Incorporating aquatic chemistry into wastewater treatment process models: A critical review of different approaches

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INTRODUCTION

In recent years the awareness of the effect of abiotic processes in wastewater and sludge treatment technologies has increased rapidly (Batstone et al., 2012). One particular aspect to consider when incorporating pH calculations is that, from a numerical point of view, the inclusion of acid-base equilibrium and the subsequent pH calculation in biochemical models can lead to the appearance of some degree of stiffness, caused by the different conversion rates considered. This may introduce numerical instabilities and slow down the simulation speed. Tackling this problem requires analysis and testing of numerical methods that deal with combined algebraic and differential equations.

OBJECTIVE

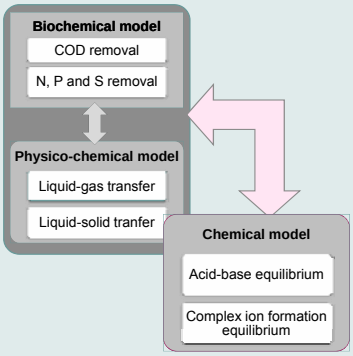
The work presented in this paper aims to introduce a methodology for incorporating aquatic chemistry into models representing wastewater treatment processes, A simulation scenario has been defined in order to carry out a comparative analysis of the different approaches in terms of the accuracy of the results and the simulation time.

Need for pH calculation

METHODOLOGY TO INCORPORATE WATER CHEMISTRY

MODEL CONSTRUCTION

The construction of the model consists of two steps

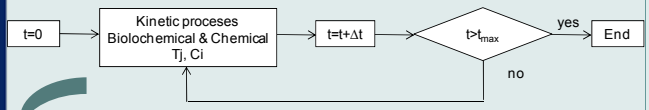


1 ***Biochemical & Physico-chemical model definition:*** Definition of components and transformations required to describe biological and physico-chemical reactions.

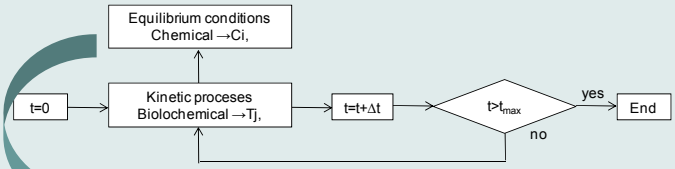
2 ***Chemical model construction*:** Based on the biochemical and physico-chemical model defined in the first step, chemical components and species are selected to construct the chemical model. Species are chemical entities taken to be physically present in the system, and for the given set of species, components are selected so that all species can be expressed as linear combination of components. Chemical equilibrium modelling consists basically of formulation of the material balance and mass action law which determine species concentrations from a mixture composition specified in terms of component concentrations.

Components			Species									
S_h	S_{TVA}	S_{Ca}	H	Mg	H_2CO_3	H_2PO_4	Hac	Hpro	CaH_2PO_4	MgH_2PO_4	$MgCO_3$	$NaHPO_4$
S_{IP}	S_{TBU}	S_{Mg}	Na	OH	HCO_3	HPO_4	Ac	Pro	$CaHCO_3$	$MgHCO_3$	$MgPO_4$	NaOH
S_{IN}	S_{TPRO}	S_{Na}	Ca	NH_3	CO_3	PO_4	Hbu	Hva	$CaHPO_4$	$MgHPO_4$	$NaCO_3$	
S_{IC}	S_{TAC}	S_{Cl}	Cl	NH_4	$CaCO_3$	CaOH	Bu	Va	$CaPO_4$	MgOH	$NaHCO_3$	

NUMERICAL RESOLUTION PROCEDURE



Ordinary differential equations (ODE):
All reactions are calculated simultaneously using ordinary differential equations

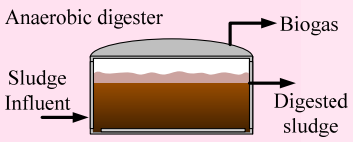


***Differential algebraic equations (DAE)**: the slower reactions are calculated by ODE and the fast reactions are calculated algebraically. Water chemistry can be solved with tailored code or using external software such as PhreeqC+ or MinteqA2*

COMPARISON OF DIFFERENT RESOLUTION APPROACHES

CASE STUDY

The objective of this study is (i) to check the capability of the model presented in the previous section to calculate aquatic chemistry equilibrium, and (ii) to carry out a comparison of the different approaches in terms of results accuracy and simulation speed. For this purpose, the anaerobic reactor in the Benchmark Simulation Model No 2 (BSM2) was selected as the simulation test case.



	Evaluation criteria	
	Simulation time (sec)	$\sum\left(K_a\cdot\{HA\}-\{H^+\}\{A^-\}\right)^2$
ODE-Kab 10^{12}	6.25	7.61^{-05}
ODE-Kab 10^{6}	3.82	7.85^{-05}
DAE-Tailored	0.96	0
DAE- PhreeqC+	23.36	0

For the ODE approach, two values for the equilibrium kinetic rate have been compared: 10^{12} and 10^{6}. When using the kinetic rate of 10^{12} the simulated results are more accurate, since the result is closer to equilibrium. Nevertheless, higher kinetic rates slow down the simulation speed.

The DAE approach using a tailored code for equilibrium calculation showed the shortest simulation time. Finally, when simulating the scenario with the external software Phreeq C+, the highest number of species was considered, but the simulations were the slowest

The methodology proposed using a tailor-made equilibrium calculation using algebraic equations, and incorporating it into the biological ODE system gave the most effective methodology, based on the simulation times of the different approaches.

CONCLUSIONS

- ✓Different approaches for calculating chemical equilibrium were presented and a critical review was undertaken.
- ✓Based on this comparison a methodology has been proposed for incorporating water chemistry into wastewater treatment process models

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