THE pHAUXOSTAT

by

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ABSTRACT

The pHauxostat technique for process control was proposed in the late nineteen fifties with a theoretical explanation done by Martin and Hempfling in 1976. The theory was extended in 1985 (Rice & Hempfling), but concluded to be incomplete. The objective of this study was to develop a theory for the pHauxostat and to investigate and explain the principles involved. This was done by investigating the pH, as the controlled output variable, and the control methodology with the feed system the manipulated input variable. Laboratory test work was conducted to verify a proposed theory by using a chemically defined substrate. The technique was thereafter applied in treating a petrochemical effluent in a demonstration plant, demonstrating the generality and applicability of the theory and the pHauxostat technique.

The controlled pH of the reactor solution was found to be a function of the weak acids and bases in the reactor solution and the strong acids and bases added to the substrate, in combination with the chemical species removed from the substrate during biodegradation. A method proposed by Loewenthal *et al.* (1991) that was developed for chemical conditioning, utilising solution and subsystem alkalinities, proved to be successful in characterising the reactor solution in combination with traditional equilibrium chemistry.

The pHauxostat control system was shown to keep the alkalinity constant, resulting in a controlled and constant difference in solution alkalinity between the reactor and the substrate solutions. The feed rate is controlled by this difference in combination with the alkalinity generation rate. The alkalinity generation rate is defined with a proposed alkalinity yield coefficient, linking water chemistry and growth kinetics. The alkalinity yield coefficient indicates the amount of alkalinity generated per substrate removed, similarly to the conventional growth yield. The alkalinity yield coefficient was successfully modelled by a theoretical alkalinity yield coefficient, based on oxidation-reduction half reactions as developed by McCarty (1975). This was shown to be true when the change in alkalinity is mainly due to substrate removal.

The developed theory is based on alkalinity, modelling the pHauxostat technique by completing a mass balance on solution alkalinity. The model proved to accurately predict the results for the

laboratory and the demonstration plant test work. The model is represented by the following formula, respectively for layouts of a chemostat and a CSTR with biomass separation:

$$i_s X_{COD} \, Y_{ALK} \, / \, Y_{obs} = S_{ALK} - S_{ALK0}$$

$$\text{and} \quad i_s X_{COD} \, Y_{ALK} \, (\tau/\theta_c) \, / \, Y_{obs} = S_{ALK} - S_{ALK0}$$

The growth limiting nutrient (S) may be a part of a weak acid/base subsystem or not, implicating two methods of control. pHauxostats were categorised on this basis, giving Category A pHauxostats with S = f(pH) and Category B pHauxostats with S ≠ f(pH). The process for Category A pHauxostats is controlled by the concentration of the growth limiting nutrient (determined by the set point pH and the substrate composition), in combination with the difference in the solution alkalinities between the substrate and reactor solutions. The growth limiting nutrient concentration for Category B pHauxostats, is not controlled but is a result of the control system which is determined by the feed rate of the growth limiting nutrient and the difference in the solution alkalinities.

The main contribution of this study is the analysis of the pHauxostat on an alkalinity basis and the subsequent proposed theory with inclusion of an alkalinity yield coefficient. The alkalinity yield coefficient is universal for biological processes in general. Calculation methods for chemical characterisation of the reactor solution were determined together with a method to predict the alkalinity yield coefficient by a theoretical alkalinity yield coefficient. The control methodology was disclosed and pHauxostats were categorised. This study makes the modelling of the pHauxostat technique possible and the implementation thereof, available to the water industry.

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SAMEVATTING

Die pHauxostat tegniek is in die laat negentien vyftigs voorgestel met 'n teoretiese beskrywing deur Martin en Hempfling in 1976. Die teorie is in 1985 verbeter, maar met die gevolgtrekking dat dit nie volledig is nie. Die doelstelling van hierdie studie was om die teorie te verbeter en die beginsels van die beheermetode te verklaar. Dit is gedoen deur die beheerde uitset-veranderlike, die pH, en die beheermetode van die gemanipuleerde inset-veranderlike, die voertempo, te ondersoek. Laboratoriumtoetse is met 'n chemies-gedefinieerde substraat voltooi om 'n voorgestelde teorie te verifieer. Die tegniek is ook in 'n demonstrasie-aanleg toegepas, met 'n petrochemieseuitvloeisel as substraat, om die algemeen toepasbaarheid van die teorie en die tegniek te demonstreer.

Dit is gevind dat die beheerde reaktor pH 'n funksie is van die swak sure en basisse in oplossing en die sterk sure en basisse in die substraat, in kombinasie met die chemiese spesies wat uit die substraat verwyder word deur biodegradering. Die reaktoroplossing kon suksesvol gekarakteriseer word met tradisionele ewewigschemie-metodes in kombinasie met 'n metode deur Loewenthal *et al.* (1991) voorgestel (vir chemiese kondisionering), wat gebaseer is op oplossing- en subsisteem-alkaliniteit.

Die beheersisteem hou die alkaliniteit in die reaktoroplossing konstant en gevolglik ook die verskil in die alkaliniteit tussen die reaktor- en substraatoplossings. Die voertempo word beheer deur hierdie verskil in kombinasie met die produksietempo van alkaliniteit. Die produksietempo van alkaliniteit word gedefinieer met 'n alkaliniteits-opbrengs-koëffisiënt, waardeur water chemie en groeikinetika gekoppel word. Die alkaliniteits-opbrengs-koëffisiënt verteenwoordig die alkaliniteit wat gegenereer word per substraat verwyder, soortgelyk aan die konvensionele selopbrengs-koëffisiënt. Die alkaliniteits-opbrengs-koëffisiënt kon suksesvol met 'n teoretiese alkaliniteits-opbrengs-koëffisiënt gemodelleer word, wat op oksidasie-reduksie halfreaksies gebaseer is, voorgestel deur McCarty (1975). Die gebruik daarvan is korrek indien die alkaliniteits-opbrengs hoofsaaklik aan substraat verwydering toegeskryf kan word.

Die voorgestelde teorie word gebaseer op alkaliniteit, waardeur die pHauxostat gemodelleer word deur 'n massabalans op alkaliniteit te voltooi. Die resultate van die laboratoriumtoetse en die

demonstrasieaanleg is suksesvol deur die model voorspel en word deur die volgende formules voorgestel, onderskeidelik vir uitlegte van 'n chemostaat en 'n volledig vermengde mengvat reaktor met selhersirkulasie :

$$i_s X_{COD} \, Y_{ALK} \, / \, Y_{obs} = S_{ALK} - S_{ALK0}$$

en $\quad i_s X_{COD} \, Y_{ALK} \, (\tau/\theta_c) \, / \, Y_{obs} = S_{ALK} - S_{ALK0}$

Die groeibeperkende nutrient (S) kan óf deel uitmaak van 'n swaksuur/basis subsisteem óf nie, wat twee moontlike beheermetodes impliseer. pHauxostate is op grond hiervan geklassifiseer met S = f(pH) vir 'n Kategorie A pHauxostat, en S ≠ f(pH) vir 'n Kategorie B pHauxostat. Die voertempo vir 'n Kategorie A pHauxostat word deur die konsentrasie van die groeibeperkende nutrient beheer, en word bepaal deur die beheerde pH-waarde en die substraat samestelling, in kombinasie met die verskil in die alkaliniteit tussen die reaktor- en substraatoplossings. Die groeibeperkende nutrient konsentrasie vir 'n Katergorie B pHauxostat word nie beheer nie maar is die gevolg van die beheersisteem, wat bepaal word deur die voertempo van die groeibeperkende nutrient en die verskil in die alkaliniteit tussen die reaktor- en substraatoplossings.

Die belangrikste bydrae van hierdie studie is die analisering van die pHauxostat op 'n alkaliniteits basis en die gevolglike voorgestelde teorie, met die insluiting van 'n alkaliniteits-opbrengs-koëffisiënt. Die alkaliniteits-opbrengs-koëffisiënt is universeel en kan in modellering van biologiese prosesse in die algemeen gebruik word. Die berekeningsmetodes vir die karakterisering van die reaktoroplossing is bepaal en 'n teoretiese alkaliniteits-opbrengs-koëffisiënt is ontwikkel vir die voorspelling van die alkaliniteits-opbrengs-koëffisiënt. Die beheermetode van die pHauxostat word in die studie verklaar en pHauxostate word gekategoriseer. Hierdie studie maak die modellering van die pHauxostat en die toepassing daarvan moontlik.

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LIST OF ACRONYMS AND SYMBOLS

A.   ACRONYMS:

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Acronym	Definition	Page no. of first reference

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Acronym	Definition	Page no. of first reference
BOH	Base (type not specified)	104
COD	Chemical Oxygen Demand	2
CSTR	Continuous Stirred Tank Reactor	4
DO	Dissolved Oxygen	7
GLN	Growth Limiting Nutrient	7
HA	Acid (type not specified)	104
HAc	Acetic Acid	17
HRT	Hydraulic Residence Time	5
PID	Proportional-Integral-Derivative	13
RO	Oxygen uptake	86
SRT	Solids Retention Time	6
SCFA	Short Chain Fatty Acid	17
TSS	Total Suspended Solids	62
VSS	Volatile Suspended Solids	62
[ANC]	Acid Neutralising Capacity	22

B.   SYMBOLS:

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Symbol	Definition	Unit	Page no. of first reference

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Symbol	Definition	Unit	Page no. of first reference
b	Decay coefficient	T^{-1}	5
C_x	Total species x concentration	$M_{mole} \, L^{-3}$	18
D	Dilution rate	T^{-1}	9
f_D	Fraction of active biomass contributing to biomass debris	-	84
f_e	Fraction of electron donor used for energy	-	37

Symbol	Definition	Unit	Page no. of first reference
f_s	Fraction of electron donor captured through synthesis	-	37
f_x	Activity coefficient x	-	19
F	Volumetric flow rate	L^3T^{-1}	5
F_o	Influent volumetric flow rate	L^3T^{-1}	5
F_w	Volumetric flow rate of biomass wastage stream	L^3T^{-1}	6
i_s	Substrate conversion factor	$M_{mole}M_{COD}^{-1}$	35
K_s	Half-saturation coefficient for substrate	ML^{-3}	3
K_x	Thermodynamic dissociation equilibrium constant x	-	19
K'_x	Apparent dissociation equilibrium constant x	-	19
Q	Air flow rate	L^3T^{-1}	5
r_{ALK}	Reaction rate for alkalinity production	$M_{mole}L^{-3}T^{-1}$	35
r_{so}	Reaction rate for dissolved oxygen	$ML^{-3}T^{-1}$	97
r_s	Reaction rate for soluble substrate	$ML^{-3}T^{-1}$	2
r_{XB}	Reaction rate for active biomass	$ML^{-3}T^{-1}$	2
r_{XD}	Reaction rate for biomass decay	$ML^{-3}T^{-1}$	114
R	Overall stoichiometric equation	-	37
R_a	Half-reaction for the electron acceptor	-	37
R_c	Half-reaction for cell material	-	37
R_d	Half-reaction for electron donor	-	37
RO	Mass rate of oxygen utilisation	MT^{-1}	86
S	The growth limiting nutrient concentration	ML^{-3}	45
S_A	Acetic acid concentration	ML^{-3}	27
S_{ALK}	Solution alkalinity reactor	$M_{mole}L^{-3}$	25
S_{ALK0}	Solution alkalinity feed	$M_{mole}L^{-3}$	25
S_o	Dissolved oxygen concentration	ML^{-3}	5
S_s	Soluble substrate concentration	ML^{-3}	3
S_{so}	Influent soluble substrate concentration	ML^{-3}	5

Symbol	Definition	Unit	Page no. of first reference
V	Reactor Volume	L^3	5
X	Biomass concentration	ML^{-3}	5
X_B	Active biomass concentration	ML^{-3}	2
X_{COD}	Biomass concentration in COD units	ML^{-3}	35
x	Alkalinity production for the electron donor and acceptor per unit substrate consumed	$M_{mole}M^{-1}_{mole}$	39
y	Alkalinity production for cell synthesis minus that of the acceptor per unit substrate consumed	$M_{mole}M^{-1}_{mole}$	39
Y	True growth yield	$M_{COD}M^{-1}_{COD}$	2
Y_{ALK}	Alkalinity yield	$M_{mole}M^{-1}_{mole}$	35
Y_{TALK}	True alkalinity yield	$M_{mole}M^{-1}_{mole}$	39
Y_{obs}	Observed growth yield	$M_{COD}M^{-1}_{COD}$	5
θ_c	Solids retention time	T	6
μ	Specific growth rate coefficient	T^{-1}	2
μ_m	Maximum specific growth rate coefficient	T^{-1}	3
τ	Hydraulic residence time	T	5
[ ]	Mass concentration	$M_{mole}L^{-3}$	18
( )	Activity concentration	$M_{mole}L^{-3}$	19

DANKBETUIGING

"Aan Hom wat op die troon sit, en aan die Lam, behoort die lof en die eer, die heerlikheid en die krag, tot in alle ewigheid."   Openbaring 5:13

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