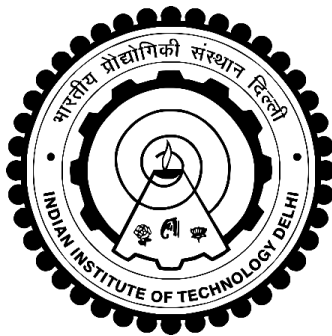


MATHEMATICAL MODELING OF THE MODIFIED TRICKLING FILTER

DEEPAK SHARMA



**DEPARTMENT OF BIOCHEMICAL ENGINEERING
AND BIOTECHNOLOGY**

INDIAN INSTITUTE OF TECHNOLOGY DELHI

MARCH 2023

© Indian Institute of Technology Delhi (IITD), New Delhi, 2023

MATHEMATICAL MODELING OF THE MODIFIED TRICKLING FILTER

by

DEEPAK SHARMA

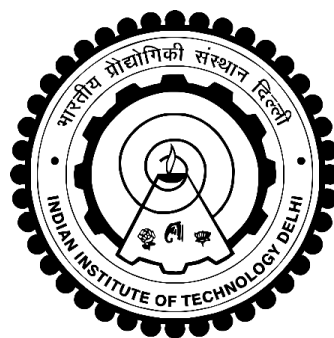
**DEPARTMENT OF BIOCHEMICAL ENGINEERING AND
BIOTECHNOLOGY**

Submitted

in the fulfillment of the requirements of the degree of

DOCTOR OF PHILOSOPHY

to the



INDIAN INSTITUTE OF TECHNOLOGY DELHI

MARCH 2023

Certificate

This is to certify that the thesis entitled “**Mathematical modeling of The Modified Trickling Filter.**” Being submitted by **Mr. Deepak Sharma** 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 the 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 or to other universities or institutes for the award of any other degree or diploma.

Dr. T. R. Sreekrishnan
Professor
Department of Biochemical Engineering
and Biotechnology
Indian Institute of Technology, Delhi

Dr. Shaikh Ziauddin Ahammad
Associate Professor
Department of Biochemical Engineering
and Biotechnology
Indian Institute of Technology, Delhi

Acknowledgments

I am incredibly grateful to my supervisors, **Dr. Shaikh Ziauddin Ahammad** and **Dr.(Prof.) T.R. Sreekrishnan** for their expert guidance and constant encouragement throughout my project. It would not have been possible at all to complete my thesis successfully within the stipulated period of time without their continuous support and motivation. I am highly indebted to them for their patience and devoting their valuable time throughout my work.

I am very thankful to prof. A.K. Srivastava, Prof. Atul Narang, Prof. Aashish Mishra, and Prof. B.J. Allapat for their valuable suggestions and encouragement.

Also, I wish to express my gratitude to each member of the Waste Treatment Lab for maintaining a friendly, encouraging, and supportive environment.

It would be a great pleasure to thank my friends Deepchandra Joshi, Partha Pritam Mondal, Abhinav Galodha, and Mahdiyar for making this long and challenging journey always joyful and easy.

Lastly, I thank almighty my spouse, my son, and my friends, who have been a constant source of inspiration during the preparation and completion of this project.

(Deepak Sharma)

Abstract

A Mathematical Model for the Modified Trickling Filter (MTF) has been developed. The MTF employs polyurethane sponge (PU sponge) as the support media for biomass growth and immobilization. PU sponge offers several advantages over conventional media such as Raschig Rings. The Mathematical model can be an excellent tool to study various aspects associated with the different parameters whose sensitivity can be used for reactor design and calculate the performance.

The model includes many steps describing the biochemical and physicochemical processes. The biochemical processes include the degradation of organic carbonaceous material and ammonia oxidation by the heterotrophs and nitrifiers, respectively. The conversion of nitrates into nitrogen is done by the facultative heterotrophs under anoxic conditions. The physicochemical processes describe mass transport processes and how substrate transport is affected by the microbial reaction within the biofilm matrix.

In brief, the model consists of the following three components:

1. A biofilm model describes the substrate conversion kinetics within the differential section of the biofilm attached to the support media. The stoichiometric equations considered were taken from the literature. The substrate utilization rates were defined using the Monod kinetics and diffusion across the biofilm matrix following Fick's Law. Microscopic mass balance was written for different components within a microscopic differential section of the biofilm. The component fluxes entering the biofilm surface can be obtained by solving the mass

balance equations. These component fluxes can be viewed as the biofilm reaction rate.

2. A Reactor Model describes how biofilm is distributed within the reactor. The compartment model is used to describe the reactor model. One compartment can be considered a Completely Mixed Biofilm Reactor (CMBR). In a CMBR, biofilm is wholly mixed within the compartment.
3. A Reactor Flow Model links the Biofilm Model and the Reactor Model. The Reactor Flow Model describes how each compartment (CMBRs) is connected. The flow model is obtained by summing up all compartments to form the complete reactor. The CMBRs are thought to be connected in series in an MTF.

The rate law expressions for the biofilm kinetics were developed. The process involves converting the Biofilm Model into the dimensionless domain. Then formulating, the rate law expression in terms of dimensionless flux, which depends on a dimensionless number named 'Biofilm Number' (B) and a dimensionless algebraic function named Biofilm Kinetic Function $\Psi(S^*)$. The concept of maximum flux has been developed, equal to the Biofilm Number's square. The effectiveness factor of the biofilm has been formulated using the Biofilm Kinetic Function.

The Mathematical Model of the MTF has been proven using the experimental data from the findings (Shukla, 2021). The spatial distribution of heterotrophs and Nitrifiers plays a vital role in the conversion. The coexistence of Heterotrophs and Nitrifiers within the same biofilm is modeled according to two hypotheses: Bilayer Biofilm and Homogenous Biofilm. The predictions of Model simulations found that Bilayer Biofilm Model is promising for the experimental data. The growth kinetics of each spec

strongly influences the structure and spatial distribution of species in the multispecies
Biofilm.

सार

संशोधित ट्रिक्लिंग फ़िल्टर (एमटीएफ) के लिए एक गणितीय मॉडल विकसित किया गया है। MTF बायोमास विकास और स्थिरीकरण के लिए समर्थन मीडिया के रूप में पॉलीयुरेथेन स्पंज (PU स्पंज) का उपयोग करता है। पीयू स्पंज रास्चिंग रिंग्स जैसे पारंपरिक मीडिया पर कई फायदे प्रदान करता है। गणितीय मॉडल विभिन्न मापदंडों से जुड़े विभिन्न पहलुओं का अध्ययन करने के लिए एक उत्कृष्ट उपकरण हो सकता है, जिनकी संवेदनशीलता का उपयोग रिएक्टर डिजाइन और प्रदर्शन की गणना के लिए किया जा सकता है।

मॉडल में जैव रासायनिक और भौतिक रासायनिक प्रक्रियाओं का वर्णन करने वाले कई चरण शामिल हैं। जैव रासायनिक प्रक्रियाओं में क्रमशः हेटरोट्रॉफ़्स और नाइट्रिफ़ायर द्वारा कार्बनिक कार्बोनेसियस सामग्री और अमोनिया ऑक्सीकरण का क्षरण शामिल है। नाइट्रेट्स का नाइट्रोजन में रूपांतरण वैकल्पिक हेटरोट्रॉफ़्स द्वारा एनोक्सिक स्थितियों के तहत किया जाता है। भौतिक-रासायनिक प्रक्रियाएं बड़े पैमाने पर परिवहन प्रक्रियाओं का वर्णन करती हैं और बायोफ़िल्म मैट्रिक्स के भीतर माइक्रोबियल प्रतिक्रिया से सब्सट्रेट परिवहन कैसे प्रभावित होता है।

संक्षेप में, मॉडल में निम्नलिखित तीन घटक होते हैं:

1. एक बायोफ़िल्म मॉडल सपोर्ट मीडिया से जुड़ी बायोफ़िल्म के डिफरेंशियल सेक्शन के भीतर सब्सट्रेट रूपांतरण कैनेटीक्स का वर्णन करता है। माना जाने वाला स्टोइकोमेट्रिक समीकरण साहित्य से लिए गए थे। फिक के नियम के बाद बायोफ़िल्म मैट्रिक्स में मोनोड कैनेटीक्स और प्रसार का उपयोग करके सब्सट्रेट उपयोग दरों को परिभाषित किया गया था। बायोफ़िल्म के एक सूक्ष्म अंतर खंड के भीतर विभिन्न घटकों के लिए सूक्ष्म द्रव्यमान संतुलन लिखा गया था। द्रव्यमान

संतुलन समीकरणों को हल करके बायोफिल्म सतह में प्रवेश करने वाले घटक फ्लक्स प्राप्त किए जा सकते हैं। इन घटक प्रवाहों को बायोफिल्म प्रतिक्रिया दर के रूप में देखा जा सकता है।

2. एक रिएक्टर मॉडल बताता है कि रिएक्टर के भीतर बायोफिल्म कैसे वितरित की जाती है। कम्पार्टमेंट मॉडल का उपयोग रिएक्टर मॉडल का वर्णन करने के लिए किया जाता है। एक कम्पार्टमेंट को पूरी तरह से मिश्रित बायोफिल्म रिएक्टर (CMBR) माना जा सकता है। एक सीएमबीआर में, बायोफिल्म पूरी तरह से डिब्बे के भीतर मिश्रित होती है।

3. एक रिएक्टर फ्लो मॉडल बायोफिल्म मॉडल और रिएक्टर मॉडल को जोड़ता है। रिएक्टर फ्लो मॉडल बताता है कि प्रत्येक कम्पार्टमेंट (सीएमबीआर) कैसे जुड़ा हुआ है। संपूर्ण रिएक्टर बनाने के लिए सभी डिब्बों को जोड़कर प्रवाह मॉडल प्राप्त किया जाता है। माना जाता है कि सीएमबीआर एक एमटीएफ में श्रृंखला में जुड़े हुए हैं।

बायोफिल्म कैनेटीक्स के लिए दर कानून के भाव विकसित किए गए थे। इस प्रक्रिया में बायोफिल्म मॉडल को डायमेंशनलेस डोमेन में बदलना शामिल है। फिर सूत्रीकरण, दर कानून अभिव्यक्ति आयाम रहित प्रवाह के संदर्भ में, जो 'बायोफिल्म नंबर' (बी) नामक एक आयाम रहित संख्या और बायोफिल्म काइनेटिक फंक्शन $\Psi(S^*)$ नामक एक आयाम रहित बीजगणितीय फंक्शन पर निर्भर करता है। बायोफिल्म संख्या के वर्ग के बराबर, अधिकतम प्रवाह की अवधारणा विकसित की गई है। बायोफिल्म काइनेटिक फंक्शन का उपयोग करके बायोफिल्म का प्रभावशीलता कारक तैयार किया गया है।

एमटीएफ का गणितीय मॉडल निष्कर्षों (शुक्ला, 2021) से प्रायोगिक डेटा का उपयोग करके सिद्ध किया गया है। हेटरोट्रॉफ्स और नाइट्रिफ़र्स का स्थानिक वितरण रूपांतरण में महत्वपूर्ण भूमिका

निभाता है। एक ही बायोफ़िल्म के भीतर हेटरोट्रॉफ़्स और नाइट्रिफ़ायर्स का सह-अस्तित्व दो परिकल्पनाओं के अनुसार तैयार किया गया है: बाइलेयर बायोफ़िल्म और होमोजेनस बायोफ़िल्म। मॉडल सिमुलेशन की भविष्यवाणियों में पाया गया कि बाइलेयर बायोफ़िल्म मॉडल प्रायोगिक डेटा के लिए आशाजनक है। प्रत्येक प्रजाति के विकास कैनेटीक्स बहु-प्रजाति बायोफ़िल्म में प्रजातियों की संरचना और स्थानिक वितरण को दृढ़ता से प्रभावित करते हैं।

CONTENTS

Certificate.....	i
Acknowledgments.....	ii
Abstract.....	iii
संर.....	vi
Contents.....	ix
List of Figures.....	xi
List of Tables.....	xiii
Nomenclature.....	xiv
Chapter -1 Introduction.....	19
1.1. Introduction.....	20
Chapter-2 Literature Review.....	24
2.1 Background.....	25
2.2 Overview of the Biofilm Models.....	28
2.3 Reactor Model.....	37
2.4 Types of Biofilm Reactors.....	39
2.5 Microbial processes in the biofilm.....	43
2.6 The Criterion of selecting the Biofilm Model.....	45
2.6.1 Characteristic time.....	45
Chapter-3 Research Gaps and Objectives.....	51
3.1 Research Gaps and motivations.....	52
3.2 Objectives.....	53
Chapter-4 Materials and Methods.....	54
4.1 Description and Operation of the Modified Trickle Filter (MTF).....	55
4.2 Simulations and Data Analysis.....	56
4.2.1 Data analysis.....	57
4.3 Procedures for estimating COD, Ammoniacal Nitrogen and Nitrate Nitrogen.....	57

Chapter-5 Results and discussion.....	60
5.1 Model Development.....	61
5.2 Biofilm Model.....	64
5.3 Solution of the Biofilm Model.....	71
5.4 Development of Rate Law expressions for Biofilm Kinetics	73
5.5 Significance of the biofilm number, B	77
5.6 Effectiveness factor of the Biofilm, η	79
5.7 Multispecies Biofilm Model.....	82
5.7.1 Bilayer Biofilm.....	83
5.7.2 Homogenous Biofilm.....	86
5.8 Denitrification Biofilm Model.....	88
5.9 Model for porous media.....	88
5.10 Reactor Model: Completely Mixed Biofilm Reactor.....	90
5.11 Reactor Flow Model: CMBRs in Series.....	91
5.11.1 Reactor Model: Calculation of HRT.....	92
5.11.2 Recycle reactor model.....	92
5.12 Solution Procedure.....	98
5.13 Experimental Validation of the Model.....	100
Chapter-6 Summary and Conclusions.....	109
References.....	115
Appendix I.....	126
Appendix II.....	137
Author's Resume.....	139

List of Figures

Figure No.	Title	Page No.
Fig. 2.1	Characteristic times of various processes occurring in a biofilm system.	47
Fig. 4.1	Diagram of Process Description of the Modified Trickling Filter (MTF).	54
Fig. 5.1	Schematic Diagram of the Modified Trickling Filter with processes taking place in the aerobic and anoxic zones.	59
Fig. 5.2	(a) Biofilm model. (b) mass balance on a volume element of biofilm of thickness Δx with surface area A .	64
Fig. 5.3	Flowchart for the solution procedure of the biofilm model.	68
Fig. 5.4	The solution of biofilm models for various Biofilm Numbers. The effect of Biofilm Number ($B=0.2, 1, 2, 5, 10, 15, 20$) for various S^* ($=0.2, 1, 2, 5, 10, 20, 50, 80, 100$) is depicted in various graphs.	70
Fig. 5.5	Flowchart for developing rate law expressions for the biofilm kinetics.	71
Fig. 5.6	The curve shows the effect of S^* on the Biofilm Kinetic Function $\Psi(S^*)$ for various values of Biofilm Number(B).	73
Fig. 5.7	The relationship between the J_F^* at $S^*=1$ and the Biofilm Number	77
Fig. 5.8	The variation of effectiveness factors for the substrate concentrations at various biofilm numbers B .	78
Fig. 5.9	(a) Bilayer Biofilm model(Blue= Heterotrophs, Green = Nitrifiers). (b) Boundary conditions for the bilayer model for Heterotrophs and Nitrifiers.	81
Fig. 5.10	(a) Homogenous Biofilm model(Blue= Heterotrophs, Green = Nitrifiers). (b) Boundary conditions for the bilayer model for Heterotrophs and Nitrifiers	84
Fig. 5.11	Model of a typical (Completely Mixed Biofilm Reactor) CMBR	88
Fig. 5.12	A model for a typical Trickling filter is a plug flow reactor.	89
Fig. 5.13	Mass Balance over differential volume element ΔV over the reactor height.	90
Fig. 5.14	A Plug Flow reactor with Recycle	93
Fig. 5.15	Modified Levenspiel Plot for Recycle System	94
Fig. 5.16	Algorithm for the Modeling of MTF.	96
Fig. 5.17	Simplified Algorithm for the Modeling of MTF.	97

Fig. 5.18	SEM Images of the Polyurethane Sponge showing the immobilization of Biomass within the pore network.(Image Source: Shukla, 2021. IIT Delhi. Ph.D Thesis[1])	102
Fig. 5.19	Parity Charts for the theoretical and Experimental removal efficiencies of Various Contaminants (X-axis: % Experimental Removal Efficiencies, Y-Axis: Theoretical Removal Efficiencies) Parity Charts for the theoretical and Experimental removal efficiencies of Various Contaminants (X-axis: % Experimental Removal Efficiencies, Y-Axis: Theoretical Removal Efficiencies)	104

List of Tables

Table No.	Title	Page No.
Table 2.1	Features of various biofilm models[2]	29
Table 2.2	Characteristic times for relevant processes in a biofilm[3][4][5][6][2] .	46
Table 5.1	The function $\Psi(S^*)$ is given by the following correlations.	74
Table 5.2	Stoichiometric Table for the microbial processes	85
Table 5.3	Biofilm Parameters used to calculate Biofilm Numbers for Heterotrophs, Nitrifiers, and Denitrifiers [7]	100
Table 5.4	Biofilm Numbers for Heterotrophs and Nitrifiers.	100
Table 5.5	Reactor Configurations [1].	101
Table 5.6	Comparison of Theoretical and Experimental removal efficiencies for the Modified Trickling Filter	103
Table 5.7	Criteria for judging a Model Prediction	104
Table 5.8	Index of agreement of goodness and Relative Error for Model Predictions and Experimental Data	105

Nomenclature

L_F	Biofilm Thickness, cm
L_H	Heterotrophic Layer thickness within the Biofilm, cm
L_N	Nitrifying Layer thickness within the Biofilm, cm
f_H	Volumetric fraction of Heterotrophs within the Biofilm
f	Volumetric fraction of Nitrifiers within the Biofilm
S_F	Substrate Concentration, mg cm^{-3}
$S_{F, \text{surf}}$	Substrate Concentration on the biofilm Surface, mg cm^{-3}
$S_{F, \text{wall}}$	Substrate Concentration at the substratum, mg cm^{-3}
S_{in}	Inlet COD concentration, mg cm^{-3}
$K_{S,H}$	Monod half-saturation constant for heterotrophs, mg cm^{-3}
$K_{S,N}$	Monod half-saturation constant for Nitrifiers, mg cm^{-3}
S_H^*	Dimensionless Substrate Concentration for heterotrophic COD
S_N^*	Dimensionless Substrate Concentration for Ammonia Substrate
S_{NO_3}	Dimensionless Substrate Concentration for Nitrate Substrate
S_{Surf}^*	Dimensionless Substrate Concentration at Biofilm surface
S_{in}	Inlet Substrate Concentration in Trickling Filter, mg cm^{-3}
$\Psi(S^*)$	Biofilm Kinetic function, dimensionless
μ_{max}	Specific growth rate (day^{-1})

X_F	Biomass Density within the biofilm, mg cm^{-1}
Y	True Yield of milligrams of biomass produced per milligrams of substrate utilized
B_H	Biofilm Number of Heterotrophs, dimensionless
B_N	Biofilm Number of Nitrifiers, dimensionless
B_{NO_3}	Biofilm Number of Denitrifiers, dimensionless
D_H	Diffusivity of the Heterotrophic substrate into biofilm, $\text{cm}^2 \text{day}^{-1}$
D_N	Diffusivity of the Ammonia substrate into biofilm, $\text{cm}^2 \text{day}^{-1}$
D_{NO_3}	Diffusivity of the Nitrate substrate into biofilm, $\text{cm}^2 \text{day}^{-1}$
x	distance normal to the biofilm surface or biofilm depth, cm
x^*	dimensionless distance normal to the biofilm surface or biofilm depth, dimensionless
$J_{F,H}$	Flux of COD substrate entering the biofilm, $\text{mg cm}^{-2} \text{day}^{-1}$
$J_{F,N}$	Flux of Ammonia substrate entering the biofilm, $\text{mg cm}^{-2} \text{day}^{-1}$
J_{F,NO_3}	Flux of Nitrate substrate entering the biofilm, $\text{mg cm}^{-2} \text{day}^{-1}$
$J_{F,H}^*$	Dimensionless COD Substrate mass flux
$J_{F,N}^*$	Dimensionless Ammonia Substrate mass flux
J_{F,NO_3}^*	Dimensionless Nitrate Substrate mass flux
θ	HRT, Hydraulic Retention Time, Hour or day
α	Group Constant
a	Specific surface area of the media, cm^{-1}

E	Porosity of the Polyurethane Sponge
τ	Tortuosity of the Polyurethane sponge
Φ	Void fraction of the Trickling Filter
X	Conversion
d	Willmot's Index of agreement
RE	Relative Error
RR	Recycle Ratio
R^2	Correlation Coefficient
R	Pearson's correlation coefficient