulation Model No. 2 (BSM2), is used as the basic platform (A0). Three different model extensions (A1, A2, A3) are implemented, simulated and evaluated. The first extension (A1) considers P transformations by accounting for the kinetic decay of polyphosphates (XPP) and potential uptake of volatile fatty acids (VFA) to produce polyhydroxyalkanoates (XPHA) by phosphorus accumulating organisms (XPAO). Two variant extensions (A2,1/A2,2) describe biological production of sulfides (SIS) by means of sulfate reducing bacteria (XSRB) utilising hydrogen only (autolithotrophically) or hydrogen plus organic acids (heterorganotrophically) as electron sources, respectively. These two approaches also consider a potential hydrogen sulfide (ZH<sub>2</sub>S) inhibition effect and stripping to the gas phase (GH<sub>2</sub>S). The third extension (A3) accounts for chemical iron (III) (SFe<sup>3+</sup>) reduction to iron (II) (SFe<sup>2+</sup>) using hydrogen (SH<sub>2</sub>) and sulfides (SIS) as electron donors. A set of pre/post interfaces between the Activated Sludge Model No. 2d (ASM2d) and ADM1 are furthermore proposed in order to allow for plant-wide (model-based) analysis and study of the interactions between the water and sludge lines. Simulation (A1 - A3) results show that the ratio between soluble/particulate P compounds strongly depends on the pH and cationic load, which determines the capacity to form (or not) precipitation products. Implementations A1 and A2,1/A2,2 lead to a reduction in the predicted methane/biogas production (and potential energy recovery) compared to reference ADM1 predictions (A0). This reduction is attributed to two factors: (1) loss of electron equivalents due to sulfate (SSO<sub>4</sub>) reduction by XSRB and storage of XPHA by XPAO; and, (2) decrease of acetoclastic and hydrogenotrophic methanogenesis due to ZH<sub>2</sub>S inhibition. Model A3 shows the potential for iron to remove free SIS (and consequently inhibition) and instead promote iron sulfide (XFeS) precipitation. It also reduces the quantities of struvite (XMgNH<sub>4</sub>PO<sub>4</sub>) and calcium phosphate (XCa<sub>3</sub>(PO<sub>4</sub>)<sub>2</sub>) that are formed due to its higher affinity for phosphate anions. This study provides a detailed analysis of the different model assumptions, the effect that operational/design conditions have on the model predictions and the practical implications of the proposed model extensions in view of plant-wide modelling/development of resource recovery strategies.

#### General information

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