

A MATHEMATICAL MODEL FOR A HYBRID ANAEROBIC REACTOR

by

V. SARAVANAN

DEPARTMENT OF BIOCHEMICAL ENGINEERING AND BIOTECHNOLOGY

Submitted

in fulfillment of the requirements of the degree of

DOCTOR OF PHILOSOPHY

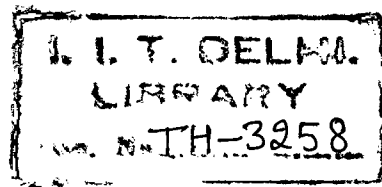
to the



**INDIAN INSTITUTE OF TECHNOLOGY DELHI
NEW DELHI – 110016, INDIA**

DECEMBER 2005

1. Hybrid anaerobic reactor
2. Anaerobic reactor



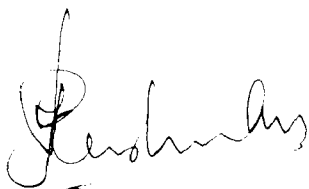
TH

574.635

SAR-M

Certificate

This is to certify that the thesis entitled “**A Mathematical Model for a Hybrid Anaerobic Reactor**” being submitted by Mr. V. Saravanan is worthy of consideration for the award of the degree of Doctor of Philosophy. The thesis has been prepared under my supervision and guidance in conformity with the rules and regulations of Indian Institute of Technology Delhi and is a record of the original bonafide research work. The results presented in this thesis have not been submitted in part or full to any other universities or institutes for the award of any other degree or diploma.



Dr. T.R. Sreekrishnan

Associate Professor

Department of Biochemical Engineering and Biotechnology

Indian Institute of Technology Delhi

Acknowledgements

I am extremely grateful to my supervisor **Dr. T. R. Sreekrishnan** for his expert guidance and constant encouragement throughout my project. It would not have been possible at all to complete my thesis successfully, within minimum period, without his continuous support and motivation. I am highly indebted to him for his patience and devoting his valuable time throughout my work.

I am very thankful to Prof. Sunil Nath, Dr. James Gomes and Prof. Mukesh Khare for their valuable suggestions and encouragements.

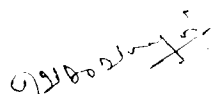
My special thanks to Prof. T.R.Rao and Prof. Subba Rao of the Chemical Engg Dept, for their advises and care.

I thank Prof. Jean-Philippe Steyer and Prof. Rene Moletta of Laboratoire de Biotechnologie de l'Environnement LBE-INRA France, for their timely help.

I wish to thank Khan Saheb, Pandit Ji, Sharma Ji, Rana Ji, VK Ji, Sapan Ji, Neera Madam, Mukesh Anand Ji, and Sitaram Ji for their technical support and cooperation.

My heartfelt thanks to my lab mates Ramesh, Mukesh, Gancsan, Nafia and Anurag for their ever-helping hands. I express my gratitude to my friends Rakesh Kumar, Satyanarayana, Periyaswami, Nitin Khanna, Partheepan, Pawan, Pankaj, Vidyanand, Vipin, Ratna Kishore, and Nagaraju for their wholehearted support throughout my stay in IIT.

It is not possible to express in words the support and love I received from my parents. Above all I thank my **Spiritual teacher and the Almighty** for their love and blessings.


V.Saravanan

ABSTRACT

A Hybrid Anaerobic Reactor (HAR) has been developed in the laboratory of Dept of Biochemical Engineering and Biotechnology, IIT Delhi. The HAR employs self-immobilized anaerobic bacterial granules under completely fluidized condition as biocatalyst. A mathematical model has been developed for this reactor. Such a model can be used to study the sensitivity of the process to various operating parameters as well as to optimize the reactor design. This model includes a number of steps describing the biochemical and physico-chemical processes. The biochemical process includes: hydrolysis of particulate matter into soluble monomers like sugars, amino acids and fatty acids; acidogenesis of sugar into volatile fatty acids like acetate, propionate and butyrate; acetogenesis of propionate and butyrate into acetate and hydrogen; and methanogenesis. i.e. conversion of acetate to methane and CO₂ and conversion of hydrogen and CO₂ into methane. The physico-chemical processes describe ion association/dissociation and gas-liquid transfer.

In brief the model consists of the following three components:

1. A biofilm model, which describes the substrate conversion kinetics within the individual granule. Glucose was used as the model substrate. The stoichiometric equations considered were taken from literature. The substrate utilization rates were defined by using Monod kinetics with substrate/product inhibition and pH inhibition. Mass balance was written for different components within a granule. By solving these equations components fluxes at the surface of a granule were obtained.
2. A bed fluidization model, which describes the distribution of biogranules inside the fluidized bed volume. Experiments were conducted to study the settling and bed

expansion characteristics of biogranules obtained from the HAR. Based on this study a new correlation relating the up flow liquid superficial velocity and bed void fraction was developed.

3. A reactor flow model, which links the biofilm and the bed fluidization models to predict the substrate and products concentrations as a function of axial position (height) within the reactor. The reactor was divided into a number of compartments. The number of granules in each compartment was calculated using bed fluidization model. The component flux at the surface of a granule was obtained from the biofilm model. Using this, component balance equations for the entire compartment were written. By solving these equations for all the compartments, component profiles were predicted. All the simulations were done using Visual C++ software.

Product inhibition and pH inhibition of each group of bacteria has been considered in the kinetic model. The spatial distribution of each group of anaerobic bacteria within the anaerobic granules has been found to play a vital role in bringing about the conversion. Experiments were conducted in the HAR using synthetic effluent containing glucose as the carbon source to study the treatment efficiency. The model was simulated for the different sets of experimental operating conditions, first assuming a layered distribution of anaerobic bacteria within granules and then homogeneous distribution of anaerobic bacteria. The predictions of model simulation with the assumption of layered structure closely represented the experimental data. This indicated that the granule structure is mainly determined by the substrate kinetics.

Contents

Page No.

Certificate	i
Acknowledgments	ii
Abstract	iii
Contents	v
List of Figures	ix
List of Tables	xi
Nomenclatures	xii
Chapter 1 Introduction and Objectives	
1.1 Introduction	1
1.2 Motivation and Objectives	3
Chapter 2 Literature Review	
2.1 Introduction	7
2.2 Models for UASB	9
2.2.1 Flow Model	10
2.2.2 Reactor Model	13
2.3 Proposed models for the structure of the biofilm	19
2.3.1 Multi-layer Model	20
2.3.2 Syntrophic Microcolony Model	21
2.3.3 Non-layered Structure Model	22
2.3.4 Granule Cluster Structure	23
2.4 Models for AFBR	26
2.4.1 Bed Fluidization Model	26
2.4.1.1 Terminal Settling Velocity	27
2.4.1.2 Fluidization Mechanics	29
2.4.1.3 Effect of Gas Production on Hydrodynamics	31
2.4.1.4 Bed Stratification	32
2.4.2 Kinetic and Reactor Sub-models	33

2.4.2.1 Stratified Biofilm Models	39
2.5 Inhibition Models	41
2.5.1 pH Inhibition	42
2.5.1.1 pH Inhibition Coupled with Substrate Inhibition	42
2.5.1.2 Independent pH Inhibition Functions	43
2.5.2 Substrate Inhibition	44
2.5.3 Product Inhibition	45
2.6 Summary	46
Chapter 3 Model Development	
3.1 Process Description	49
3.2 Biofilm Model	50
3.2.1 Growth Kinetics	51
3.2.1.1 Acidogenesis	51
3.2.1.2 Acetogenesis	51
3.2.1.3 Methanogenesis	52
3.2.2 Biofilm Model for 3-layered Structure	53
3.2.2.1 Outer Layer Mass Balance	53
3.2.2.2 Middle Layer Mass Balance	57
3.2.2.3 Inner Layer Mass Balance	60
3.2.3 Biofilm Model for Homogeneous Structure	61
3.2.4 Biofilm Model for Two-layer Structure	64
3.2.4.1 Outer Layer Mass Balance	64
3.2.4.2 Inner Layer Mass Balance	66
3.3 Physico-chemical Reaction System	67
3.3.1 pH Modeling	68
3.3.2 Gas-liquid Transfer	73
3.4 Reactor Model	73
3.4.1 Compartmental Model	73

	3.5 Model Parameters	74
	3.5.1 Kinetic Constants	74
	3.5.2 Biomass Composition	76
Chapter 4	Experimental Methodology and Analytical Procedure	
	4.1 Materials	77
	4.1.1 Effluents	77
	4.1.2 Experimental Setup of the Hybrid Anaerobic Reactor	77
	4.1.3 Biogranules	78
	4.2 Methodology	79
	4.2.1 Density of Biogranules	79
	4.2.2 Terminal Settling Velocity of Biogranules	79
	4.2.3 Bed Expansion Characteristics	80
	4.2.4 Analytical Methods	81
	4.2.4.1 Chemical Oxygen Demand (COD)	81
	4.2.4.2 Glucose Estimation	82
	4.2.4.3 Volatile Fatty Acids (VFA) Concentration	82
Chapter 5	Results and Discussion	
	5.1 Biofilm Model	83
	5.1.1 Methods Adopted for Solving the Biofilm Model	
	Equations	83
	5.1.2 pH Inhibition Kinetics	84
	5.2 Bed Fluidization Model	85
	5.2.1 Density Variation of Biogranules of Different Sizes	86
	5.2.2 Biogranule Terminal Settling Velocity	86
	5.2.3 Bed Expansion Characteristics of Bio-bed 1	90
	5.2.4 Bed Expansion Characteristics of Bio-bed 2	94
	5.2.5 Algorithm to Predict the Fluidized Bed Voidage	98
	5.3 pH Estimation	100
	5.4 Reactor Model	100

5.4.1 Components Balance for a Compartment	101
5.4.2 Components Profile along the Reactor Height with Recycle	103
5.5 Experimental Study on HAR	105
5.6 Model Validation with Experimental Data	106
Chapter 6 Summary and Conclusions	
6.1 Summary and Conclusions	109
References	111
Appendices	
Appendix A: Programme Codes Written in VC++	127
Appendix B: Author's Resume	181