MODELING, STATISTICAL ANALYSES, AND LIFE CYCLE ASSESSMENT OF ANAEROBIC BIOREACTORS FOR THE TREATMENT OF ORGANIC WASTES AND RESOURCE RECOVERY

by

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ABSTRACT

Increased application of anaerobic bioreactors can accelerate the transformation of wastewater treatment to energy-efficient resource recovery. These technologies are viable alternatives to traditional aerobic wastewater treatment practices due to their ability to generate methane-rich biogas from the microbial decomposition of organic matter within waste without the need for costly aeration. The biogas can be captured and used in heating or electricity production, potentially eliminating the need for consumption of external fossil fuel-based electricity or natural gas. Barriers to implementation of anaerobic treatment methods may include costs associated with upgrading existing facilities, lack of knowledge of how the treatment processes work or not knowing how adoption may benefit a particular facility. To overcome these barriers and bring anaerobic bioreactors into mainstream use, decision support tools are needed. Computer models and simulations, including life-cycle analysis for environmental impacts, can generate predictions regarding treatment abilities, methane production, carbon dioxide emissions, and costs. These predictions can be used by decision makers to help determine if implementation of anaerobic bioreactors is the best decision for them.

To address these research needs, this dissertation creates decision support tools through multiple modeling methods of anaerobic bioreactors, including computer simulation, statistical analyses, waste characterization, and life cycle assessment. The bioreactors examined during the research included three pilot-scale anaerobic baffled reactors (ABRs) treating wastewater in Colorado and full-scale anaerobic co-digestion at a water resource recovery facility in New York. Outcomes of the study of the ABRs include successful modeling of constituent removal and methane generation within 9% through identification and modification of key default parameters within a commonly used wastewater treatment computer simulation program. Additionally, statistical analysis of the wastewater characteristics and performance of the three ABRs identified distinct differences between the systems, but also average constituent removal efficiencies, effluent concentrations, and methane generation. These results can be used to assist with the design and operation of future pilot- or full-scale ABRs operating in colder climates. Finally, three waste streams (wastewater sludge, food, and fats, oils, and grease wastes) were characterized and used to develop a stoichiometric model for methane generation, energy production, and environmental impacts associated with anaerobic co-digestion, with adjustable parameters for use in future research.

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LIST OF ABBREVIATIONS

Activated sludge model	ASM
Anaerobic baffled bioreactors	ABR
Anaerobic co-digestion	AnCoD
Anaerobic digestion model	ADM
Anaerobic digestion.	AnD
Analysis of variance	ANOVA
Atmospheres	atm
Biochemical oxygen demand (5-day)	BOD (BOD_5)
British Thermal Unit	BTU
Carbon dioxide	CO_2
Celsius	°C
Centrum voor Milieukunde Leiden (Institute of Environmental Sciences Leiden)	CML
Chemical oxygen demand	COD
Combined heat and power	CHP
Cubic meter	m^3
Day	d
Department of Defense	DoD
Dissolved organic carbon	DOC
Engineering Research Center for Reinventing the Nation's Urban Water Infrastructure	ReNUWIt
Environmental Security Technology Certification Program	ESTCP
Expanded granular sludge blanket	EGSB
Fats, oils, and grease	FOG
Gallons per day, million gallons per day	gpd/MGD
Gas chromatography – mass spectrometry	GC-MS
Global warming potential	GWP
Greenhouse gas	GHG
Hydraulic residence time	HRT
Hour	h
Inorganic, non-volatile, or fixed solids	IS
International Organization for Standardization	ISO
Ion chromatography	IC

Iron . . . . Fe

Joule, Megajoule . . . . J, MJ

Kilowatt, Megawatt . . . . kW, MW

LCA for Experts (software) . . . . LCAFE

Life cycle assessment . . . . LCA

Life cycle costing LCC

Life cycle impact assessment . . . . LCIA

Life cycle inventory LCI

Liter L

Methane . . . . CH_4

Milligram, Gram, Kilogram . . . . mg, g, kg

Mines Park . . . . MP

National Science Foundation . . . . NSF

Ordinary heterotrophic organisms . . . . OHO

Particulate COD . . . . pCOD

Plum Creek . . . . PC

Readily biodegradable COD . . . . rbCOD

Solids residence time . . . . SRT

Soluble COD . . . . sCOD

South Platte . . . . SP

Sulfate . . . . SO_4^{2-}

Target Hill . . . . TH

Techno-economic assessment . . . . TEA

Tool for Reduction and Assessment of Chemicals and other Environmental Impacts . . . TRACI

Total COD . . . . tCOD

Total solids . . . . TS

Total suspended solids . . . . TSS

Upflow anaerobic sludge blanket . . . . UASB

U.S. Environmental Protection Agency . . . . EPA

Volatile fatty acids . . . . VFA

Volatile solids . . . . VS

Volatile suspended solids . . . . VSS

Water resource recovery facility . . . . WRRF

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CHAPTER 1
INTRODUCTION

Over the past decade, there has been a significant shift in how wastewater is treated. It used to be seen as a simple process of removing contaminants and releasing treated water into the environment. However, wastewater is now recognized to contain valuable resources that can be recovered. This transformation encourages the reuse of treated wastewater, which helps protect our freshwater supplies. Moreover, it allows recovery of energy, nutrients, and biosolids, leading to both environmental and financial benefits in wastewater treatment [1, 2]. Anaerobic treatment processes allow for the microbial degradation of organic matter to methane-rich biogas, which can be used as a renewable energy source when coupled with heat and power recovery technologies. Additionally, the nutrients found in wastewater can be extracted and sold as fertilizers to farmers and the agriculture industry, thereby enhancing crop productivity. Furthermore, the biosolids can be utilized for land application to promote composting, growth, and restoration of disturbed lands [1]. Studies and modeling of anaerobic bioreactors, co-digestion (the simultaneous anaerobic digestion of multiple organic wastes), and factors affecting biogas production can provide insight into the design and operation of anaerobic processes for wastewater and solids treatment.

1.1 Research Background

1.1.1 Anaerobic Digesters and Bioreactors

For domestic wastewater treatment, conventional aerobic treatment uses activated sludge systems where oxygen is provided to support the biological treatment by microorganisms. The aeration requirements can account for 35-75% of a wastewater treatment plant's energy consumption, depending on size of the aeration tanks, solids retention times, and facility elevation [1]. Traditional primary and secondary treatment methods generate biosolids, which require thickening, dewatering, stabilization, and disposal at additional costs to the treatment facility. Anaerobic digestion is a commonly used approach for stabilizing primary wastewater sludge and waste sludge generated from conventional activated treatment processes [2, 3].

Research showed that anaerobic processes could be used to treat raw domestic wastewater, not just sludge produced from aerobic systems [4, 5]. Bioreactors that employ anaerobic microbiota to treat raw domestic wastewater represent a potential energy-positive alternative to traditional aerobic wastewater treatment due to the use of passive anaerobic sludge blanket bioreactors without the costly aeration requirements. This treatment method has low complexity and also reduces the amount of biosolids generated while simultaneously generating methane-rich biogas [6–8]. In anaerobic sludge blanket bioreactors, wastewater flows upward from the bottom of the bioreactor through a dense sludge layer with high microbial activity. As wastewater passes through the sludge, anaerobic microorganisms degrade complex wastewater organics to simple compounds (e.g., monomers or volatile fatty acids) and then to methane and carbon dioxide. The methane produced can be captured and converted to heat and/or electrical energy with use of reuse technologies [9].

Currently, full-scale anaerobic sludge blanket bioreactors are primarily implemented in tropical climates, such as in areas of South America and Asia [8, 10, 11]. However, the development of viable low-temperature anaerobic sludge blanket bioreactors that meet the effluent goals for wastewater treatment is an area of on-going research [6, 8, 12, 13]. The most commonly studied anaerobic sludge blanket bioreactors include the upflow anaerobic sludge blanket (UASB), the anaerobic baffled reactor (ABR), and the expanded granular sludge blanket (EGSB) bioreactor [11]. Of these systems, ABRs have a simple design, low capital and operating costs and provide better retention of solids in response to load variations than single compartment UASB or EGSB reactors [11, 14].

1.1.2 Co-Digestion

Anaerobic bioreactors are not limited to the treatment of raw domestic wastewater. Anaerobic digestion of sludge has been employed in some water resource recovery facilities (WRRF; formerly known as wastewater treatment facilities) for over a century. Anaerobic digestion of primary sludge and waste activated sludge is well-studied; however, an area of research is anaerobic co-digestion of multiple organic wastes. Energy-rich food waste, including fats, oils, and grease (FOG), can help balance carbon and nutrients in wastewater sludge streams, increasing the efficiency of waste degradation and increasing biogas production [15–17]. Recovery of methane from the biogas provides increased renewable energy for heat, power, and fuel. In addition, co-digestion of food waste, the most common solid waste, diverts the amount of waste material deposited at landfills [18, 19].

As of 2018, of the ~17,000 WRRF in the U.S., less than 10% utilize anaerobic digestion for the treatment of the wastewater sludge. Approximately 71% of the facilities that use anaerobic digestion simply flare the biogas and do not recover any energy or heat [18, 20, 21]. For those facilities with existing digester capacity, flaring the biogas results in a loss of energy, which can instead be recovered for heat and/or electricity. Additionally, those facilities with digesters should consider co-digestion with wastewater solids as it presents an opportunity for the facilities to increase biogas production. Due to the high energy content, biogas yields increase by 25-50% when food waste, especially FOG, are included in the anaerobic digester [20, 22]. However, only 1 in 10 of the existing facilities with anaerobic digesters in use take advantage of co-digestion [18]. In addition to increased methane yield, co-digestion of wastewater sludge with food waste can improve digester stability resulting in synergistic reactions from balanced nutrients, trace elements, and carbon/nitrogen ratios in comparison to digesting one product alone [23]. With states, including New York, adopting landfill disposal bans for organic waste or mandatory food scrap recycling [24], anaerobic co-digestion will become a likely alternative. Modeling of co-digestion processes is limited in literature but can help treatment facilities make informed decisions regarding infrastructure upgrades, a common barrier to implementation [20].

1.1.3 Modeling and Simulations

Model and simulation development involve identification of the key processes involved in a system, identification of the controlling equations, parameter estimation based on prior knowledge, sensitivity analysis to determine the parameters with the strongest influence, calibration based on selected experimental data, and validation of the model using different conditions from the experimental data used for calibration [25–27]. Models characterizing the ABR were first proposed when the bioreactor was initially presented at bench-scale [14]. Over time, modeling efforts have continued to improve and have integrated more parameters, creating more complex models; however, the fundamentals of the modeling framework, and subsequent implementation into computer-based simulation software, have remained similar. In general, bioreactor model construction is based on using data from real-world systems to determine which kinetics and stoichiometry are important to include. Once initial models are constructed, sensitivity analyses can be used to help determine the most influential processes or parameters, which can then lead to model improvements and increased predictive ability. Reformulation of the design, model, and parameters is an iterative, continual process [25, 27, 28]. Experimental procedures can sometimes be expensive and time consuming, and results may be inaccurate. Successful simulation of an anaerobic bioreactor can improve understanding of the complex biological and chemical processes without the costs of time and resources needed to build and operate additional physical test beds. Further, a simulation capable of predicting performance and resource recovery (e.g., methane generation) can assist in designing or upgrading a treatment system and inform research technology transfer to industry while advancing sustainability [29–31].

1.1.4 Life Cycle Assessment

Life cycle assessments are tools that can be used to compare competing systems for environmental performance and impacts and are usually divided into four phases: goal and scope definition, inventory analysis, impact assessment and interpretation phase [32, 33]. Defining the goal of the LCA, including setting system boundaries and defining the functional unit, will set the stage for a study that provides enough detail to address the goal (e.g., what process causes the least amount of environmental impact). The life cycle inventory identifies the relevant energy and material inputs and environmental releases, and the life cycle impact analysis evaluates the potential environmental impacts associated with the identified inputs and releases. The final portion of the LCA involves interpreting the results to help inform decision makers regarding their options and potential impacts [32, 34]. A life cycle analysis comparing real-world data from a small-scale WRRF using anaerobic co-digestion to a conventional anaerobic digestion is needed to understand environmental impacts and further assess the efficacy of co-digestion.

1.2 Research Questions, Objectives, and Dissertation Structure

The goal of this dissertation research was to further the existing body of knowledge concerning the use of anaerobic bioreactors in the treatment of wastewater and organic solids. In support of this goal, I worked in conjunction with other researchers to characterize, compare and model the performance of three pilot-scale ABRs treating domestic wastewater in Colorado. In addition, I worked with faculty and installation staff of the U.S. Military Academy (USMA) at West Point, NY, to characterize and model waste-to-energy through anaerobic co-digestion at the installation WRRF.

The following research questions guided the research:

(1) What modifications to default operating parameters and system characterizations are required for BioWin, a wastewater computer simulation software program, to predict the removal of chemical oxygen demand and suspended solids and methane generation of anaerobic bioreactors receiving domestic wastewater?

(2) How do the differing flow rates, operating temperature, and influent characteristics between three similar treatment systems impact the performance (chemical oxygen demand (COD) and suspended solids removal and methane generation) of anaerobic reactors treating domestic wastewater?

(3) What are the environmental impacts from the increase in biogas and energy generation when anaerobic digestion is upgraded to co-digestion?

The following objectives supported the research questions:

(1) Construct and validate a BioWin computer simulation to predict the removal of chemical oxygen demand and suspended solids and methane generation of a pilot-scale ABR with varying temperature within 10% of the observed performance.

(2) Characterize and compare the wastewater characteristics and performance of three multi-compartment pilot-scale anaerobic reactors treating different domestic wastewater streams.

(3) Characterize, assess, and model the performance of West Point’s anaerobic co-digestion process for stabilization of wastewater sludge, food scrap waste, and FOG for energy production.

This dissertation is a culmination of the research objectives and organized into four additional chapters. CHAPTER 2is a published paper in *Bioresource Technology Reports* describing the modifications to BioWin default parameters necessary to successfully predict the performance characteristics of a pilot-scale ABR operated at the Mines Park Advanced Water Technology Center, Golden, CO. CHAPTER 3is a manuscript submitted to *Water Environment Research* documenting the statistical analysis and comparative findings from the Mines Park ABR in comparison to two additional pilot-scale ABRs located in Castle Rock and Englewood, CO. CHAPTER 4describes research of anaerobic co-digestion for renewable energy at West Point’s WRRF in support of development for a decision support tool to be used at other DoD installations. Conclusions and suggestions for future work are summarized in CHAPTER 5and the appendices provide supporting information for each chapter.

CHAPTER 2

BIOWIN® MODELING OF ANAEROBIC SLUDGE BLANKET TREATMENT OF DOMESTIC WASTEWATER

Modified from a paper published in *Bioresource Technology Reports*[1].

Jennie L. Callahan[2,3], Andrew R. Pfluger[4], Linda A. Figueroa[5], Junko Munakata-Marr[6]

2.1 Abstract

Anaerobic bioreactors treating wastewater have lower operating costs and waste sludge generation and produce more energy-rich methane than traditional aerobic systems. The ability to simulate performance of anaerobic mainstream treatment allows for comparison to the existing aerobic treatment paradigm. Required modifications were determined for a computer simulation tool, BioWin, to predict wastewater treatment performance of a multi-compartment anaerobic baffled reactor system. The model was calibrated using one month of data and validated using two years of data pooled into three temperature regimes. The validation results were within 10 percent of actual, measured values recorded from a multi-year study of a pilot-scale anaerobic bioreactor treating domestic wastewater. Sensitivity analysis showed the simulation was most sensitive to changes to the influent wastewater characteristics and acetogen and methanogen kinetic parameters. Thus, using BioWin, anaerobic domestic wastewater treatment can be integrated into wastewater facility design scenarios.

2.2 Introduction

Mesophilic anaerobic digestion is a commonly used approach for stabilizing primary wastewater sludge and waste sludge generated from conventional aerobic wastewater treatment processes, such as

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activated sludge and trickling filter systems [5]. Bioreactors that employ anaerobic microbiota to treat raw domestic wastewater represent a viable alternative to traditional aerobic wastewater treatment due to their low complexity, ability to generate methane-rich biogas with little or no energy input, and reduced production of waste sludge [6]. In anaerobic baffled bioreactors (ABRs), wastewater flows upward from the bottom of the bioreactor through a dense sludge layer with high microbial activity. As wastewater passes through the sludge, anaerobic microorganisms degrade complex wastewater organics to simple compounds (e.g., monomers or volatile fatty acids) and then to methane and carbon dioxide. The methane produced can be captured and converted to electrical and heat energy with use of combined heat and power technology [9].

Model and simulation development involves identification of the key processes involved in a system, identification of the controlling equations, parameter estimation based on prior knowledge, sensitivity analysis to determine the parameters with the strongest influence, calibration based on selected experimental data and validation of the model using different conditions from the experimental data used for calibration [25–27]. Modeling efforts have continued to improve and have integrated more parameters, creating more complex models; however, the fundamentals of the modeling framework, and subsequent implementation into computer-based simulation software, have remained similar. In general, bioreactor models are constructed using real-world data, which help determine important kinetics and stoichiometry. Once initial models are constructed, sensitivity analyses can be used to identify the most influential processes or parameters, which can then lead to model improvements and increased predictive ability. Reformulation of the design, model, and parameters is an iterative, continual process [25, 27, 28]. BioWin, a program developed by EnviroSim Associates Limited in Ontario, Canada, is the wastewater treatment process simulator chosen for this study due to its frequent industry use in the United States.

Few pilot-scale and no full-scale ABRs treat domestic wastewater at ambient wastewater temperatures in temperate climates. Further, very few publications describe adaptations of BioWin for anaerobic treatment of raw wastewater. A study completed by Schalk et al. (2019) between 2012 and 2017, examined an eight compartment ABR with a wastewater flowrate of 5,000 to 14,000 L/d at temperatures between 8 and 24 °C; however, insufficient data was publicly available for influent characterization and no simulation efforts were discovered [35]. Simulation of an upflow anaerobic sludge blanket reactor using BioWin was presented in a newsletter published by EnviroSim Associates Ltd. (2011). An anaerobic digester element coupled to a point clarifier element, which allowed for the simulation of a sludge bed for accumulating solids to create a UASB, a process that is not pre-defined in BioWin [36]. As the ABR is often characterized as a collection of UASB in series [6, 11, 37], the UASB example was used as the basis to model the ABR. Sönmez et al. (2011) and Midkiff (2016) attempted to use BioWin simulations to determine the theoretical performance of anaerobic treatment technologies [38, 39]. However, the authors had little information regarding the wastewater characteristics, limited primarily to flow rate, chemical oxygen demand (COD), biological oxygen demand (BOD), and suspended solids concentrations. With remaining characteristics based on literature or BioWin default values, the simulation predictions were inaccurate. Li et al. (2016) utilized BioWin to simulate the performance of a bench-scale modified anaerobic baffled reactor [40]. The configuration used four separate compartments; however, the total volume of the system utilized by Li was approximately 55 L, operated at 30 °C, and used synthetic wastewater. The authors characterized the influent wastewater (based on data collected over 40 days of operation) and adjusted the default parameters in BioWin. Subsequently, their ABR BioWin model simulated effluent total COD and total suspended solids (TSS) concentrations, biogas flow and pH within 13% of observed values.

The goal of this research was to establish a modeling framework for mainstream anaerobic processes using the widely employed BioWin simulation software. The objective was to determine required modifications to BioWin default setting in order to predict the removal of COD and suspended solids and the methane generation of a pilot-scale ABR under varying temperature within 10% of observed performance. The simulation of the ABR improves on previous efforts by utilizing a more comprehensive data set obtained from a system treating actual wastewater at varying temperatures. Successful simulation of an anaerobic bioreactor can improve understanding of the complex biological and chemical processes without the costs of time and resources needed to build and operate additional physical test beds. Further, a simulation capable of predicting performance and resource recovery (e.g., methane generation) can assist in designing or upgrading a treatment system and inform research technology transfer to industry while advancing sustainability [29–31].

2.3 Materials and Methods

2.3.1 ABR Description and Performance

The Mines Park ABR (depicted in Figure 2.1, p. 9) consisted of three equal-sized cylindrical compartments (0.152 m radius and 3.66 m height), each containing 240 L of wastewater. A fourth cylindrical compartment (same radius and 1.22 m height) was added as a fixed-film reactor containing approximately 30 L of polyethylene wheels as media for biofilm growth, leading to a total hydraulic volume of 800 L. The system operated at a 26.7-hour hydraulic residence time when the fourth compartment was added. The influent was pumped from a 2500-gallon holding tank with a submerged grinder pump and 2 mm screen containing domestic wastewater from the 250-unit Mines Park housing complex in Golden, CO. The treatment system operated year-round at ambient air temperatures ranging from -20 to 37 °C, with an average temperature of 12 °C at 0.82 atm. Wastewater temperatures varied between 6 and 27 °C with an average of 18 °C. During school breaks, when fewer students occupied the housing complex, the influent wastewater contained lower concentrations of constituents such as COD and solids. The Mines Park ABR removed an average of 54% of organics (as COD) and 75% of suspended solids, exceeding the performance of conventional primary treatment and achieving secondary discharge standards for suspended solids at warmer wastewater temperatures (20 to 27 °C) [6]. The full operational history of these digesters and analytical methods for key operational parameters including COD removal and daily biogas production have been described in detail elsewhere [6, 41].

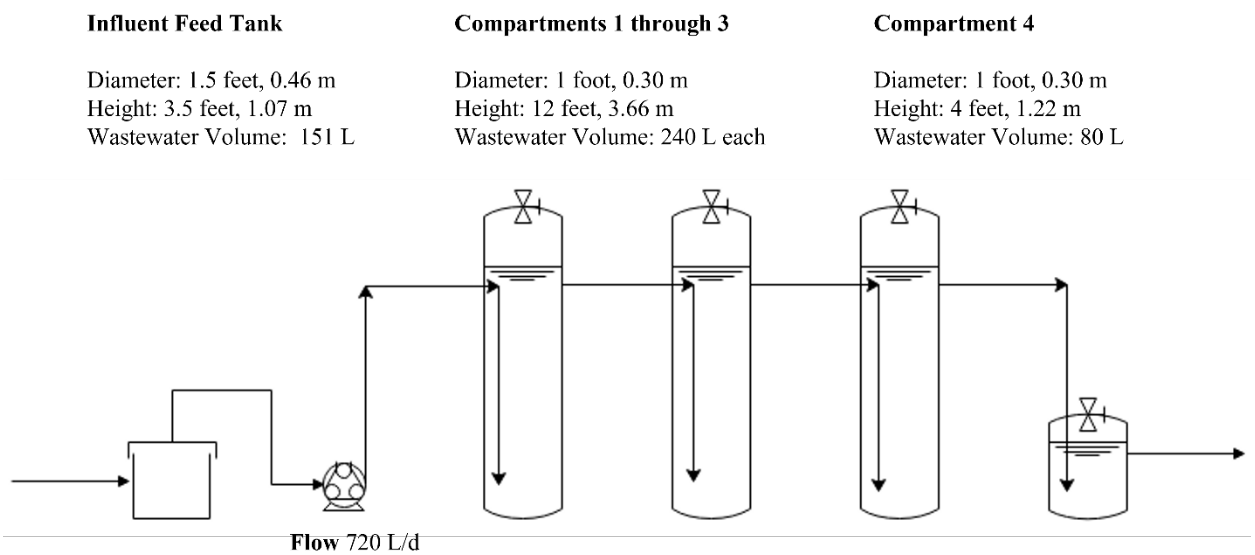


Figure 2.1 Mines Park ABR Flow Schematic.

The key wastewater constituents of interest for modeling included total, soluble and particulate COD (tCOD, sCOD, pCOD), volatile fatty acids (VFAs), and methane. TSS volatile suspended solids (VSS), and 5-day biochemical oxygen demand (BOD_5) were also considered. These constituents were selected based on their relevance to the wastewater treatment industry, as well as their significance to this anaerobic treatment model. BOD_5 and TSS standards are used by the U.S. Environmental Protection Agency to regulate wastewater discharge. However, COD is more consistent than BOD_5 for measuring wastewater organic strength. The anaerobic microbial communities utilize VFAs for the production of methane. The average, standard deviation and medians for each wastewater component concentration, temperature, and pH were determined using values from the overall dataset. The mean typically was greater than the median for all constituents, indicating a positive skew. Sometimes this skew resulted in substantial differences, especially for influent suspended solids concentrations (e.g., median of 117 mg/L and mean of 171 mg/L). It is best to use median when the distribution of data values is skewed or when there are clear outliers [42]. The median of the values within one standard deviation of the mean were subsequently used for analysis. In treatment systems without outliers or skewed data, the average may better characterize the performance [42]. The month of April 2018 was used for calibration of the simulation because the system performance (including constituent concentrations, operating temperature, and removal rates) was closest to the overall system median and the system operation was stable. During this month, school was in session and the Mines Park residences were at full capacity. Additionally, all compartments of the treatment system had been operational for at least 12 months, allowing them to stabilize, and all testing and monitoring equipment was fully operational. The constituent median values for April 2018 are listed in Table 2.1.

Table 2.1 Mines Park ABR median influent and effluent characteristics for April 2018.

	Influent	**Effluent**
tCOD (mg/L)	428	191
pCOD (mg/L)	243	78
sCOD (mg/L)	185	113
Acetate (mg COD/L)	34.5	2.8
Propionate (mg COD/L)	16.5	2.6
BOD_5 (mg/L)	209	68
TSS (mg/L)	125	37
VSS (mg/L)	113	35
dCH_4 (mg/L)[1]	0	24
Total CH_4 (L/d)[1, 2]		63

[1] Overall system median, not specific to April 2018

[2] Includes gaseous methane from all 4 compartments

2.3.2 BioWin Software and Model Construction

BioWin is a wastewater treatment process simulator (EnviroSim Associates Limited, Ontario, Canada) that uses proprietary biological models supplemented with other process models such as water chemistry and mass transfer gas-liquid interactions. The biological model in BioWin is built upon the activated sludge model (ASM) and the anaerobic digestion model (ADM). BioWin incorporates four function-based microbial populations to model anaerobic systems: heterotrophs for hydrolysis and fermentation; acetogens for acetogenesis; and both acetoclastic and hydrogenotrophic methanogens for methane generation [43]. BioWin (Version 5.3) was selected for Mines Park simulation modeling due to its frequent industry use in the United States.

BioWin can run two types of simulations: steady state and dynamic. Steady state is based on the flow and average influent loading to the system, while dynamic uses time-varying system or operational responses (e.g., seasonal loading characteristics, temperature changes, system start-up development). All model solutions in this study were determined using steady-state simulations. The Mines Park ABR simulation was built using five types of elements within BioWin: the anaerobic digester, point clarifier, influent, effluent, and pipes (Figure 2.2). The anaerobic digester element in BioWin is designed to model the digestion of primary and waste activated sludge. However, when used in conjunction with a point clarifier, the coupled elements represent the design of the UASB or a single compartment of an ABR. Specifically, the point clarifier is used to simulate recirculation of the sludge and allows for the accumulation of suspended solids, creating the sludge bed and decoupling HRT and SRT – a characteristic of ABR treatment systems [36].

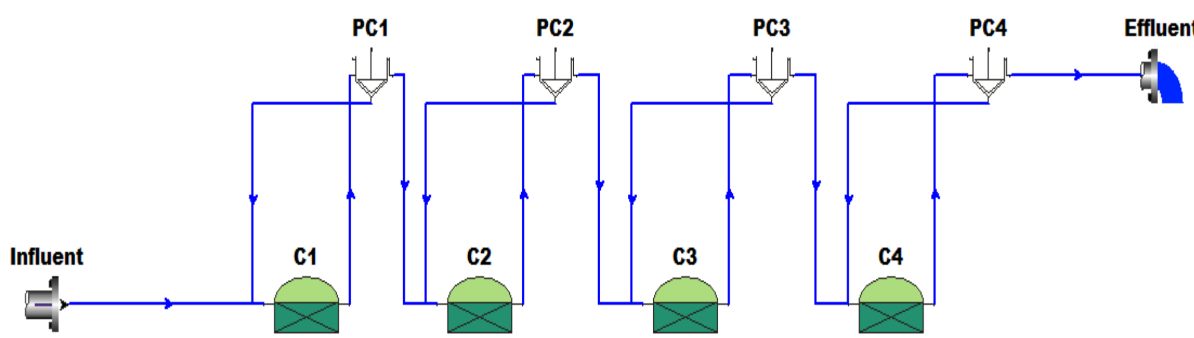


Figure 2.2 Flow schematic from BioWin simulator showing four compartments (each represented by the anerobic digester element combined with the point clarifier element) in series to represent the ABR.

A sensitivity analysis was conducted with initial BioWin configurations constructed using the coupled anaerobic digester, point clarifier, influent, effluent, and pipe elements, to describe a singular ABR compartment. The anaerobic digester element was adjusted to the size of a single ABR compartment, and the wastewater characteristics and flow were adjusted to approximate the ABR influent. The sensitivity analysis was further divided into three key categories: physical characteristics (flow, digester volume, etc.), kinetic values, and influent wastewater fractions. The analysis was conducted using a Morris One-at-a-Time (OAT) approach wherein a single BioWin parameter was altered by 10 to 50% from baseline values to determine the parameters with the largest impact on key constituents of concern [44–46]. The variations were normalized, generating a sensitivity coefficient ($S_{i,j}$)

from the ratio of the relative percentage change in the output variable (constituent concentrations or y_i) to the relative percentage change in the input variable (BioWin parameter or x_i) using the following equation [44, 45]:

$$S_{i,j} = \left|\frac{\Delta y_i / y_i}{\Delta x_i / x_i}\right| \tag{2.1}$$

A parameter with a high sensitivity was one that resulted in a large variation of the predicted concentrations from a small variation in the input parameter from the baseline values. A uniform scale of $S_{i,j}$ values for labeling parameters as highly or moderately sensitive was not developed due to the variations between the three categories. Subsequently, the parameters with highest $S_{i,j}$ values (generally, the top 5) by category, location and constituent were considered most sensitive. The wastewater characterization and BioWin component settings used in the sensitivity analyses can be found in the supplementary material.

Once sensitive parameters were identified, a four-compartment ABR (Figure 2.2, p. 11) was constructed in BioWin using design parameters and influent wastewater characteristics listed in Table 2.2 (p. 13), which leveraged representative data from April 2018. Four coupled anaerobic digester elements coupled with point clarifier elements in series represented the four-compartment ABR. Three types of BioWin influent elements (COD- or BOD-based, and user-defined) can be used to input wastewater flow and characteristics. The COD- and BOD-based influent elements use default wastewater components and fractions to partition the total aggregated organic concentrations. The user-defined influent element can be tailored to input specific substrates [43]. Both the COD-based and user-defined influent elements were used in this study, with better predictive results from the user-defined influent with the manual addition of propionate, which is not available in the COD-based influent element. The model was calibrated by adjusting the kinetic and stoichiometric parameters identified in the sensitivity analysis to minimize the percent difference between the simulation results and the experimental data for April 2018 listed in Table 2.1 (p. 10). BioWin default values were used for the parameters identified during the sensitivity analysis as either irrelevant for this study or as having little influence (less than 2%) on performance. Additionally, changes were made to as few parameters as possible. For example, parameters pertaining to the endogenous product decay rate, hydrolysis rate constant, and hydrogenotrophic methanogen kinetics were not altered due to lack of supporting pilot data or conflicting literature information.

Table 2.2 Reactor design and operational information used in BioWin ABR simulation.

System Parameters	Value
HRT (hours)	27
Anaerobic Digester Elements	
Water Volume (Compartments 1-3) (L)	240
Water Volume (Compartment 4) (L)	80
Head Space Volume (1-3) (L)	22
Head Space Volume (4) (L)	10
Head Space Pressure (kPa)	84.1
Temperature (°C)	17.2*
Point Clarifier Elements	
Underflow (L/d)	1440
Influent Characteristics	
Influent Flow (L/d)	720
Total COD (mg COD/L)	428
Total Kjeldahl Nitrogen (mg N/L)	70
Total P (mg P/L)	7.8
Nitrate N (mg N/L)	0
pH	7.57
Alkalinity (mmol/L)	4.66
Influent Inorganic Suspended Solids (mg ISS/L)	11.1
Calcium (mg/L)	27.7
Magnesium (mg/L)	7.1
Dissolved O_2 (mg/L)	0

The calibrated model was validated by targeting simulated removal percentages within 10% of the observed removal rates from median values from three data sets based on three water temperature ranges (less than 16, 16 to 20, and greater than 20 °C), representing ambient temperatures during colder, median, and warmer months. The data used for validation did not include the April 2018 data used in calibration. Because calibration solutions were non-unique, calibration and validation were conducted iteratively to achieve the validation metrics. Once the initial BioWin simulation was completed, additional calibration utilizing the same April 2018 data was conducted for adjustment of the hydrolysis rate constant Arrhenius factor. The simulation utilizing the adjusted Arrhenius factor was validated using the same three water temperature data sets as the initial simulation.

2.4 Results and Discussion

2.4.1 Sensitivity Analyses

Given the number of constituents, parameters, and equations available in BioWin, identifying the most important constituents of concern and which kinetic and stoichiometric parameters affect those concentrations is essential. The initial one-compartment sensitivity analysis was useful for determining the key parameters that would affect major constituents, such as COD and TSS. However, the extent to which these parameters affected the effluent changed with the inclusion of additional compartments. For example, additional compartments resulted in an accumulation of inert suspended solids and volatile fatty acids above measured values, which required additional modifications to the microbial kinetic rates (discussed in the following kinetics section). Re-evaluation of the sensitive parameters may be required if a simulation increases in complexity.

Sensitivity analysis findings are not typically reported for anaerobic wastewater treatment simulations. The basic UASB simulation developed by EnviroSim (2011) was for a theoretical high-strength organic waste with a goal of supporting start-up and control strategies [36]. Sönmez et al. 2011 developed BioWin simulations for a coupled clarifier, ABR and anaerobic filter system using influent and effluent data only with a goal of evaluation effect of sanitation options on treatment design and costs [38]. The Li et al. (2016) simulation was for a lab scale modified ABR and observed that the range of under- and over-prediction was ± 20% when default parameters were used [40]. Li et al. (2016) adjusted four kinetic parameters for the anaerobic digester element: maximum specific growth rate and half-saturation for ordinary heterotrophic organisms, acetogen half-saturation and anaerobic decay. The parameters were adjusted to achieve an absolute relative error of less than 15% between data and model simulation. Midkiff (2016) conducted a sensitivity analysis of a simulated Imhoff tank represented by a sedimentation chamber coupled to an anaerobic digester element followed by trickling filter polishing [39]. Measured data was influent and effluent BOD and TSS of the complete system. Eight parameters were selected for the sensitivity analysis: sedimentation underflow and percent TSS removal, tricking filter air flow and wastewater influent characterization parameters (F_{us}, F_{bs}, and F_{up}), VSS/TSS ratio, and cBOD/BOD ratio for the BOD influent element. The effect on BOD and TSS removal was studied using parameter reductions of 10, 20 and 50%. Percent TSS removal was identified as the most important parameter for both BOD and TSS removal which aligns with the sensitivity of the point clarifier solids removal efficiency in our study.

Sensitivity analyses were completed on three data categories: physical characteristics, kinetic values of the anaerobic digester element, and influent wastewater fractions. The most sensitive parameters (those with the highest $S_{i,j}$ value) for the effluent concentrations of COD, suspended solids, acetate, and BOD_5 for each parameter category are listed in Table 2.3. Additional values of $S_{i,j}$ for other constituents and locations are provided in the supplementary material.

Table 2.3 The values of $S_{i,j}$ for the most sensitive parameters in three categories for key effluent constituents. Higher values indicate higher sensitivity. A down arrow indicates a decrease in the BioWin parameter and an up arrow indicates an increase in the BioWin parameter. Parameters are defined in the text.

Parameters	**$S_{i,j}$**						
	tCOD	***pCOD***	***sCOD***	***TSS***	***VSS***	***Acetate***	***BOD_5***
Physical							
PC % Removal ↑	58.80	32.57	69.22	26.99	35.36	97.81	106.51
PC % Removal ↓	80.78	14.24	107.14	11.59	15.24	152.32	148.11
AD pH ↓	1.07	0.12	1.54	0.10	0.14	2.19	1.97
AD Area ↓	0.72	0.09	0.97	0.07	0.09	1.38	1.32
AD Diameter ↓	0.72	0.09	0.97	0.07	0.09	1.37	1.32
Kinetic							
$\mu_{max, Meth}$ ↓	1.45	0.17	2.68	0.14	0.69	3.00	2.68
$b_{Meth, anaerob}$ ↑	1.42	0.17	2.62	0.14	0.69	2.93	2.62
$b_{Meth, anaerob}$ ↓	0.55	0.15	1.03	0.13	0.19	1.19	1.03
$\mu_{max, Meth}$ ↑	0.51		0.95			1.07	0.95
K_{Meth} ↑	0.51		0.94			1.05	0.94
k_{hyd} ↓		0.72		0.48	0.69		
HF_{AD} ↓		0.72		0.48	0.69		
Influent Fractionation							
F_{up} ↑	0.19	0.67		0.45	0.64		
F_{us} ↑	0.19		0.28				
F_{ac} ↓						0.05	0.07

Table 2.3 Continued

Parameters	$S_{i,j}$						
	tCOD	***pCOD***	***sCOD***	***TSS***	***VSS***	***Acetate***	***BOD_5***
F_{bs} ↓	0.08	0.16	0.04	0.12	0.16	0.05	0.10

Sensitivity analysis of the physical characteristics revealed the point clarifier (PC) percent removal and the digester pH impacted system performance the most relative to the constituents of interest. For example, the point clarifier percent removal baseline was 99.6%. Increasing the percentage to 99.9% resulted in a 250% increase of tCOD in the point clarifier underflow and digester elements ($S_{i,j}$ values of 840) and decreased the effluent tCOD by 18% ($S_{i,j}$ value of 59). In contrast, reducing the percent removal to 99.3% resulted in tCOD concentrations being reduced by half in the point clarifier underflow and digester elements ($S_{i,j}$ values of 128), while the effluent concentration increased by 24% ($S_{i,j}$ value of 81). Other variables such as the physical size of the anaerobic digester element, flow and temperature also had an effect but were set to the actual system dimensions and values.

In BioWin, anaerobic digester element performance is governed by 111 kinetic parameters, divided into 11 categories. Of those, concentrations of COD, TSS, VSS, acetate and methane were most affected by the following kinetic parameters: hydrolysis rate constant (k_{hyd}), anaerobic hydrolysis factor (HF_{AD}) and methanogen kinetic parameters (anaerobic decay rate ($b_{Meth,\ anaerob}$), substrate half-saturation ($K_{S,\ Meth}$), and maximum specific growth rate ($\mu_{max,\ Meth}$)), resulting in the highest $S_{i,j}$ values.

Influent wastewater characterization using the COD influent element in BioWin is determined by modifying default descriptive fractions, such as the fraction of readily biodegradable COD (rbCOD) to tCOD (labeled "F_{bs}" in BioWin). The fractions for F_{bs} and unbiodegradable particulate COD (F_{up}) had the greatest impact on the influent concentrations of pCOD, suspended solids, and BOD_5 components, resulting in the highest $S_{i,j}$ values. The fraction of unbiodegradable soluble COD (F_{us}) was the only influent fraction with an $S_{i,j}$ value higher than 0.05 making it the most relevant fraction for altering the concentration of influent soluble COD despite the comparatively low $S_{i,j}$ value. An important fraction for methane generation was the concentration of volatile fatty acids (primarily acetate and propionate). The fraction of volatile fatty acids (F_{ac}) in the COD influent element characterization includes only acetate. However, if the user-defined influent element is employed, volatile fatty acids can include propionate as well. The fraction of COD that is slowly biodegradable (F_{xsp}) was not determined to be an important fraction during the one compartment sensitivity analysis; however, over the course of the four compartments, F_{xsp} was important for the effluent pCOD to tCOD ratio. Full descriptions of these categories and fractions are available in the BioWin help manuals; in addition, a reference chart created for this study is available in the supplementary material.

A complication of the sensitivity analysis was the asymmetric impacts of some parameter changes on dependent variables (or $S_{i,j}$ values) equally across all BioWin elements (i.e., point clarifier or anaerobic digestor). An example of this was provided in the Results section for the percent removal of particulate matter in the point clarifier element; however, such asymmetry was noted in other categories and parameters, as well. Another example is the decrease of the acetoclastic methanogen maximum specific growth rate. The effluent tCOD concentration has an $S_{i,j}$ value of 1.4, but the same alteration results in an $S_{i,j}$ value of only 0.1 in the anaerobic digester element. Subsequently, both increases and decreases in parameters for the influent, effluent, anaerobic digestor, and point clarifier elements were analyzed using the $S_{i,j}$ formula.

2.4.2 Calibration

2.4.2.1 Influent Fractionation

The COD influent element in BioWin does not allow for the addition of propionate, a key volatile fatty acid in this simulation. Without including propionate in the model, the concentration of complex readily biodegradable COD increases and does not account for the prior hydrolysis and subsequent fermentation of particulate matter to other short chain fatty acids. Increasing the fraction of acetate (F_{ac}) to increase the acetate concentration to account for the propionate resulted in a buildup of acetate. Thus, the user-defined influent element was implemented to add propionate and correct for these shortcomings.

While the COD influent element allows a user to characterize their influent with the use of two simple tables with calculations performed automatically, the user-defined influent element requires input of the concentrations of the specified constituents. A user is provided with an editable list of 50 state variables (including four blank user defined components). To change the concentration of propionate in the influent to 16.5 mg COD/L, for example, readily biodegradable complex COD would need to be reduced (by 16.5 mg/L) to maintain the same concentrations of pCOD and sCOD, otherwise sCOD and tCOD would increase beyond the target values recorded for the Mines Park ABR. Similar changes to the slowly biodegradable and soluble inert COD concentrations, each with two components in the list of 50 state variables, were required for changes to F_{xsp}, F_{up} and F_{us}. A spreadsheet with COD-based and user-defined influent element characteristics was useful for calculating fractions and necessary concentrations. An example of the differences between the COD influent element and the user-defined influent element is provided in the supplementary material. Table 2.4 (p. 18) lists the equivalent fractions utilized for the user-defined influent element in the calibrated model.

Table 2.4 Fractions for April 2018 influent composition adjusted for the user-defined influent element. Default values were retained for all other wastewater fractions. The fractions used in three other studies are included here for comparison. Values were rounded to two decimal places for clarity.

Fraction	Default	Li et al.[1]	Izadi et al.[1]	Oleyiblo et al.[2]	User-Defined Stream[3]
Readily biodegradable COD, F_{bs} (g COD/g tCOD)	0.16	0.78	0.22	0.20	0.12
Slowly biodegradable particulate COD, F_{xsp} (g COD/g slowly degradable COD)	0.75	0.75	0.75	0.75	0.79
Acetate, F_{ac} (g COD/g rbCOD)	0.15	0.03	0.15	0.19	0.68
Non-biodegradable soluble COD, F_{us} (g COD/g tCOD)	0.05	0.08	0.12	0.05	0.17
Non-biodegradable particulate COD, F_{up} (g COD/g tCOD)	0.13	0.05	0.65	0.13	0.01

[1] The data reported by Li et al. (2016) and Izadi et al. (2022) were for synthetic wastewater created for use in pilot-scale experiments.
[2] The data reported by Oleyiblo et al. (2015) is for influent to a wastewater treatment plant in Anhui Province, China, utilizing oxidation ditches proceeded by anaerobic and anoxic tanks for treatment.
[3] As the user-defined influent element does not use wastewater fractions, these values are the fractional equivalents based on the concentrations utilized.

Of all of the variables within BioWin, the fractions that determine the composition of the influent COD are the most important. Specifically, the fractions identify what portions of the wastewater can be degraded or utilized as substrate for the microbial populations. If a model is to provide reasonable predictions of system behavior, the influent wastewater must be sufficiently characterized [25]. The user-defined influent element does not use the automated influent characterization fractions from the COD-based influent element and all constituent concentrations must be entered manually. However, the manually entered values still reflect the influent fractions. For example, manually entering 13.2 mg/L of rbCOD (complex), 34.5 mg COD/L of acetate and 16.5 mg/L of propionate results in 64.2 mg of readily biodegradable COD or an F_{bs} of 0.15 (15% of the tCOD).

The descriptive fractions most essential to the Mines Park ABR, as well as the ABR studied by Li et al. (2016), included F_{bs}, F_{ac}, F_{us}, F_{up}, and F_{xsp}, which are all interrelated to the tCOD, pCOD and sCOD concentrations [40]. For example, if the F_{bs} is lowered from 0.15 to 0.14, the F_{us} must be increased from

0.22 to 0.23 to keep the same desired initial sCOD concentration. Additionally, a user can achieve the same influent tCOD, pCOD and sCOD concentrations with different fractions of readily and slowly biodegradable or inert COD. Table 2.4 (p. 18) depicts the equivalent fractions utilized for the calibrated model. However, similar COD and BOD influent concentrations can be achieved with an F_{us} of 0.14, F_{up} of 0.02 and F_{xsp} of 0.75, though fractions have effects not just on the influent COD, but also on BOD and suspended solids concentrations throughout subsequent treatment compartments. These seemingly minor changes result in simulated influent and effluent BOD concentrations within 2% of the measured values. However, the simulated suspended solids and BOD removal is reduced to 65% from the measured 70%. The final result after four treatment compartments is quite different in the ratios of particulate and soluble COD. The effluent sCOD:pCOD ratio is reduced from 1.2 to 1 and the removal percentages for these constituents are also altered by 5% due to the lower concentration values. As mentioned previously, F_{xsp} was not initially considered a sensitive parameter. A 10% change in the default value of 0.75 only resulted in a 5% change in influent pCOD and VSS concentrations ($S_{i,j}$ values of 0.53) and a 0.01% change in effluent concentrations ($S_{i,j}$ values of 0.0014). However, the 5% change of the default F_{xsp} value from 0.75 to 0.79 used in this simulation resulted in a 17% decrease in the effluent pCOD:tCOD ratio (an $S_{i,j}$ value of 3.11).

In general, lowering the influent F_{bs} decreases the simulated amount of propionate, pCOD, suspended solids, BOD, BOD removal percentage and pCOD:tCOD ratio over the course of the four compartments and subsequently the effluent. Simultaneously, the pCOD:VSS, VSS:TSS and sCOD:pCOD ratios all increase. Lowering the F_{xsp} fraction results in increased BOD, pCOD, and suspended solids concentrations. In addition, BOD removal and the pCOD:tCOD, pCOD:VSS and VSS:TSS ratios also increase. Decreasing the F_{up} fraction decreases sCOD (increasing pCOD), BOD and the BOD percent removal. However, suspended solids concentrations change minimally.

2.4.2.2 Kinetic Parameters

In addition to the influent characterization of the user-defined influent element, successful calibration required modifications to the point clarifier percent removal, inert conversion module, microbial kinetic rates constants, and methane mass transfer rate. The project-level default and modified values are listed in Table 2.5 (p. 20). All simulated influent and effluent concentrations, as well as removal percentages, were within 7% of the measured values. Table 2.6 (p. 20) summarizes the influent and effluent concentrations and the percent difference between them.

Table 2.5 Project default and utilized values.

	Default	Calibration Values			
Methane Mass Transfer Rate (Kl) (m/d)	8	2			
Particulate Substrate and Inert COD Ratios (mg COD/mg VSS)	1.6	2.2			
Inert Conversion					
Kd_Xi	-	0.05			
Kd_ISS	-	0.03			
Kd_ZE	-	0.1			
		C1	**C2**	**C3**	**C4**
Point Clarifier Removal Percentage	99.8	99.675	99.73	91.5	99.28
Acetoclastic Methanogens					
Maximum Specific Growth Rate (μ_{max}) (1/d)	0.3	0.459	0.489	0.33	0.525
Substrate Half-Saturation (K_S) (mg COD/L)	100	47	37	90	25
Anaerobic Decay Rate (b) (1/d)	0.13	0.061	0.048	0.12	0.033
Acetogens					
Maximum Specific Growth Rate (μ_{max}) (1/d)	0.25	0.22			
Substrate Half-Saturation (K_S) (mg COD/L)	10	11.2			
Anaerobic Decay Rate (b) (1/d)	0.05	0.056			

Table 2.6 Comparison of April 2018 data and simulated values.

	Influent			Effluent		
Arrhenius factor 1.029	Measured	Simulation	% Diff	Measured	Simulation	% Diff
tCOD (mg/L)	428	428	0%	192	190	1%
pCOD (mg/L)	243	243	0%	79	76	3%
sCOD (mg/L)	185	185	0%	113	113	0%
Acetate (mg COD/L)	34.5	34.5	0%	2.8	2.9	3%
Propionate (mg COD/L)	16.5	16.5	0%	2.6	2.4	6%
dCH4 (mg/L)	0	0	0%	24	23	5%
TSS (mg/L)	125	124	0%	37	39	6%
VSS(mg/L)	113	113	0%	35	37	6%
ISS (mg/L)	11.8	11.6	1%	2.5	2.6	4%
BOD_5 (mg/L)	209	207	1%	68	69	1%

Table 2.6 Continued

	Influent			Effluent		
Arrhenius factor 1.037	Measured	Simulation	% Diff	Measured	Simulation	% Diff
tCOD (mg/L)	428	428	0%	192	192	0%
pCOD (mg/L)	243	243	0%	79	76	3%
sCOD (mg/L)	185	185	0%	113	116	2%
Acetate (mg COD/L)	34.5	34.5	0%	2.8	2.6	7%
Propionate (mg COD/L)	16.5	16.5	0%	2.6	2.5	4%
dCH_4 (mg/L)	0	0	0%	24	24	0%
TSS (mg/L)	125	124	0%	37	39	4%
VSS(mg/L)	113	113	0%	35	36	3%
ISS (mg/L)	11.8	11.6	1%	2.5	2.5	0%
BOD_5 (mg/L)	209	207	1%	68	70	3%

The default value point clarifier percent removal of 99.8% for COD was high in comparison to the actual removal rate of the compartments, so each of the point clarifier percent removal values was lowered to match the removal rates of the experimental data. Lowering the kinetic rate constants of the acetogens produced less acetate and propionate, while increasing the kinetic rates of the methanogens consumed more acetate and produced more methane. The inert conversion module, an add-on from the BioWin Model Builder cabinet, was enabled primarily to increase the removal of ISS throughout the compartments. Failure to implement the inert conversions results in concentrations building up in the compartments in contrast to the removal seen in the pilot data.

BioWin has no model elements for mainstream anaerobic bioreactors receiving wastewater, and the original anaerobic digester element within BioWin was designed for the treatment of sludge (high concentrations of COD with a large fraction of recalcitrant particulates). Thus, the need to adjust many of the wastewater composition and microbial kinetic parameters from default values was expected. To adjust for discrepancies, outliers were removed and median values, as opposed to average values, were used in the model. In the Mines Park ABR, the increased soluble COD concentrations (including acetate), suspended solids removal and the kinetic rates of the microbial community necessitated the adjustments of the default variables.

BioWin allows for the alteration of variables at both project level and digester element level. Project-level parameters are applied for calculations across the entire treatment system and are not altered for each digester [43]. Model predictions improved by utilizing the user-defined influent element and digester-level parameters. The user-defined influent element allows for manual inclusion of propionate and dissolved methane concentrations while digester level adjustments permit the creation of unique operating environments (e.g., one ABR compartment) within a treatment system However, they both increase the complexity of designing the simulation. If data are insufficient to support the use of additional parameters, increasing the complexity may not meaningfully improve the model.

Removal of the COD and solids varied from compartment to compartment and season to season. Mean tCOD removal was 55%, decreasing to 45% in colder temperatures and increasing to 65% during warmer temperatures. Median TSS removal was 73%, decreasing to 60% in colder temperatures and increasing to 83% under warmer temperatures. Changes to the predicted removal percentages in the model are primarily accomplished by adjusting the percent removal of particulate material within each of the point clarifiers. To achieve the observed removal percentages, the average percent removal for the point clarifier elements was 97%; however, higher than average values (99.6%) were noted in the first and second compartments and lower average values (92%) in the third compartment. Because the percent removal for the point clarifiers includes all particulate material, these removal percentages were necessary to achieve the observed 55% and 73% tCOD and TSS removal rates during calibration.

Changes in acetate, propionate, and methane within each of the compartments are dictated by the microbial kinetic rates. In this study, the kinetic rates were altered using the digester-level parameters to match varying amounts of substrate by compartments. The microbial kinetic rates (and substrate utilization) can be altered by changing the maximum specific growth rate, substrate half-saturation and anaerobic decay rate constants. In contrast to this publication, for which all three of the most sensitive kinetic parameters were altered by the same percentage, Li et al. (2016) altered only one parameter for two different microbial communities (acetogen half-saturation constant and OHO maximum specific growth rate) [40]. To increase methane production and acetate consumption in this study, acetoclastic methanogen activity was increased by increasing the default growth rate and decreasing the half-saturation and decay rates by approximately 50%. The new parameter values listed in Table 2.5 (p. 20) are within previously observed values for acetoclastic methanogens [47, 48].

During the initial stages of reactor stabilization (i.e., the first 180 days of operation), the measured VFA concentrations increased from the influent to the effluent with the largest concentration of acetate observed in the middle compartment and being removed in the final compartment [49]. However, over the course of two years of operation, measured acetate and propionate concentrations generally decreased by 50% from the previous compartment, suggesting increased acetate-consuming activity across all compartments in comparison to the stabilization period. An exception to this is noted in the third compartment, which generally saw a 20% increase in the VFA concentrations and also produced the least gaseous methane (in comparison to similar sized compartments) in all but colder temperatures, when it produced the largest amount of methane accompanied by a minimal increase (3%) of acetate from compartment 2. The compartment 3 differences suggest a larger acetoclastic methanogen population than the BioWin default that required less modification to the default kinetic parameters. Therefore, acetoclastic methanogen kinetics were increased by 53% in the first compartment, 63% for the second, 10% for the third, and 75% for the final compartment. Propionate concentrations were too low and not sufficiently different to complicate the model by modifying the acetogen kinetic rates per compartment. In general, the model benefited by a system-wide decrease in kinetic parameters of the acetogens by 12%.

Accurate prediction of methane generation is important for any ABR model, as the methane recovery and combustion facilitate energy production. However, the dCH_4 concentrations were not a large contributing factor to the selection of BioWin parameters, which were modified as version 5.3 did not include dissolved methane in the total or soluble COD concentrations. Methane is a calculated state variable reported as mg CH_4/L and also calculated as a percentage of biogas emitted but was not included in the calculations for solution phase COD. Dissolved methane does comprise some portion of sCOD, but how much is difficult to determine [50–52]. Part of this problem is related to over-saturation of methane in the liquid phase [52–54]. The phenomenon results in dCH_4 concentrations 1.33 to 1.7 times higher than stoichiometrically feasible for similar treatment systems [6, 12, 55]. Thus, the BioWin mass transfer rate for methane was altered from 8 to 2 m/d to create dCH_4 concentrations near the effluent median concentration of 24 mg/L.

Excluding dissolved methane and with the default Arrhenius factor of 1.029 for hydrolysis, the total system methane production for the simulations was below the actual production for the April 2018 (1%) and warmer models (7%). For cooler temperatures, the simulated methane production was 8% over the observed production. Additionally, the Mines Park ABR experienced a 17% decrease in methane production in the cooler temperatures and a 25% increase in warmer temperatures. The simulation predictions varied by -10% in the cooler temperatures and +17% in warmer temperatures. The distribution of the methane generation between cells was also inconsistent with the actual data. The experimental data revealed compartment 1 produced approximately 30% of the total gaseous methane, and compartments 2 and 3 each produced approximately 25% [6]. Distribution of gaseous methane production in a similar system increased from 20 to 35% incrementally through the compartments, with the fourth compartment producing the largest percentage [12]. The simulations predicted a distribution in which methane generation was highest (approximately 43%) in the first compartment and decreased through the compartments so that the fourth compartment only produced 6% of the total gaseous methane. Measured biogas composition of the Mines Park ABR was typically 70% methane [6]. However, the simulations predicted concentrations greater than 80%.

The reasons for these differences are unknown, and efforts to change the BioWin parameters for additional simulations did not substantially improve the distribution or methane production. Based on the changes required in the acetogen and methanogen kinetic variables, the discrepancy may be linked to the active microbial population and diversity. Recent analysis of the microbial population of the first 275 days of the Mines Park ABR revealed initial methanogen populations were dominated by *Methanobrevibacter*, a hydrogenotrophic methanogen, in the first two compartments while *Methanosaeta*, an acetoclastic methanogen, dominated the third compartment [49]. Over the course of the first 200 days of operation, the population of *Methanosaeta* increased and came to dominate the methanogen population in the second compartment. As the fourth compartment was seeded from the sludge bed of the third compartment, *Methanosaeta* likely dominated there as well. This information validates the decision to alter only the acetoclastic methanogen kinetic rates as the dominant methane producers. However, the product yields associated with the different microbial populations in the Mines Park ABR are unknown. If the population of hydrogenotrophic methanogens is larger than the BioWin default values, then a larger portion of the methane produced would originate from them. Such a population shift, not modeled in BioWin, may contribute to the disparity of the percentage of methane generated by compartment. Additionally, BioWin does not account for the potential transfer of both aqueous and gaseous methane between compartments, which was likely (but not measured) between the interconnected compartments of the Mines Park ABR.

2.4.3 Validation

Validation was conducted by extending the calibrated BioWin simulation to the experimental data based on the seasonal performance medians of the ABR under warmer and colder conditions. Performance was divided into temperature quartile ranges, less than 16 °C (Q1), 16 to 20 °C (interquartile range Q3-Q1 (IQR)), and greater than 20 °C (Q3). The median temperature was 13.6 °C for the lowest quartile of water temperatures and 23.5 °C for the highest quartile. The median temperature was 18 °C, which was similar to the temperature of April 2018 measured values of 17.2 °C and validation mirrored the calibration results. Validation using the 16 to 20 °C quartile range is available in the supplementary material. The operating temperatures of each compartment of the BioWin model were changed to reflect the median temperatures for each quartile range. Simulated removal percentages were within 10% of the measured removal percentages (Figure 2.3(a), p. 25).

In the Mines Park ABR system, the influent wastewater characteristics change based on student population and removal rates vary with temperature. In winter, when the temperatures are generally below 16 °C, more students are present than during the summer (when temperatures are greater than 20 °C), contributing to the increased COD concentrations. These colder temperatures result in depressed microbial kinetic rates leading to decreased COD removal. During median temperature periods (16-20 °C), tCOD removal is 51%, pCOD removal is 61%, and sCOD removal is 40%. However, in colder months, tCOD removal is only 45%, pCOD removal is 55% and sCOD removal is 33%. In contrast, at temperatures above 20 °C, tCOD removal is 65%, pCOD removal is 78% and sCOD removal is 50%. These variations in the wastewater characteristics make removal, rather than specific constituent concentrations, easier to compare.

The original calibrated and validated model, which used the Arrhenius factor of 1.029, achieved removal percentages within 2% for the April 2018 data. While only adjusting the operating temperature of the anaerobic digester elements for the validation, median removal percentages were within 5%, and warmer and colder temperature removal percentages were within 10%. However, the predicted removal percentages at warmer temperatures were 10% below the observed removal and were 10% over that measured in colder temperatures.

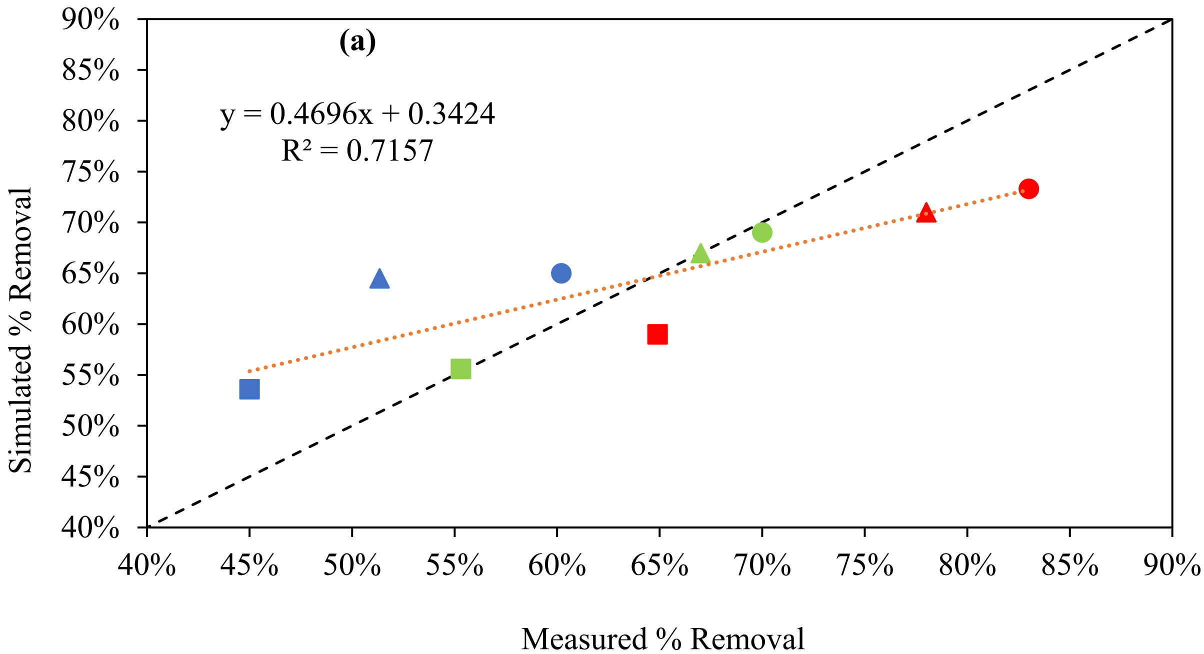
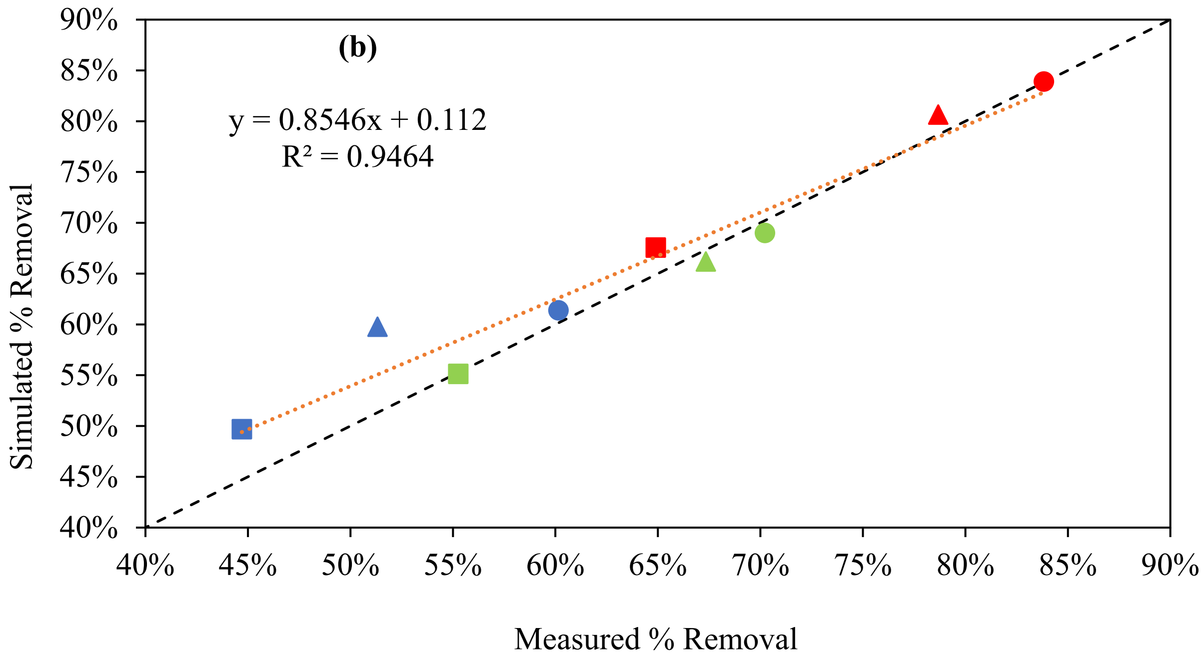


Figure 2.3 Simulated vs. measured percent removal using BioWin default hydrolysis Arrhenius factor of 1.029 (a) and using calibrated hydrolysis Arrhenius factor of 1.037 (b). April 2018 values are in green, cool temperature values are in blue and warm temperature values are in red. Removal percentages for tCOD are squares, TSS are circles, and BOD are triangles. The dashed black line represents an exact match between the simulated and measured removals. The dotted orange line is the trendline, the equation for which appears on the figure.

Figure 2.3 Continued



2.4.4 Arrhenius Factor Correction

While the initial validated model produced removal percentages within the goal of 10% of the observed values, it appeared the model accuracy could be improved with corrections for temperature by adjusting the Arrhenius factor. Subsequently, the model was recalibrated utilizing the April 2018 data, optimizing the Arrhenius factor for hydrolysis from the BioWin default of 1.029 to 1.037 for each of the compartments. The new calibrated model was then validated, producing the results in Table 2.6 (p. 20) and Figure 2.3(b), based on the colder, median, and warmer temperature data sets used in the initial simulation.

Because the initial simulation over-predicted removal in the colder temperatures and under-predicted in warmer temperatures, the hydrolysis Arrhenius factor was increased to reproduce the increased change of COD, suspended solids, and BOD_5 removal between the temperature ranges. The simulation removal rate accuracy was improved by increasing the Arrhenius factor for the hydrolysis rate of all compartments. Temperature affects reaction rates, such as hydrolysis, generally by increasing rates of reaction in warmer temperatures and slowing rates during colder temperatures [29, 48]. The Arrhenius factor is included in rate reactions to account for these temperature differences. Wastewater treatment and anaerobic digestion are generally presumed to occur at or near the same temperature, 20 and 35 °C, respectively, without variations beyond 10 °C [25, 29, 56]. Due to the broader wastewater temperature range (6 – 27 °C) seen in the Mines Park ABR in comparison to typical treatment systems, a higher

Arrhenius factor (1.037) than the default value of 1.029 was necessary. The Arrhenius factor for treatment varies in literature from 0.939 to 1.29 depending on the kinetic rate being manipulated, operating temperature ranges and whether the process is aerobic or anaerobic [56–58]. In this study, only the modification of the hydrolysis Arrhenius factor was determined to be necessary and alteration of the Arrhenius factor for other anaerobic kinetic processes (e.g., maximum specific growth rate of acetoclastic methanogens) failed to decrease the disparity with temperature. One of the first processes in the degradation of wastewater organics is the hydrolysis of particulate organic material. In a multicompartment treatment system, such as the ABR, this primarily occurs in the first compartment [11, 59]. This phenomenon was observed in the Mines Park ABR as approximately 60% of the overall reduction of pCOD occurred in the first compartment.

With the hydrolysis Arrhenius factor correction to 1.037, total system methane production also changed from the original validated model. Production for April 2018 was 2% lower in the calibrated simulation than the observed values. Validation using colder temperatures (less than 16 °C) resulted in simulated methane production 1% under the observed production and validation using warmer temperatures (greater than 20 °C) resulted in simulated methane production 8% over the observed methane production. While the percentages are similar to the original simulation that used an Arrhenius factor of 1.029, the modified production more closely follows the observed 17% decrease in methane production in the cooler temperatures and 25% increase in warmer temperatures.

2.4.5 Prospective Application

This research provides a method used to successfully characterize, model, and simulate mainstream anaerobic wastewater treatment. As indicated, influent wastewater characteristics differ between treatment systems; however, once influent wastewater is properly characterized, the modeling utilized by BioWin can be adapted to predict constituent removal and biogas generation. These performance attributes can assist in designing or modifying wastewater treatment systems that incorporate sustainable anaerobic treatment technologies. Traditional aerobic wastewater treatment facilities would be able to estimate the potential advantages from methane generation and reuse, diminished solids removal, and reduction of costs from the removal of aeration requirements. Additionally, the simulation indicates which BioWin parameters are relevant to anaerobic bioreactors and adaptations for temperate climates. With this, researchers can reduce the amount of time spent developing accurate simulations and minimize physical experiments.

2.5 Conclusions

This study demonstrates the use of a computer simulation tool, BioWin, to simulate performance of wastewater treatment using an anaerobic baffled reactor. Kinetic and stoichiometric parameters identified during the sensitivity analysis were calibrated based on concentrations for a specific month. Successful validation was accomplished through comparison of the simulation's projections to the target constituent removal percentages within 9% at different temperatures. Results from the BioWin simulations can provide predictive operating performance of unique anaerobic reactor processes for domestic wastewater treatment facilitating the design, system analysis, and assessment of resource recovery options of sustainable wastewater treatment practices, such as the ABR.

2.6 Acknowledgements

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CHAPTER 3

PERFORMANCE ANALYSIS OF THREE PILOT-SCALE MULTI-COMPARTMENT ANAEROBIC BAFFLED REACTORS TREATING DOMESTIC WASTEWATER AT PSYCHROPHILIC TEMPERATURES IN COLORADO

A manuscript submitted to *Water Environment Research*.

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3.1 Abstract

A transition from inefficient aerobic wastewater treatment methods to sustainable approaches is needed. Anaerobic bioreactors are a viable solution as they consume less energy, reduce biosolid production, and provide a source of renewable methane-rich biogas. A barrier to widespread implementation of anaerobic technologies is the lack of design guidance, especially in colder climates. This study bridges this knowledge gap by presenting design principles derived from three long-running pilot-scale anaerobic baffled reactors (ABRs) operating under psychrophilic conditions. To elucidate design principles, relationships between influent parameters, operational variables, and performance were explored. The ABRs removed 56% and 80% chemical oxygen demand (COD) and suspended solids, respectively, with a methane yield of 0.21 L CH_4/g COD_{rem}. Results suggest that ABRs can treat a range of wastewater strengths with near stoichiometric methane production, that ABRs require infrequent sludge wasting but the ability to waste sludge is needed, and that ABR dimensions need further optimization.

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3.2 Introduction

Over the last decade, researchers and practitioners have begun to view wastewater as a resource rather than simply a waste stream. This philosophical transformation promotes the reuse of treated wastewater, preserving freshwater resources, and the reclamation of energy, nutrients, and biosolids, creating an opportunity for environmental and financial sustainability in wastewater treatment [1, 2]. For domestic wastewater treatment, conventional aerobic treatment uses activated sludge systems where oxygen is provided to support the biological treatment by microorganisms. The aeration requirements can account for 35-75% of a facility's energy consumption, depending on size of the aeration tanks, solids retention times, and facility elevation [1]. Traditional primary and secondary treatment methods generate biosolids, which require thickening, dewatering, stabilization, and disposal at additional cost to the treatment facility. Anaerobic digestion is a commonly used approach for stabilizing wastewater sludge generated from conventional treatment processes and producing biogas [2, 3]. Anaerobic digestion bioreactors treating domestic wastewater and sludges facilitate the microbial degradation of organic matter to methane-rich biogas, which can be used as a renewable energy source when coupled with combined heat and power technologies. However, sludge blanket wastewater treatment methods have low complexity and also reduce the amount of biosolids generated with the simultaneous generation of methane [7, 8].

Currently, full-scale anaerobic sludge blanket bioreactors are primarily implemented in tropical climates, such as in areas of South America and Asia [8, 10, 11]. However, the development of viable low-temperature anaerobic sludge blanket bioreactors that meet the effluent goals for wastewater treatment is an area of on-going research [6, 8, 12, 13]. The most commonly studied anaerobic sludge blanket bioreactors include the upflow anaerobic sludge blanket (UASB), the anaerobic baffled reactor (ABR), and the expanded granular sludge blanket (EGSB) bioreactor [11]. Of these systems, ABRs have a simple design, low capital and operating costs and provide better retention of solids in response to load variations than single compartment UASB or EGSB reactors [11, 14]. Currently, few pilot-scale and no full-scale ABRs treat domestic wastewater at ambient wastewater temperatures in temperate climates. Further, limited consistent or sufficient data and analysis inhibit development of design guidelines for ABRs. This study explores the performance of three pilot-scale ABRs receiving wastewater from three different locations within Colorado. The goal is to provide insights into similarly configured ABRs with different influent substrate compositions in an effort to bridge the knowledge gap between ABR performance and design by analyzing the operational variables and system performances.

3.3 Methods and Materials

3.3.1 ABR Descriptions

Three pilot-scale, multi-compartment ABRs were operated in three different locations near Denver, Colorado between 2012 and 2022, each receiving screened and degritted raw domestic wastewater from their surrounding communities. The systems varied in volume from 720 to 1440 L and were cylindrical or rectangular in shape with different aspect ratios, generally following the schematic depicted in Figure 3.1 (p. 32). The primary differences between the systems are highlighted here.

The Plum Creek (PC) system was in operation in Castle Rock, CO, between 2012 and 2017, receiving wastewater from Plum Creek Water Reclamation Authority, a water resource recovery facility (WRRF). The ABR consisted of four equal-sized rectangular compartments 0.46 m in width and length and a height of 1.22 m, each with a hydraulic volume of 217 L (869 L total hydraulic volume). The ABR received wastewater from a 910 L continuously mixed feed tank with a flowrate of 869 L/d and operated at a 24-hour hydraulic retention time (HRT) between March 2016 and August 2017. Additional operational information for the PC system can be found in previous publications [12, 60].

The Mines Park (MP) system was in operation in Golden, CO, between 2015 and 2022, receiving domestic wastewater from a 250-unit Colorado School of Mines campus housing complex. The ABR consisted of three equal-sized cylindrical compartments with a 0.3 m diameter and a height of 3.66 m, each with a hydraulic volume of 240 L. Each compartment contained a gas-liquid-solid separator that was located above the sludge bed but below the water surface. The ABR received wastewater from a 9,500 L holding tank that was pumped to a 150 L holding tank via a submerged grinder pump before entering the ABR. The Mines Park system primarily treated 720 L/d with a 24-hour HRT. Additional operational information for the MP system can be found in previous publications [6, 41].

The South Platte (SP) system was in operation in Englewood, CO, between 2019 and 2021 receiving wastewater from South Platte Renew, a WRRF. The system was mobile, operated from a 16' trailer, and was comprised of four cylindrical tanks 1.14 m tall with a 0.69 m diameter. The hydraulic volume of each compartment was 360 L with a total system volume of 1,440 L operated with a flowrate of 1,440 L/d or 24-hour HRT.

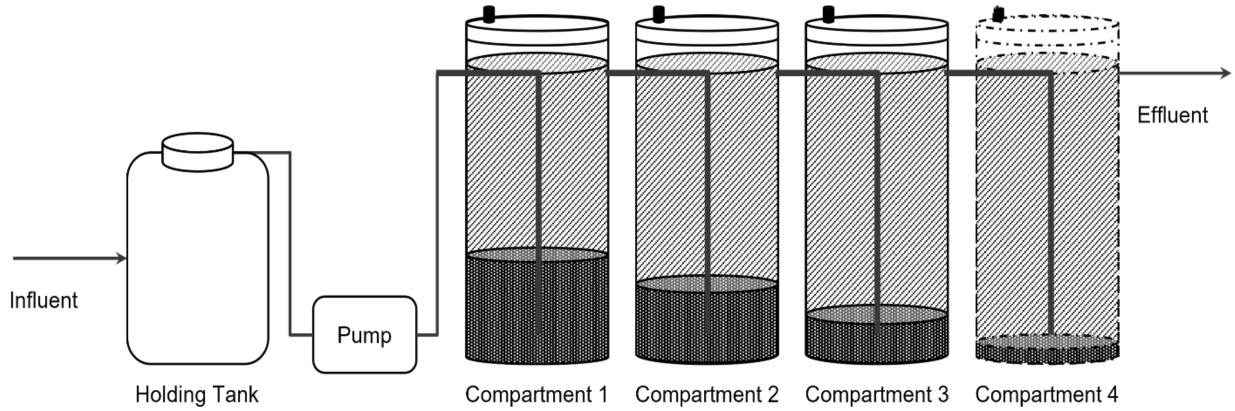

Figure 3.1 Generic schematic of a four-compartment ABR. The Mines Park ABR consisted of three compartments.

3.3.2 Data Collection and Analyses

Performance parameters and operational characteristics were measured throughout the duration of each study in accordance with the Standard Methods for the Examination of Water and Wastewater [61] or previously developed protocols. Data included probe-based temperature and pH measurements, chemical oxygen demand (total - tCOD, soluble – sCOD, and particulate – pCOD), suspended solids (total – TSS, volatile – VSS, and inorganic or fixed – ISS), sludge solids (total – TS, volatile – VS, and inorganic or fixed – IS), gas chromatography – mass spectrometry for biogas composition of CO_2 and CH_4, ion chromatography for dissolved sulfate anions (dSO_4^{2-}), Shimadzu combustion catalytic oxidation method for dissolved organic carbon (DOC), and inductively coupled plasma – atomic emission spectroscopy for dissolved elements. Specific model information for probes and equipment for each system are provided in Appendix C.1 (p. 96). Gas volumes were originally recorded based on the atmospheric pressure and laboratory temperature in Golden, CO, where analysis was performed. For this study, gas volumes were normalized to a standard temperature of 0 °C and standard pressure of 1 atm.

3.3.3 Statistical Analyses

Analysis primarily focused on the influent and effluent (final compartment) concentrations to determine the removal or accumulation for COD, suspended solids, sludge bed solids, sulfate, sulfur, and iron during 24-hour HRT operations. Compartment volumes and wastewater flowrates were utilized in converting the recorded concentrations in mg/L to loading rates (kg/m^3·d). Analysis of the intermediate compartments was completed for biogas and methane generation. All statistical analyses were performed using R (version 4.2) and RStudio (version 2022.2). Additional packages included readxl, tidyr, and dplyr for raw data manipulation; ggplot2 for graph generation; and psych and DescTools for additional statistical packages. Initial analysis included univariate descriptive statistics including central tendency (e.g., mean and median), dispersion and distribution (e.g., range and standard deviation), and measures of position (e.g., interquartile ranges and outliers). Statistically significant differences between the mean values of the three ABRs were explored using analysis of variance (ANOVA). Linear regression and correlation analysis was used for multivariate statistics to determine the relationship between variables. When data were not available for comparison of multiple constituents on the same date (e.g., methane production and COD concentrations), monthly averages were used. For data that were continuously monitored (i.e., temperature and pH), daily averages were utilized.

3.4 Results and Discussion

3.4.1 Descriptive Statistics

This section describes general statistical findings from the three ABRs. Constituent concentrations and temperatures for influent wastewater and treated effluent are tabulated in Appendix C.2 (p. 101). The Plum Creek and South Platte ABRs treated higher strength wastewater based on influent COD and suspended solids concentrations compared to Mines Park. The South Platte ABR influent contained almost 3 times as much sulfate as the other two ABR influents. ANOVA showed a statistically significant difference in the means of the three systems for effluent wastewater temperature and some of the influent constituent concentrations such as COD and suspended solids. The principal operating temperature range of the ABRs, based on first and third quartiles of the effluent wastewater temperature, was between 15 and 22 °C, with an average of 18.3 °C. Even though all ABRs operated near Denver, CO, the average South Platte effluent wastewater temperatures were statistically lower by 0.4 °C and 1.6 °C than Mines Park and Plum Creek, respectively. Though the differences between average values are less than 2 °C, closer examination shows the Plum Creek wastewater temperature never dropped below 10 °C, while the Mines Park and South Platte ABRs operated at temperatures below 10 °C approximately 4% and 6% of the operational days, respectively, which may have impacted performance. Additional details pertaining to the ANOVA results are provided in Appendix C.3 (p. 102).

Generally, influent data are skewed right with more frequent higher-than-average concentrations and median values less than the average. Sulfate and temperature are exceptions indicating more frequent lower-than-average values. The skewness decreases from the influent to the effluent resulting in data that follow a more normal distribution. The skewness and difference between average and median are important for determining typical concentrations observed in the ABRs. When the data are skewed, the average may not represent the typical. For example, the South Platte median influent tCOD concentration was approximately 500 mg/L, while the average was approximately 700 mg/L due to occasional high tCOD concentrations. These surges of tCOD may have occurred for multiple reasons, such as sampling differences, unit process failure (e.g., pump), or temporary increased loading, and therefore may not be indicative of typical influent characteristics. The difference of 200 mg/L may be important when modeling or estimating potential performance. Therefore, caution should be taken to ensure that typical values, not necessarily averages, are utilized.

Another area for caution is consistency in data collection and calculations. For these ABRs, samples for all constituents were not always taken on the same date. For example, biogas measurements may have been recorded on Mondays, while tCOD measurements were obtained on Fridays. Direct comparison of some constituents, such as methane production and tCOD removal, is thus difficult, so weekly or monthly average calculations are required. In addition, the point at which total biogas production or tCOD removal is calculated may change the values, and the differences are compounded by increasing the number of calculations. Using the South Platte ABR methane production as an example, average total gaseous methane production (sum of all compartments) was between 22 and 25 L/d depending on whether monthly or daily averages were used. Average tCOD removal varied between 623 and 661 g/d depending on whether the average was calculated from daily or monthly values and whether the removal calculation was computed daily or based on final average influent and effluent values. Subsequently, this results in multiple "averages" of L CH_4 produced/g tCOD removed varying between 0.04 and 0.12, all from the same data. In this study, calculations were performed first, and averages of those calculations are reported. The varying concentrations between the three systems, displayed in Table C.1 (p. 98) and Table C.2 (p. 99), coupled with ANOVA (Figures C.1-C.6, p. 103-106), depict the differences in influent wastewater characteristics and system performance. Additional differences pertaining to methane generation, constituent ratios, effluent concentrations, and removal performance are discussed in further detail in subsequent sections.

3.4.2 Biogas and Methane Production

One of the key performance indicators for anaerobic treatment systems is the ability to produce methane-rich biogas for subsequent recovery of the energy for heat or power. Anaerobic treatment processes generate biogas that is 55-70% methane [3, 11, 62]. The average percentage of methane in the biogas for all three ABRs was 63%, indicating the biogas has a high energy content and is amenable to beneficial use for electricity generation, natural gas vehicles or pipeline injection. However, the percentage varied from 5 to 98% for the three systems. Percent methane in biogas can vary widely depending on wastewater composition, environmental and operational conditions, which should be characterized to optimize production of methane and achieve a consistent quality of biogas.

The volumetric output of methane of the ABRs is depicted in Figure 3.2. As methane generation is a function of the wastewater composition and the system size, performance should be normalized to COD removal for more readily comparable results. Stoichiometrically two moles of oxygen (as O_2) are required to convert one mole of methane to carbon dioxide and water, so that 1 mole of methane is equal to 64 g of COD. Where a mole of an ideal gas at 0 °C and 1 atm (STP) occupies 22.4 L, the theoretical amount of methane produced per gram of COD converted is 22.4 L/64 g COD or 0.35 L/g COD [3, 11]. Average gaseous methane yields (at STP) normalized to the amount of tCOD removed for the three ABRs ranged from 0.12 to 0.25 L CH_4/g $tCOD_{rem}$. Combined, the average for all three ABRs was 0.21 L CH_4/g $tCOD_{rem}$.

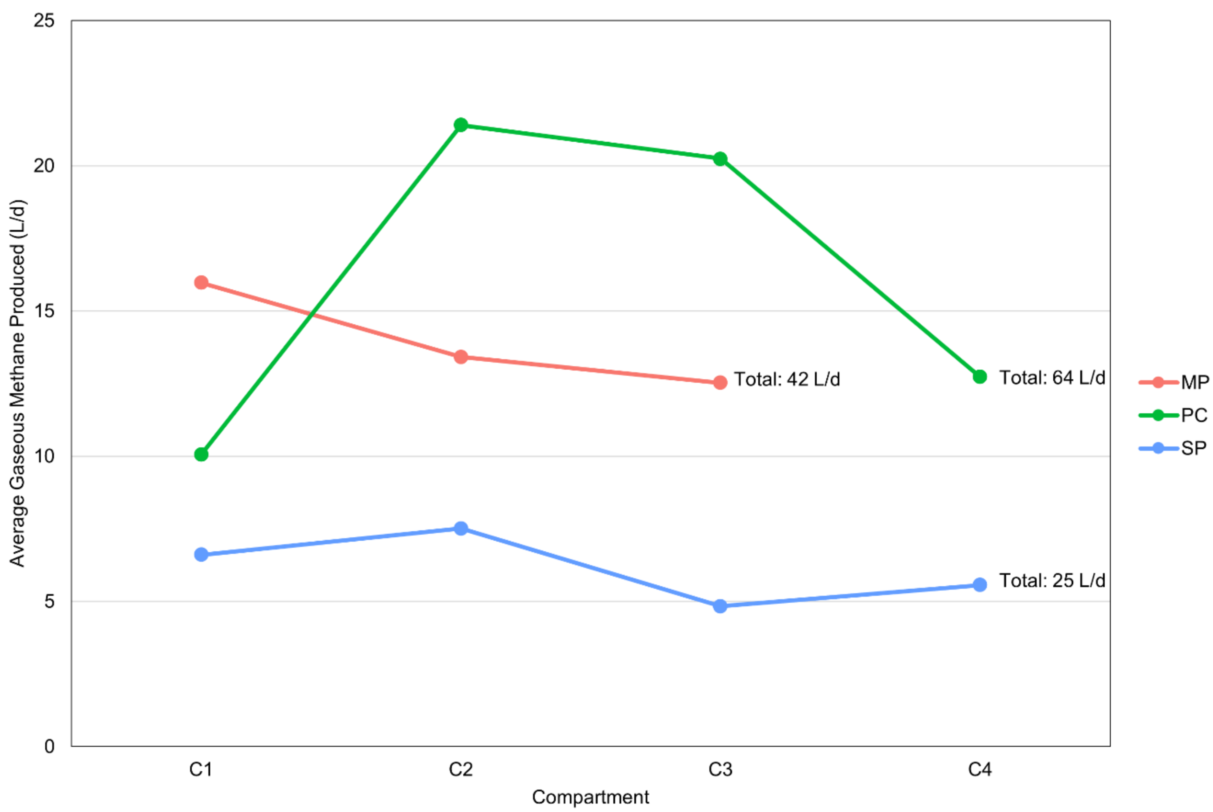

Figure 3.2 Average methane production by compartment and ABR location.

Dissolved methane within the effluent wastewater was not included in this study due to insufficient data for all three ABRs. However, inclusion of effluent dissolved methane concentrations would likely result in methane yield closer to the stoichiometric value. Any future examination of methane production should include dissolved methane concentrations as the dissolved portion can make up a large percentage (22 - 75 %) of total methane production [12, 55, 63, 64], with increased solubility of methane at lower temperatures, lower salinity and higher pressure [65, 66]. These values are important for determining total potential energy production in cases where dissolved methane is recovered (i.e., air stripping or membrane separation), but are also important for determining potential environmental impacts if not recovered [67, 68].

Mines Park produced methane near the stoichiometric value, but methane yields in all three systems were similar to those observed in other studies. Lettinga et al. (1983) observed methane yields between 0.12 and 0.44 L CH_4/g $tCOD_{rem}$ using a 120 L UASB operated at ambient temperatures between 6.5 and 19.5 °C treating domestic wastewater with influent COD concentrations similar to those in this study. Lettinga's study showed an increase of methane yield with increased temperature, which was not observed in this study. Yang & Chou (1985) observed methane yields between 0.04 and 0.27 L CH_4/g $tCOD_{added}$ while treating dilute swine waste using a 20 L baffled reactor at an ambient temperature of 30 °C; note that their results were reported as L CH_4 per gram of tCOD added, while results in this paper are reported per gram of tCOD removed. Yang and Chou provided sufficient information to calculate methane yield based on tCOD removed, 0.09 to 0.48 L CH_4/g $tCOD_{rem}$. Their highest yield was observed with a tCOD organic loading rate (OLR) of 0.92 kg/m^3·d and a 120-hour HRT. In contrast, the lowest yield was with an OLR of 13.5 kg/m^3·d and a 6-hour HRT, indicating that a longer HRT and/or lower OLR produces higher yield. In this study, methane yield was negatively correlated with tCOD loading (R^2 = 0.22, p = 1.3E-5). As a cautionary note, many publications reviewed for this study did not contain sufficient information to determine methane yield. Further, when methane production was provided, often it was uncertain whether dissolved methane concentrations were included and under what conditions methane calculations were performed (i.e., STP or local pressure and temperature). When using the Ideal Gas Law to calculate methane generation, the number of moles (or volume) increases with increased temperature or decreased atmospheric pressure and may account for the reported methane yields greater than the theoretical (0.35 L CH_4/g COD_{rem}). As noted by Shoener et al. (2014) in their review of the energy potential of anerobic wastewater treatment technologies, hundreds of papers may be screened for inclusion in an analysis but few may actually be utilized due to insufficient data meeting inclusion criteria (e.g., 3 ABR papers of 225 reviewed).

No strong correlations (i.e., $r < -0.7$, $r > 0.7$ or $R^2 > 0.49$) were apparent between gaseous methane generation (or methane yield) and any other daily recorded values or monthly averages across all three ABRs. Individual ABR systems showed isolated correlations between methane generation or yield and factors such as temperature and TSS concentration, but nothing consistent (indeed, sometimes opposite correlations) across the reactors. A weak correlation (R^2 = 0.24) was noted for total volumetric methane production and sulfate loading (Figure 3.3, p. 37). Additionally, the amount of tCOD removed (g/d) and the amount of methane produced (L/d) were only weakly correlated, with an R^2 = 0.28 (Figure

3.4.A, p. 38). However, by forcing the linear regression through the origin, a stronger relationship is observed with R^2 values between 0.67 and 0.9 for the individual ABRs (Figure 3.4.B, p. 38). The coefficients (or slopes) of the different ABR linear models are lower than the average values discussed previously; however, this approach highlights the difference in performance where the Mines Park ABR generated the most methane per COD removal and the South Platte ABR generated the least.

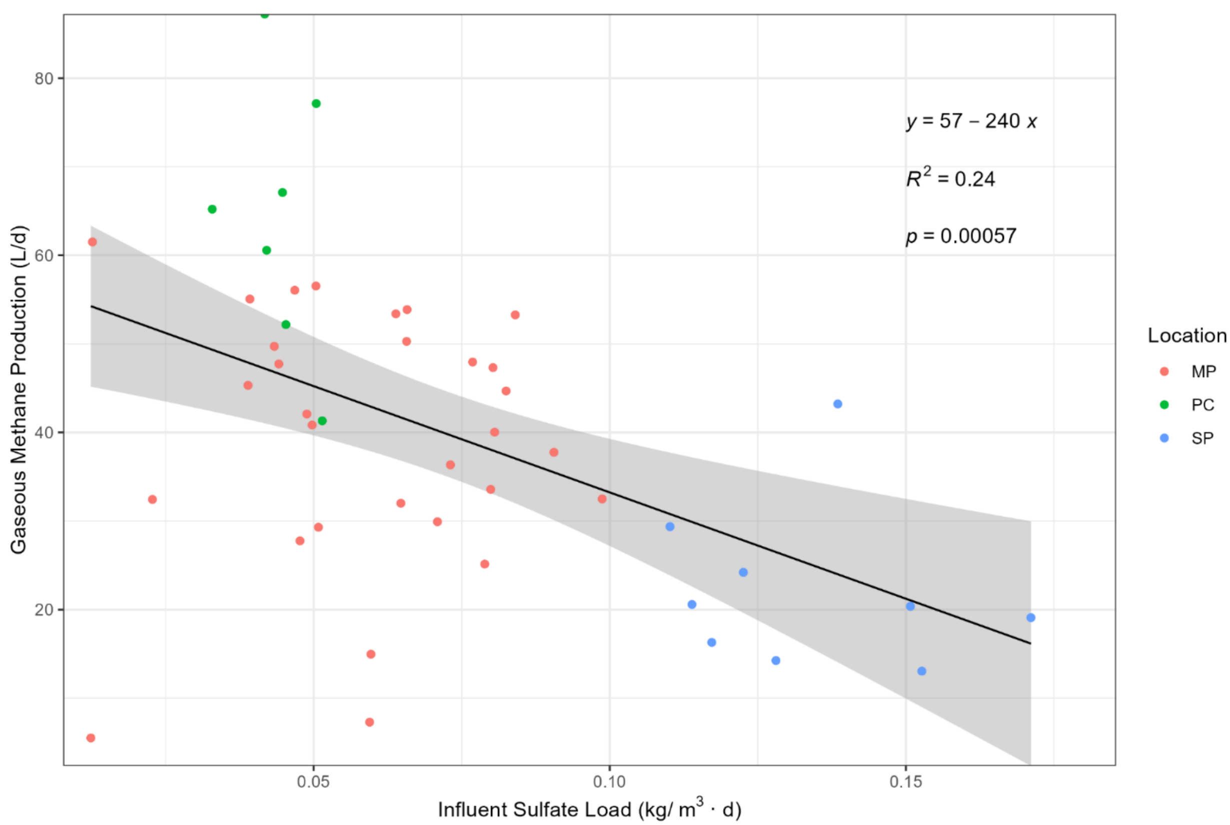

Figure 3.3 Linear model of monthly average influent sulfate loading as a predictor of total system volumetric methane production.

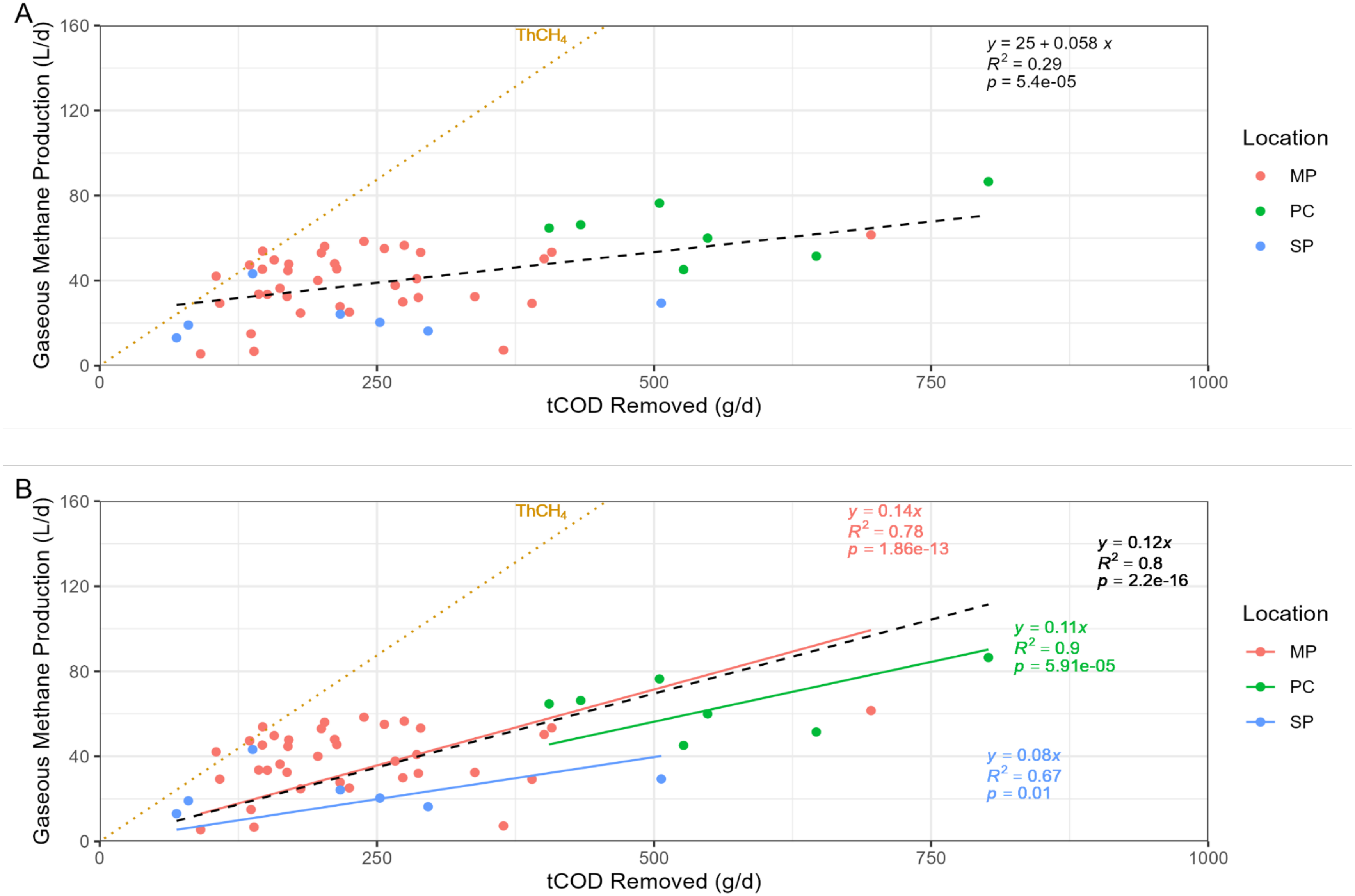

Figure 3.4 Average monthly tCOD removal as a predictor of total methane production. (A) linear model and (B) linear model through the origin. B includes the equations, R^2 and p-values for each system separately, with the combination of the systems in black.

Given the lack of strong correlation data, the higher average methane yield observed in Mines Park compared to the other systems may be due to the differing influent wastewater characteristics. Influent wastewater to the Mines Park ABR originated from a septic tank where hydrolysis of the particulate matter may have occurred, leading to the increased sCOD and VFA concentrations. Similar hydrolysis would have occurred in the first compartments of the Plum Creek and South Platte ABRs, leading to one less compartment suitable for higher methane production. One factor not observable in the combined data set was that the compartment with the highest average incoming sCOD concentration produced the largest volume of gaseous methane in each of the ABRs. The second compartment produced the most biogas and gaseous methane for the Plum Creek and South Platte ABRs, while the first compartment produced the most in the Mines Park ABR.

Additionally, high concentrations of influent sulfate, as observed in the South Platte influent, have been shown to inhibit methane production in anaerobic systems due to competition for electron donors (e.g., hydrogen and acetate) between sulfate-reducing bacteria and methanogens or sulfide toxicity [71, 72]. Further, the more energetically favorable anaerobic oxidation of methane and sulfidogenic reactions can contribute to the reduced percentage of methane and increased carbon dioxide in the biogas [72–74]. Median tCOD/sulfate ratios in all compartments (including the influent) at South Platte were between 2.5 and 5 (sCOD/sulfate between 0.8 and 2.7); tCOD/sulfate ratios of less than 10 are known to reduce methane production [71, 72]. In contrast, the tCOD/sulfate ratios for the other ABRs were between 10 and 30 (sCOD/sulfate between 4 and 17). No correlations were noted for the tCOD/sulfate ratio; however, a higher influent sCOD/sulfate ratio improved methane production ($r = 0.6$). The average influent concentration for the South Platte ABR was approximately 140 mg SO_4^{2-}/L but varied between 110 and 185 SO_4^{2-}/L. The sulfate concentration was reduced to an effluent concentration averaging 60 mg SO_4^{2-}/L (average removal 80 mg SO_4^{2-}/L or 60%). The largest concentration reduction of sulfate occurred in the first compartment, with the removal of an average of 40 mg SO_4^{2-}/L, with each subsequent compartment removing half again as much. As the concentration of VFAs increased in the compartment (particularly acetate and propionate), sulfate removal also increased ($r > 0.88$). The increase in sulfate reduction appeared associated with the decrease of the percentage of methane in the biogas ($r = -0.63$) as well as the overall yield of methane per gram of tCOD removed ($r = -0.55$). Increased availability of sCOD (and VFAs) through potential pre-ABR hydrolysis or lack of competition for the substrate by sulfate reduction appears to improve methane generation performance when the three ABRs are compared together. However, other factors may affect an individual reactor's performance, such as temperature, HRT, OLR, and suspended solids.

3.4.3 Oxygen Demand

Another performance indicator for anaerobic treatment of wastewater is the ability of the system to remove organics and associated oxygen demand. When examining available substrates for microbial activity, tCOD can be divided into biodegradable and nonbiodegradable matter. Both biodegradable and nonbiodegradable COD are observable as particulate and soluble forms of the total. The particulate biodegradable COD is considered slowly biodegradable as the material must be further degraded or hydrolyzed into the biodegradable soluble form of COD. The resulting sCOD, primarily comprised of volatile fatty acids, is readily available for further fermentation and/or uptake and use by the methanogen populations for production of methane [3, 25]. Subsequently, influent wastewater with higher percentages of pCOD (of the total) have less readily available substrate and the additional hydrolysis required will be observed through increased biodegradable pCOD removal, principally in the initial compartments of ABRs.

The total, particulate, and soluble COD influent loading and removal efficiency (percentage removed) varied between systems; however, the three systems all produced similar tCOD effluent values (when normalized to flow and volume) near 0.23 $kg/m^3 \cdot d$. Figure 3.5 (p. 41) depicts loading and removal of COD for each of the ABRs (additional details available in Table C.3, p. 106). Generally, the highest tCOD removal rate (averaging 0.58 $kg/m^3 \cdot d$ and 71%) was observed in the Plum Creek ABR, while the Mines Park and South Platte ABRs removed ~48%. Together, there was no correlation with temperature ($R^2 = 0.07$, $p = 6.9E\text{-}8$). Closer examination of the ABRs independently showed Mines Park and Plum Creek percent tCOD removal was positively correlated with wastewater temperature ($R^2 = 0.34$, $p = 7.3E\text{-}7$) while South Platte was not ($R^2 = 0.02$, $p = 0.57$).

Similar removal efficiencies (50-90%) have been observed in bench-scale (< 100 L) ABR studies [75–77] treating domestic wastewater operated at ambient temperatures (3-35 °C). However, the ABR efficiencies in this study were lower than the 90%+ observed in pilot ABR studies [78–80] using synthetic wastewaters at temperatures between 15 and 30 °C. The anaerobic system studied by Yang & Chou (1985) averaged removal efficiencies between 42 and 81% while treating diluted swine wastewater at 30 °C with varying tCOD OLR (all > 0.92 $kg/m^3 \cdot d$) and HRT between 6 and 120 hours; highest removal efficiencies were noted for HRTs between 19 and 32 hours. Foxon et al. (2006) utilized a 3000 L ABR to treat wastewater in two different locations in South Africa. At the first location, Umbilo, the ABR was operated at an average loading rate of 0.85 $kg/m^3 \cdot d$, HRT of 20 hours, and removed an average of 62% of the tCOD (unspecified operating temperature). The tCOD removal was lower (47%) with a longer HRT (60 hours) and lower OLR (0.3 $kg/m^3 \cdot d$), which may have been due to ABR start-up and stabilization. While detailed wastewater composition was not provided, the influent wastewater in the first

Foxon location (Umbilo) contained a mixture of domestic and industrial wastewater. In the second location, Kingsburgh, where only domestic wastewater was treated, average tCOD removal was 57% with an OLR of 0.84 kg/m^3·d and HRT of 20 hours and average ambient temperature of 22 °C. In contrast to the Umbilo location, removal efficiency increased to an average of 81% with increased HRT (40 hours) and decreased loading (0.4 kg/m^3·d). However, neither longer HRT nor increased temperature appeared to be a factor in improving tCOD removal efficiency in the reviewed studies. As the percent tCOD removal for the Colorado ABRs (interquartile range between 40 and 69% with 53% average) was within the range of values observed in other studies treating wastewater (non-synthetic) at ambient temperatures, increasing HRT or temperature may have no significant effect. However, the variations in the tCOD removal rates and efficiencies between the three ABRs in this study and those reported in other studies emphasize the need for pilot or bench-scale studies using the same wastewater and operating conditions of any proposed full scale treatment system.

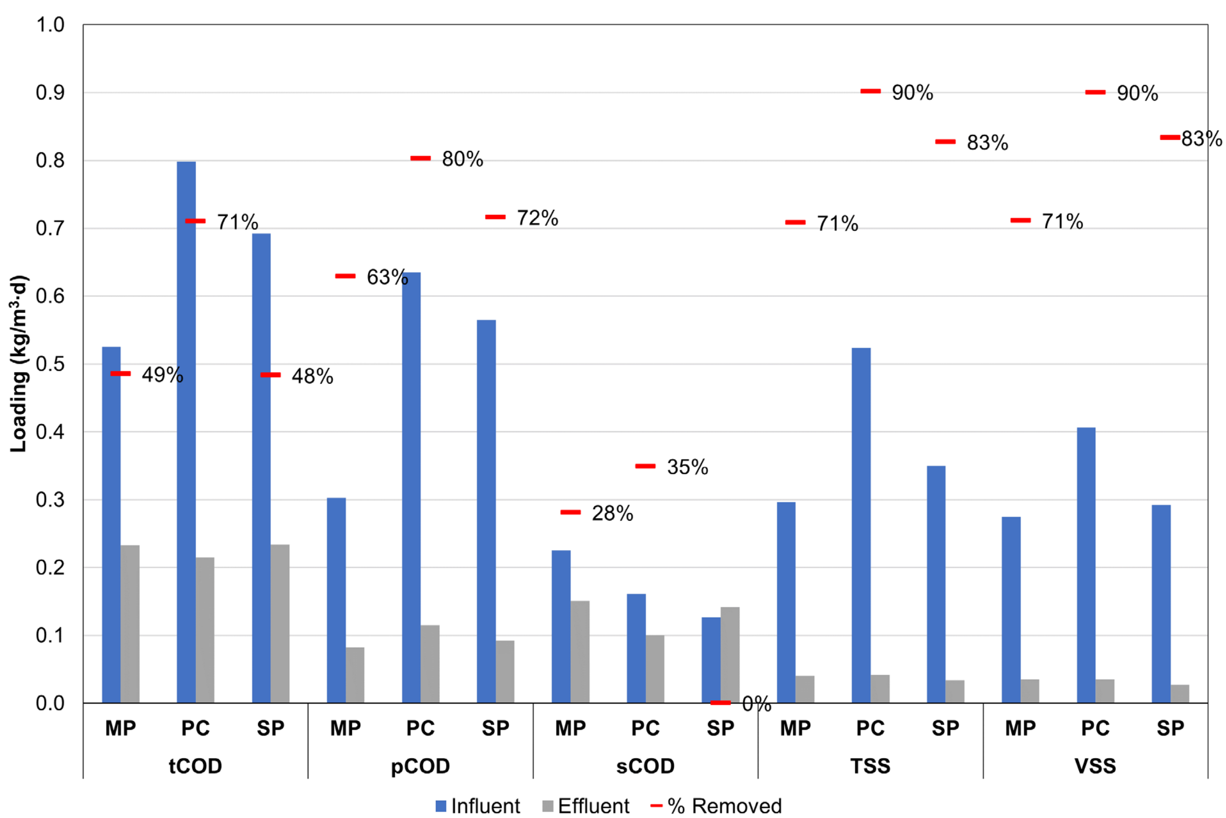

Figure 3.5 Average tCOD, pCOD, sCOD, TSS and VSS loading (kg/m^3·d) and percent removal (red lines) by location. The supporting table is located in Appendix C.4 (p. 106).

While much literature reviewed for this study reported a decrease in removal efficiency with increased tCOD loading or decreased temperature, the three Colorado ABRs saw increased percent removal efficiency with increased influent tCOD loading (depicted in Figure 3.6.A, p. 44). Since influent loading is a component of the calculation for removal efficiency, a test for collinearity was conducted and determined not to be problematic (documented in Appendix C.5, p. 107). However, the correlation is likely subject to maximum OLR or removal efficiency. The Plum Creek ABR, with the highest tCOD OLR and removal rates, indicates the limit may be near 1.1 $kg/m^3 \cdot d$ and 83% (maximum values, excluding outliers). Additionally, the decrease in removal efficiency observed by Yang and Chou (1985) and Yu and Anderson (1996) was for increasing OLR between 0.92 to 13.52 $kg/m^3 \cdot d$. In contrast, the ABRs for this study generally observed lower tCOD OLR with an interquartile range between 0.38 and 0.68 $kg/m^3 \cdot d$.

As pCOD is a component of tCOD and the biodegradable portion of pCOD is converted to sCOD, it is unsurprising that all three ABRs had higher pCOD removal efficiency than tCOD or sCOD. For literature reporting particulate COD (and/or soluble COD), this is a commonly observed occurrence where pCOD removal efficiency is approximately 5-10% higher than tCOD [35, 78, 82–84]. However, pCOD may also settle to the sludge bed and thereby reduce the concentrations observed in the wastewater samples. COD concentrations in the sludge beds of the three ABRs were not recorded during the 24-hr HRT but based on available data for sludge bed height and solids concentrations, no accumulation of solids was apparent. The increase in the sCOD concentrations (and sCOD:tCOD ratios), with no solids wasting or accumulation, indicates pCOD was being transformed, rather than just settling. The most substantial difference between the ABRs in this study was the pCOD and sCOD percentages of the tCOD in both the influent and effluent. For Mines Park, sCOD comprised 47% of influent tCOD and 66% of effluent. While Mines Park influent sCOD comprised just less than half of influent tCOD, sCOD exceeded pCOD beginning with the first ABR compartment. In contrast, the Plum Creek and South Platte ABR influents consisted of 80% pCOD. Therefore, the South Platte and Plum Creek upstream compartments were dominated by the process of hydrolysis and the conversion of pCOD to sCOD. The Plum Creek ABR system effluent tCOD remained approximately 50% sCOD, while the South Platte ABR continued to hydrolyze pCOD throughout the system so that approximately 20% of the remaining pCOD was removed from each subsequent cell and sCOD comprised 61% of effluent. As mentioned previously, the higher influent sCOD concentrations observed in the Mines Park ABR likely contributed to the increased methane production in the first compartment in comparison to the other two ABRs (Figure 3.2, p. 35). Additionally, the high conversion of pCOD to sCOD in the South Platte and Plum Creek ABRs accounted for the increased pCOD removal efficiency observed in those systems. It cannot be determined exactly how much sCOD and VFAs were created and how much was utilized as samples collected only provide a snapshot of the concentration at that moment. However, sCOD concentration generally decreased from the influent to the effluent in the Mines Park and Plum Creek ABRs, whereas sCOD increased in the South Platte ABR. The sCOD concentration at South Platte increased in the system as indicated by the low tCOD removal and shift in pCOD:tCOD ratio from 0.78 in the influent to 0.39 in the effluent. As the Plum Creek ABR generated substantially higher methane than the South Platte ABR, the methanogen population at Plum Creek was likely more active, more efficient, or experienced less competition for the substrate.

One final important component of COD removal correlations was sulfate concentrations. Combined, there was no correlation between influent sulfate concentrations or sulfate loading and system tCOD removal for the three ABRs. Generally, all COD removal efficiencies declined with increased influent sulfate concentrations in the ABRs, but with low R^2 values and high p-values. In the Mines Park and Plum Creek ABRs, negative correlations (r between -0.68 and -0.01) with system tCOD removal efficiency were also observed when comparing sulfate concentrations in subsequent compartments. No other correlations were noted with the compartments beyond the decreased biogas and methane production previously discussed. In contrast, the South Platte tCOD removal had positive r values (between 0.05 and 0.64) with subsequent compartment sulfate concentrations, and additional correlations were found with sulfate removal and sludge bed solids. In the South Platte ABR, the largest reduction of sulfate occurred in the first compartment, with approximately 55-60% drop in concentration. Subsequent compartmental sulfate concentrations and removal were lower, with less than 20 mg SO_4^{2-}/L and less than 30% removal. When biogas and methane production increase from the microbial conversion of soluble VFAs, sCOD would also be reduced. However, the sulfide produced by sulfate reduction would exert an oxygen demand (leading to decreased tCOD removal efficiency and higher sCOD concentrations). As the system sulfate removal increased, the amount of non-volatile (inorganic) sludge bed solids increased and as the solids increased, COD removal decreased. South Platte COD removal appeared inhibited by the presence of high inorganic sludge solids, especially in the third and fourth compartments, which comprised the largest percentage of total sludge bed solids for the system (Figure 3.7, p. 45). Future study is recommended to investigate the use of recirculation of the high sCOD effluent, a longer residence time holding tank or an additional treatment compartment, and periodic removal of the sludge bed solids to improve methane generation and removal of COD and solids in ABR systems with significant influent sulfate.

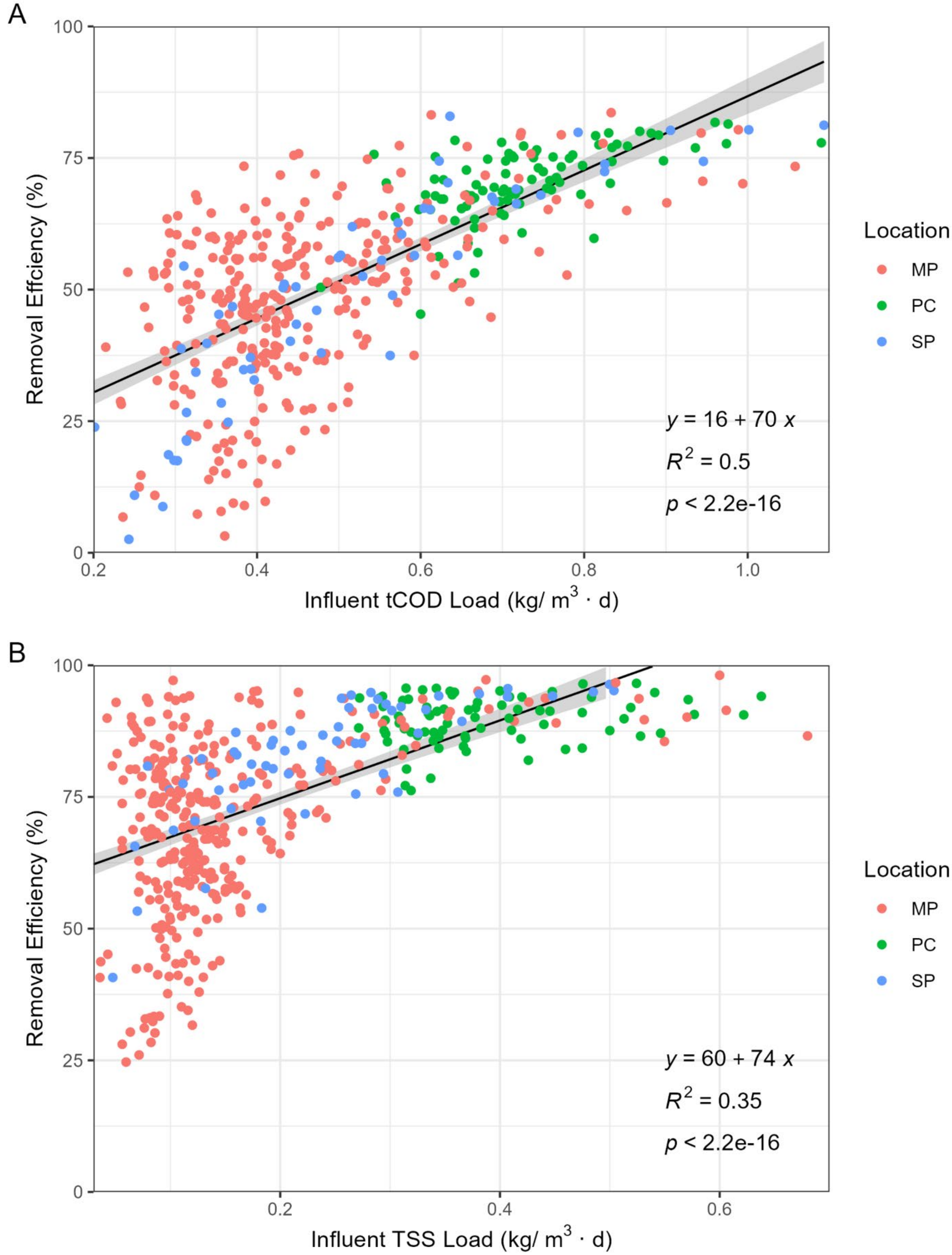

Figure 3.6 Linear model of the system removal capacity in relation to average influent loading of tCOD (A) and TSS (B).

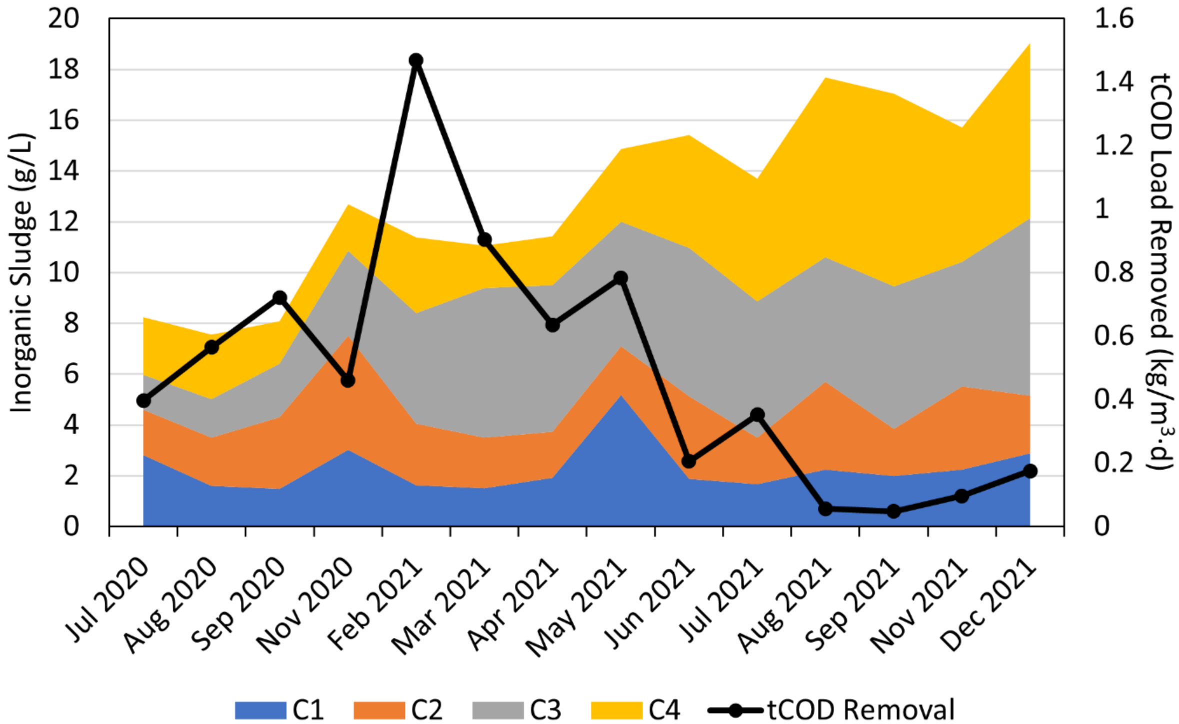

Figure 3.7 tCOD removal for the South Platte ABR decreased as the inorganic sludge concentration increased in the compartments, especially in C3 and C4.

3.4.4 Suspended Solids

The final area of performance examined in this study was removal of suspended solids, which is important for reducing turbidity and preventing sludge deposits when effluent is discharged to the environment [3]. In the U.S., suspended solids performance is judged based on removal efficiency, like COD, but also on the ability to meet the U.S. Environmental Protection Agency's (USEPA) secondary treatment standards for effluent TSS of 30 mg/L [85]. As with the division of tCOD into biodegradable and non-biodegradable discussed above, TSS is sub-divided into organic and inorganic matter, with the organic matter representing the portion available for microbial degradation. Although some organic matter may not volatilize and some inorganic matter may volatilize at the standard temperature of 550 °C used to differentiate between the two, the VSS measurement is generally accepted as the organic (though not necessarily the biodegradable) portion of TSS and ISS as the inorganic [3, 25, 61]. Wastewater with higher percentages of VSS indicate substrate-rich material including microorganisms. Because microbial biomass is primarily organic material, VSS is often used to measure biomass growth. The yield for aerobic biological treatment process is approximately 0.4 g VSS/g COD removed [3]. However, in anaerobic treatment systems, the yield is even smaller in comparison to COD removal, where anaerobic fermenters may produce between only 0.06 and 0.12 g VSS/g COD used and methanogens even less with approximately 0.04 g VSS/g COD used [3, 86]. Thus, despite the VSS yield of microorganisms, the yield is not expected to exceed the removal of organic matter as COD or VSS.

Figure 3.8 (p. 47) depicts the linear regression models for the monthly average influent and effluent concentrations of VSS as a fraction of TSS for each of the ABRs, demonstrating the strong linear relationship between TSS and VSS as indicated by low p-value and high R^2 values. At Mines Park, VSS comprised approximately 90% of the TSS influent and effluent. At South Platte, ABR VSS comprised approximately 83% of the influent and effluent TSS. Only in the Plum Creek ABR did the percentage of VSS increase, from 82% of the TSS in the influent to 86% in the effluent. Despite the higher percentages of influent ISS in the Plum Creek and South Platte ABRs, sufficient organic matter and active biomass was present to achieve high TSS removal efficiencies (90% and 83%, respectively, compared to 71% observed at Mines Park; Figure 3.5, p. 41). As the TSS was primarily comprised of VSS and the linearity was so strong, the correlation of factors relevant to both TSS and VSS removal were the same. Similar to tCOD, the removal efficiency was positively correlated with influent loading for all three systems (Figure 3.6.B, p. 44). As system tCOD and pCOD removal efficiencies increased, suspended solids removal efficiencies also increased ($r \sim 0.74$); however, no other strong positive or negative correlations were observed.

Plum Creek received the highest influent concentration and suspended solids loading, while Mines Park received the lowest. Even with 90% removal efficiency, due to the high loading Plum Creek was unable to meet the USEPA secondary treatment standards, averaging effluent TSS concentration of 42 mg/L. The Mines Park ABR effluent TSS concentration averaged 40 mg/L, achieving concentrations below the USEPA standard approximately 35% of the time. While no strong correlation existed between temperature and effluent concentrations ($r < -0.41$) or removal efficiency ($r < 0.3$), compartmental wastewater temperatures were usually above 21 °C when effluent concentrations were below 30 mg/L at Mines Park. The South Platte ABR also exceeded the standard approximately 50% of the time, with an average effluent concentration of 34 mg/L.

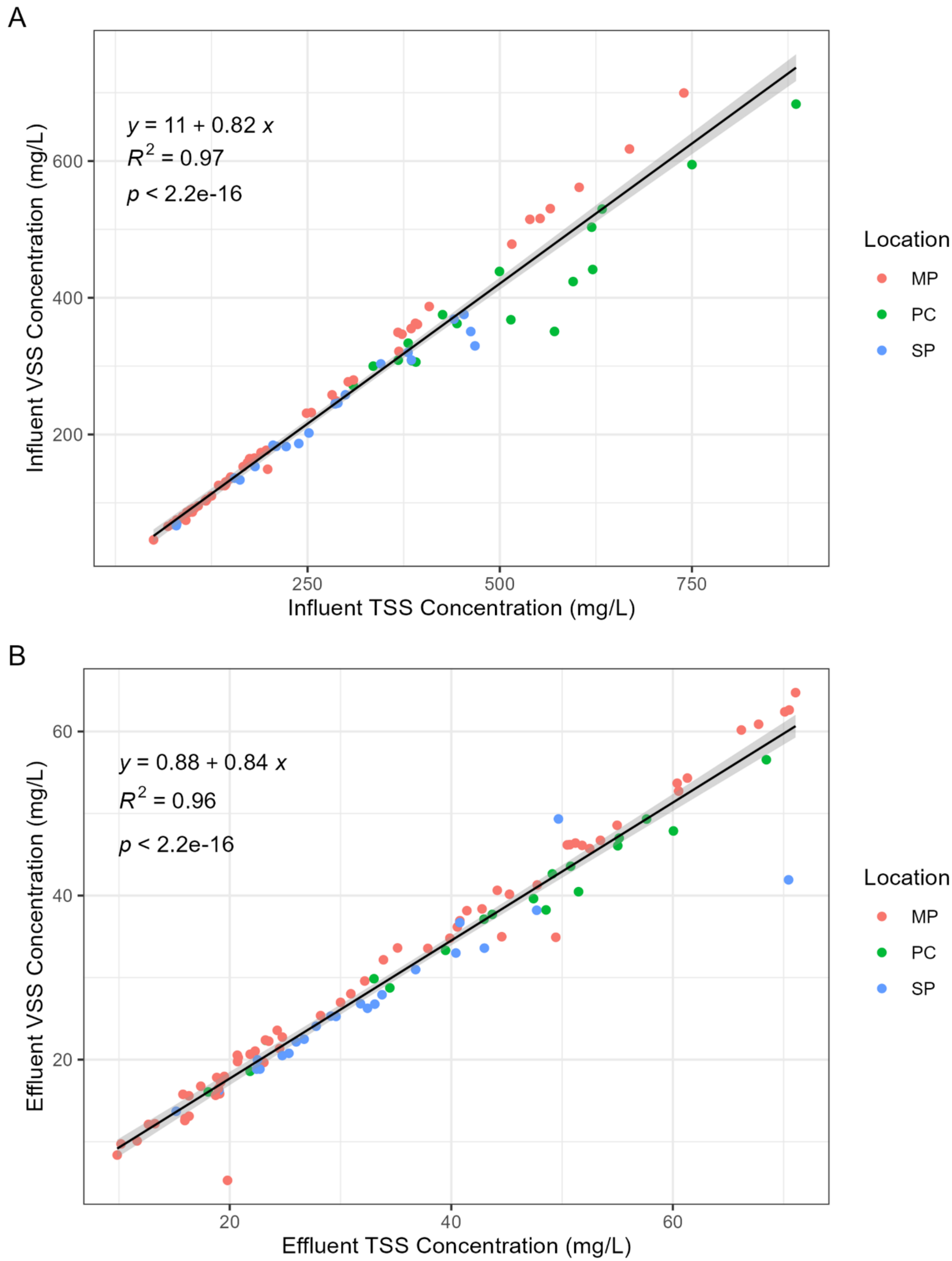

Figure 3.8 Linear models for influent (A) and effluent (B) average monthly TSS and VSS concentrations for all locations.

While average effluent concentrations were not consistently below the requisite 30 mg/L, the TSS removal efficiencies were similar to other ABRs and consistently higher than the average of 60% seen in traditional primary settling tanks [3]. Gopala Krishna et al. (2008) and Manariotis & Grigoropoulos (2002) observed TSS removal percentages between 74 and 92% using synthetic wastewater with average influent suspended solids concentrations below 210 mg/L. Yang & Chou (1985) observed removal efficiencies between 36 and 88% with varying influent TSS concentrations between 250 and 1450 mg/L in diluted swine wastewater, which generally increased with increased HRT. Wade (2015) observed higher removal efficiencies (95%) with lower HRT (~13 hours) with influent TSS concentrations between 112 and 305 mg/L. However, wastewater temperature was controlled at 15 and 20 °C. In contrast, Foxon et al. (2004) and Schalk et al. (2019) observed lower TSS removal efficiencies of 53 and 42%, respectively, in their larger scale (3000 and 9800 L) ABRs treating domestic wastewater at ambient temperatures in South Africa and Germany. The largest difference between the Schalk and Foxon studies was that influent TSS concentrations for Schalk were near the ABRs in this study (~140 mg/L) and the Foxon study observed an average influent concentration of 480 mg/L. The Foxon study was one of the few reviewed to report VSS values and showed an average of 64% VSS of TSS. Other domestic wastewater studies that reported VSS concentrations or percentages of TSS were between 80 and 91% [83, 88]. The influent TSS concentrations for the ABRs in this study varied between 40 and 680 mg/L while generally achieving removal efficiencies greater than 64% (Q1) and average effluent concentrations of 40 mg/L. However, the percentage of VSS was never below 73% of the TSS. Subsequently, higher loading rates or lower VSS:TSS ratios may warrant increased HRT or influent holding to allow for an increased percentage of VSS or TSS removal.

One final note about suspended solids removal involves the ISS. Typical wastewater concentrations of ISS vary between 10 to 100 mg/L depending on whether the wastewater is raw or settled, with the lower concentrations observed following primary treatment [3, 25]. These inorganic or non-biodegradable portions of the total suspended solids are generally expected to remain in and possibly accumulate in traditional aerobic treatment systems absent good solids management. In anaerobic treatment systems, which typically have longer HRTs than aerobic systems and extended solids retention times, the ISS retained in the compartments is likely degraded, although slowly. This conversion of non-biodegradable to biodegradable may be evidenced by the reduction in ISS concentrations in all three ABRs. Plum Creek average influent ISS concentration was 120 mg/L with 89% removal, South Platte average influent ISS concentration was 57 mg/L with 80% removal, and Mines Park average influent ISS concentration was 23 mg/L with 68% removal. The ISS removal may have occurred due to settling into the sludge beds. However, the IS concentrations in the Mines Park ABR sludge beds averaged ~5 g/L without substantial variations (based on first and third quartiles between 2 and 7 g/L) and no active solids wasting throughout the experiment. Limited sludge bed data were available for the Plum Creek ABR, however during the three years of 12-hour HRT operation, sludge bed IS concentrations remained between 0.4 and 5 g/L, again with no active solids wasting. Even in the South Platte ABR, which did accumulate inorganic matter in the sludge beds of the two latter compartments, the accumulation and decreased ISS removal performance did not occur until after 18 months of operation. ISS removal was observed in other ABR studies with efficiencies between 44 and 100%, but sludge bed inorganic data were not provided [78, 81, 83]. While data are limited, this removal of ISS coupled with established lower VSS yields by methanogens in comparison to aerobic microbial communities show the decreased requirement of solids treatment in comparison to traditional aerobic treatment practices requiring constant active wasting.

3.5 Conclusions

This study examined the performance of three ABRs treating wastewater under similar operating conditions in Colorado. Despite sharing location, temperature, and HRT, the ABRs displayed distinct performances, highlighting the significance of influent wastewater characteristics. For example, temperature and sulfate concentrations appeared to negatively impact tCOD removal for Mines Park and Plum Creek, while the South Platte ABR showed a different trend, where increased effluent sCOD concentrations, sulfate removal, and inorganic sludge bed solids negatively impacted tCOD removal performance. Importantly, the size and shape of the ABR did not appear to significantly affect performance. The Plum Creek ABR, composed of short square compartments, exceeded the removal efficiencies for COD and suspended solids and volumetric methane production of the other two ABRs. While the short cylinders of the South Platte ABR and the tall cylinders of Mines Park showed comparable results. However, all ABRs may have benefitted from diffusion of influent substrate across the sludge bed, common in other anaerobic sludge bed designs, to maximize the microbiota to substrate contact.

Gaseous methane yield for all ABRs averaged 0.21 L CH_4/g $tCOD_{rem}$. Notably, Mines Park achieved the highest methane yield (0.25 L CH_4/g $tCOD_{rem}$), possibly due to upstream septic tank hydrolysis, resulting in 47% of influent tCOD being sCOD, and lower sulfate concentrations. The South Platte ABR, with the highest percentage of pCOD in the influent tCOD and the highest concentration of sulfate, produced the least methane. Sulfate loading and the sCOD to sulfate ratio influenced methane production, accounting for 24% and 36% of the variability, respectively. This analysis showed that even at psychrophilic temperatures, approximately 60% of the biogas generated is expected to be methane and methane yield can be near stoichiometric values. Methane production can be improved with increased influent sCOD concentrations and decreased sulfate concentrations. When considering full-scale design, this can potentially be achieved through recirculation of high sCOD effluent, such as with the South Platte ABR, or the use of a holding tank or equalization basin where preliminary settling and microbial activity can increase the sCOD to tCOD or sulfate ratios, as observed in the Mines Park ABR. Future studies or designs should include effluent dissolved methane concentrations as the dissolved portion can make up a large percentage of total methane production and is relevant to both methane use or greenhouse gas emissions.

Additionally, this study demonstrated the ability of ABRs to handle a variety of COD and solids loadings while producing consistent effluent concentrations. COD loading ranged between 0.1 and 3.8 $kg/m^3 \cdot d$ between the ABRs, all achieving an average effluent concentration of 230 mg/L (± 66 mg/L). TSS loading varied between 0.03 and 4.5 $kg/m^3 \cdot d$, achieving average effluent concentrations of 40 mg/L (± 21 mg/L). In addition to the high TSS removal efficiency, ~80%, designs for ABRs can expect seldom active sludge wasting compared to the constant daily wasting rates of aerobic systems due to the substantially lower anaerobic microbial growth rates and ISS removal. ABRs designed for higher removal rates should consider HRTs longer than 24 hours or the same potential pre-treatment for improving methane production.

While these general design principles can be interpreted from the results of this study, the variations observed between the three ABRs underscore the importance of conducting further study for any proposed full-scale treatment system using on-site wastewater. Additional studies enable designers to identify crucial variables, such as temperature, sCOD, or sulfate concentrations, that may uniquely impact ABR performance. By carefully assessing these factors, the design and optimization of ABR systems can be tailored to specific wastewater characteristics, leading to more efficient and reliable wastewater treatment processes.

3.6 Acknowledgements

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CHAPTER 4

ANAEROBIC CO-DIGESTION FOR DOD INSTALLATION ENERGY SECURITY – MODELING ENERGY PRODUCTION AND CARBON EMISSION REDUCTION

A manuscript in preparation for *Cleaner Environmental Systems*.

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4.1 Abstract

This study presents a consequential life cycle assessment (LCA) of anaerobic co-digestion (AnCoD) as a renewable energy solution for wastewater treatment plants at military installations. The LCA was conducted in accordance with the International Organization for Standardization (ISO) 14040 and 14044 framework using Sphera's Life Cycle Assessment for Experts (LCAFE) software and supplemented with information from the ecoinvent database. The goal was to determine if AnCoD generates sufficient high-quality biogas to warrant biogas capture and use. The study focuses on the solids handling phase of wastewater treatment plants, specifically the anaerobic digestion of waste sludge, with the addition of food and fats for co-digestion. The functional unit is 1,340 kg of influent total solids (TS) in the sludge received at the digester per day, with an expanded functional unit to account for varying energy content in the waste streams. Data from literature reviews and databases were used to model biogas production, carbon emissions, and energy production. Findings for recovery and use of the biogas for digester heating or electricity generation indicate that AnCoD can be beneficial for large military bases with independent wastewater treatment, planned renovations, and available land for expansion. By offsetting capital costs, AnCoD offers potential cost savings for wastewater treatment plant upgrades. However, its feasibility as a potential renewable energy source varies based on individual installation requirements and costs. While AnCoD shows promise as a renewable energy solution, careful evaluation of the specific installation context is necessary to determine its suitability. The study highlights the

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importance of data accuracy in LCA models, as emissions estimation may vary significantly based on several factors, such as inclusion or exclusion of biogenic carbon emissions, attributional or consequential modeling, accurate energy consumption, and different grid electricity sources. Future research should focus on refining the LCA model, gathering site-specific data, and evaluating AnCoD's potential application in various military installations. These findings contribute to sustainable decision-making in wastewater treatment processes, supporting the Department of Defense's commitment to renewable energy adoption and environmental stewardship.

4.2 Introduction

4.2.1 Energy Security on Department of Defense Installations

Military installations experience a wide variety of acute stressors that can impact the performance of energy generation systems. Such stressors include, but are not limited to, extreme weather, climate change impacts, natural disturbances or disasters, degraded infrastructure, and changing interactions with local power authorities. Installations are like small towns or college campuses, which are often self-contained, but can be wholly reliant on external service providers such as electrical grids to provide energy. Further, current back-up energy plans for many installations require external supplies of oil and gasoline for fossil fuel run generators. Therefore, installations are continually at risk of electrical and thermal energy loss. A lack of energy can impair installation and tenant unit leaders in training, preparing, and executing missions.

U.S. Department of Defense (DoD) and its subordinate service branches fully recognize the importance of energy security. As such, the current national defense strategy requires DoD entities to increase readiness through implementation of resilient and cyber-secure fuel and power for both operational forces and permanent installations. Compliance with the strategy is measured through reduction of energy consumption and greenhouse gas (GHG) emissions, which includes adoption of more efficient and clean energy technologies. Additionally, permanent DoD installations have a requirement to be able to provide at least 14 days of energy for continuous operations in case of disruption [89–92]. Despite emphasis on energy security, many DoD installations maintain degrading infrastructure and vulnerable ties to external energy grids; therefore, DoD is exploring options to upgrade energy infrastructure, create renewable energy onsite, and enhance energy security.

4.2.2 Anaerobic Co-Digestion of Organic Wastes

Anaerobic co-digestion of organic wastes including wastewater sludge, food scrap waste, and fats, oils, and grease (FOG) is a potential renewable energy technology to create methane-rich biogas at water resource recovery facilities (WRRFs). Anaerobic digestion (AnD) of wastewater sludge generated during the wastewater treatment process has been employed for over a century; however, adoption is not widespread in the U.S., with less than 10% of treatment facilities using the technology [20]. The facilities using AnD are more likely to be large scale, treating over 10 million gallons wastewater per day (MGD), rather than smaller scale facilities (less than 10 MGD) as found on DoD installations [20, 93]. Co-digestion of wastewater sludge with organic food waste and FOG has recently gained popularity due to increased methane generation (relative to anaerobic digestion of wastewater sludge only). Heat and electrical energy can be produced from methane through combined heat and power technologies. Despite the energy benefits, co-digestion is not commonly implemented in the U.S. At present, approximately 1 in 10 WRRFs using anaerobic digestion also co-digest additional organic streams beyond wastewater sludge [20]. No DoD installation currently uses anaerobic co-digestion.

AnCoD at DoD installations presents an opportunity to meet resilience and security goals, reduce reliance on external energy providers, promote consumption of renewable fuel, and reduce GHG emissions through recovery and beneficial use of the biogas generated. As DoD installations create a large volume of organic wastes, almost all of which currently goes to landfills, there is an opportunity for anaerobic co-digestion to contribute to DoD installation energy security requirements.

4.2.3 Anaerobic Co-Digestion at the U.S. Military Academy

Researchers at the U.S. Military Academy at West Point were recently awarded a DoD Environmental Security Technology Certification Program (ESTCP) grant to study all aspects of an anaerobic co-digester currently undergoing construction at West Point's Target Hill Wastewater Treatment Plant (THWWTP). American Water signed a 50-year contract agreement in 2019 to become West Point's privatized partner for water and wastewater services, assuming the duties previously belonging to the installation's Department of Public Works. American Water received $70 million to upgrade the existing 1.7 MGD WRRF to a 2.3 MGD facility. A portion of the funds was allocated to construct a new food and FOG waste receiving area and co-digester, which will be linked to existing primary and secondary anaerobic digesters. The upgraded THWWTP is scheduled to begin startup procedures, including food scrap waste and FOG processing and co-digestion, in November 2023. As start-up and steady state of the new system has not been achieved, usable measurements for performance (e.g., biogas production or solids removal) are not yet available.

This study is the first examination of AnCoD on a DoD installation and provides a unique contribution to the literature. Of note, obtaining data for the generation and characterization of food and FOG waste at West Point was difficult as existing measurements are almost nonexistent; therefore, a literature review was necessary to fill gaps and develop unique flows and unit processes with adjustable parameters for use in Sphera's LCAFE software. Literature review provided the necessary characterization for water, solids, carbohydrate, protein, and lipids content of the three unique influent flows. The median values were used to feed a stoichiometric model for the conversion of hydrogen, carbon, and oxygen to methane and carbon dioxide, which are the principal components of biogas generated in the AnD process. The biogas is then disposed of through unit processes in one of five ways: uncontrolled release, flaring, reuse in a boiler, reuse in a combined heat and power (CHP) unit, and cleaning to biomethane for natural gas line injection. Additionally, the treated organic solids are transformed to biosolids which undergo dewatering and offsite transport for disposal. The emissions and credits from these processes and the emissions from the fuel and electrical energy required to treat the organic waste become the basis for examination of the environmental impacts. The modeled biogas, potential energy production, and environmental LCA results will feed a decision support tool used by DoD installations to determine if AnCoD is a viable renewable energy alternative. The portion of the study documented here includes the waste characterization, energy production estimations, and potential emissions associated with uncontrolled release and flaring of biogas. This study presents an adaptable anaerobic digestion and sludge treatment model that can be refined when additional primary data from THWWTP become available. This model allows for exportation to additional applications, such as the decision support tool. The decision support tool will be designed for extended accessibility and will not require the complexity involved in learning and properly using existing LCA software with fixed and often proprietary flows and processes.

4.3 Methods and Materials

4.3.1 Lifecycle Assessment of Greenhouse Gas Emissions

This study was conducted in accordance with the Lifecycle Assessment Framework (provided in ISO 14040 and 14044) and was applied using Sphera's LCAFE software v. 10.7.0.183 and included the ecoinvent v. 3.9.1 database. The following methods and materials are supplemented by Appendix D.1 (p. 109), which includes a detailed primer of the LCA process. This primer will be included in the decision support tool created for DoD users.

4.3.1.1 Goal Statement

The goal of the LCA is to provide comparative life cycle analysis of biogas generated in anaerobic digestion of wastewater sludge, food waste and FOG waste, focusing on climate change impacts. Comparative scenarios include the impacts of one, two or three waste inputs (sludge, sludge and food, or sludge, food, and FOG) and the subsequent disposition of the generated biogas. The intended application is for provisioning in a final decision support tool designed for installation commanders to determine if the incorporation of additional waste streams of food and FOG to a wastewater treatment plant sludge stream to the anaerobic digesters will generate sufficient quantity and quality of biogas to warrant subsequent biogas capture and use. In addition to the environmental impacts of emissions from the production of biogas from anaerobic digestion, future research will examine the costs and additional emissions associated with the various biogas disposition equipment, biosolids treatment and disposition, and rerouting food and FOG wastes from the landfill to the THWTTP. The increased information will augment the LCA findings allowing for the development of a more robust decision support tool. Additional details regarding the requirements of LCA goal statements are provided in Appendix D.1.1.1 (p. 110) and details regarding future work are in Section 4.6.2 (p. 74).

4.3.1.2 Scope

The product system analyzed in this study is the solids handling phase of wastewater treatment plants, specifically the anaerobic digestion of waste sludge and subsequent beneficial use or disposal of the biogas generated during the digestion process. The function of this product system is to treat the sludge by stabilizing the content to biosolids in accordance with Federal Code of Regulations, 40 CFR 503. The THWTTP permit is for Class B solids, which is the minimum standard for pathogen removal prior to land application (e.g., agricultural, reclamation sites, or landfill cover) of the biosolids [94]. Stabilization of the waste occurs through the reduction of pathogens, mass, offensive odors and potential for putrefaction [3]. This study includes two additional waste streams of food and FOG waste for consideration of co-digestion with the AnD of wastewater primary and waste activated sludge.

For WRRF studies discussing sludge and biosolids handling, the most common functional units involve solids characteristics [95, 96]. The functional unit selected for this study is 1,340 kg of influent TS in the sludge received at the digester per day. However, the functional unit is expanded to be representative of the differing energy content in the three waste streams through percentages. The combined flow for the first scenario is comprised of 1,340 kg TS from sludge/d, 0 kg from food waste, and 0 kg from FOG waste, resulting in 100% sludge, 0% food waste and 0% FOG. The combined flow for the second scenario is comprised of 1,340 kg TS from sludge/d, 631 kg from food waste, and 0 kg from FOG waste, resulting in 68% sludge, 32% food waste and 0% FOG. The combined flow for the third scenario is comprised of 1,340 kg TS from sludge/d, 631 kg from food waste, and 39 kg from FOG waste, resulting in 67% sludge, 31% food waste and 2% FOG. The expanded functional unit is used to provide clarity and reduce uncertainty in complex LCAs [34, 96] and has been applied in several other anaerobic digestion studies [97–100]. Additional details regarding the selection of the functional unit are provided in Appendix D.1.1.2.2 (p. 111).

This study focuses on the anaerobic digestion process for the treatment of solid waste streams and the subsequent disposition of the biosolids and biogas generated. This study explores the upgrade of the THWWTP and will inherently contain site-specific information (e.g., cost and mix of electricity). AnD of wastewater sludge serves as the baseline for comparison to the second and third scenarios, incorporating the digestion of food waste and food waste and FOG, respectively. The current boundary flow diagram depicted in Figure 4.1 (p. 57) shows the modeled portion of this study, which includes anaerobic digestion of wastewater sludge, food and FOG and the uncontrolled release and flaring of the biogas. Additional details regarding boundary selection are provided in Appendix D.1.1.2.3 (p. 112).

In this study, wastewater treatment and upstream processes for the creation of waste streams remain the same for all scenarios and are excluded from the comparison. Influent streams to the digester, the quantity and quality of biogas, and the quantity and quality of biosolids products are different for each scenario and are therefore included in the extended boundary (Appendix D.2, p. 123). End of life treatment of biosolids for Target Hill is currently transportation to a composting facility approximately 30 miles from the installation, where it is composted with wood chips and used in land application. This process remains the same throughout all scenarios; however, transportation factors (such as weight and vehicle emissions) will change with the variable influent organic loads. Alternate biosolids waste treatment and/or disposal approaches (e.g., incineration or landfilling) are not included in the current analysis. Other exclusions are: (1) digestate from the anaerobic digestion and centrate from solids dewatering processes (assumed to be returned to headworks); (2) hydrogen sulfide and nitrous oxide gases generated in the anaerobic digestion process; (3) construction, maintenance, or upgrades of existing infrastructure within the boundary; (4) energy consumption and equipment moving the waste within the boundaries; (5) indoor emissions; (6) administrative tasks; and (7) chemical additions (e.g., for thickening or alkalinity control). These exclusions are generally not required in LCAs or are inconsistent with the current goal and scope [3, 34, 96, 101–103].

The upgraded THWWTP is scheduled to begin startup procedures in November 2023, which will include food scrap waste and FOG processing and co-digestion. As this is a new system for THWWTP, relevant measurements of carbon, oxygen demand, solids, and biogas production are not yet available. Usable measurements for the new system will not be available until after co-digestor start-up and steady state is achieved – likely in the spring of 2024. Accordingly, this study uses background data for THWWTP and literature data to create an initial LCA model, which will be updated and refined in 2024. Sources of data for this study predominantly originated from literature review of primary sources and the use of secondary source databases created and maintained for the purpose of conducting an LCA. Additional details regarding data collection and quality are located in Appendix D.1.1.2.6 (p. 118).

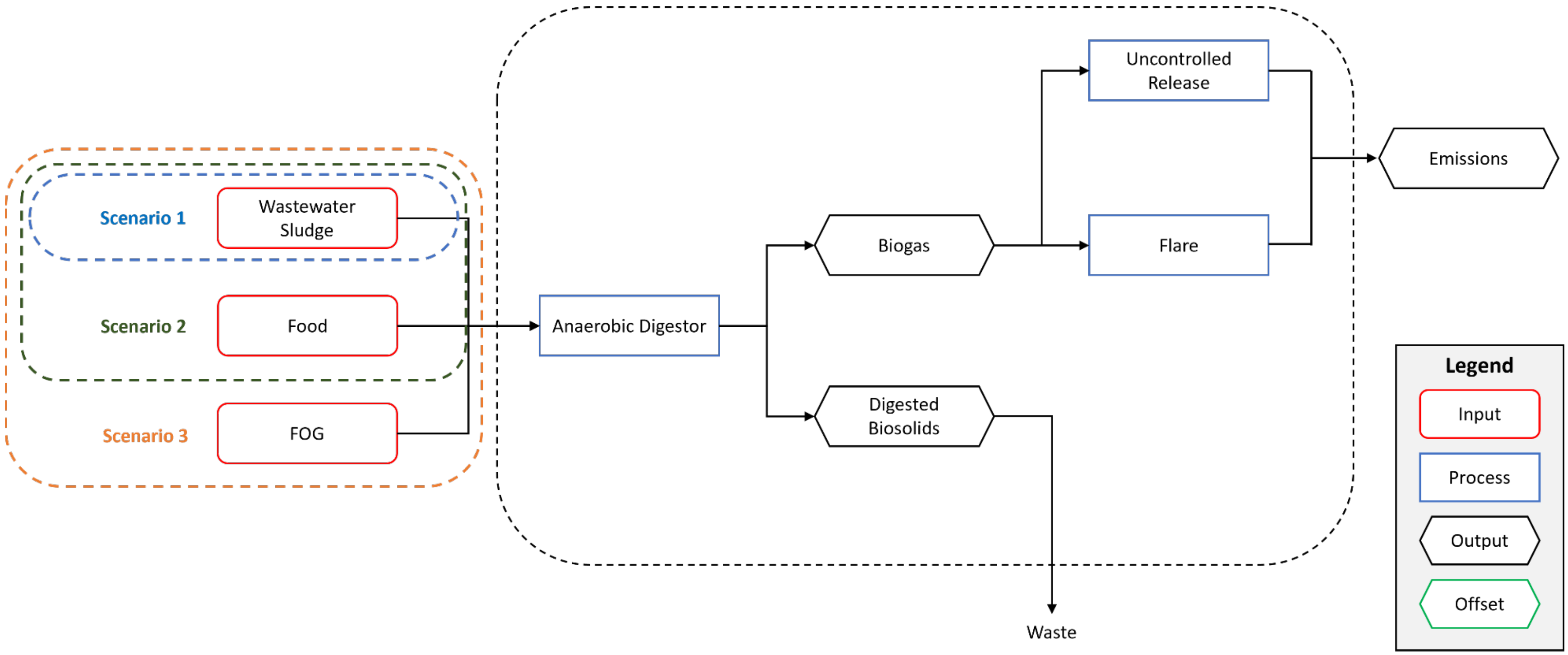

Figure 4.1 System boundary diagram for uncontrolled release and flaring of the three different influent streams. The composition of the influent streams for the three scenarios are indicated by the colored dashed lines encircling them.

To limit potential bias and to support development of a custom-built model, effort was made to review the original source of primary data when discovered in secondary sources. Effort was also made to confine the review to published information within the last 10 years to ensure the most recent technological improvements were included; however, it was not always possible, and some sources are between 10 and 20 years of this study. The software program used in this study, which included paid databases for relevant processes, are updated frequently and are considered reliable and of good quality; however, these data are sometimes limited due to proprietary ownership. To address this shortcoming, flows and processes were created using an independent set of values based on stoichiometric calculations and supported by statistical analysis of existing data reviewed. This approach facilitates the transfer of the LCA inventory and impact assessment into a spreadsheet-based decision support tool for DoD users. Additionally, use of equations for calculating unknown values for which there are no measurement is common [97, 104–107]. For example, similar to this study, Alyaseri et al., (2019) conducted a statistical review of literature and used the results for their LCA model [108].

This study is conducted as a consequential life cycle assessment, to include the impact assessment method TRACI v. 2.1, developed by the U.S. Environmental Protection Agency (USEPA), chosen for its relevance to LCAs in North America [109]. Additional details regarding impact assessment methods are located in Appendix D.1.1.2.5 (p. 115). The LCA is consequentially based due to the change in market demand from solids treatment in anerobic digestion to resource recovery in the form of usable energy converted from biogas. The potential biogas dispositions represent the possible decision-based principles, which may change whether the stakeholder prefers a business-as-usual scenario, a cost saving scenario, an energy independence scenario, or a pollution reduction scenario. Finally, this study uses system expansion by subtraction (also known as substitution or avoided burden), which involves crediting the system with the output of a dual product process (e.g., electrical and heat energy from the CHP process) and is common in consequential LCAs to avoid allocation (or partitioning) of the inputs and outputs. Additional details regarding allocation procedures are provided in Appendix D.1.1.2.4 (p. 114) and D.1.1.2.7 (p. 120).

4.3.2 Waste Characterization

Analysis was focused on the characterization of the organic waste (sludge, food, and FOG) based on solids, moisture content, and classification of carbohydrate, protein, or lipid portions (the most commonly reported characteristics). When available, oxygen demand, elemental composition, density, and heating values were retained as additional characterization factors. Sources specific to characterization were lengthy and are provided in a supplemental data file documented in Appendix D.3 (p. 124). Estimated volumetric flow for the food and FOG wastes were based on a combination of literature review and coordination with the producing entities. Estimated volumetric flow for primary and waste activated sludge were based on scaling from the historical averages at 1.7 MGD to a 35% increase (or 2.3 MGD). Data acquired for description of the intermediate flow of biogas and biosolids were based on well-established equations (found in Section 4.3.3). Variables and constants for each equation were obtained from literature and database reviews, and included basic statistical analysis (mean, median, range, etc.) of differing values. Based on comparable values between studies (i.e., unit conversion to the same metric), the median was utilized as the indicator of the midpoint value. The sludge waste flow included a percentage of biomass to account for the microbial growth that occurs during the aerobic treatment of wastewater. Generic chemical formulas were used for the volatile compounds (carbohydrate, protein, or lipids) [3]. The final category of waste characterization, denoted as "other", included both slowly biodegradable carbohydrates, such as cellulose or lignin, and non-biodegradable material. During literature review, non-biodegradable naming convention varied between ash, inert, and non-volatile. Based on the input data, output analysis focused on the carbon emissions (i.e., carbon dioxide and methane) to the atmosphere.

4.3.3 Biogas and Energy Production Modeling

Modeled biogas production and resulting emissions were based on stoichiometric and industry accepted calculations for estimates of the treatment of the waste streams (e.g., reduction in solids and oxygen demand). Owing to the complexity of the waste streams, this study focused on atmospheric CO_2 and CH_4 emissions or biogas beneficial use compared to fossil fuel energy consumption. Two major assumptions were required for the underlying LCA model. First, all volatile solids removed during the digestion process are consumed as organic material resulting in the production of either CO_2 or CH_4, with none being retained in the wastewater. Second, for simplicity and adaptation of adjustable parameters in the LCA software, microbial kinetic rates for the conversion of organics are not included in the calculations. However, an example using the theoretical conversion of chemical oxygen demand (COD) to methane using microbial efficiency, yield, and decay rate (described below) is included in Section 4.4.1 for comparison to the underlying LCA model.

Within the anerobic digestion unit process, the intermediate product of biogas was calculated mathematically based on the stoichiometric conversion of the organic matter to carbon dioxide, methane, ammonia, and hydrogen sulfide (Equation 4.1) [3]. The fraction of methane in the biogas was also calculated using Equation 4.2 [3]. As ammonia and hydrogen sulfide were excluded from this analysis (see Section 4.3.1.2), the percentage of carbon dioxide was assumed to be the remaining fraction of the biogas. The Ideal Gas Law (Equation 4.3) was used to convert moles (n) to volume (V) at the digester temperature 35 °C (308 K) and 1 atm for atmospheric pressure in New York.

$$C_vH_wO_xN_yS_z + \left(v - \frac{w}{4} - \frac{x}{2} + \frac{3y}{4} + \frac{z}{2}\right) H_2O \rightarrow$$
$$\left(\frac{v}{2} + \frac{w}{8} - \frac{x}{4} - \frac{3y}{8} - \frac{z}{4}\right) CH_4 + \left(\frac{v}{2} - \frac{w}{8} + \frac{x}{4} + \frac{3y}{8} + \frac{z}{4}\right) CO_2 + yNH_3 + zH_2S \tag{4.1}$$

$$Fraction\ of\ CH_4 = \frac{4v + w - 2x - 2z}{8(v + z)} \tag{4.2}$$

$$V = \frac{n\left(0.08206 \frac{atm \cdot L}{g \cdot mol}\right) 308\ K}{1\ atm} \tag{4.3}$$

Another commonly used approach to theoretical methane production involves the conversion of biodegradable chemical oxygen demand (bCOD) to volume of methane based on Equations 4.4 and 4.5 [3]. In this study, the concentration of influent 5-day carbonaceous biochemical oxygen demand ($cBOD_5$) was estimated from the waste flowrates, estimated total COD concentrations and default parameters from computer software wastewater simulation tool BioWin (v. 6.2, EnviroSim Associates, Ltd.). $cBOD_5$ was then converted to bCOD using a conversion factor of 1 mg bCOD = 0.63 mg $cBOD_5$ [41]. Effluent bCOD was calculated using a value of 0.6 for the efficiency (E) of waste utilization [3]. Default values of the yield and decay coefficients and SRT are listed below in parentheses. Specific values used for tCOD, $cBOD_5$, S_0, S and Q can be found in Appendix D.4 (p. 125).

$$V_{CH4} = (0.4)(S_0 - S)(Q)\left(\frac{1\ kg}{10^3\ g}\right) - 1.42P_x \tag{4.4}$$

$$P_x = \frac{YQ(S_0 - S)\left(\frac{1\ kg}{10^3\ g}\right)}{1 + b(SRT)} \tag{4.5}$$

where V_{CH4} = volume of methane produced at 35 °C and 1 atm, m^3/d

0.4 = theoretical conversion factor of methane (m^3) from 1 kg bCOD

Q = waste flowrate, m^3/d

S_0 = bCOD in influent, g/m^3

S = bCOD in effluent, g/m^3

P_x = net mass of cell tissue produced per day, kg/d

Y = yield coefficient, g VSS/g bCOD (0.08)

b = decay coefficient, 1/d (0.03)

SRT = solids retention time, d (30)

Once calculated, the estimated biogas is connected to a dummy process (a simulated unit process used for the conversion of an intermediate flow) for the simulation of uncontrolled release. In this process the percentage of methane and carbon dioxide in the biogas is converted to mass-based emissions. In the case of flaring, the CH_4 content of the biogas is converted to kg CO_2 in a different (flaring) dummy process. Volumetric methane production is converted to energy based on a lower heating value of 50 MJ/kg (35.85 MJ/m^3) and further converted to electricity based on a conversion factor of 3.6 MJ/kWh (0.223 kWh/mol) [8, 26, (see also Appendix D.3, p. 124)].

4.4 Results

4.4.1 Modeled Organic Composition and Methane Production

The life cycle inventory (LCI) includes the elementary flows that enter or exit the boundary and also includes intermediate flows (comprised of the elementary flows) within the boundary. The boundary for the baseline scenario contained one unit process for anerobic digestion. The input to this unit process was “waste” characterized by the percentage of combined primary and waste activated sludge, food, and FOG. The percentage of food and FOG waste in Scenario 1 was 0 resulting in a 100% waste stream of sludge as depicted in Table 4.1 (p. 62). Design sludge flows for the upgraded plant (2.3 MGD) included approximately 20 m^3/d (5,300 gpd) from primary treatment and 16 m^3/d (4,300 gpd) from waste activated sludge. The resulting sludge feed rate to the digesters was 36 m^3/d (9,513 gpd). Total solids for the combined sludge stream were 1,340 kg/d with 75% volatile solids (of the TS). Approximately 19,000 kg of food scrap waste and approximately 800 kg of FOG are generated at West Point per week. Much of the waste originates from the Cadet Mess Hall, which feeds 4,400 USMA Cadets several times daily. Food scrap and FOG waste contributions from the Cadet Mess Hall and other installation facilities are listed in Appendix D.5 (p. 126). In Scenario 2, food waste is added to the sludge flow resulting in 1,340 kg TS from sludge, plus an additional 631 kg TS from food. Scenario 3 includes the sludge and food streams, plus an additional 39 kg TS from FOG/d. The percentage of these contributions to the waste stream from each scenario are also depicted in Table 4.1 (p. 62).

Median composition of wet food waste was determined to contain 77% moisture and 23% TS; 91% of the total solids was volatile (VS). Median FOG waste was 66% moisture and 34% total solids;

98% of the total solids was volatile. Sludge was 96% moisture and 4% total solids; 75% of the total solids was volatile. Volatile solids were subdivided into carbohydrates, proteins, and fats. Median volatile characterization percentages for sludge were 9% lipids, 15% carbohydrates, and 35% proteins. Table 4.1 also depicts the composition of the food and FOG streams, as well as the percentage of each stream for the three influent scenarios, which are the default values for the adjustable parameters for the LCI.

Table 4.1 Compositional characteristics of the influent waste streams.

	Sludge	Food	FOG
Biomass ($C_5H_7NO_2$)	9%	-	-
Lipid ($C_{18}H_{33}O_2$)	9%	13%	85%
Carbohydrate ($C_6H_{10}O_5$)	15%	40%	7%
Protein ($C_{11}H_{24}O_5N_4$)	35%	15%	2%
Other (cellulose, lignin, inert)	32%	32%	6%
Scenario 1	100%	0%	0%
Scenario 2	68%	32%	0%
Scenario 3	67%	31%	2%

Based on the percentages of the organic matter, one mole of sludge VS resulted in an estimated chemical formula of $C_{6.8}H_{13.5}O_{2.9}N_{1.5}S_0$ (molecular weight = 163 g/mol), which results in approximately 3.8 moles of CH_4, 3 moles of CO_2 and biogas which is 64.3% CH_4 using Equations 4.1 and 4.2. The estimated flow rate of the sludge to the Target Hill digesters (36 m^3/d, and 1,340 kg TS/d) results in 5,602 moles of VS in the sludge per day. Conversion of all of the organic matter produces 21,472 moles CH_4/d; however, an assumption of 65% efficiency (an additional adjustable parameter for the LCA model) for solids removal was presumed for the anaerobic digesters based on an solids retention time (SRT) of 30 days [3]. Using this model produced 549 m^3 biogas/d with 353 m^3 CH_4/d. The yield was 0.84 m^3 biogas/kg VS_{rem}, which is within the typical range of 0.75-1.12 m^3 biogas/kg VS_{rem} [3, 111]. Table 4.2 (p. 63) depicts the percentage of methane in the biogas and volumetric production of methane using the same modeled process described above based on the TS in the waste stream for each of the scenarios.

Table 4.2 Total solids flow rate, percentage of methane in the biogas and methane production.

	Scenario 1	Scenario 2	Scenario 3
Waste Stream (kg TS/d)	1340	1971	2009
Sludge	1340	1340	1340
Food	0	631	631
FOG	0	0	39
% CH_4 in biogas	64.3%	63.4%	63.5%
m^3 CH_4/d	353	534	560

Table 4.3 (p. 64) depicts the results of the bCOD model (Equations 4.4 and 4.5, p. 60) for the three scenarios. The model predicted volumetric methane production within 6% of the LCA model. A possible cause for the discrepancies may be related to using separate formulas for primary and waste activated sludge in the bCOD model in comparison to the LCA model, which combines the two streams. Additionally, using a conversion factor of 0.63 cBOD5 to bCOD for all waste streams may also contribute to the differences. The largest percentage of the waste stream volume is sludge, which is expected to contain a lower fraction of bCOD in comparison to food or FOG. In comparison to percentage of flow, percentage of bCOD is skewed the other way with FOG representing 63% of the total and food 26%. Finally, the use of a single tCOD concentration estimate from a limited study period may not accurately characterize the sludge waste streams. The LCA model created for this report was based on statistical findings (n = 33) from the characterization of combined sludge resulting in a tCOD concentration of 55 g/L (very near the weighted concentration of 51 g/L used in the bCOD model). Changing the BioWin tCOD concentration to the median tCOD concentration from the literature review of combined sludge in this study, results in 45 g bCOD/m^3, 41 kg biomass/d, and 362 m^3 CH_4/d for Scenario 1 (a -3% difference from the LCA model). Specific values used to obtain these results are in Appendix D.4 (p. 125).

Table 4.3 bCOD theoretical conversion to methane model results.

	Scenario 1	Scenario 2	Scenario 3
Waste Flowrate (m^3/d)	36	41	42
Primary sludge	20	20	20
Waste activated sludge	16	16	16
Food	0	5.5	5.5
FOG	0	0	0.13
P_x (kg/d)	37	63	65
V_{CH4} m^3/d	332	564	577
% Diff CH_4 from LCA Model	6%	-6%	-3%

4.4.2 Carbon Emissions

This section details the findings of the impact assessment using the TRACI v. 2.1 method and GWP impact category in LCAFE from the three scenarios and the uncontrolled release and flaring biogas dispositions. Additional analysis compares differences between including or excluding biogenic carbon emissions and variation of results based on attributional or consequential LCA formats using the ecoinvent process "anaerobic digestion of sewage sludge."

Figure 4.2 (p. 65) depicts the process diagram as generated in the LCAFE software based on the calculations discussed in the previous section and depicted in Table 4.2 (p. 63). The emissions for the baseline scenario are 341 kg CO_2 and 224 kg CH_4. In the case of flaring, the CH_4 content of the biogas is converted to kg CO_2 emissions in another dummy process, resulting in 565 kg CO_2. The inventory for the remaining scenarios adding food and FOG were calculated using each of the biogas disposition scenarios in the same manner. The mass emissions were then used to examine the environmental impacts.

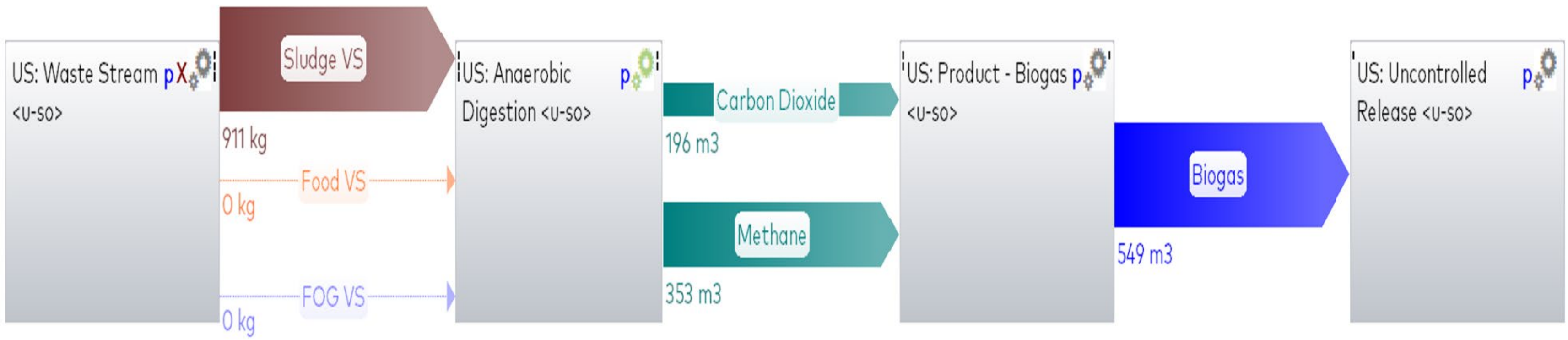

Figure 4.2 LCAFE process flow diagram for the baseline scenario. Inventory values shown are per day. Influent sludge, food and FOG TS masses are not shown, but are inputs to the "US: Waste Stream" process. Outputs from the "US: Waste Stream" process and inputs to the "US: Anaerobic Digestion" process are mass of VS.

The results of the impact assessment for the anaerobic digestion of 1,340 kg sludge TS/d, with and without biogenic distinctions, are depicted in Figure 4.3. For additional details regarding biogenic and inorganic carbon distinction impact assessment methods, see Appendix D.1.1.2.5 (p. 115). In this study, no distinction is made between $CH_{4,fossil}$ and $CH_{4,bio}$. This results in the full 224 kg CH_4 from Scenario 1 being assigned a characterization factor of 25 resulting in 5,597 kg CO_2-eq. The 341 kg CO_2 is assigned a factor of 1, resulting in 341 kg CO_2-eq (sum total of 5,939 kg CO_2-eq). The TRACI method in LCAFE assigns a characterization factor of 22.25 for $CH_{4,bio}$, which results in 4,982 kg CO_2-eq for Scenario 1a (a 10% difference). While not used in this study, certain impact assessment methods (i.e., CML2001 and EF 3.1) use a characterization factor of 0 for $CO_{2,bio}$, which would result in no global warming impacts for the flaring scenarios. The impact assessment results for the remaining scenarios are also depicted in Figure 4.3. Scenario 3a (sludge, food, and FOG with uncontrolled release of the biogas) had the largest CO_2-eq emissions and subsequently the largest negative impact to the environment.

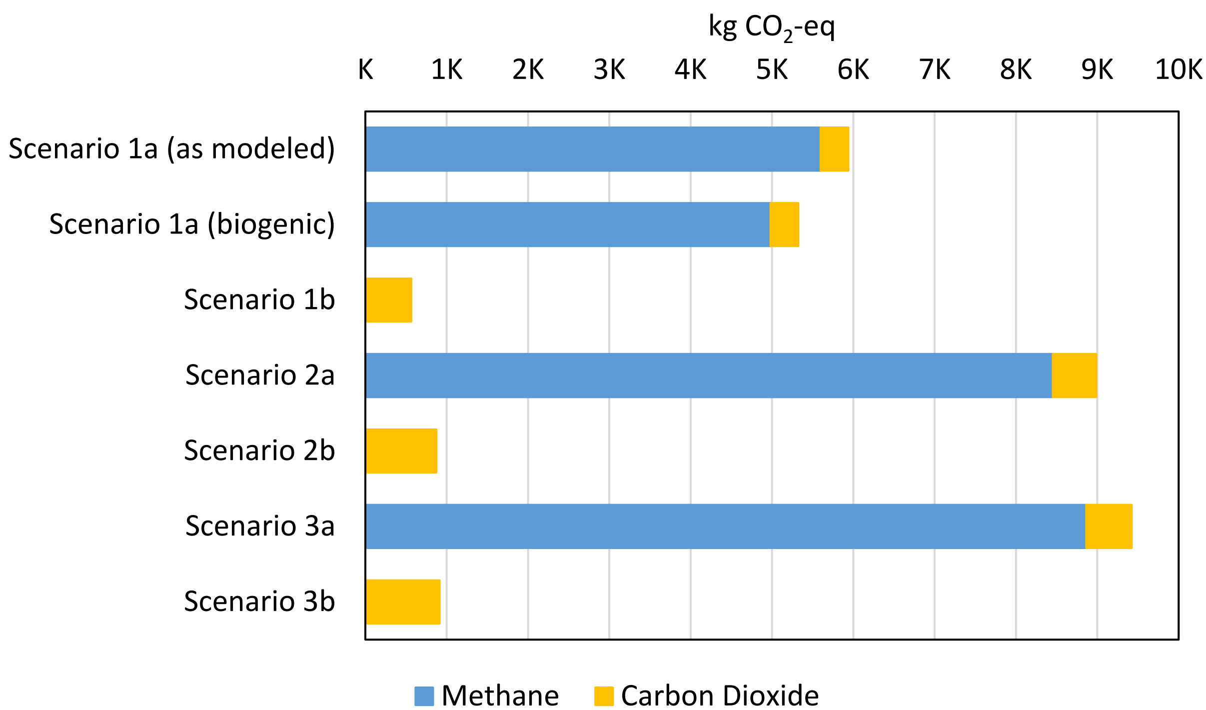

Figure 4.3 GWP using TRACI in LCAFE. Categories labeled with “as modeled” or with no label do not distinguish between biogenic and fossil carbon emissions. Scenarios with an “a” are uncontrolled release and “b” are flaring.

The results of the LCI and LCIA for the baseline scenario equate to approximately 9.5 kg CO_2, 6.2 kg CH_4, and 165 kg CO_2-eq per m^3 of sludge. It is notable to compare these modeled results with existing databases to identify potential errors or differences. As described in Appendix D.1.1.2.6 (p. 118), the LCAFE databases are aggregated for the entire wastewater treatment plant and the unit processes for treatment, such as anaerobic digestion, are unavailable. However, the ecoinvent v. 3.9.1 database contains both unit processes and aggregated LCI and LCIA for the anaerobic digestion of 1 m^3 of sewage sludge [112]. The undefined unit process (no upstream or downstream emissions) shows that treatment results in 16.6 m^3 biogas, with 1.66 kg CO_2 and 0.056 kg CH_4 as biogenic emissions to air. The documentation for the processes reveals the model originated from literature review (primarily in 2002) of large scale facilities in Switzerland. The activity starts with the reception of the sludge at the AnD plant and ends at the plant gate (i.e., wastewater treatment and raw sludge production are excluded), similar to this study. Important modeling information identified included the fact that digesters were mesophilic (~35 °C), 4-6% of the wet waste was TS, and the digesters averaged 45% TS removal. One cubic meter of sludge required approximately 4 kWh of electricity for sludge mixing and 67 MJ for sludge heating [112]. At first glance, the results of the ecoinvent model and the model in this study appear substantially different; however, the difference mainly lies in the treatment of the biogas.

The ecoinvent process for AnD does not include biogas, or the components within, as emissions, but rather as a valuable resource regardless of how the biogas is used. Additional system model processes are created from the undefined unit process and each of these processes treat the biogas and emissions differently. Cut-off unit processes allocate the entire emission burden from the treatment of the sludge to the entity treating it [113]. This results in two products, treated sludge and biogas. In cut-off models, the entity treating the sludge is not able to use the biogas or receive credits. Any other entity may use the produced biogas (e.g., a resident heating their home) without any upstream emissions, also known as burden free. In contrast, allocation at the point of substitution (APOS) gives an allocated portion of the emissions to the entity treating the sludge and another allocated portion to the entity using the produced biogas [113]. The final method is the consequential method. Consequential LCAs, such as this one, avoid allocation through system expansion (or avoided burdens) where the produced biogas is used as credit towards the emissions (see Appendix D.1.1.2.4, p. 114 and D.1.1.2.7, p. 120). The consequences of the different ecoinvent models are depicted in Figure 4.4 (p. 68) based on the GWP category of the TRACI v. 2.1 assessment method. Only the consequential method results in no impact or potential credit (indicated by the negative value) with approximately -9 kg CO_2-eq/m^3 and the attributional methods result in 7.5 kg CO_2-eq/m^3.

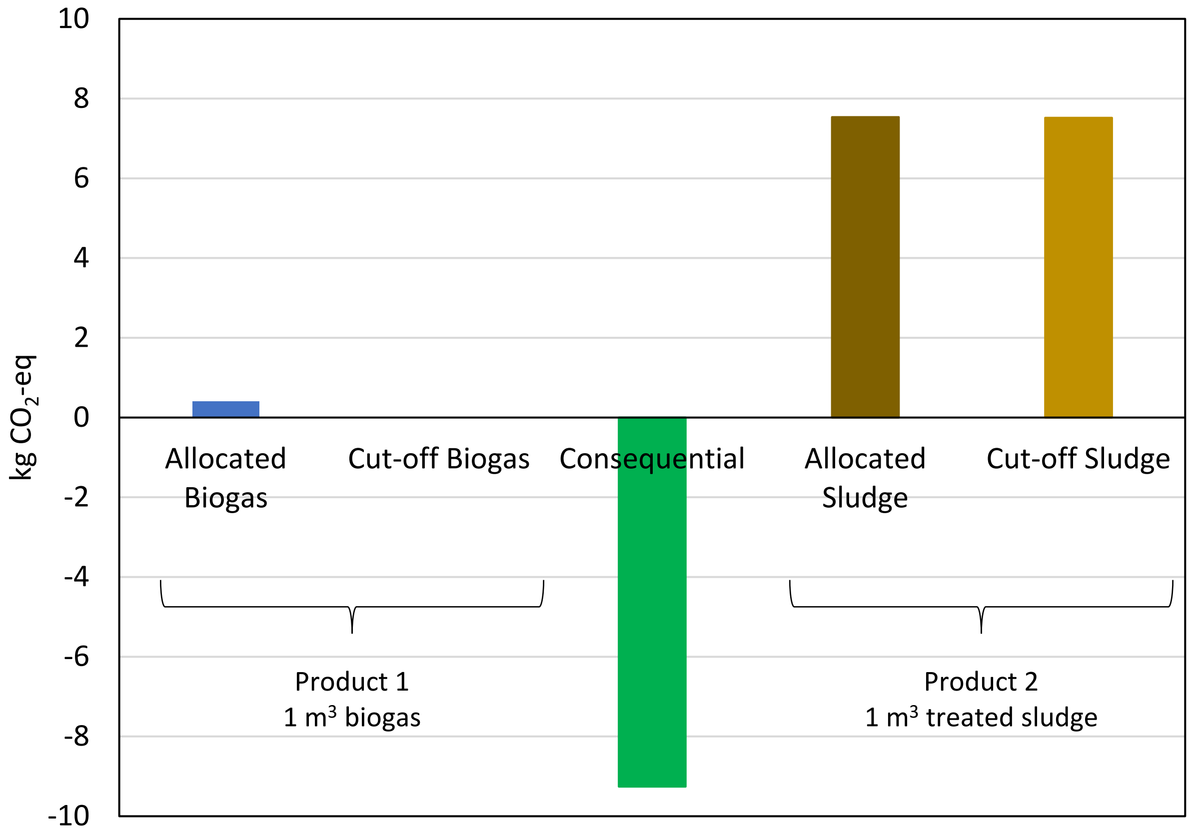

Figure 4.4 LCIA results for the ecoinvent process of anaerobic digestion of 1 m^3 of sewage sludge, using three system models [114].

Since biogas is a valuable product, and not considered an emission within the ecoinvent database, additional analysis (and modification) of the processes is required to allow for equitable comparison between the LCA model in this study and the ecoinvent model. Assuming the same methane content in the biogas as the LCA model (64.3%) results in 11 m^3 CH_4 (6.8 kg at 35 °C and 1 atm) and 6 m^3 CO_2 (10.3 kg). Adding these values, to simulate uncontrolled release of the biogas, to the previous emissions (without biogas) results in 6.8 kg CH_4 and 12 kg CO_2. Conversion of the masses to kg CO_2-eq without biogenic distinction results in 171 kg CO_2-eq/m^3 of sludge. This value is approximately 10% higher than the 165 kg CO_2-eq/m^3 of sludge calculated in the LCA model. These impacts are quite similar considering the ecoinvent model was designed from average values of large-scale treatment facilities in Europe and may not have been considered characteristic of small-scale facilities in the U.S. However, the actual mass and volume of methane are unknown and the parameters for determining them were not provided in the ecoinvent data.

4.4.3 Onsite Energy Production

Modeling results indicate that co-digestion of primary and waste activated sludge coupled with the estimated food and FOG flows will result in approximately 355 kg (560 m^3) of methane per day. Conversion of the methane to energy results in ~18,000 MJ of energy/d. This value is based on the energy content of the methane only, not the biogas as a whole, which is generally between 19 and 22 MJ/m^3 [111]. Conversion of the methane to electricity with a 33% efficient microturbine results in an approximately 1,630 kWh/d. More specific results for each scenario are depicted in Table 4.4.

Table 4.4 Onsite energy production results for the three influent scenarios using conversion factors of 50 MJ/kg CH_4, 0.28 kWh/MJ and a 33% efficient microturbine.

	kg CH_4/d	MJ/d	kWh/d
Scenario 1	224	11,195	1,026
Scenario 2	339	16,943	1,553
Scenario 3	355	17,766	1,629

4.5 Discussion

This initial analysis discussed will be refined with additional primary data when it becomes available and incorporated into the decision support tool. Interpretation of issues, evaluation of data, and final recommendations are also subject to further refinement; however, findings from the initial study warrant further analysis and point to the viability of anaerobic co-digestion for DOD installations. With a focus on energy costs, energy production, and grid electricity source selection, this section discusses the potential cost savings and improvements in energy security and also examines implications to the overall analysis resulting from inaccurate grid energy mix.

4.5.1 Facility Energy Consumption and Production

Based on the size of the facility, THWWTP should require an estimated 5,100 kWh of electricity per day to treat approximately 2 MGD of wastewater [115, 116]. However, recent data showed THWWTP averaged 1.3 MGD and consumed 2,600 kWh/d in 2022. This historical electricity usage does not account for increased loading from the addition of food and FOG waste, increased aeration requirements for an improved larger biological treatment system and storage facilities, active heating of five digesters, or any of the energy consuming processes inherent in upgrading the facility. Accordingly, the higher estimate of 5,100 kWh was used as a conservative estimate for comparison in this initial study.

Historical data for the consumption by individual processes or treatment trains was not directly measured by West Point. However, an estimated 724 kWh/d (or 20 kWh/m^3 of sludge) is necessary for anaerobic digestion assuming approximately 14% of a plant's electricity consumption [2]. This value is consistent with the ecoinvent anaerobic digestion process, 23 kWh/m^3, after converting the required heat energy (MJ) to electricity (kWh) and assuming 100% efficiency in conversion [112]. Additionally, the upgraded plant will incorporate the use of natural gas for the boiler units used for heating the food and FOG waste, as well as the digesters. Using the 67 MJ/m^3 of sludge heating requirements from the ecoinvent process, this is approximately 2,800 MJ of heat required per day [112]. However, the design specifications for the four new heat exchanger/boiler units being installed at Target Hill require an estimated 25,000 MJ/d, a tenfold increase. Subsequently, the increased heating requirements may not reduce the overall energy consumption or costs of the facility, but additional evaluation is required.

The average cost of 1 kWh of electricity was $0.23 and the average cost of piped utility gas was $0.65 per cubic meter for the New York area in December 2022 [117]. THWWTP currently uses all electrical energy (no natural gas or renewable energy sources), which results in an estimated cost of $1,178/d to operate the treatment facility ($167/d for the AnD). Based on the potential electricity production from the use of biogas in a CHP unit (between 1,026 and 1,629 kWh/d from Table 4.4, p. 69), this results in a potential savings of $237 to $376/d for the three scenarios. Use of the biogas from all scenarios results in the production of enough electricity for the anaerobic digestion process with excess to contribute to the WWTP's total electricity consumption. However, if energy consumption remains at the measured 2022 values (2,600 kWh/d), the 32% savings observed with Scenario 3 is increased to 63% (Figure 4.5, p. 71). In addition to the potential cost savings, CHP provides a source of electricity independent of the utility company resulting in improved energy security. While the electricity is insufficient to power the entire plant at full operational capacity, sufficient energy may be produced to operate limited processes required for minimal treatment in the event of a utility power outage.

Assuming all four of the anaerobic digestors are heating sludge 24-hours a day (at a rate of 150 gal/min, as designed) this results in an estimated cost of $443/d for natural gas consumption. Daily savings for the use of digester gas, rather than natural gas, are between $230 and $365 or approximately 52 to 82% of the expected consumption based on the design specifications. Similar to electricity consumption, heating requirements will likely fall somewhere in between the two estimations (2,800 to 25,000 MJ/d). Once the upgraded facility becomes fully operational, the anaerobic digestors may not require all four of the digesters to be heated or designed recirculation rates may be unnecessarily high to maintain the desired 35 °C operating temperature. If heating requirements are as low as the ecoinvent estimations, biogas utilization in a boiler unit results in 4 to 6 times more thermal energy produced than required, even assuming only 85% heat recovery efficiency. However, excess thermal energy is not as versatile as excess electricity in supporting WWTP operations beyond the digestion process. Thermal energy could be redirected to heat buildings or water; however, this usage would likely only be required during colder months.

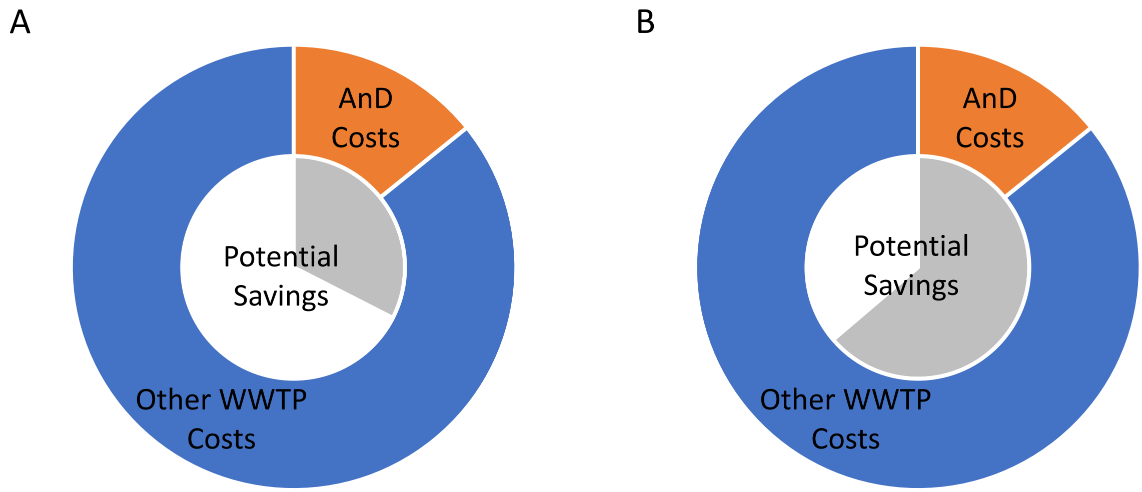

Figure 4.5 Electricity costs and potential savings for 5,100 kWh/d (A) and 2,600 kWh/d (B). Anaerobic digestion costs are 14% of the total and potential savings are based on Scenario 3 ($376/d) for both.

As the potential savings between the recovery of energy electricity and for heat are similar, the amount of electricity generated based on existing equipment efficiencies may not warrant the cost of purchase, installation, and maintenance of a CHP unit. Boiler processes are more efficient (75-85%) for heat recovery than CHP units; however, the combined electrical and heat recovery efficiencies can be equal to boilers [118, 119]. Depending on emissions from boiler and CHP processes, recovered biogas directly at the digester with fewer losses from transport of the gas and boiler efficiency may be recommended and is the most common use of biogas in wastewater treatment plants [20]. However, the usefulness of surplus electricity offers more diverse opportunities for renewable energy consumption and year-round energy security.

4.5.2 Grid Energy Emissions

Electricity use measurements are required for further development of the existing LCA model. In the LCAFE software, this involves finding a process termed “electricity grid mix” or (some variation) and connecting it to the anaerobic digester as an input flow. This process provides state, region, and/or country wide averages for the required inputs, outputs, and emissions in the production of electrical power without having to know all of the unit processes involved. Databases may also include different values based on whether the electricity emissions are direct (power company only) or indirect (emissions from upstream process). In the case of LCAFE, the three processes for the electricity grid mix for the West Point region (termed NYUP by USEPA Emissions & Generation Resource Integrated Database (eGRID) substation nomenclature) are direct, indirect and no additional qualifier, which is the sum of the previous two processes [120]. Reliance on such generalized processes is useful, especially when developing a general tool to be used anywhere in the world; however, attention needs to be paid to the inputs and outputs to ensure the values are a good match for the system under study.

Closer examination of the inorganic portion of direct carbon dioxide emissions revealed an emission amount of 0.205 kg CO_2/kWh. In comparison, the most recent values from eGRID showed a value of 0.106 kg total CO_2/kWh for the same region [121]. Part of the discrepancy could arise from the fact that the metadata in the LCAFE process lists eGRID2012 v. 1.0 as a reference to build the dataset, with updates from 2020; however, the current version is eGRID2021, with updated values released in January 2023. Another source of inconsistency could be that eGRID data reports that zero part of the NYUP energy is derived from coal; however, the LCAFE metadata shows that 0.11% is derived from hard coal and is listed in the inputs. Figure 4.6 (p. 73) depicts the emissions of kg CO_2 based on the consumption of 724 kWh/d for the anaerobic digestion process. As a matter of interest, the U.S. average is 19.5% coal derived electricity, which would certainly produce inaccurate results for electricity emissions in NY but may be a relevant value for the creation of a decision support tool used more widely across the U.S.

Regardless, the difference between NYUP emissions is significant as the current eGRID total emissions are less than half of the LCAFE emissions. This becomes especially important when considering the 5,100 kWh/d estimated total consumption of the plant and/or the offset emissions in the reuse of biogas for electricity generation. As an example, production of the 1,629 kWh/d in Scenario 3 offsets the grid electricity CO_2 emissions by 415 kg CO_2/d using the LCAFE emissions and 172 kg CO_2/d using the eGRID emissions (approximately 32% of the total WWTP electricity emissions). Both emissions result in a credit for the anaerobic digestion process; however, the -246 kg CO_2/d credit based on the LCAFE emissions results in an inaccurate and biased result compared to the actual -96 kg CO_2/d based on the eGRID emissions. These types of errors are easily identifiable and avoidable with sufficient research into the underlying data used in the LCA, lending more credibility to the study.

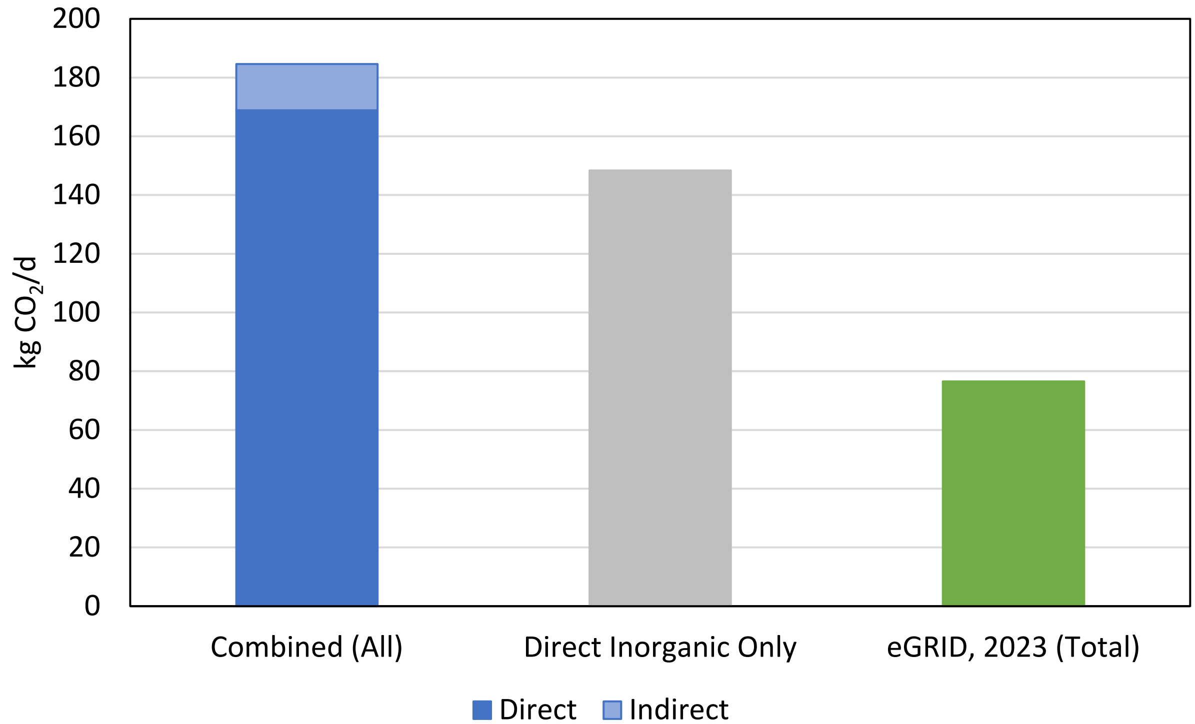

Figure 4.6 Difference in CO_2 emissions utilizing the existing NYUP electricity grid mix in LCAFE in comparison to more recent and accurate values from eGRID. The first bar contains all CO_2 emissions from the LCAFE data, with distinction between direct emissions from the power plant in dark blue and upstream indirect emissions in light blue. The second bar depicts inorganic CO_2 from direct emissions only and is used to highlight the difference in emissions with biogenic carbon distinction. In contrast, the final bar showing emissions data from eGRID includes the total CO_2 emissions.

4.6 Conclusions and Future Work

4.6.1 Conclusions

This life cycle assessment of AnCoD as a renewable energy solution for wastewater treatment plants at DoD installations has yielded valuable insights and key findings. We evaluated three waste input scenarios: sludge alone, sludge with food waste, and sludge with food and FOG, to assess the feasibility and benefits of AnCoD. Our results indicate that AnCoD holds promise as a renewable energy solution for military installations with independent wastewater treatment facilities, planned renovations, and ample available land. AnCoD can prove advantageous by offsetting capital costs and yielding potential cost savings for wastewater treatment plant upgrades. The ability to utilize existing waste streams, such as food and FOG, enhances biogas production, contributing to increased energy generation and potential energy savings. However, it is essential to recognize that the applicability of AnCoD varies depending on the specific circumstances of each installation. Costs associated with new or upgraded equipment, land availability, and local energy prices should be carefully weighed against the potential energy savings to determine the economic viability of AnCoD implementation. The study also emphasizes the importance of data accuracy in LCA models. Notably, variations in data and method selections can significantly impact carbon emissions estimations. As such, adjustable parameters were created to ensure the use of up-to-date, region-specific data to yield more accurate results in energy production predictions and impact assessments.

Overall, the findings underscore the potential role of AnCoD as a sustainable approach to energy generation in wastewater treatment plants, even at small-scale facilities treating less than 10 MGD. By capturing and utilizing biogas, AnCoD can contribute to the reduction of greenhouse gas emissions and enhance energy security for military installations. This study lays the groundwork for exploring AnCoD as a renewable energy solution, but to further enhance the reliability and applicability of AnCoD, future research should focus on refining the LCA model by incorporating site-specific data from diverse military installations. Understanding the variations in waste composition and treatment processes will aid in optimizing biogas production and energy recovery. By promoting sustainable practices and reducing environmental impact, AnCoD aligns with DoD's commitment to energy security and resiliency. As the LCA continues to evolve, further exploration and validation of AnCoD's potential across a wider range of military installations will facilitate informed and sustainable decision-making for the future.

4.6.2 Future Work

This section identifies the remaining analysis required for the completion of the final LCA. These tasks are ongoing and expected completion for the LCA model is in December 2023. Updated, site specific revisions to the LCA model and further development of the support tool are expected in 2024.

- Modifications to the existing baseline model include adding the heat and energy requirements and their emissions for the digestion process with potential inclusion of minor fugitive CH_4 emissions characteristic with AnD and flaring.
- In each of the 3 other biogas disposition scenarios for the differing influent scenarios, the dummy processes (i.e., uncontrolled release or flaring) are removed and substituted with a new unit process (boiler, CHP, and cleaning for natural gas upgrade). These processes produce valuable resources as energy (heat and/or electricity) and become offsets or credits to the system as a whole. The resulting emissions and credits are used in the impact assessment. The proposed extended boundary diagram for the final LCA, which will be integrated into the final decision support tool, is provided in Appendix D.2 (p. 123).

- The heating requirements and subsequent development of the boiler unit process will be modeled from the new boiler and heat exchanger combination equipment (JVD model H355C42) being installed, which can be operated from biogas (minimum 600 BTU/ft^3 and at least 60% methane). The equipment requires natural gas input, which will be offset by the biogas production in the boiler scenarios.
- Development of a CHP unit process in the LCA model will be based on existing unit processes in the ecoinvent database, supported with available literature findings. Several CHP manufacturers utilize engines to support direct biogas without cleaning, similar to the boiler.
- The final unit process to be added will be for cleaning the biogas (removing water, siloxanes, hydrogen sulfide and carbon dioxide) to purify the gas to biomethane to the extent needed for reuse in natural gas injection. Natural gas injection is not currently supported in the West Point area. Subsequently, site specific credits or refunds are unavailable, and a state or national average will be used.

- The food and FOG waste requires transport (fuel consumption and emissions) to THWWTP and food pre-processing (heat and electricity), which are not currently within the system boundary. Expansion of the boundary or modeling in the decision support tool are likely. Preliminary ideas for including these values in the model include determining the distance of farthest donator of food or FOG to THWTTP compared with distance of farthest waste pickup to the landfill. Heat and electricity requirements for food and FOG waste will be based on the receiving station equipment being installed (e.g., FOG processing is the JWC Honey Monster).
- Post digestion solids (biosolids) are currently treated as waste with no additional processing steps. In the future, biosolids will be connected between the AnD and a dewatering process. The dewatering unit process will include an additional electrical input (with emissions) and an output of an intermediate product, dewatered biosolids. The dewatered biosolids will be connected to truck transport with fuel input and emissions from driving 30 miles to Rockland, NY.
  - Additional consideration was given for calculating and tracking nitrogen and phosphorus in the biosolids for nutrient credits in land applied biosolids; however, this was determined to be problematic and not relevant to the goal and scope of this study. Regulations, permits, and N and P offsets will all vary by location and type of fertilizer the biosolids would be substituted for (i.e., Class A or Class B biosolids) [96]. Heimersson et al., (2016) provides a list of varying N and P ratios found in literature

review and additionally recommends credits be allotted to the entity not using the fertilizer, rather than the solids treatment plant [122].

- Impact assessment results using ReCiPe 2016 Midpoint (H) and IPCC AR6 2021 methods for the remaining scenarios and biogas dispositions will be incorporated. ReCiPe is selected for its global acceptance and predominance in reviewed LCA publications [95, 96, 123], and IPCC for its recent update and extensive research [124]. Median midpoint global warming categories (i.e., 100 years) are the focus of the assessment results. Preliminary results for Scenario 1a show a 40% difference in kg CO_2-eq for methane using the ReCiPe method. The impact category for ReCiPe is climate change (rather than GWP) and the conversion factor is 36. Results differ by only 16% using the IPCC AR6 method for GWP 100-year. The most likely cause for the minimal difference is that the LCA model does not distinguish between biogenic and fossil carbon emissions and characterization factors for methane are similar (25 with TRACI and 29.8 for AR6). It is a generally accepted practice that assessment results with differences in alternatives that are small (less than 20%) are excluded as not significant [96, 125]. Subsequently, the GWP 20-year category (a 220% difference) may be adopted to highlight the difference between individualist and hierarchical approaches.
- The existing interpretation section of the LCA will be expanded to include discussion of significant issues, evaluation of the results of the inventory and assessment, and final conclusions and recommendations based on the findings. The significant issues section will highlight relative contributions (the highest and lowest CO_2 equivalents) and differences between impact assessment methods. Additionally, emphasis will be placed on the use of recoverable energy products in comparison to the business-as-usual method of uncontrolled release.
- Future evaluation of the data will include the results of the Monte Carlo uncertainty analysis and sensitivity analysis, both of which are available tools embedded in LCAFE. Sensitivity analysis will include energy mixes (e.g., U.S. vs NY average mix) and carbon content and waste mixing ratios (e.g., higher fat vs. higher non-biodegradable content). Chiu and Lo (2018) found the most sensitive parameters were the lower heating value of CH_4, efficiency of electricity generating equipment and percentage of CH_4 in the biogas when comparing the differences between scenarios using the same influent. These identified parameters will also be examined due to the similarity between the AnCoD LCAs.
- Completeness of data was not considered lacking in that numerous peer-reviewed publications and databases were referenced for characterization of the model parameters. Sources of data were chosen based on their quality, including recent publications in comparable regions of the world,

and using industry accepted practices. However, lack of the most relevant data, primary foreground data from THWWTP, makes this the primary limitation. As this was an LCA for that facility, the use of modeled data from average values from all over the world limits the applicability to just Target Hill but supports use in the decision support tool. Additionally, the data reviewed from published journal articles and databases were variable, requiring additional statistical and uncertainty calculations to improve the confidence of central tendency and ranges. Not having the original raw data creates a potential source of error or bias from the original author. Lastly, the method of modeling used does not include all potential modeling equations (i.e., microbial kinetic rates, thermodynamic changes, etc.). Subsequently, the results of this study, including potential impacts, are estimations and not scientific measurements. Additional limitations include:

  - Limitation from boundary selection. This study does not provide full impacts (e.g., upstream wastewater treatment and emissions) but these impacts would still exist regardless of the treatment of sludge, food waste and FOG. The existing boundary also does not include land use or the impacts to solid waste facilities (i.e., X kg of food waste diverted from landfill, conserving X m^3 of land). Inclusion of these impacts could provide detail regarding the environmental impacts of anaerobic co-digestion and biogas reuse in comparison to other processes.
  - The decision to limit the study to a single environmental impact category means it does not address all emissions or account for all ecological effects. While global warming is a significant impact category, especially when considering only greenhouse gas emissions, the lack of other categories does not show the significance and robustness of the results, nor does it allow the identification of trade-offs among environmental areas of concern.

- This study does not address financial, economic, or social impacts. These are not required components of an LCA; however, additional information from including these factors could provide more insight. Specifically, life cycle costing is a useful tool for the decision-making process and is a required component DoD Sustainability Analysis [34, 96, 125, 126]. Future research will include life cycle costing LCC or a techno-economic assessment (TEA) for THWWTP and development of scaling factors for inclusion in the decision support tool for DoD facilities world-wide. The results from the final LCA can be used in conjunction with the results of the economic analysis. For example, if the electricity produced by a CHP unit is insufficient to warrant the higher cost identified in a TEA, a decision maker could decline to purchase such a unit and instead purchase a boiler with lower cost and better heat efficiency accepting the loss of electricity.

- For development of the decision support tool, the goal is to limit the amount of geographical or temporal confinement by creating adjustable parameters for use in other regions and excluding processes unique to Target Hill, such as the quantity, efficiency, and energy consumption of a specific number or type of pump being installed.

CHAPTER 5

CONCLUSIONS AND FUTURE WORK

5.1 Conclusions

The overall conclusion of this work is that treatment of domestic wastewater using multiple-compartment anaerobic bioreactors below mesophilic temperatures is a viable alternative to conventional primary treatment approaches and is a path forward for energy-efficient wastewater treatment. Furthermore, the addition high organic food and fats, oils, and grease (FOG) waste can improve methane generation in anaerobic co-digestion (AnCoD) of wastewater sludge while reducing or eliminating costs associated with landfilling the waste, natural gas for heating, or electricity for treatment processes. Both treatment systems can be modeled with existing tools through modification of key parameters, such as microbial kinetic rates or organic carbon content, based on site-specific factors such as influent characteristics.

In Chapter 2, I demonstrated the ability to simulate performance of anaerobic mainstream wastewater treatment using a common industry computer simulation tool, BioWin. The results of the sensitivity analysis identified the essential default operating, stoichiometric, and kinetic parameters that need to be modified for successful calibration and validation of the model. These parameters included adjustments to the influent wastewater characterization and acetogenic and methanogenic kinetic rates to achieve predictions within 10% of the modeled system. This research allows for predictive operating performance of unique anaerobic reactor processes facilitating the design, system analysis, and assessment of resource recovery options. Additionally, the simulation allows for comparison to existing aerobic treatment practices highlighting the benefits of anaerobic treatment such as lower operating costs and waste sludge generation and the ability to produce more methane-rich biogas.

As described in Chapter 3, I investigated the performance of three anaerobic baffled reactors (ABRs) treating wastewater under similar operating conditions in Colorado. Despite sharing location, temperature, and hydraulic retention time, the ABRs exhibited distinct performance in methane generation and removal of chemical oxygen demand (COD) and solids. Lower sulfate concentrations and upstream hydrolysis (resulting in a higher percentage soluble COD) led to increased performance. Additionally, this study showcased the versatility of ABRs in handling various COD and solids loadings while producing consistent effluent concentrations. Designs for ABRs can expect less active sludge wasting compared to aerobic systems, owing to the lower anaerobic microbial growth rates and inert suspended solids removal. While the study provides general design principles, the observed variations between the ABRs underscore the need for further investigation in full-scale treatment systems with emphasis on influent wastewater characteristics. Additional site-specific studies allow designers to identify crucial variables, such as temperature or sulfate and soluble COD concentrations, that uniquely impact ABR performance. By carefully assessing these factors, the design and optimization of ABR systems can be tailored to specific wastewater characteristics, leading to more efficient and reliable wastewater treatment processes.

In Chapter 4, characterization of three influent waste streams (sludge, food scrap waste, and FOG) was used to model methane and carbon dioxide in biogas generated from AnCoD. The results were coupled with a life cycle assessment (LCA) to determine the feasibility and benefits of biogas recovery and use as potential fuel and electricity sources at wastewater treatment facilities on Department of Defense (DoD) installations. Overall, our findings highlight the potential role of AnCoD as a sustainable approach to energy generation in wastewater treatment plants, even at small-scale facilities treating less than 10 MGD. By capturing and utilizing biogas, AnCoD can contribute to reducing greenhouse gas emissions and enhancing energy security for military installations, which aligns with the DoD's commitment to energy security and resiliency. In addition, this study emphasizes the significance of data accuracy in LCA models as variations in data and method selections can substantially impact carbon emissions estimations. Adjustable LCA model parameters were incorporated to allow for up-to-date, region-specific data yielding more accurate results in energy production predictions and impact assessments. The research establishes the foundation for additional investigation of AnCoD as a renewable energy solution. To enhance reliability and applicability, future research will focus on refining the LCA model by incorporating site-specific data from military installations to provision a decision support tool to be used by leaders at other DoD installations facilitating informed and sustainable decision-making for the future.

5.2 Future Work

To produce an accurate model or simulation of an anerobic treatment system, the more plentiful and accurate the underlying data, the more successful the predictions will be. However, discharge permits typically only require accounting of BOD, suspended solids and sometimes nitrogen concentrations. Unfortunately, these become the only constituent concentrations that are quantified and monitored. Subsequently, it is recommended additional study be conducted to fully characterize the influent waste stream of a new treatment system to include non-traditional constituents, such a readily biodegradable COD or sulfur containing compounds. For existing systems attempting to model or improve performance, full characterization between treatment processes or compartments could provide necessary information for relevant system (or system model) parameters. The parameters adjusted in the BioWin model were based on a combination of sensitivity analysis and observed data. Some of the most sensitive parameters in the ABR model were the methanogenic kinetic rates (decay, growth, utilization); however, these parameters were increased or decreased based on observable acetate and methane concentrations, not recorded data for methanogen activity. Therefore, increased and long-term microbial community characterization through genomic DNA extraction and analysis are recommended for better identification of accurate parameter adjustments. Additionally, observation of biochemical methane potential for decreased or increased kinetic rates under differing circumstances (e.g., changes in sCOD, sulfate or temperature) could also support variations in parameter values for specific treatment systems. While the three ABRs used in this study are no longer operational, any future research of other treatment systems could benefit from full characterization of influent and microbial kinetics.

For overall improved ABR performance, additional study is recommended for (1) the examination of influent wastewater holding prior to entry into the treatment system to increase sCOD concentrations and (2) the study of periodic sludge bed disturbance and solids wasting to eliminate inorganic sludge bed accumulation. These two factors may have played an important role in the improved performance of the Mines Park ABR in comparison to the South Platte or Plum Creek ABRs. Additionally, when only the South Platte ABR was examined, negative effects of increased influent sulfate concentrations were not observable. However, in comparison to the two other ABRs operated at similar conditions (e.g., temperature, pressure, elevation), higher influent sulfate concentrations appeared to be a factor in the observed decreased performance. Additional study is recommended to examine the effects of sulfate concentrations on systems to determine if the microbial community (e.g., sulfate reducing bacteria and methanogens) interact in a synergistic relationship enhancing methane production or if the increased sulfate reduction is detrimental to the methanogen population thereby reducing methane production.

Recommendations for future work regarding co-digestion modeling are significant given the relatively few existing studies or reference texts. For the Target Hill treatment facility, comparison of the theoretical performance of anaerobic co-digestion to actual data obtained once construction is complete and the treatment process is stable is the largest area of study remaining. However, co-digestion modeling in general can only be improved with increased information regarding important concepts such as accurate influent waste characterization, pre-processing of food and FOG waste, mixing ratios, solids residence time, and recorded emissions from treatment processes.

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APPENDIX A
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APPENDIX B

SUPPLEMENTAL DATA FOR CHAPTER 2

B.1 Supplemental Data

The supplemental files referenced in Chapter 2 may be found in supplemental file Chapter_2_Files.zip or https://doi.org/10.1016/j.biteb.2022.10123.

APPENDIX C

SUPPLEMENTAL DATA FOR CHAPTER 3

C.1 Wastewater Analysis Equipment

Biogas Composition (gas chromatography – mass spectrometry (GC-MS))

PC: Shimadzu GC-17A and a Shimadzu GC-8A with TCD detectors and a Haysep Q 80/100 column with UHP helium carrier gas at 30 mL/min, Columbia, MD.

MP and SP: Hewlett Packard 6890 with Agilent 5973 Mass Selective Detector with an Agilent 113-3133 GS-Carbonplot capillary column, and helium carrier gas, Santa Clara, CA

Biogas Flowrate

PC: Cole-Parmer 0 to 500 SSCM gas flow meters, Vernon Hills, IL

MP: Agilent Digital Flow Meter – Optiflow 520, Santa Clara, CA

SP: Agilent Precision Gas Flow Meter – 5067-0223, Santa Clara, CA

COD

All systems: Hach ® TNTplus Vial Test 822 or 825 (mercury free) in accordance with Standard Methods (SM) 5220 D

DOC

All systems: Shimadzu TOC-L CSH with NTM-L, Columbia, MD (SM5301B)

Ion chromatography (IC)

All systems: ThermoFisher Dionex ICS-900 with Dionex IonPac, Sunnyvale, CA (SM4110B)

Inductively coupled plasma – atomic emission spectroscopy (ICP-AES)

All systems: Perkin Elmer ICP-AES, Optima 5300, Fremont, CA (SM3120B)

pH

PC: Broadly James pH ProcessProbes, Irvine, CA

MP: Cole-Parmer pH electrodes (100 Ohm Pt RTD, EW-27003-23), Vernon Hills, IL

SP: Cole-Parmer pH electrodes (1000 Ohm RTD, EW-27003-04), Vernon Hills, IL

Suspended Solids

All systems: SM2540B, D and E

Sludge Solids

All systems: SM2540G

Temperature

PC: HOBO Temp Pro V2, Bourne, MA

MP and SP: Labjack EI1034 Temperature Probe, Lakewood, CO

VFA

PC and MP: Shimadzu LC-20AT liquid chromatograph with Agilent Zorbax StableBond, Columbia, MD and Hewlett Packard 6890 with flame ionization detector, Santa Clara, CA (SM5560D)

SP: Hewlett Packard 6890 with flame ionization detector, Santa Clara, CA (SM5560D)

C.2 Influent and Effluent Statistics

Table C.1 Basic statistics of the influent data.

Water Parameter	Average	Std Dev	Median	Minimum	Maximum	Skewness	Q1 (25%)	Q3 (75%)	n
tCOD (mg/L)									
MP	525	318	429	215	2,024	2.94	365	555	360
PC	798	293	715	478	2,400	3.23	662	814	98
SP	692	624	509	143	3,766	2.73	342	717	70
pCOD (mg/L)									
MP	303	289	218	43.0	1,794	3.48	173	298	352
PC	635	274	566	364	2,116	3.38	517	629	97
SP	565	580	388	80	3,441	2.88	265	565	70
sCOD (mg/L)									
MP	225	93.8	205	86.9	1,238	5.23	176	251	352
PC	161	38.3	156	101	338	1.78	138	174	97
SP	127	72.1	119	47.7	473	1.99	69.5	158	70
TSS (mg/L)									
MP	297	595	124	35.9	4,500	4.46	94.9	180	366
PC	524	426	383	271	3,747	4.89	335	528	101
SP	350	478	245	33.0	3,804	5.54	162	331	70
VSS (mg/L)									
MP	275	565	111	33.3	4,268	4.45	82.7	167	365

Table C.1 Continued

Water Parameter	Average	Std Dev	Median	Minimum	Maximum	Skewness	Q1 (25%)	Q3 (75%)	n
VSS (mg/L)									
PC	406	261	333	239	2,175	4.29	291	414	100
SP	292	428	213	29.8	3,513	6.15	138	292	70
dSO_4^{2-} (mg/L)									
MP	60.0	24.1	58.7	0.10	106	-0.30	46.2	77.9	68
PC	44.9	6.90	46.6	27.8	58.7	-0.88	41.8	49.0	37
SP	140	25.8	140	88.8	188	0.11	123	159	35
DOC (mg/L)									
MP	56.9	19.9	53.7	24.0	151	1.77	44.2	63.5	68
PC	58.6	12.6	55.6	30.7	87.1	0.22	50.5	67.4	31
SP	40.0	24.8	34.3	14.2	118	1.38	21.6	48.9	34

Table C.2 Basic statistics of the effluent data.

Water Parameter	Average	Std Dev	Median	Minimum	Maximum	Skewness	Q1 (25%)	Q3 (75%)	n
tCOD (mg/L)									
MP	233	73.0	225	102	524	0.65	97.0	181	357
PC	215	43.3	211	132	412	1.41	184	233	98
SP	234	47.1	230	108	420	0.85	211	252	72
pCOD (mg/L)									
MP	82.0	35.2	82.0	1.00	228	0.13	56.0	106	352

Table C.2 Continued

Water Parameter	Average	Std Dev	Median	Minimum	Maximum	Skewness	Q1 (25%)	Q3 (75%)	n
pCOD (mg/L)									
PC	115	38.3	109	50.0	332	2.25	94.5	127	96
SP	91.5	34.0	93.9	30.1	286	2.51	73.4	104	72
sCOD (mg/L)									
MP	151	49.3	146	61.1	333	0.67	113	181	352
PC	100	19.9	94.0	61.0	146	0.68	86.0	110	97
SP	142	31.2	140	78.3	229	0.49	120	157	72
TSS (mg/L)									
MP	40.0	20.4	40.4	2.94	123	0.52	23.4	52.9	367
PC	41.8	24.1	37.6	13.6	175	2.48	27.0	50.0	101
SP	33.6	14.5	31.7	14.6	84.4	1.33	24.2	38.9	73
VSS (mg/L)									
MP	35.4	17.9	36.2	0.00	112	0.41	21.0	47.5	364
PC	35.3	18.7	32.8	12.5	139	2.28	23.4	43.2	100
SP	27.3	10.0	26.2	12.9	59.0	0.95	20.4	33.1	73
dSO_4^{2-} (mg/L)									
MP	11.8	8.52	8.78	2.00	45.0	1.33	5.70	17.5	71
PC	5.76	2.35	5.21	1.46	11.7	0.66	4.67	7.00	37
SP	59.6	30.7	55.7	13.3	112	0.06	36.0	84.8	35

Table C.2 Continued

Water Parameter	Average	Std Dev	Median	Minimum	Maximum	Skewness	Q1 (25%)	Q3 (75%)	n
DOC (mg/L)									
MP	29.5	16.8	25.6	5	69.9	0.59	15.4	40.7	69
PC	22.9	7.56	22.4	11.9	51.1	1.72	18.4	25.8	32
SP	29.5	8.35	29.7	13.2	50.3	0.03	24.7	35.1	33
Temp (°C)									
MP	18.4	3.77	17.9	8.45	30.1	0.10	15.3	21.7	1,928
PC	19.4	2.82	19.9	9.23	24.6	-0.62	17.4	21.3	152
SP	17.9	5.34	17.1	0.36	29.4	-0.10	14.4	22.6	524

C.3 ANOVA Analysis

C.3.1 Wastewater Temperature

Mean effluent operating temperatures for the three systems are located in Table C.1 (p. 98) and show the value to be approximately 18-19 °C. The null hypothesis being tested is that the means are equal, and the significance level tested is 5% ($\alpha = 0.05$, 95% CI). When the p-value is less than the significance level, the null hypothesis is rejected and there is a statistically significant difference in the means. Conducting an analysis of variance (one-way) in R base produces results that identify whether the means under consideration are the same, but it does not tell which particular means are different nor how they differ. An example of the R code and output for the collective temperature data (all.temp) is depicted below:

P < 0.05, reject H_0 and there is a statistically significant difference between means

```
anova <- aov(Result ~ Location, data = all.temp)
summary(anova)

              Df Sum Sq Mean Sq F value   Pr(>F)
Location       2    278  138.86   8.309 0.000253 ***
Residuals   2601  43465   16.71
---
Signif. codes:  0 ‘***’ 0.001 ‘**’ 0.01 ‘*’ 0.05 ‘.’ 0.1 ‘ ’ 1
```

Tukey multiple comparisons of means (a.k.a. honest significant difference test) allows comparison of pairs of sample means using their absolute differences based on the equation below:

$$T = q_{\alpha(c, n_1 - c)} * \sqrt{\frac{MSE}{n_2}} \quad (1)$$

T – Tukey criteria

q – studentized range distribution

MSE – Mean Squared Error from ANOVA table (16.71 above)

c – number of factors (3 systems)

n_1 – total sample size (2,604 total observations for the 3 systems)

n_2 – smallest sample size (152 for PC)

The Tukey criteria is then compared to the absolute value of means between pairs. If the difference is greater than the criteria, the difference between the pair is significant at the 0.05 significance level. If the difference value is less than the Tukey criteria, that means there is no evidence the means are different. The R output shows the difference between the pairs, the 95% CI, and the p-value of the pairwise comparison and can be plotted for easy visual reference (Figure C.1, p. 103).

```
alpha = 0.05 # 95% confidence interval
tukey <- TukeyHSD(x = anova, conf.level= 1-alpha)
tukey
plot(tukey, las = 1, col = "orangered")

  Tukey multiple comparisons of means
    95% family-wise confidence level

Fit: aov(formula = Result ~ Location, data = all.temp)

$Location
            diff        lwr        upr     p adj
PC-MP  1.0777529  0.2701309  1.8853749 0.0050359
SP-MP -0.4432675 -0.9155402  0.0290052 0.0711756
SP-PC -1.5210204 -2.4041770 -0.6378639 0.0001634
```

$P > 0.05$, do not reject H_0 and there is no statistically significant difference between means of SP and MP.

Figure C.1 Tukey Plot of mean effluent wastewater temperatures.

Similar analyses were conducted on tCOD, pCOD, sCOD, TSS and VSS for normalized influent and effluent mass flow ("influent and effluent loading") rates and system percent removal efficiency. The average values are available in Table C.1 (p. 98) and Table C.2 (p. 99). The Tukey plots are available in Figures C.2-C.6 (p. 104-106), below:

C.3.2 tCOD

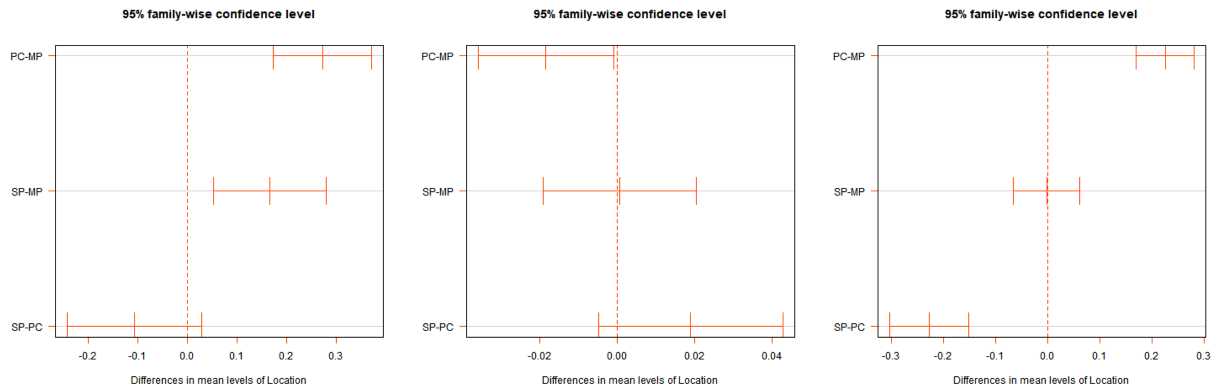

Figure C.2 Tukey plots for average tCOD influent and effluent loading (kg/m^3·d) and percent removal efficiency.

C.3.3 pCOD

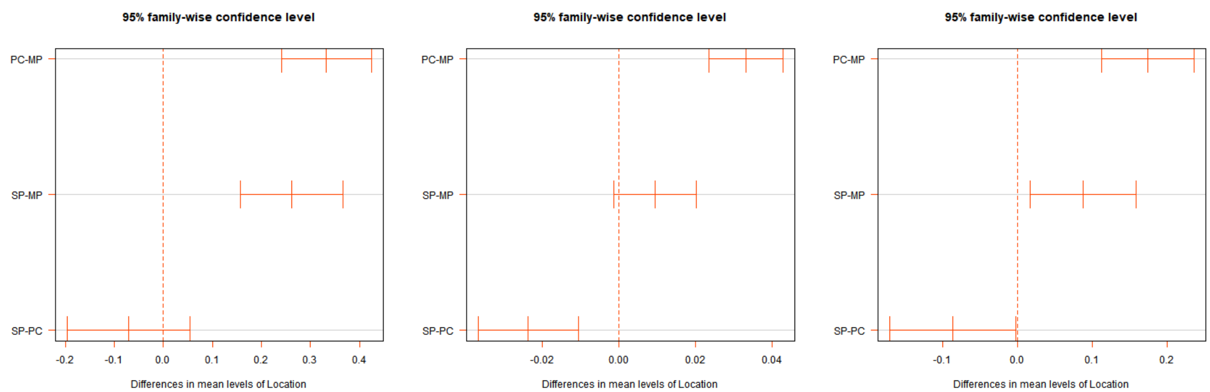

Figure C.3 Tukey plots for average pCOD influent and effluent loading (kg/m^3·d) and percent removal efficiency.

C.3.4 sCOD

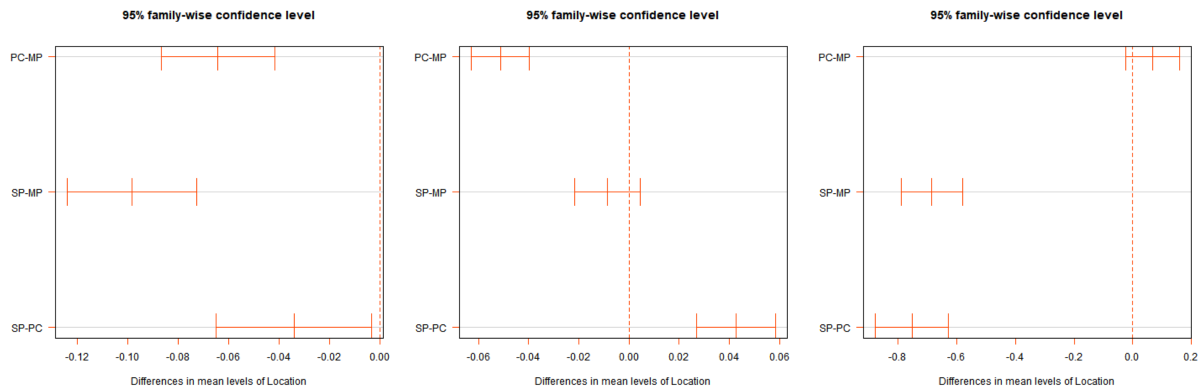

Figure C.4 Tukey plots for average sCOD influent and effluent loading (kg/m^3·d) and percent removal efficiency.

C.3.5 TSS

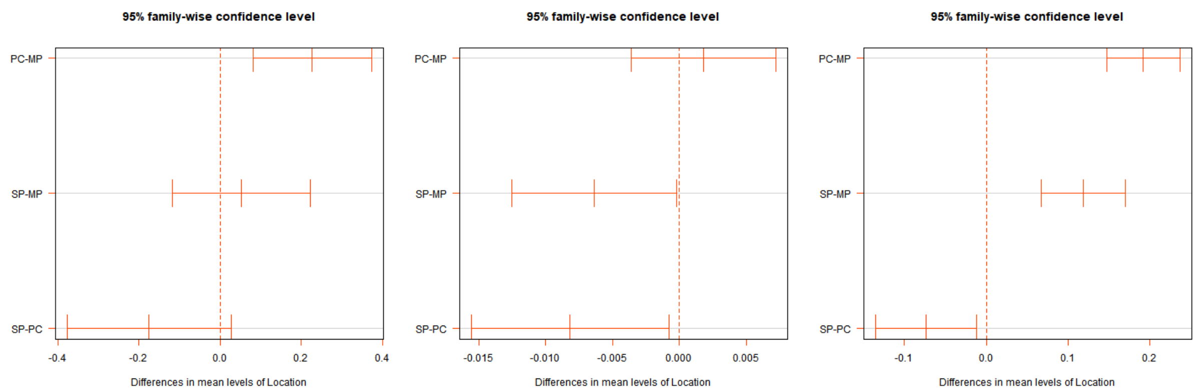

Figure C.5 Tukey plots for average TSS influent and effluent loading (kg/m^3·d) and percent removal efficiency.

C.3.6 VSS

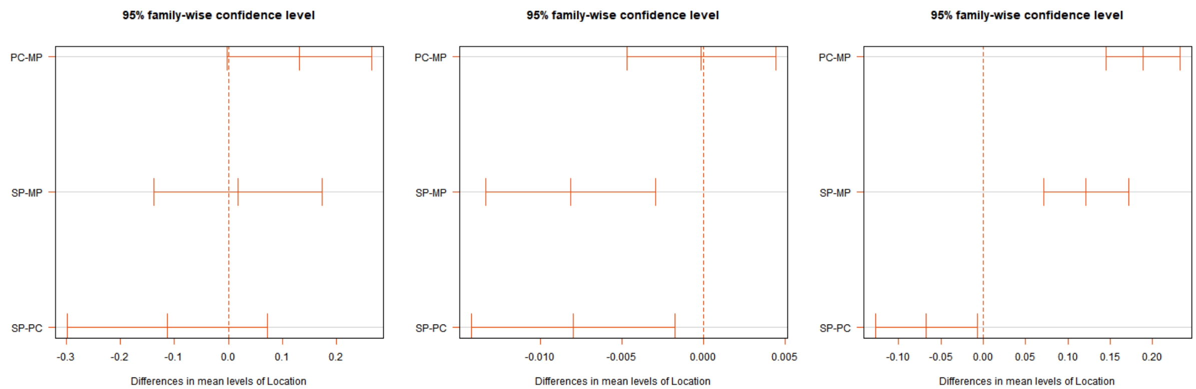

Figure C.6 Tukey plots for average VSS influent and effluent loading (kg/m^3·d) and percent removal efficiency.

C.4 Loading Table

Table C.3 Average tCOD, pCOD, sCOD, TSS and VSS loading (kg/m^3·d) and removal by location. Negative value indicates an increase in effluent load.

	Location	Influent	Removed	Effluent	% Removed[1]
tCOD	MP	0.525	0.292	0.233	48.5%
	PC	0.798	0.583	0.215	71.0%
	SP	0.692	0.459	0.234	48.3%
pCOD	MP	0.303	0.221	0.082	62.9%
	PC	0.635	0.521	0.115	80.3%
	SP	0.565	0.472	0.092	71.6%
sCOD	MP	0.225	0.073	0.151	28.1%
	PC	0.161	0.061	0.100	34.9%
	SP	0.127	-0.013	0.142	-40.4%[1]
TSS	MP	0.297	0.257	0.040	70.8%
	PC	0.524	0.483	0.042	90.1%
	SP	0.350	0.316	0.034	82.7%
VSS	MP	0.275	0.240	0.035	71.1%
	PC	0.406	0.370	0.035	90.0%
	SP	0.292	0.266	0.027	83.3%

C.5 Collinearity

Collinearity occurs when two variables are near perfect linear combinations of one another and the value of one variable depends on the value of the other, usually indicated by the "perfect" r-value (or R^2) of 1. Collinearity itself is not problematic; however, in regression models use of collinear variables may create a problem of multicollinearity. Multicollinearity exists when two or more predictor variables are highly correlated to each other so that they do not provide any unique or independent information to the model [127, 128]. An example of multicollinearity for wastewater might be tCOD and pCOD, as pCOD is calculated from the difference of tCOD and sCOD (sCOD is independent of tCOD, but pCOD is not). Attempting to determine the linear regression model for tCOD (as the response variable) from the predictor variables, sCOD and pCOD, creates potential problems with validity of the model. In the code below, the coefficients for sCOD and pCOD are both 1, with a near 0 intercept. The F-statistic is extremely large and the R^2 is 1. This near perfect model indicates a problem with multicollinearity and a warning is given by the lm package.

```
Warning: essentially perfect fit: summary may be unreliable
Call:
lm(formula = Inf.tCOD_mg_L ~ Inf.sCOD_mg_L + Inf.pCOD_mg_L, data = all2)

Residuals:
       Min         1Q     Median         3Q        Max 
-7.327e-12 -6.800e-15  1.420e-14  3.590e-14  4.024e-12 

Coefficients:
                Estimate Std. Error    t value Pr(>|t|)    
(Intercept)   -3.996e-14  7.202e-14 -5.550e-01    0.579    
Inf.sCOD_mg_L  1.000e+00  3.063e-16  3.264e+15   <2e-16 ***
Inf.pCOD_mg_L  1.000e+00  7.602e-17  1.316e+16   <2e-16 ***
---
Signif. codes:  0 ‘***’ 0.001 ‘**’ 0.01 ‘*’ 0.05 ‘.’ 0.1 ‘ ’ 1

Residual standard error: 6.359e-13 on 515 degrees of freedom
  (2186 observations deleted due to missingness)
Multiple R-squared:      1,	Adjusted R-squared:      1 
F-statistic: 9.542e+31 on 2 and 515 DF,  p-value: < 2.2e-16
```

In contrast to the example above, the regression model for tCOD loading and removal efficiency involves only one predictor variable (loading) and one response variable (removal). The correlation between the two is only $r = 0.71$, not 1. In the code below, "Total.Inf_tCOD_Load" is the system tCOD OLR, "Total.Eff_tCOD_Load" is equivalent to the effluent loading and "Total.tCOD_PR" is the percent removal or removal efficiency.

```
> cor(all2[,c("Total.Inf_tCOD_Load", "Total.Eff_tCOD_Load",
"Total.tCOD_PR")], use = "na.or.complete")

                  Total.Inf_tCOD_Load Total.Eff_tCOD_Load Total.tCOD_PR
Total.Inf_tCOD_Load           1.0000000           0.1191113     0.7097486
Total.Eff_tCOD_Load           0.1191113           1.0000000    -0.5338280
Total.tCOD_PR                 0.7097486          -0.5338280     1.0000000
```

In the case of multiple predictor variables, R offers numerous packages to test for multicollinearity. While not co-predictors, a modified test for the variance inflation factor (VIF), which measures how much the variance of a regression coefficient is inflated due to multicollinearity [127, 128], is used to compare the influent tCOD loading and removal efficiency. A VIF starts at a value of 1 (no multicollinearity) and values above 5 or 10 indicate potentially problematic correlation [127, 128]. In the code below, all values are below 3.2, indicating moderate correlation, but not severe or problematic:

```
> model1 <- lm(Total.tCOD_LR ~ Total.Inf_tCOD_Load + Total.Eff_tCOD_Load +
Total.tCOD_PR, data = all2)

> car::vif(model1)

Total.Inf_tCOD_Load Total.Eff_tCOD_Load       Total.tCOD_PR
           2.468758            1.996754            3.205895
```

The same tests were repeated for influent TSS loading and TSS removal efficiency, again resulting in no potential problems.

```
>cor(all2[,c("Total.Inf_TSS_Load", "Total.Eff_TSS_Load", "Total.TSS_PR")],
use = "na.or.complete")

                   Total.Inf_TSS_Load Total.Eff_TSS_Load Total.TSS_PR
Total.Inf_TSS_Load          1.0000000          0.1697681    0.4209277
Total.Eff_TSS_Load          0.1697681          1.0000000   -0.4693720
Total.TSS_PR                0.4209277         -0.4693720    1.0000000

> model2 <- lm(Total.TSS_LR ~ Total.Inf_TSS_Load + Total.Eff_TSS_Load +
Total.TSS_PR, data = all2)

> car::vif(model2)

Total.Inf_TSS_Load Total.Eff_TSS_Load       Total.TSS_PR
          1.539046           1.624181           1.917030
```

APPENDIX D
SUPPLEMENTAL DATA FOR CHAPTER 4

D.1 Life Cycle Assessment Primer

The life cycle assessment (LCA) is one of several approaches used to inform decision makers regarding the adoption of particular waste treatment practices. Generally, the LCA addresses the environmental aspects and potential impacts of the manufacture, use, and final disposition (e.g., disposal or recycling) of a product or process [33, 125, 129]. However, an assessment can cover any spectrum of a product's life, from the initial creation from elemental materials (known as "cradle"), to the product leaving a manufacturing plant ("gate"), to an end-user disposing of the product in the local landfill (grave). The portion of the life cycle being examined is known as the system boundary. A proper LCA quantifies the potential environmental impacts of the processes involved within the chosen boundary, which can then be used to identify problem areas and/or compare alternatives. The LCA itself is not a solution, but can help inform solutions by identifying the amounts of hazardous waste, contaminants or pollutants being released to the environment and the subsequent effects of the releases [34, 125]. The results of the LCA can be used in conjunction with other approaches, such as life cycle costing (LCC), techno-economic assessment (TEA), or site-specific environmental impact assessments, to assist decision makers in evaluating sustainability of a practice and examine trade-offs [34, 125, 129].

LCAs follow guidance provided in the International Organization for Standardization (ISO) 14040, Environmental management – Life cycle assessment – Principles and framework, and ISO 14044, Environmental management – Life cycle assessment – requirements and guidelines to be considered ISO compliant. These references help standardize terminology, formatting, and reporting requirements of an LCA, which are globally accepted. In accordance with these ISOs, the LCA should conform to a four-part framework including the goal and scope definition, inventory analysis, impact assessment and interpretation [32, 129]. Defining the goal of the LCA, including setting system boundaries, and defining the functional unit, will set the stage for a study that provides enough detail to address the goal (e.g., what process causes the least amount of environmental impact). The life cycle inventory identifies the relevant energy and material inputs and environmental releases, and the life cycle impact analysis evaluates the potential environmental impacts associated with the identified inputs and releases. The final portion of the LCA involves interpreting the results to help inform decision makers regarding their options and potential impacts [32, 34, 125]. The format of this appendix section follows the four-part ISO framework, individually addressing the required components of the LCA.

D.1.1 Goal and Scope Definition

D.1.1.1 Goal Statement

The goal statement of an LCA is more than a mere introduction to the study, it helps shape the remainder of the phases within the framework so that the information provided is compatible and sufficient to address the goal [34, 130]. The goal of the study should unambiguously state (using keywords) the reason for study, intended application, target audience, whether it is a comparison study, and whether the results will be made publicly available [32, 125]. These specific distinctions become important in identifying additional requirements of the study, which readers would expect to find. For example, publicly available LCAs require a critical review of the study by a panel consisting of at least 3 members [32, 34]. Additionally, when conducting a comparison study, a complete LCA must be performed to include the impact assessment with sensitivity analysis [32, 125]. In contrast to an LCA, a life cycle inventory (LCI) excludes the assessment phase and merely provides an accounting of the inputs and outputs without discussion of the environmental impacts [125]. When conducting a study, all phases within the framework may be re-addressed and modified, often due to availability of data or changing assumptions [32, 34, 125]. During these iterations, it is important to return to the goal statement and ensure that the information, assumptions and results continue to support the goal [34, 129]. The goal statement for this LCA is provided in Section 4.3.1.1 of the manuscript.

D.1.1.2 Scope

The scope of the LCA provides qualitative and quantitative statements indicating what information is included in the study and what methods were used to obtain the information [32, 125]. The ISOs guide practitioners of LCAs to address 12 topics within the scope section. Generally, these topics include descriptions of the system being studied (including function, functional unit, boundaries), data (requirements, assumptions, limitations), and data handling methods (impact assessment method, quality reviews, and format) [32]. After the review of 121 published articles regarding wastewater treatment LCAs, Corominas et al. (2020) additionally recommend identifying the level of detail to be included. For example, an LCA likely to be used at the planning level, requiring only low to medium level of detail, would differ from analysis of an existing wastewater facility for operation and optimization, which would require a high level of detail [96]. Corominas et al. (2020) and Curran et al. (2017) also recommend including additional information regarding the methods, such as whether the LCA is attributional, consequential, process or input-output (IO) based, or defined by spatial or temporal boundaries [34, 96].

The scope for this LCA is provided in Section 4.3.1.2 of the manuscript and the requirements of the ISO scope are discussed in more detail in the following sections.

D.1.1.2.1 Product System and Function

The product system describes the processes that provide a particular function, and the function describes what the process system is designed to accomplish or do [125].

D.1.1.2.2 Functional Unit

The functional unit is a key parameter for the LCA as it provides a basis for how the remaining portions of the LCA are mapped, including data collection, inventories, impact assessments, and final analysis of the results. ISO 14044 states that the functional unit normalizes the modeled inputs and outputs to a single reference. The functional unit should be consistent with the goal and scope of the study and also be clearly defined and measurable. Most importantly, for comparison studies the reference flow defined from the functional unit must be the same so that all scenarios are comparable [32]. Authors of common references for creating proper life cycle assessments provide additional guidance that the choice of the functional unit should bridge the inputs and outputs of the analyzed systems and should be linked to the function of the product consistent with all scenarios being examined (i.e., equivalent use) [34, 125]. Additionally, the functional unit should be scaled to provide easily observable differences in the inputs and outputs of the reference flows (e.g., production per day, week, or year) [34]. The functional unit should be able to describe what is needed, how much, for how long, where and how well [131]. A common example is a power plant whose function is to generate electricity [125]. The functional unit could be 1 kWh of electricity generated to provide 115 V AC and 60 Hz frequency to consumers in New York. In this simple case, the input and output would be bridged by the reference flow (1 kWh) normalizing the amount of raw materials needed to produce the electricity (e.g., 1 kg coal/1 kWh) and the emissions from the electricity (e.g., 1 kg CO_2/1 kWh). The functional unit in the example provides the necessary details of what (electricity), where (New York), how much (1 kW), how long (1 hour), and how well (US standard of 115 V, 60 Hz).

In wastewater treatment or resource recovery facilities, the most commonly used functional units are based on flows, such as such as 1 m^3 of wastewater [95, 96]. Functional units are sometimes expanded to include treatment to a specific standard (e.g., discharge permits), so that the reference flow would be 1 m^3 of treated wastewater to permit specifications or normalized to population. Of note, energy production should not be used as a functional unit as seen in Isola et al. (2018), Bartocci, et al. (2020), and Mayer et al. (2021) as energy form and recovery are normally not common across all assessed scenarios [97, 101, 132, 133]. For WRRF studies discussing sludge and biosolids handling, the most common functional units involve solids characteristics [95, 96]. For LCAs of this industry, it is important to note whether volumes and masses used are for the influent, effluent, wet or dry weight, conversion factors, etc., as these values appear to differ between studies. Difficulty arises when the modeled system contains multiple inputs and outputs due to differing processes contained within the boundary. In this study, three influent sludge flows need to be distinguished between each other and an additional five effluent end of life flows for the biogas. The common link between the 15 scenarios examined is the treatment of the primary and waste activated sludge. The functional unit selected for this study is 1,340 kg of influent total solids (TS) in the combined primary and waste activated sludge received at the digester per day. However, the functional unit is expanded to be representative of the differing energy content in the three waste streams through percentages. For example, the combined flow for the third scenario is comprised of 1,340 kg TS from sludge/d, 631 kg from food waste, and 39 kg from FOG waste, resulting in 67% sludge, 31% food and 2% FOG. The expanded functional unit is used to provide clarity and reduce uncertainty in complex LCAs [34, 96] and has been observed in several other anaerobic digestion studies [97–100].

D.1.1.2.3 System Boundary

The system boundary determines which unit processes are included in the LCA and should be consistent with the goal and scope. Decisions regarding the boundary (e.g., size, processes, or exclusions of life cycle stages) need to be identified and explained [32]. Ideally, a life cycle assessment would include all life cycle stages (i.e., cradle-to-grave) [32, 125]; however, the boundary identifies the subset of processes simplifying the amount of information relevant for the focus of the study [34, 96, 125]. This study focuses on the anaerobic digestion process for the treatment of solid waste streams and the subsequent disposition of the biosolids and biogas generated. The anaerobic digestion process becomes the gate (manufacturing process), and the disposition of the treated solids and biogas becomes the grave, creating a gate-to-grave or waste management LCA. Subsequently, this LCA focuses on the direct effects of those processes. Inclusion of indirect effects for the influent waste streams, or those which happen prior to the anaerobic digestion process, would overly complicate the model, fail to address the goal of this LCA and are not generally included for input flows considered waste streams [34, 125, 134]. For example, indirect effects, or an expanded system boundary, could require emissions reporting for how the food waste stream originated, such as emissions from growth, processing, packaging, transport to grocery store, consumer emissions from transport from grocery store, preparation of meal, consumption, waste, transport of waste to a waste facility, treatment by waste facility, etc. Finally, geographical and temporal considerations may be relevant factors in an LCA and should be identified in the scope [96, 125]. In wastewater treatment analyses comparing different treatment options for a WWTP, the resulting reports are likely specific to that site based on local conditions and standards, which could include factors such as population, surrounding environment, legislation, or life expectancy of the facilities and equipment, that are not applicable in another location [96]. This study explores the upgrade of the THWWTP and inherently contains site-specific information (e.g., cost and mix of electricity).

AnD of wastewater sludge serves as the baseline for comparison to the second and third scenarios, incorporating the digestion of food waste and food waste and FOG, respectively. Each scenario of the completed LCA examines 5 options for the biogas generated from the system: uncontrolled release, flaring, boiler, combined heat and power (CHP), and cleaning for natural gas upgrade, for a total of 15 permutations. The proposed extended boundary diagram for the final LCA, which will be integrated into the final decision support tool, is depicted in Figure D.2 (p. 123).

Other previous studies have incorporated the wastewater treatment portion of modeled facilities within their system boundaries. However, the goal of these studies are typically to compare integrated management of wastewater and waste, or options for upgrading existing facilities [98, 100, 104, 135]. Studies pertaining to solids handling have used a smaller boundary, which enables the focus to be the comparison of waste handling technologies [97, 99, 136, 137]. Additionally, a study by Møller et al. (2009) determined that the downstream emissions from anaerobic digestion were the most important, while direct emissions from the digestion process and upstream emissions were less important to impact analysis [102]. In this study, wastewater treatment and upstream processes for the creation of waste streams remain the same for all scenarios and are excluded from the comparison. Influent streams to the digester, the quantity and quality of biogas, and the quantity and quality of biosolids products are different for each scenario and are therefore included in the boundary. End of life treatment of biosolids for Target Hill is currently transportation to a composting facility approximately 30 miles from the installation, where it is composted with wood chips and used in land application. This process remains the same through all scenarios; however, transportation factors (such as weight and vehicle emissions) change with the variable influent organic loads. Alternate biosolids waste treatment and/or disposal approaches (e.g., incineration or landfilling) are not included in the current analysis. Other exclusions are: (1) digestate from the anaerobic digestion and centrate from solids dewatering processes (assumed to be returned to headworks); (2) construction, maintenance, or upgrades of existing infrastructure within the boundary; (3) energy consumption and equipment moving the waste within the boundaries; (4) indoor emissions; (5) administrative tasks; and (6) chemical additions (e.g., for thickening or alkalinity control). Each of these are generally not required in LCA (due to negligible emissions) or difficult to determine for non-site specific information [34, 96, 101].

In addition to exclusions, discussion of the boundary requires identification of cut-off criteria, which is the limit of relevance assigned by the LCA practitioner for exclusion in the study [32, 125].

These are quantitative reference points distinguishing between relevant and non-relevant data for a particular study [34]. Ordinarily, cut-off criteria should be avoided as the argument could be made that the data in the study is biased or incomplete; however, it is still observed in practice in the selection of system boundaries [131, 134]. Determination of what flows are relevant and which are not is usually based on mass, energy, or environmental significance, but also includes exclusion of processes from a study [32]. Common practice is to exclude values for these categories that amount to less than 1% of the total contribution [34, 125]. If cut-off criteria are included in an LCA, the impacts to the LCA from implementing the criteria need also be addressed in the interpretation stage of the final report. Beyond the exclusions already discussed in setting the boundary around the anerobic digestion and biogas treatment processes, additional cut-off exclusions are hydrogen sulfide and nitrous oxide gases generated in the anaerobic digestion process. The substances are generally accepted as insignificant contributor to emissions from wastewater treatment processes, including anaerobic digestion, and preliminary calculations reveal the average sulfur content of the waste streams is less than 0.2% [3, 103].

D.1.1.2.4 Allocation Procedures

Allocation is the partitioning of an input or output flow to different products generated from the same process [32]. Allocation determines what portion of the input and output flows are attributed to the subprocess and is typically based on a physical characteristic, such as mass or energy content, where the system total needs to equal the sum of the allocated totals [32, 125]. For a process where the co-production of two products is fixed, allocation can be easily based on the ratio (e.g., 30% of a input material goes to one portion of the process and 70% to another) [125]. Regardless of the number of processes, when comparing outputs, including emissions, the resulting products need to be fair and based on equivalent functions [125].

Of note, the ISO and several reference texts recommend that allocation situations in LCA studies should be avoided when possible, but also recognize processes that generate one or more co-products are common [32, 34, 125]. One form of avoidance is disaggregating the original process into smaller sub-processes, so that each sub-process had a single product [125, 134]. Another common method for allocation avoidance is system expansion (by addition or subtraction) [32, 34, 125, 134]. System expansion by addition involves adding a process to an existing process that only produces one product, so that it can be directly compared to a different process that produces two products. System expansion by subtraction (also known as substitution or avoided burden) involves crediting the system with the output of a dual product process and is common in consequential LCAs (discussed in more detail in Section D.1.1.2.7) [32, 34, 125].

In this study, the CHP process results in the production of both heat energy and electrical energy. In the CHP, a microturbine (or other CHP technology) uses a portion of the input fuel (methane-rich biogas) for generating electricity through combustion of the fuel source to drive an electric generator. Exhaust from the combustion process also produces thermal energy, which is captured to increase the efficiency in the turbine, but can be used for external heating (i.e., liquid in a boiler or space heating). Each subprocess within the CHP creates its own product, either heat or electricity, and each with their own efficiency and share of the emissions. In the case of CHP, the two products have two different functions (one to provide heat and one to provide electricity) and are not directly comparable as they are two different forms of energy. Additionally, comparing the ability of a CHP unit to produce heat with the ability of a single process designed only for heat production (e.g., a boiler) could seem unfair. The heat recovery efficiency of a CHP unit has been observed as varying between 35 and 50%; however, the heat recovery efficiency of the boiler in this study is approximately 80%. The intent of the analysis is not to directly compare the ability of a selected CHP unit to produce heat with that of a boiler to produce heat, but to show the difference between heat generated from the biogas with sludge, sludge and food, and sludge food and FOG as inputs.

Mehmeti and Canaj (2022) conducted a review of 59 LCAs for wastewater treatment and reuse between 2010 and 2022. Approximately, 17% of the reviewed articles used system expansion by addition and 19% used avoided burden (system expansion by subtraction) with the remaining 64% not clearly stating either allocation approach. Literature review for this study resulted in 10% of articles using economic based allocation, 20% using system expansion by avoidance, 40% not specifically addressing allocation, but appeared to use avoidance, and the remaining 30% of studies providing no information regarding their selection. In the current study, allocation by physical apportionment for the heat and electricity generated from CHP or boilers is not necessary. However, the resulting output of the two products (heat and electricity) is necessary to compare the differences between the three influent streams. These products, and emissions, are credited to the system as avoided burdens of grid electricity and natural gas heating. The values of the differing functions of all of the products are still reported in the LCI findings; however, direct comparisons between them are based on the same energy type and units (e.g., kWh for electricity production) or the same process (e.g., boiler heat recovery from the three streams).

D.1.1.2.5 Impact Assessment Interpretation Methods

Impact assessment methods categorize the outputs from the modeled processes into categories based on their environmental impacts [125]. A particular category title may change slightly depending upon the specific method used, but generally they include impacts to climate change via global warming, damages to the atmosphere and ozone layers, pollution in waters or soils, non-renewable resource use, energy consumption, and effects on human health (e.g., carcinogens or particulate matter in the air). The impact categories chosen for a study should be explicitly stated along with the selected method (including version). Many factors can affect the decision for which method to use, but generally include relevance to the goal/scope, geographic location, time, and industry [34, 96, 125]. Common methods include ReCiPe, CML, and TRACI, although many different methods are available depending upon region and environmental focus [34, 96, 125, 138]. Once the relevant categories within a method are identified then the data is characterized by a specific factor. This normally is a mathematical conversion of the inventory data into impact category indicators based on pre-existing scientific studies. The resulting characterized value becomes the basis for comparison between alternative scenarios and subject to assessment in the final interpretation phase of the study. Optional treatment of the impact assessment profile may also include normalization (e.g., to population), grouping, or weighting, but use of the additional transformations may introduce uncertainty or bias in the study and make them difficult to compare with other studies [125]. However, a common optional classification includes grouping and weighting based on endpoint factors. Endpoint factors adjust the values obtained from the impact assessment (known as midpoint) to potentially more easily understood damage categories such as how global warming may affect human health represented by the disability adjusted life-years (essentially, years of human life lost due to GHG emissions) [96, 125, 139]. ReCiPe and IMPACT 2002+ methods include both midpoint and endpoint analysis for comparison in a LCA [123, 139, 140].

Generation of methane gas during the anaerobic digestion process generates environmental impacts. For example, if inventory results show there is a flow of 300 m^3 CH_4/kg of TS exiting the anaerobic digestion process, this gas must be captured or released to the atmosphere. When released to the atmosphere, methane gas is considered a greenhouse gas (GHG). GHGs retained in the atmosphere trap heat causing increased temperatures, a phenomenon known as global warming, which can induce climate change (long-term shift in temperature and weather resulting from global warming). The distinction between GHG and climate change is noted here because different impact assessment methods label their categories differently and resulting impacts need to be comparable. For example, the adopted standard in Europe (EN15804+A2) uses the impact category “climate change” and the Intergovernmental Panel for Climate Change (IPCC) differentiates between global temperature change potential (GTP) and global warming potential (GWP); however, all impact values are listed in the same units, as kg of CO_2-equivalents.

Returning to the hypothetical inventory result of 300 m^3 CH_4 / kg of TS, the methane must be converted to an impact category’s characterized units for global warming or climate change potential (kg CO_2-eq). Methane is considered a more potent GHG in comparison to carbon dioxide, so the characterization factor is a number multiplied by the amount of methane in the inventory. The characterization factor differs between different methods and may also vary depending on how far in the future the researcher wants to model the environmental impacts. Temporal categories are based on cultural theory: individualist (I) considers short-term interests (e.g., 20 years) with more certain impacts; hierarchical (H) is considered the default or medium view (e.g., 100 years) with a consensus regarding impacts based on existing policies and technologies; and egalitarian (E) is the long-term view (e.g., 500 years) considering impacts with less certainty and a pessimistic stance on management and technology [125, 141]. Returning to methane, the conversion factor could be anywhere from 7.95 to 86 (kg CO_2-eq/kg CH_4) depending upon near- or long-term considerations or which IPCC assessment report the factors are based on (e.g., 4th from 2007, 5th from 2013-14, or 6th from 2021-22).

Beginning in the 1990's, additional categories were created differentiating between carbon dioxide and methane emissions to the air generated from the combustion of fossil fuels versus those generated from the combustion of biogenic sources (such as wood or other organic matter), which can complicate an analysis [103, 142]. The theory is based on the carbon cycle where biogenic carbon emissions (e.g., carbon dioxide and methane from AnD) are released into the air and plants and trees sequester carbon for photosynthesis. Biogenic carbon can move to soil through decomposition or biological consumption, which can in-turn return the carbon to the atmosphere from breathing or decomposition. Several studies indicate that carbon emissions generated from downstream organic matter sequestration should not count against the greenhouse gas inventory [103, 143]. Over the years the practice has become common place and is evident in most existing assessment methods. However, caution should be taken as adaptation of distinguishing between fossil and biogenic carbon is not consistent. Some methods choose to credit $CO_{2,\ bio}$ in the inventory (reducing $CO_{2,\ fossil}$) some assign a factor of zero, and some do not distinguish between biogenic or fossil. $CH_{4,\ bio}$ emissions may still be counted as a GHG emission and/or or may be assigned a different factor. Finally, LCA software such as Sphera's LCAFE, Pré Sustainability's SimaPro, and GreenDelta GmbH's openLCA have elected to create additional methods based off existing methods for compatibility with their databases. For example, the original TRACI v. 2.1 does not distinguish between fossil and biogenic emissions and assigns a characterization factor of 25 to convert methane to carbon dioxide [109, 144]. However, all three of the software tools mentioned previously have created "TRACI v. 2.1" impact assessment methods which differentiate between the methane or use different characterization factors (e.g., 22.25 for $CH_{4,bio}$ vs. 25 $CH_{4,fossil}$) [120, 145, 146]. Examples of these differences are highlighted in Figure D.1 (p. 118).

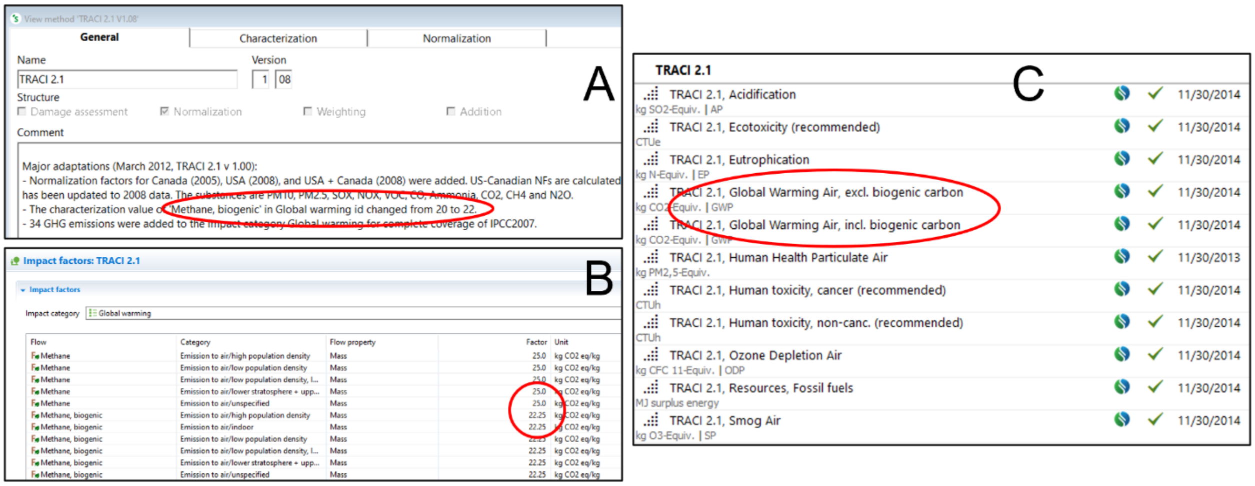

Figure D.1 Software screen captures depicting the different treatment of fossil and biogenic carbon emissions (SimaPro in the top left (A), openLCA in the bottom left (B), and LCAFE in the right (C)) in comparison to the original TRACI impact assessment method, which does not differentiate, using a fixed conversion factor of 25.

The differences in methane and carbon dioxide emissions from biogas between the 15 scenarios are the focus of this study and subsequently, one impact category is considered, climate change. Given the number of scenarios and the desire of the Department of Defense (DoD) stakeholder to only understand carbon-related impacts, this study emphasizes the differences of climate change or global warming potential impacts for each scenario. Focusing impact results to those the stakeholder is most concerned with is a vetted approach [34, 96] and is also observed in other published modeling studies and decision support tools [99, 132, 147]. Even in studies that include multiple impact categories, climate change or global warming are topics of specific focus [97, 101, 106, 148, 149]. Land use, especially in the context of avoiding organic waste in landfills, is also of interest. However, due to likely variations in volume, location, and distance from other military WRRFs, inclusion of this category would require future study for implementation in a decision support tool (and could possibly be outside the overall scope of the study).

D.1.1.2.6 Data Collection and Data Quality Requirements

Data collected for an LCA may include a mixture of measured values from the system being studied, calculated values based on equations, or estimated based on literature review and statistical information [32]. In this portion of the scope, data quality requirements should be specified. Requirements provide information regarding the quality (e.g., precision, completeness, consistency, and reproducibility) of the sources, as well quantifiable measures (e.g., technology, location, time period, and uncertainty) [32, 125]. Data can generally be described as originating from primary or secondary sources and categorized as either foreground or background information [34, 125]. Foreground materials are those that are determined specifically for the study, such as measuring biogas flowrate and composition of the THWTTP digesters or obtaining manufacturer's documents for a piece of equipment. Background materials are those not created exclusively for the study, but are relevant and provide representative information, such as publications pertaining to anaerobic co-digestion [34]. Additionally, issues concerning the data are revisited in the final interpretation phase, where results regarding sensitivity and uncertainty analyses may have impacted the results.

The upgraded THWWTP is scheduled to begin startup procedures in November 2023, which will include food scrap waste and FOG processing and co-digestion. As this is a new system for THWWTP, relevant measurements of carbon, oxygen demand, solids, and biogas production are not yet available. Usable measurements for the new system will not be available until after co-digestor start-up and steady state is achieved – likely in the spring of 2024. Accordingly, this study uses background data for THWWTP and literature data to create an initial LCA model, which will be updated and refined in 2024. Sources of data predominantly originated from literature review of primary sources and the use of secondary source databases created and maintained for the purpose of conducting an initial LCA. In an effort to limit potential bias and to support development of a custom-built model, effort was made to review the original source of primary data when discovered in secondary sources. Effort was also made to confine the review to published information within the last 10 years to ensure the most recent technological improvements were included; however, it was not always possible, and some sources are between 10 and 20 years of this study. For example, the supporting documentation and database contents of USEPA TRACI assessment model were originally released in 2012 (with data from the ICCP AR3, 2001), and only one update for normalization factors in 2014 [109].

The software program used in this study was LCAFE, which included paid databases for relevant processes (e.g., end of life treatment of waste products and energy use) developed by Sphera, and ecoinvent version 3.9.1, a life cycle inventory database maintained by a non-profit organization in Switzerland. The software and supporting databases are updated frequently and are considered reliable and of good quality; however, these data are sometimes limited due to proprietary ownership. For example, Sphera created an aggregate process (a group of smaller unit processes for a total system LCI), which provides all inputs and outputs (including all emissions) for the entire wastewater treatment plant combined. A user enters in the amount of wastewater treated and the apportionment of where the treated sludge should end up (incineration, landfill, or agricultural land use). From these user defined settings, the quantity of emissions is then calculated. This is very convenient for modeling wastewater treatment in general, but not for looking at individual unit processes such as anerobic digestion or sludge drying. The underlying unit processes with their relevant inputs and outputs are proprietary, unavailable, and unverifiable; therefore, each must also be examined outside LCAFE. To address this shortcoming, flows and processes were created using an independent set of values based on stoichiometric calculations and supported by statistical analysis of existing data reviewed. This approach facilitates the transfer of the LCA inventory and impact assessment into a spreadsheet-based decision support tool for DoD users. Additionally, use of equations for calculating unknown values for which there are no measurement is common [97, 104–107]. For example, similar to this study, Alyaseri et al. (2019) conducted a statistical review of literature and used the results for their LCA model [108]. Other than lack of primary data from THWTTP and limitations inherently created from selection of the boundary and assessment method, no additional limitations were identified and considered.

D.1.1.2.7 Type, Format and Review of the LCA

According to ISO 14044, the scope of an LCA needs to describe the “type and format of the report required by the study” [32]. ISO 14040 defines two types of studies, life cycle inventory and life cycle assessment studies. The difference in these two study types is distinguished by the inclusion of the impact assessment phase [129]. In a life cycle inventory analysis, the inventory results (inputs and outputs only) are the final data that are discussed in the interpretation phase (analogous to the results, discussion, and conclusion sections of a scientific journal article) and are not categorized by a particular assessment method nor are values converted into characterized values (e.g., kg CO_2 eq.). Many studies may terminate at this phase, but a full life cycle assessment includes the impact assessment phase [34, 125].

The type of LCA may also be defined by two main modeling principles where inventories are considered attributional or consequential [34, 150]. Attributional models depict a product system either as it currently is, or what it will look like in some future scenario. Data in attributional model inventories allow for comparison of the relative contributions of each process within an entire system. Attributional models are more confined analyses, focusing on the material balances. Attributional models address the environmental impacts of a specific property of a product or process [34]. Additionally, the modeling of the background data is based on average industry data and those processes with co-products are treated by allocation (or possibly system expansion) [131].

In contrast, a consequential model examines the same inventories, but recognizes the values are no longer fixed and may fluctuate based on social or economic demand [34, 150]. Values could include strictly financial factors, such as costs or supply and demand, but could also include shifting ideals, such as the paradigm swing from waste disposal to treatment to recovery of valuable resources. Consequential models examine the forecasted environmental consequences of different actions or decisions, by using marginal process background data (processes employed in response to a change in demand) and system expansion is used for all multi-functional processes [34, 131].

The distinction between attributional and consequential LCAs is rather abstract, especially since there are no definitive guidelines; however, numerous authors of LCA reference manuals try to clear up the decision to use one or the other, or even a combination [34, 131, 150]. Heimersson et al. (2019) published a study where both consequential and attributional methods were used, highlighting the distinctions between them but also showing how the data may overlap. The example they provide is that a consequential LCA, identifying differing environmental impacts for differing treatment options for solids handling at a wastewater treatment plant (system boundary for the entire plant) will provide information to a decision maker regarding the sustainability of one process over another. However, the same data may be used by managers to establish the impacts of specific subsystems within wastewater (e.g., aerobic biological treatment vs. solids handling) [151].

This study is primarily conducted as a consequential life cycle assessment, to include the impact assessment reviewed in the interpretation phases. It is consequentially based due to the change in market demand from solids treatment in anerobic digestion to resource recovery in the form of usable energy converted from biogas. The five potential biogas dispositions represent the possible decision-based principles, which may change whether the stakeholder prefers a business-as-usual scenario, a cost saving scenario, an energy independence scenario, or a pollution reduction scenario. Finally, this study uses system expansion by subtraction (also known as substitution or avoided burden) which involves crediting the system with the output of a dual product process (e.g., electrical and heat energy from the CHP process) and is common in consequential LCAs to avoid allocation (or partitioning) of the inputs and outputs. With fixed flows based on the actual state of the system and limited analysis regarding alternate disposal methods, this LCA is also attributional in regard to the food and FOG waste. However, the developed flows in this study were built with user-definable parameters; additional future research will include alternative disposal methods for food, FOG, and biosolids.

D.1.2 Life Cycle Inventory

Details regarding the equations used to calculate the inventory are located in Sections 4.3.2 and 4.3.3 of the manuscript, while the inventory is located in Section 4.4.

D.1.3 Impact Assessment

Details regarding the results of the impact assessment are located in Section 4.4.2.

D.1.4 Interpretation

The final phase of an LCA, interpretation, contains three main subsections: identification of significant issues, evaluation of the results, and a discussion regarding the conclusions, limitations, and recommendations [5]. In this section, the results of the previous phases (inventory and impact assessment) are analyzed together in relation to the goal and scope, as well as findings pertaining to assumptions and uncertainty and sensitivity analyses [4, 16]. Identification of significant issues involves highlighting the most important findings, such as key processes and flows and their relative contributions to impact categories. It may also address issues stemming from assumptions, boundaries, functional unit, or allocation [16]. For example, the choice to use "kg wastewater sludge/d" versus "kg waste TS/d" as a functional unit or not including the electricity consumption for FOG processing should be examined considering results. Results evaluation also involves checking the data for completeness, identifying sensitive components, and evaluating consistency of findings against the goal and scope [16]. If a particular part of the inventory is missing data or data are too uncertain, adjustment to the boundary (as well as a discussion as to how and why the boundary was altered) may be required. The most common approach for uncertainty analysis is Monte Carlo. Morris one-at-a-time or Spearman correlation coefficients are the most common sensitivity analysis methods. The results (e.g., probability distribution functions, ranges, most sensitive parameters) should be included in the discussion [13]. Finally, the conclusions and recommendations section provides logical and reasonable assertions while acknowledging the limitations of the study. Conclusions need to be made based on the inventory and impact assessment results and consistent with the goal and scope [4, 13].

D.2 Expanded System Boundary

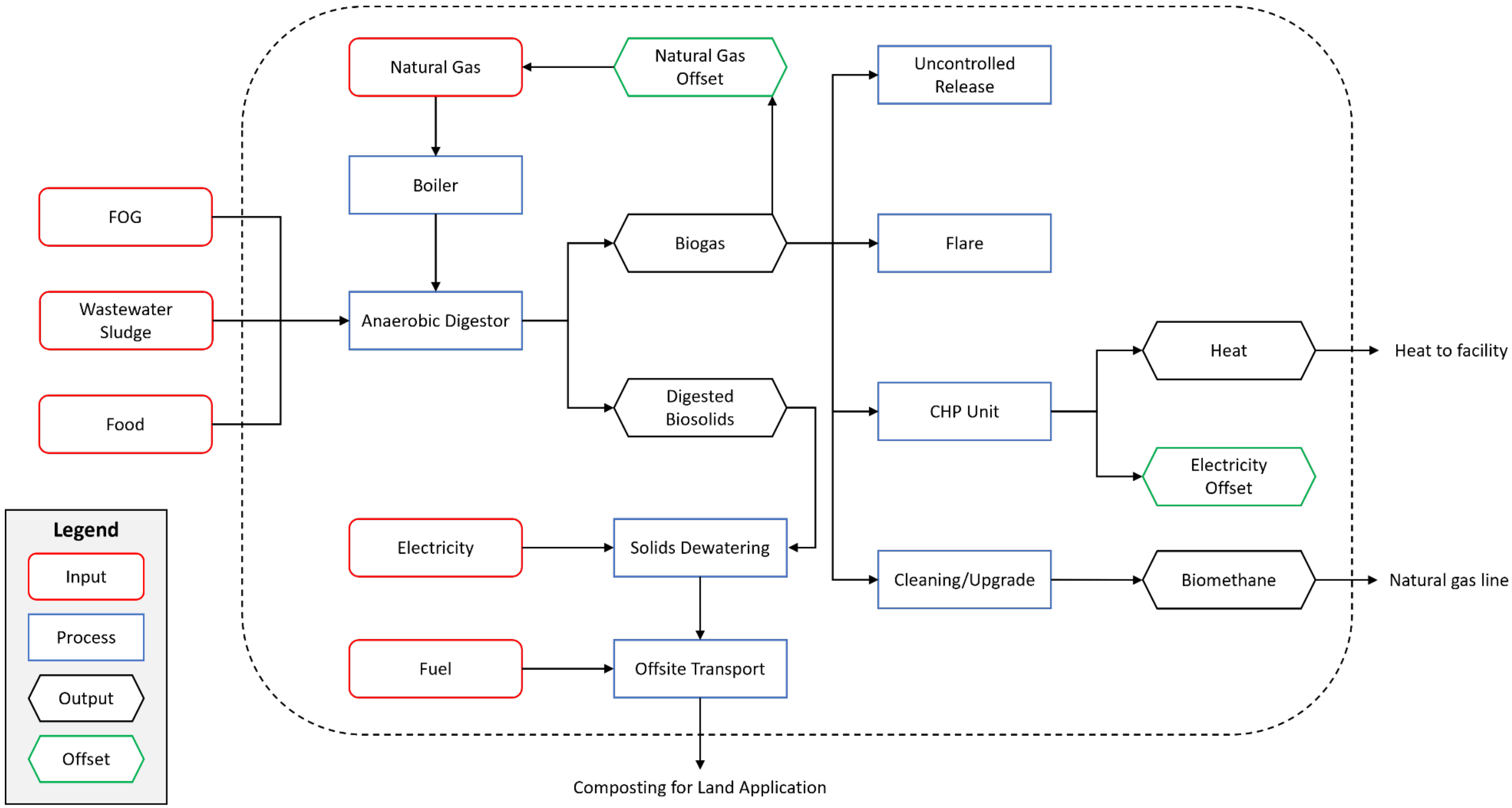

Figure D.2 Proposed extended system boundary including all three influent streams and five biogas dispositions.

D.3 Supplemental Data

Sources not cited in the text but used to characterize the wastewater sludge, food, and FOG may be found in the supplemental file Chapter_4_Additional_Sources.xlsx.

D.4 Alternate Model Values

Table D.1 Values used and resulting calculated values using the alternate model (Section 4.3.3, Equation (4.4, and Equation (4.5)

	Feed rate (m^3/d)	tCOD (mg/L)	$cBOD_5$ (mg/L)	bCOD (g/m^3) (S_0)	bCOD (kg/d)	$bCOD_{eff}$ (g/m^3) (S)	$bCOD_{eff}$ (kg/d)	P_x (kg/d)	m^3 CH_4/d (@35C)
Primary	19.97	41,246	20,929	33,221	663	13,288	265	17	150
WAS	16.04	62,445	31,688	50,298	807	20,119	323	20	182
Food	5.46	242,354	118,877	188,694	1,030	75,477	412	26	232
FOG	0.13	597,860	293,219	465,427	58	186,171	23	1	13
Combined Sludge	36.01	55,350	28,085	44,579	1,605	17,832	642	41	362

D.5 Estimated Food and FOG Waste Contributors and Flows

Table D.2 Food scrap and FOG waste generators on West Point with estimated generation rates.

Generator	Generation Rates	
	Food Waste (kg/week)	FOG Waste (kg/week)
Bowling Alley	144	16
Thayer Hotel	188	44
Commissary	1,500	NA
Post Exchange Burger King	171	44
Child Development Center	27	NA
Michie Stadium and Holleder Sports Center	207	44
Grant Hall	108	22
Cadet Mess Hall	13,870	532
West Point Club	119	18
Firstie Club	29	11
Eisenhower Hall	30	14
Subway / Starbucks	79	11
Elementary School	54	9
Keller Hospital	48	9
USMAPS (Prep School)	629	29
Residential Areas	1,987	NA
Total	**19,191**	**801**