WATER RESEARCH 74 (2015) 239–256

Available online at www.sciencedirect.com

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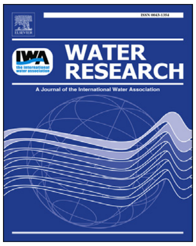
journal homepage: www.elsevier.com/locate/watres



A new general methodology for incorporating physico-chemical transformations into multi-phase wastewater treatment process models

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ARTICLE INFO

Article history:
Received 27 August 2014
Received in revised form
19 January 2015
Accepted 21 January 2015
Available online 12 February 2015

Keywords:
Abiotic processes
Mathematical modelling
pH calculation
Plant-wide modelling
Water chemistry

ABSTRACT

This paper introduces a new general methodology for incorporating physico-chemical and chemical transformations into multi-phase wastewater treatment process models in a systematic and rigorous way under a Plant-Wide modelling (PWM) framework. The methodology presented in this paper requires the selection of the relevant biochemical, chemical and physico-chemical transformations taking place and the definition of the mass transport for the co-existing phases. As an example a mathematical model has been constructed to describe a system for biological COD, nitrogen and phosphorus removal, liquid–gas transfer, precipitation processes, and chemical reactions. The capability of the model has been tested by comparing simulated and experimental results for a nutrient removal system with sludge digestion. Finally, a scenario analysis has been undertaken to show the potential of the obtained mathematical model to study phosphorus recovery.

1. Introduction

Traditionally, WWTPs have been operated to guarantee a certain effluent quality and consequently the main focus has been the biological processes taking place for COD and nutrient removal. However, nowadays, the general concern about climate change and scarcity of natural resources is encouraging operating the processes in a more sustainable and environmental-friendly way seeking the reduction of energy consumption, recovery of valuable materials and minimization of greenhouse gas emissions. With this purpose, WWTPs are incorporating novel technologies and ways of design and operation where physico-chemical and

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http://dx.doi.org/10.1016/j.watres.2015.01.031

List of abbreviations

AD	Anaerobic digestion
ADM1	Anaerobic digestion model No 1
ASM1/2d/3	Activated sludge model No 1, 2d and 3
ASMs	Activated sludge models
ASU	Activated sludge unit
BNRM	Biological nutrient removal model
CEIT	Centro de estudios e investigaciones técnicas de Gipuzkoa
COD	Chemical oxygen demand
DAE	Differential algebraic equations
DO	Dissolved oxygen
E-PWM	Extended plant-wide model
IAP	Ion activity coefficient
IWA	International water association
LT	List of transformations
NDBERP	Nitrification–denitrification biological excess phosphorous removal
ODE	Ordinary differential equations
PAO	Phosphorous accumulating organisms
PHA	Polyhydroxyalkanoates
PWM	Plant-wide model
TAC	Total acetate
TBU	Total butyrate
T-HS	Total hydrogen sulphide
TIC	Total inorganic carbon
TIN	Total inorganic nitrogen
TIP	Total inorganic phosphorous
T-NO$_2$	Total nitrite
T-NO$_3$	Total nitrate
TPRO	Total propionate
TSO$_4$	Total sulphate
TVA	Total valerate
UCT	University of Cape Town
UCTADMP	University of Cape Town anaerobic digestion model
VFA	Volatile fatty acids
WWTP	Wastewater treatment plant

List of symbols

a	Contact area between liquid and gaseous phases (m^2)
a_{ij}	Stoichiometric relationship of species i and component j
A	Debye–Huckel constant
C_i	Concentration of component i (mol m^{-3})
d_B	Diameter of the bubbles (m)
$D_{L,i}$	Diffusivity of component i in liquid phase (m^2 d^{-1})
D_{L,O_2}	Diffusivity of component oxygen in liquid phase (m^2 d^{-1})
$E_{ghu,w}$	Stoichiometry of interaction between water and gas hold up in gas hold up
$E_{w,ghu}$	Stoichiometry of interaction between water and gas hold up in water phase
I	Ionic strength
K'	Kinetic rate for precipitation (d^{-1})
K_a	Equilibrium constant (mol L^{-1})
K_{ab}	Kinetic rate constant for chemical equilibrium (d^{-1})
K_H	Henry's constant (mol atm^{-1} L^{-1})
$K_{H,i}$	Henry's constant for component I (mol atm^{-1} L^{-1})
$k_{L/G}$	Mass transfer rate constant (d^{-1})
$k_{L/G,i}$	Mass transfer rate constant for component i (d^{-1})
$k_{L/G,NH_3}$	Mass transfer rate constant for ammonia (d^{-1})
$k_{L/G,O_2}$	Mass transfer rate constant for oxygen (d^{-1})
k_G	Mass transfer rate constant limited by gaseous phase (d^{-1})
k_{G,NH_3}	Mass transfer rate constant limited by gaseous phase for ammonia (d^{-1})
k_L	Mass transfer rate constant limited by liquid phase (d^{-1})
k_{L,O_2}	Mass transfer rate constant limited by liquid phase for oxygen (d^{-1})
$k_{L,i}$	Mass transfer rate constant limited by liquid phase for component i (d^{-1})
K_{sp}	Supersaturation coefficient (mol L^{-1})
M_i	Molality of species i (mol L^{-1})
n_{ghu}	Total moles contained in gas hold-up (mol)
P_i	Partial pressure of component i (atm)
P_{ghu}	Pressure of gas hold-up (atm)
P_{goff}	Pressure of contact atmosphere (atm)
$\{S\}$	Activity of species S
$[S]$	Molality of species S (mol L^{-1})
S_{A-}	Total anion equivalent concentration (mol L^{-1})
S_{C+}	Total cation equivalent concentration (mol L^{-1})
T_j	Molality of component j given by the process model mass balance (mol L^{-1})
V_{ghu}	Gas hold up volume (m^3)
Z_i	Charge of species i

Greek symbols

γ_S	Activity coefficient of S
ρ	Kinetic rate (d^{-1})
υ_r	Slip velocity between liquid and gaseous phase (m s^{-1})
$\psi\ k_L$	proportionality factor

chemical processes are becoming increasingly important and cannot be neglected when making decisions.

Referring to *energy consumption reduction* in WWTPs, the optimization of aeration systems is a key factor as it may represent 50% of the total energy consumption in a WWTP (Olsson, 2013). Several aspects such as type and state of diffusers, reactor geometry, wastewater characteristics, operational temperature or air composition may have a great impact on aeration systems and consequently on energy consumption. In this respect, work has been carried out to optimize aeration systems (Beltran et al., 2013; Thunberg et al., 2009) with the aim of reducing energy consumption. Another example is the use of high purity oxygen aeration as alternative to conventional aeration systems in industrial sector (Irizar et al., 2012) as a way to improve the efficiency of the process and consequently reduce energy costs (Irizar et al., 2012).

The concern of scarcity of natural resources is also driving *resource recovery* at WWTP. As an example, some studies