Bioreactor Treatment Tool
Literature Review and Data Set Specification

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Study Context

Two-stage bioreactor filtration technology is uniquely suitable for nitrogen removal in local small scale wastewater treatment systems. Initial field evaluation of bioreactor designs demonstrated 97% total nitrogen removal from onsite wastewater (Smith, 2009a). Ongoing pilot testing is confirming initial performance results and expanding knowledge of the nitrogen removal capabilities of bioreactor filters for onsite treatment (Smith, 2009b). The goal of this study is to develop a bioreactor treatment tool for onsite nitrogen removal design that is straightforward to apply but which is based on model simulations of fundamental physical, chemical, and biochemical processes occurring within the treatment bioreactors.

Bioreactor filters flow wastewater though porous media, and nitrogen removal within the bioreactor is inherently complex. System design must facilitate a successful assemblage of multiple interacting processes (Figure 1). The bioreactors that have successfully removed nitrogen have to this point been designed based on critical analysis of state of the art knowledge and the application of scientific and engineering judgment (Smith, 2008). While these treatment systems have performed very effectively, their fundamental treatment processes are not fully understood and their designs have not been fully optimized. Knowledge gaps have been identified with important performance and economic implications (Smith et al., 2008).

A standard tool for systematizing the design and evaluation of engineered systems is quantitative simulation (modeling), in which mathematical equations are used to represent physical, chemical and biochemical processes. Modeling will predict the effluent nitrogen concentration from highly complex nitrogen removal bioreactors when the model is supplied values for inputs such as bioreactor filtration rate, media depth and influent nitrogen concentration. Modeling of nitrogen removal bioreactors provides the critical link between performance assessment and design analysis. The key factor for developing predictive design capabilities that can be used with confidence is a modeling approach that explicitly describes the functional dynamics of microbially mediated biochemical reactions. Model simulations can be used to more fully elucidate the hydraulic and nitrogen loadings which can be effectively treated by onsite bioreactor filters. Standardized bioreactor design platforms can be developed that reduce the economic and performance uncertainties of these engineered systems.

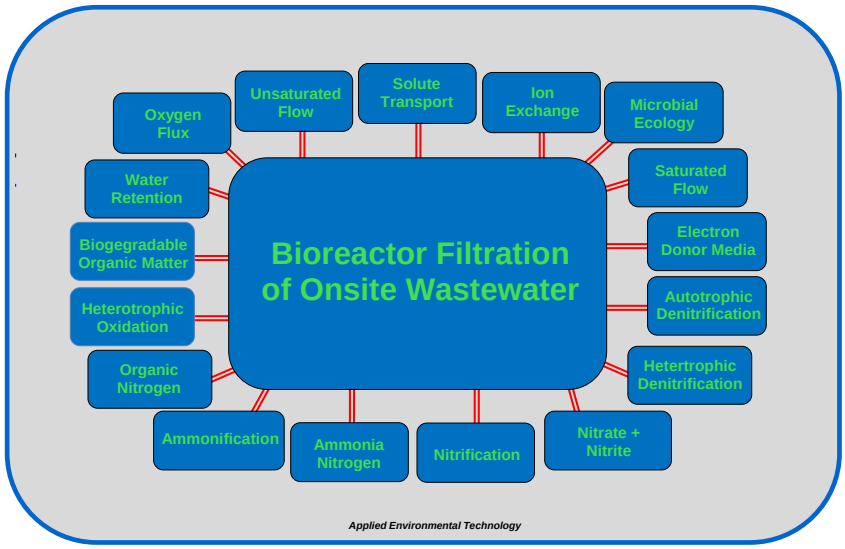

Figure 1. Bioreactor Filtration Treatment of Onsite Wastewater

Objectives

The project will implement a spreadsheet based Bioreactor Treatment Tool (BTT) for design of two-stage bioreactor filter systems for onsite wastewater nitrogen removal systems. Stage 1 is an unsaturated porous media bioreactor that supports microbial nitrification under aerobic conditions, while Stage 2 is a saturated porous media bioreactor that is supplied with electron donor to support microbial denitrification. Applying the Bioreactor Treatment Tool will be relatively straightforward, with limited inputs for wastewater fow and quality characterisitics and bioreactor filter design. The Bioreactor Treatment Tool predicts effluent nitrogen concentrations and removal efficiencies. The Bioreactor Treatment Tool will be based on more complex model simulations of Stage 1 (unsaturated) and Stage 2 (saturated) bioreactors that include saturated and unsaturated water flow, solute transport, and microbially mediated biochemical reactions including heterotrohic oxidation, ammonification, nitrification and heterotrophic and autotrophic denitrification (Figure 1). The results of complex model simulations will be the basis for the spreadsheet based Bioreactor Treatment Tool.

The objectives of Task 1 are:

- Describe Bioreactor Treatment Tool development
- Identify data sets for calibrating treatment process models which are the basis for Bioreactor Treatment Tool algorithms
- Select process simulation model(s) that predict nitrogen removal performance of saturated and unsaturated bioreactors

Development of Bioreactor Treatment Tool

The Bioreactor Treatment Tool (BTT) will be structured as a spreadsheet based module into which are entered basic inputs and which outputs bioreactor designs and effluent nitrogen. BTT inputs are influent wastewater characteristics, Stage 1 design parameters, and Stage 2 design

parameters. BTT outputs are the bioreactor sizings, effluent nitrogen concentrations and nitrogen removal efficiency. The Bioreactor Treatment Tool will enter influent wastewater parameters (i.e. primary effluent) as average values. The BTT will include performance algorithms that are conservatively derived from complex model simulations and that account for imput parameter variabilities. BTT inputs are:

- Primary effluent (input to the two-stage bioreactor system)
  - Flowrate
  - Carbonaceous biochemical oxygen demand, five day
  - Total kjeldahl nitrogen
- Stage 1 bioreactor (unsaturated, nitrification)
  - Media type: expanded clay, clinoptilolite, sand
  - Total media depth (six to 30 inch)
  - Surface loading rate (gallons per square feet per day)
  - Dose cycle time (0.5 to 6 hour)
- Stage 2 bioreactor (saturated, denitrification)
  - Electron donor media: lignocellulosic material, elemental sulfur
  - Total media depth (12 to 144 inch)
  - Media composition, Percent of electron donor in media in bioreactor: 20 to 80 based on experiemntal testing in PNRS 1 and PNRS 2
  - Surface loading rate (gallons per square feet per day)
  - Dose cycle time (0.5 to 6 hour)

The Bioreactor Treatment Tool will calculate Stage 1 effuent nitrogen concentrations of organic, ammonium, and NO_x nitrogen. BTT will internally specify Stage 1 effluent nitrogen concentrations as influent values to the Stage 2 bioreactor; external specification will not be required. The Bioreactor Treatment Tool will have an input interface with default values that enble the user to independently change any input value. .

The Bioreactor Treatment Tool contains algorithms that convert the bioreactor input data to effluent concentrations for each stage. The Bioreactor Treatment Tool calculates the Stage 1 effluent nitrogen from the Stage 1 influent data, provides Stage 1 effluent nitrogen as the influent to Stage 2, and calculated Stage 2 effluent nitrogen based on the input data to Stage 2. Effluent from the Stage 2 bioreactor is the final effluent from the two-stage bioreactor system. The Bioreactor Treatment Tool then calculates nitrogen removal efficiency and other treatment results based on the influent data and Stage 2 effluent outputs. The output of the Bioreactor Treatment Tool are the bioreactor design sizes, final effluent nitrogen concentrations, removal efficiencies, and mass loadings:

- Organic nitrogen
- Ammonia nitrogen
- Oxidized nitrogen (nitrate+nitrite)
- Total nitrogen
- Total kjeldahl nitrogen
- Nitrogen removal efficiency

- Nitrogen mass loading rate

The output interface of the Bioreactor Treatment Tool will display all BTT output results including average effluent nitrogen concentrations and average nitrogen removal efficiency for the entered flowrate, influent nitrogen concentrations, and bioreactor design.

The Bioreactor Treatment Tool is based on calibrations of complex biological treatment simulation models of Stage 1 (unsaturated) and Stage 2 (saturated) bioreactors. The calibrated simulation models generate the core algorithms in the Bioreactor Treatment Tool that predict effluent nitrogen. The following describes the implemention structure and progression from the complex process simulation modeling to the Bioreactor Treatment Tool.

The unsaturated and saturated bioreactor models will be calibrated using data identified in the following section. The unsaturated and saturated models will be operated in a one dimensional mode. Prior to performing calibrations, it will be verified that the simulation codes are being accurately executed by comparing simulation results for pseudo flowrate and influent concentration cases with analytical solutions or hand calculations. The unsaturated bioreactor model will be calibrated first for effluent flowrate for repeating doses at the cycle intervals, using effluent flowrate data sets and the applied dose flows (volumes). Saturated hydraulic conductivity and water retention parameters will be used as calibration parameters, and an these will be correlated with the physcial characteristics of the selected bioreactor filter media. The flow calibration will be followed by calibration for organics and nitrogen reductions using measured datasets for influent and effluent concentrations of biochemical oxygen demand and nitrogen (organic, ammonia and oxidized nitrogen. The specific substrate utilization rates from organics and nitrification systems and possibly other biokinetic parameters will be used as calibration fitting parameters.

The saturated bioreactor model will be calibrated mainly for oxidized nitrogen (i.e. NO_x, nitrate + nitrite). For the saturated bioreactors, specific substrate utilization rates will likely be significant fitting parameters for saturated bioreactor calibrations, and will be parameterized as areal biochemical rates with a dependency on electron acceptor concentrations (i.e. O_2 and NO_x). An attempt will be made to relate parameters to media characteristics, such as specific surface area, grain size, or porosity. Model calibration will evaluate goodness of fit using regressions of paired experimental and simulation data (sum of square residuals) or other techniques. Single parameter sensitivity analyses will be performed on calibration parameters using base calibrations.

The calibrated unsaturated bioreactor process model and the calibrated saturated bioreactor process model will each be used (separately) to generate predictive results which span a matrix of the treatment application range of interest. The matrix of simulation results bioreactor will be compiled and regression equations will be derived for three forms of nitrogen: organic nitrogen, ammonia nitrogen, and oxidized nitrogen. For the unsaturated bioreactor, nine regressions will be produced for three media (expanded clay, clinoptilolite, and sand) and three nitrogen forms (i.e. 3x3). The anticipated form of the unsaturated bioreactor correlations for each media are:

Organic N = function (Total media depth, Surface loading rate,
Dose cycle time, Influent TKN)

Ammonia N = function (Total media depth, Surface loading rate, Dose cycle time, Influent TKN)

Oxidized N = function (Total media depth, Surface loading rate, Dose cycle time, Influent TKN

For the saturated bioreactor, six regressions will be produced, for two media (lignocellulosic material, elemental sulfur) and three nitrogen forms (2x3). The anticipated form of the unsaturated bioreactor correlations for each electron donor media are:

Organic N = function (Total media depth, Percent electron donor media, Surface loading rate, Dose cycle time, Influent Organic N)

Ammonia N = function (Total media depth, Percent electron donor media, Surface loading rate, Dose cycle time, Influent Organic N, Influent ammonia)

Oxidized N = function (Total media depth, Percent electron donor media Surface loading rate, Dose cycle time, Influent NO_x)

Regession will be based on non-linear least squares techniques such as Marquardt-Levenberg algorithm. Inspection of the complex simulation results may indicate phenomena, such as threshhold values, that will limit the regession to subsets of the simulation results. The regression results will be interpreted conservatively (i.e. err on the side of higher effluent nitrogen concentrations); depending on regression results, 90% upper confidence levels or other conservative performance estimates fmay be used. The conservatively derived results will be incorporated into algorithms within the Bioreactor Treatment Tool that calculate total effluent nitrogen (Total N = organic N + ammonia-N = oxidized N), nitrogen removal efficiencies for the two-stage bioreactor system, and other process parameters.

Data Set Specification

A review was conducted to identify data sets for process model simulations. The scope of review was initial and ongoing passive nitrogen removal studies (PNRS 1 and PNRS 2), studies cited in the literature review (Smith et al., 2008), and any other available data. It was determined that the PNRS 1 and PNRS 2 field demonstration projects have produced the most useful data sets for development of the Bioreactor Treatment Tool. Other studies do not provide bioreactor design, operation and treatment results in a full and consistent manner that is needed for model calibration objectives. The chosen calibration data are listed in Table 1 and consist entirely of data from PNRS 1 and PNRS 2. The Table 1 data encompass detailed treatment performance measurements from numerous well-characterized bioreactor filters, for both unsaturated and saturated media, and for a variety of media types, media depths and layers, media percentages, and surface loading rates. The data sets represent an excellent data compilation for the development and truth testing of the Bioreactor Treatment Tool.

Table 1. Data Sets

Water Saturation	Biofilter	Project	Media	Media Depth, inch	Media Size Layers	Surface Loading Rate, gal/ft^2-day	Number of Data Sets
Unsaturated	1A	PNRS 1	Clinoptilolite	24	3	3	10
Unsaturated	1B	PNRS 1	Expanded Clay	24	3	3	8
Unsaturated	UNSAT-EC1	PNRS 2	Expanded Clay	15	2	3	6
Unsaturated	UNSAT-EC3	PNRS 2	Expanded Clay	30	2	3	6
Unsaturated	UNSAT-CL1	PNRS 2	Clinoptilolite	15	2	3	6
Unsaturated	UNSAT-CL3	PNRS 2	Clinoptilolite	30	2	3	6
Unsaturated	UNSAT-SA2	PNRS 2	Sand	30	2	3	6
Unsaturated	UNSAT-EC4	PNRS 2	Expanded Clay	30	2	3	6
Unsaturated	UNSAT-CL2	PNRS 2	Clinoptilolite	15	2	3	6
Unsaturated	UNSAT-CL4	PNRS 2	Clinoptilolite	30	2	3	6
Saturated	2A	PNRS 1	Elemental Sulfur (75%)	24	1	12	10
Saturated	2B	PNRS 1	Elemental Sulfur (60%)	24	1	12	10
Saturated	2C	PNRS 1	Elemental Sulfur (45%)	24	1	12	10
Saturated	DENIT-SU4	PNRS 2	Elemental Sulfur (30%)	24	1	5.6	6
Saturated	DENIT-LS3	PNRS 2	Southern Yellow Pine (50%)	24	1	5.6	6
Saturated	DENIT-SU2	PNRS 2	Elemental Sulfur (80%)	24	1	5.6	6
Saturated	DENIT-LS2	PNRS 2	Southern Yellow Pine (25%)	24	1	5.6	6
Saturated	DENIT-LS4	PNRS 2	Southern Yellow Pine (30%)	24	1	5.6	6
Saturated	DENIT-GL1	PNRS 2	Expanded Clay (100%), Glycerol	72	1	10	6
Saturated	DENIT-LS1	PNRS 2	Southern Yellow Pine (50%)	72	1	10	6
Saturated	DENIT-SU2	PNRS 2	Elemental Sulfur (30%)	72	1	10	6
Saturated	DENIT-SU1	PNRS 2	Elemental Sulfur (80%)	72	1	10	6

Model Selection

A review was conducted to identify and select model codes for simulation of Stage 1 (unsaturated) and Stage 2 (saturated) bioreactor filters. Multi-component reactive transport codes are needed to simulate bioreactor filter preformance. Information on model codes was procured from a wide variety of sources, including peer reviewed articles, conference proceedings, websites, and project reports. Numerous codes were reviewed. Many were not considered for a variety of reasons including their development for only narrow situations, inability to customize, simulation of only steady state flow, and highly simplified kinetics. Other model considerations are its stucture and suitability for describing the significant physcial, chemical, and biological processes occurring in the bioreactor filters; the availability of the code for use, model documentation describing its technical basis, input, and output platforms, and previous model applications.

The model features required for bioreactor filter simulations include:

- Biochemical reactions for organic matter and for individual nitrogen species, which are absolutely required for meaningful simulations of bioreactors
- Dependent variable microbial population for organic matter and for individual nitrogen species, which are required for meaningful simulations of bioreactors
- Non-steady unsaturated flow, which is required for intermittently loaded Stage 1 bioreactors
- Ability to simulate multiple layers of filter media, which is the basis of Stage 1 bioreactor media designs
- Saturated flow and reactive solute transport for Stage 2 bioreactors
- Ability to incorporate electron donors in Stage 2 as solid phase (elemental sulfur, lignocellulosic material)

Numerous model codes were eliminated because they did not consider one or more of the required model features listed above or their inadaptability to specific needs of the project. Selected candidate model codes for use are listed in Table 2. All but one of the Table 2 codes incorporate a representation of unsaturated flow with solute degradation. Friere et al., 2010 uses CSTRs in series for flow representation but is inappropriate due to its single component degradation. McGechan et al., 2005 and Giraldi et al., 2010 employ multiple bioreactions but use a multiple horizontal layer approach for flow simulation, in which the horizontal layers are hydraulic simulation layers not consistent with the media characteristics of the bioreactor filters. Four model codes use the Richards Equation for transient water flow in variably saturated media and convective-dispersive solute transport in the mobile compartment of the liquid phase. Wanko et al., 2006 does not include nitrogen reactions. The Ojeda et al., 2008 model appears to have potential but is neither genrally available nor documented. The CWM1 model (Langergraber, 2009) and CW2D (Langergraber and Simunek, 2005) are the only identified model codes that are publicly available, well documented, and that are capable of simulating biochemical transformations of both organic matter and individual nitrogen species. The newer CWM1 includes anoxic denitrification, anaerobic reactions of fermentation, and sulfides. This analysis suggests that CWM1 is the most appropriate model code for meeting the objectives of the Bioreactor Treatment Tool and is the code selected for unsaturated bioreactor simulations (Stage

1). CWM1 may also be operated in a saturated mode in which case it could provide a platform for simulations of saturated bioreactors (Stage 2). The ability of CWM1 to simulate multiple bioreactions with solid phase electron donors is currently under evaluation and the incorporation of solid phase electron donors into the CWM1 code is under discussion with the developer. An alternative option for saturated bioreactor modeling is the Denitrification Bioreactor Filter Model (DBFM), which is a reactive transport model that was specifically developed by AET to simulate saturated flow denitrification bioreactors that contain solid phase electron donor. To the author's knowledge, DBFM is the only code that has developed to perform such simulations. DBFM model results were included in a presentation of PNRS 1 results that was made at the Water Environment Federation Technical Exhibition and Conference (Smith, 2009c). DBFM is the model code selected for saturated bioreactor simulations (Stage 2), pending possible developments with the CWM1 code. Use of DBFM or a modification of CWM1 would entail initial testing to assure that the code is being properly executed and is representing the salient processes, and standard calibration and verification practices.

Table 2 Model Codes

Source	Water Status	Water Transport	Structure and Biochemical Reactions
Friere at al, 2010	Saturated/ unsaturated	CSTR is series, dead zones	Degradation of only single component
McGechan et al, 2005	Saturated/ unsaturated	Multiple horizontal layers for flow simulation	Organic matter pools, ammonium, nitrate and oxygen, microbial reactions
Giraldi at al., 2010	Saturated/ unsaturated	Multiple horizontal layers for flow simulation	FITOVERT: carbon and nitrogen microbial reactions in matrix notation
CWM1, Langergaber, 2009	Saturated/ unsaturated	Advection/ Dispersion, Richards equation	Matrix format aerobic and anaerobic reactions, biochemical reactions for organic matter, nitrogen species, and anerobic reactions
CW2D, Langergaber, 2001, Langergaber and Simunek, 2005	Saturated/ unsaturated	Advection/ Dispersion, Richards equation	Matrix format aerobic reactions, biochemical reactions for heterotrophic organic matter utilization, ammonium and nitrite oxidation
Wanko et al., 2006	Saturated/ unsaturated	Advection/ Dispersion, Richards equation	Organic matter and oxygen transport in vertical flow filters
Ojeda et al., 2008	Saturated/ unsaturated	Advection/ Dispersion, Richards equation	Simplified description of reactions for organic matter, nitrogen and sulfur, RCB flow model
DBFM, Smith, 2009c	Saturated	Advection	Oxygen utilization, denitrification with solid phase electron donor

Summary

The project will develop a spreadsheet based Bioreactor Treatment Tool for process design of onsite nitrogen removal bioreactors. The Bioreactor Treatment Tool will be based on complex model simulations of biochemical nitrogen transformations and physical and chemical processes. The approach to Bioreactor Treatment Tool development was presented, and simulation models and calibration data sets were identified. The CWM1 model was chosen for simulation because of its ability to model biochemical transformations in bioreactors with variably saturated porous media. and a modified CWM1 model or DBFM were selected for simulation of saturated bioreactors containing solid phase electron donor.

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