System Studies of Anaerobic Co-digestion Processes

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SYSTEM STUDIES OF ANAEROBIC CO-DIGESTION PROCESSES

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Abstract

Production of biogas through anaerobic digestion is one pathway to achieving the European Union (EU) goals of reducing greenhouse gas emissions, increasing the share of renewable energy, and improving energy efficiency. In this thesis, two different models (Anaerobic Digestion Model No. 1 and an artificial neural network) are used to simulate a full-scale co-digester in order to evaluate the feasibility of such models. This thesis also includes models of two systems to study the inclusion of microalgae in biogas plants and wastewater treatment plants. One of the studies is a life-cycle assessment in which replacement of the ley crop with microalgae is evaluated. The other study concerns the inclusion of microalgae in case studies of biological treatment in three wastewater treatment plants. Finally, the co-digestion between microalgae and sewage sludge has been simulated to evaluate the effect on biogas and methane yield. The results showed that Anaerobic Digestion Model No.1 and the artificial neural network are suitable for replicating the dynamics of a full-scale co-digestion plant. For the tested period, the artificial neural network showed a better fit for biogas and methane content than the Anaerobic Digestion Model No. 1. Simulations showed that co-digestion with microalgae tended to reduce biomethane production. However, this depended on the species and biodegradability of the microalgae. The results also showed that inclusion of microalgae could decrease carbon dioxide emissions in both types of plants and decrease the energy demand of the studied wastewater treatment plants. The extent of the decrease in the wastewater treatment plants depended on surface volume. In the biogas plant, the inclusion of microalgae led to a lower net energy ratio for the methane compared to when using ley crop silage. Both studies show that microalgae cultivation is best suited for use in summer in the northern climate.
Dedicated to my family
Acknowledgement

This thesis is the end product of a long journey. I want to thank my supervisors, Jinyue Yan and Eva Thorin, who have been with me all this time. Thank you very much for all your comments on my papers and all your input and for not giving up on me. Special thanks to Eva for being available to meet on short notice many times.

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I also want to thank Jesus Zambrano for many valuable discussions regarding modelling and for help with LaTeX. I also want to thank all my other colleagues not mentioned here for many interesting conversations in the coffee room and valuable information, such as the colour code of "IKEA white".

These years have been some of the most eventful in my life, with regard to both my PhD studies and my private life. I am grateful to my friends and family for their support. Last, but not least, I want to thank Jim Nordlander, my partner in everything and the love of my life. I could not have done it without you.
Summary

To achieve the European Union (EU) goals of reducing greenhouse gas emissions, increasing the share of renewable energy, and improving energy efficiency, a broad perspective is needed. The production of biogas through anaerobic digestion has the potential to contribute to achieving this goal. It is important that the biogas is produced as efficiently as possible and with low emissions of greenhouse gases. Anaerobic digestion is used in several different systems, both in stand-alone biogas plants primarily intended for biogas production and also in wastewater treatment to treat sewage sludge.

The objective of this thesis is to evaluate different ways of improving processes containing anaerobic digestion. Modelling and simulation are tools that can be used to improve the operation of processes. In this thesis, a full-scale digester has been simulated using two different models, an artificial neural network model and the Anaerobic Digestion Model No. 1. The overall aim for the full-scale modelling has been to determine the feasibility of using such models for a full-scale digester. Another way of improving the energy balance for such systems is to reconsider the substrates that should be used. This thesis also includes studies of two systems. The first is a life-cycle assessment of a biogas plant in which replacing the ley crop with microalgae is evaluated. The second system studied concerns the inclusion of microalgae in the biological treatment of three wastewater treatment plants. Further, the co-digestion between microalgae and sewage sludge has been simulated to evaluate the effect on biogas and methane yield.

Results show that both the artificial neural network and the Anaerobic Digestion Model No.1 could successfully simulate the raw biogas outflow and the methane content of that biogas. The greatest hindrance in using the models was in measuring parameters related to the characterisation of the substrates. The Anaerobic Digestion Model No.1 requires a detailed characterisation of the substrates, which is challenging and not covered by measurements usually made at the biogas plant. Furthermore, it would be beneficial for both models if more of the input parameters could be measured online, both for characterisation of the inputs as well as validation of the models.

Studying the inclusion of microalgae at the wastewater treatment plant showed that the microalgae had the potential to reduce both energy use and greenhouse gas emissions for the three wastewater treatment plants. However, to get a reduction greater than 10%, the land requirement of the current biological treatment needs to be increased several times. At the biogas plant, the co-digestion with microalgae would require greater energy use from a life-cycle
perspective than co-digestion with the ley crop silage. However the land use would be less with microalgae compared to ley crop silage. The microalgae, if cultivated without greenhouse heating, also have the potential to reduce greenhouse gas emissions. The largest reduction in greenhouse gas emissions for both wastewater treatment plants and biogas plants were shown to occur when the microalgae is cultivated during the summer period compared to during the entire year.

Findings from the simulations of co-digestion with microalgae and sewage sludge showed a reduction in biogas and methane production when replacing part of the incoming waste activated sludge with microalgae. However, this seems to be dependent on the composition and species of microalgae as values taken from literature on another species of microalgae gave more biogas and methane than the comparative waste activated sludge.
Sammanfattning

EUs klimatmål innebär att till 2030 ska utsläppen av växthusgaser minska, andelen förnyelsebar energi öka och energianvändningen ska bli mer effektiv. Produktion av biogas genom anaerob rötning är en väg för att nå dessa mål. Det räcker dock inte att bara producera biogas, den borde även produceras så effektivt som möjligt och med så låga utsläpp av växthusgaser som möjligt. Anaerob rötning används i flera olika system, både i enskilda biogasanläggningar vars främsta mål är att producera biogas och som en del i reningsverk. Syftet med den här avhandlingen är att titta på olika sätt att förbättra processer som använder sig av anaerob rötning.


Resultaten visar att både det artificiella neurala nätverket och Anaerobic Digestion Model No.1 kan förutsätta utförs av rå biogas och metanhalten hos biogasan. Det största hindret mot användningen av modellerna är relaterat till karaktäriseringen av substraten. Anaerobic Digestion Model No.1 kräver en detaljerad karaktärisering av substraten som är svår att utföra och som inkluderar analyser som inte normalt utförds vid biogasanläggningen. Dessutom skulle det vara fördelaktigt för båda modellerna om mer av de parametrar som krävs till indata och till validering kunde mätas kontinuerligt.

Systemstudien av inkludering av mikroalger vid reningsverken visar att mikroalger har potential att reducera energianvändningen såväl som utsläppen av växthusgaser. Emellertid, för att få en större reduciering krävs att marknävändningen för den nuvarande biologiska reningen ökar flera gånger om. Systemstudien för biogasanläggningen visar att inkludering av mikroalger skulle kräva mer energi i ett livscykelperspektiv än ensilage, däremot skulle en
mindre yta krävas för odling. Om mikroalgerna odlas under sommarmånader-
na utan uppvärmning av växthusen så blir utsläppen av växthusgaser mindre
jämfört mot användning av ensilage. För båda systemstudierna gäller att den
bästa effekten för mikroalger uppnås när mikroalgerna odlas under sommar-
perioden, jämfört med odling under hela året.

Slutligen så visade simuleringen av samrötning mellan mikroalger och av-
loppsslam att när en del av den inkommande organiska torrsubstansen för se-
kundärsen ersätts med mikroalger så minskar biogas- och metanproduktio-
gen. Däremot så verkar det vara beroende av sammansättningen hos mikroal-
gerna/mikroalgart. För en av de mikroalgarter vars värden togs från litteratu-
ren, så blev resultaten att en större mängd biogas och metan skulle produceras
jämfört med sekundärsslam.
List of Papers

Publications Included in the Thesis

I Nordlander, E., Thorin, E., Yan, J. (2017). Investigating the possibility of applying an ADM1 based model to a full-scale co-digestion plant. *Biochemical Engineering Journal*, 120: 73-83


III Nordlander, E., Thorin, E., Yan, J. (2017). Simulation of co-digestion of microalgae and sludge. *Manuscript*


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Author’s Contribution

I Planning of study, data collection, modelling, analysis of the result as well as the writing the majority of the paper

II Planning of study, data collection, modelling, analysis of the result as well as the writing the majority of the paper

III Planning of study, modelling, analysis of the result as well as the writing the majority of the paper

IV Participated in the data collection, did the modelling and calculations, the majority of the analysis as well as writing the majority of the paper
V Performed a large part of the data collection and participated in the analysis and the revision of the draft

Publications not Included in the Thesis


V Ericson, E., Thorin, E., Yan, J. (2010). Exploring the possibility of using a simple neural network for the prediction of biogas production of a solid waste digester. *12th World Congress on Anaerobic Digestion*, Oct 31 - Nov 4, Guadalajara, Mexico


Some papers were written under the author’s birth name "Ericson".
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Nomenclature

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<tr>
<td>ADM1</td>
<td>Anaerobic Digestion Model No.1</td>
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<td>ANN</td>
<td>Artificial Neural Network</td>
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<td>BMP</td>
<td>Biomethane Potential</td>
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<td>BOD</td>
<td>Biological Oxygen Demand</td>
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<td>COD</td>
<td>Chemical Oxygen Demand</td>
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<tr>
<td>CODp</td>
<td>Particulate Chemical Oxygen Demand</td>
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<tr>
<td>CODs</td>
<td>Soluble Chemical Oxygen Demand</td>
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<td>GHG</td>
<td>Greenhouse Gas</td>
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<td>HRT</td>
<td>Hydraulic Retention Time</td>
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<td>HRAP</td>
<td>High-Rate Algal Pond</td>
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<td>LCA</td>
<td>Life-cycle Assessment</td>
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<td>LCFA</td>
<td>Long-chain Fatty Acids</td>
</tr>
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<td>LCS</td>
<td>Ley Crop Silage</td>
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<td>MS</td>
<td>Mixed Substrate</td>
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<tr>
<td>NARX</td>
<td>Nonlinear Autoregressive Neural Network with External Input</td>
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<td>NER</td>
<td>Net Energy Ratio</td>
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<td>NIRS</td>
<td>Near-infrared Spectroscopy</td>
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<td>OFMSW</td>
<td>Organic Fraction of Municipal Solid Waste</td>
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<tr>
<td>OLR</td>
<td>Organic Loading Rate</td>
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<tr>
<td>PBR</td>
<td>Photobioreactor</td>
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<tr>
<td>PPF</td>
<td>Photosynthetic Photon Flux</td>
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<tr>
<td>PPFD</td>
<td>Photosynthetic Photon Flux Density</td>
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<td>RK1</td>
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<td>ThOD</td>
<td>Theoretical Oxygen Demand</td>
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<td>TS</td>
<td>Total Solids</td>
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<tr>
<td>VFA</td>
<td>Volatile Fatty Acids</td>
</tr>
<tr>
<td>VS</td>
<td>Volatile Solids</td>
</tr>
<tr>
<td>VSS</td>
<td>Volatile Suspended Solids</td>
</tr>
<tr>
<td>WAS</td>
<td>Waste Activated Sludge</td>
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<td>WWTP</td>
<td>Wastewater Treatment Plant</td>
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Symbols and Units

\[ E_{LC} \quad \text{Life Cycle Energy (MJ)} \]
$E_P$ Amount of Energy in the Product (MJ)
$\text{GHGLC}$ Life Cycle Greenhouse Gas Emission (CO$_2$e)
$IoA$ Index of Agreement (-)
$k_{hyd,\text{ch}}$ Hydrolysis First-rate Coefficient for Carbohydrates ($d^{-1}$)
$k_{hyd,\text{ch, microalgae}}$ Hydrolysis First-rate Coefficient for Carbohydrates for the Microalgae ($d^{-1}$)
$k_{hyd,\text{ch, sludge}}$ Hydrolysis First-rate Coefficient for Carbohydrates for the Sewage Sludge ($d^{-1}$)
$k_{hyd,\text{li}}$ Hydrolysis First-rate Coefficient for Lipids ($d^{-1}$)
$k_{hyd,\text{li, microalgae}}$ Hydrolysis First-rate Coefficient for Lipids for the Microalgae ($d^{-1}$)
$k_{hyd,\text{li, sludge}}$ Hydrolysis First-rate Coefficient for Lipids for the Sewage Sludge ($d^{-1}$)
$k_{hyd, pr}$ Hydrolysis First-rate Coefficient for Proteins ($d^{-1}$)
$k_{hyd, pr, microalgae}$ Hydrolysis First-rate Coefficient for Proteins for the Microalgae ($d^{-1}$)
$k_{hyd, pr, sludge}$ Hydrolysis First-rate Coefficient for Proteins for the Sewage Sludge ($d^{-1}$)
$k_{hyd, lcs}$ Hydrolysis First-rate Coefficient for the Ley Crop Silage ($d^{-1}$)
$k_{hyd, ms}$ Hydrolysis First-rate Coefficient for the Mixed Substrate ($d^{-1}$)
$k_{m, ac}$ Monod Maximum Specific Uptake Rate for Acetate (kg COD kg$^{-1}$d$^{-1}$)
$k_{m, h2}$ Monod Maximum Specific Uptake Rate for Hydrogen (kg COD kg$^{-1}$d$^{-1}$)
$k_{S, ac}$ Half-saturation Value for Acetate (kg COD m$^{-3}$)
$k_{S, h2}$ Half-saturation Value for Hydrogen (kg COD m$^{-3}$)
$\text{NRMSD}$ Normalised Rot Mean Squared Deviation (-)
$\text{PE}$ Population Equivalent (1 PE = 70g BOD$_7$ d$^{-1}$)
$R$ Pearson Correlation Coefficient (-)
$S_{\text{IN}}$ Soluble Inorganic Nitrogen (ADM1 state) (kmol m$^{-3}$)
$X_C$ Composite Particulate Matter (ADM1 state) (kgCOD m$^{-3}$)
$Y_{\text{obs}}$ Observed Bacterial Biomass Yield (kg VS sludge kg$^{-1}$BOD)
1. Introduction

To mitigate climate change, reduce the dependency on energy imports, and increase the security of energy supplies, the European Union (EU) has adopted the 2030 climate and energy framework [1]. The framework sets three key targets:

- At least 40% cuts in greenhouse gas emissions (from 1990 levels)
- At least 27% share for renewable energy
- At least 27% improvement in energy efficiency

In this context, biogas can play an important role as a source of renewable energy. The production and use of biogas has a long history, with Louis Pasteur producing biogas from horse dung in 1884 to power the street lights of Paris [2]. The large availability of cheap oil more or less killed the interest in biogas in the 1950s, but during and after the oil crisis [2], the need for waste treatment and renewable fuels reignited the interest. Anaerobic digestion (the process generating the biogas) has, from a historical perspective, mainly been focused on the stabilisation of sludge generated by treating domestic wastewater [3, 4]. However, biogas can be produced from a wide range of different substrates apart from sewage sludge, such as food waste, energy crops, and manure. Biogas can either be burned directly to produce heat and electricity or be upgraded to be used as a vehicle fuel.

In 2013, almost 13.4 million tonnes of oil equivalent of biogas were produced in the EU [5]. Biogas from landfills makes up 22% of the biogas, 9% of the biogas came from sewage sludge treatment, and the rest of the biogas came from stand-alone plants and plants that co-digests sewage sludge with other substrates [5]. To increase the amount of biogas produced from these plants, there are a number of different measures that can be taken. Co-digesting two or more substrates can give more biogas than mono-digestion of the same substrates, as the right combination can balance the nutrients, produce the correct moisture level, reduce toxic components, etc. [4]. For the co-digestion system, the right substrates need to be combined and in the right ratios to produce as much biogas as possible. To increase the yield from an existing plant, the anaerobic digester, as well as the plant as a whole, needs to be operated as efficiently as possible. Modelling and simulation is an important tool that can be used to find the right ratios for co-digestion [4] as well as for improving existing plant operations.

Another way to increase biogas production is to find new substrates. One substrate that has received increasing attention is microalgae. Microalgae have
shown promise as a protein rich co-substrate [6, 7]. Microalgae can also give other benefits to the plant apart from additional biogas from co-digestion. Today, wastewater treatment plants (WWTPs) use energy to treat domestic wastewater. However, several studies envision that the WWTP can be transformed into a facility that recovers energy and nutrients [8, 9]. In this context, microalgae have shown promise as a way of reducing the energy use for aeration and aiding the transformation of the WWTP from a net energy user to a net energy producer [10].

Microalgae can also play a part in fulfilling the third and last of the key targets of the EU climate and energy framework. Many species of microalgae require carbon dioxide (CO2) to grow. The raw biogas produced mainly contains methane (CH4) (the energy carrier and desired product) and CO2. The CO2 is released both from combustion of the biogas for heat and electricity production and from upgrading of the biogas to vehicle fuel. This means that both the biogas plants and the WWTPs are sources of greenhouse gas (GHG) emissions. This CO2 could be used for the growth of the microalgae instead of being released to the atmosphere. Apart from nutrients and CO2, most species of microalgae also need light to be able to grow. The light can either be natural sunlight or artificial light. However, artificial light will consume electricity. To fully understand the impact of microalgae on the plant, a system perspective is needed to evaluate how the microalgae will impact both energy use and GHG emissions.

The objective of this thesis is to study different ways of improving the anaerobic digestion process and other processes where anaerobic digestion is an integral component. Modelling and simulation of the system helps the understanding of the processes. Models can be used for process diagnostics, for better control of the system, and to investigate new substrates and other changes to the system before they are implemented. There have been many simulation studies done, though few have been conducted on full-scale co-digestion. In this thesis, a full-scale anaerobic digester has been modelled using two different models to study the practicality of such models in a full-scale system. A lab-scale experiment has also been simulated to evaluate the effect of co-digesting microalgae with sewage sludge on biogas and CH4 yields. The experimental study is then extended by simulating a full-scale system. The simulation of the full-scale system also includes data on microalgae from other studies. Evaluating the whole system can find the pathway that uses the least energy and leads to the lowest climate impact. Biodiesel from microalgae system have been the focus of many life-cycle assessments (LCA) related to microalgae. In this thesis, a LCA is instead focused on a case study of a co-digestion plant with replacement of one of the substrates, the ley crop, with microalgae. In addition, three case studies of systems for the inclusion of microalgae in the biological treatment at three WWTPs have been developed within the scope of the thesis. The focus is on the effect on energy use and
CO₂ emissions to complement previous studies that have been more focused on nutrients and/or other process solutions.

1.1 Research Questions
The research questions studied in this thesis are the following:

1. How does the performance of the Anaerobic Digestion Model No. 1 (ADM1) compare with an artificial neural network for simulating a full-scale co-digestion plant? (Paper I-II)
2. What will be the effect of the addition of microalgae on biomethane yield from anaerobic digestion of sewage sludge? (Paper III)
3. How will the energy balance and carbon dioxide emission of biogas plants and WWTPs be affected by the inclusion of microalgae? (Paper IV-V)

1.2 Thesis Structure
This thesis is based on five scientific papers (papers I-V). Paper I and Paper II are focused on the simulation of full-scale digestion and how modelling and simulation can be used as tools for process improvement. Paper III presents how the microalgae will affect the anaerobic digestion through simulation of the digester. Paper IV and Paper V are focused on how the microalgae will affect the energy use and CO₂ emissions of the entire plant. Figure 1.1 illustrates how the papers are related to each other.

Figure 1.1. Overview of the thesis and the included papers
2. Literature Review

In this section, the background related to the subject and the methods used in the thesis are given along with references to similar studies.

2.1 Anaerobic Digestion

Anaerobic digestion is the degradation of organic matter in the absence of oxygen. A large number of different microorganisms are involved in this process. Anaerobic digestion can be divided into four different process steps: hydrolysis, acidogenesis, acetogenesis, and methanogenesis, as shown in Figure 2.1.

Before the anaerobic digestion, there is also a fifth step called disintegration. Disintegration is not a biological process, but it is necessary in order for the anaerobic digestion to proceed.

Some of the microorganisms compete with each other for the same resources, and some of them are inhibited by substances in the resources or substances produced by themselves or the other microorganisms. There are also several possible pathways for degradation of the substrate. All these factors add to the complexity of the process [2]. A number of different gases are produced or can be produced in anaerobic digestion, with the two main gases being CH\(_4\) and CO\(_2\). CH\(_4\) often comprises 60-65 % of the volume of biogas, while CO\(_2\) will comprise 35-40 % [11]. However, the amount and composition of the biogas depends on the substrate and operating conditions [11].

![Figure 2.1. Overview of the processes involved in anaerobic digestion](image-url)
2.1.1 Factors Influencing the Process

Important factors for anaerobic digestion include temperature, biodegradability of substrate(s), mixing conditions, presence of inhibitors, and availability of micro- and macronutrients.

Biodegradability depends on a number of different physical, chemical, and physiological factors [12]. The structure of the substrate is important, as the compounds can be easily accessible or be part of a complex. If it is a complex substrate particle, surface area is also important, since a biofilm needs to be formed on the particle surface [12]. Pre-treatment of the substrate can increase the biodegradability [13]. Examples of substrates with strong cell walls that can benefit from pre-treatment are ley crop and microalgae [14, 15].

Mixing is important in an anaerobic digester for a number of reasons, including moderating the temperature and distributing microorganisms and nutrients. Furthermore, the mixing cannot be too vigorous, or the microorganisms will be damaged [16].

The rate of anaerobic digestion is dependent on the temperature. Anaerobic digestion can occur from about 10 °C to over 70 °C, with two optimal points, one around 35 °C (mesophilic conditions) and one around 55 °C (thermophilic conditions) [13]. Thermophilic conditions offer better methane yields, but the drawback is greater energy use for heating as well as lower process stability [13].

When it comes to macronutrients, the Carbon (C):Nitrogen (N) ratio is an important factor for digestion. The optimal C:N ratios is about 15-30 [17]. Some substrates have a C:N ratio that is too high, and others have a C:N ratio that is too low. Apart from macronutrients, there are also nutrients required in a small quantity for growth. These are called micronutrients and include vitamins, sulphur, and traces of minerals [13].

A number of compounds can inhibit anaerobic digestion above a certain threshold, including volatile fatty acids (VFAs) [13, 18], ammonia [13, 19], nitrate [19], heavy metals [20], and hydrogen sulphur [13]. VFAs are one of the intermediate products in anaerobic digestion. A substrate with a high level of easily degradable carbohydrates can lead to an accumulation of VFAs in the digester that will decrease the pH and suppress the methanogensis [21]. Ammonia is both an important source of N in anaerobic digestion as well as a strong inhibitor at high concentrations [19]. The concentration at which ammonia becomes toxic is uncertain and is probably dependent on the difference in operating conditions. The reported range of ammonia concentration is 1.7-14 g L⁻¹ [19].

2.1.2 Substrates

In 2015, the total biogas production in Sweden was 19.5 TWh [22]. The majority of this biogas came from co-digestion plants [22]. The second largest
contributor was WWTPs. The four largest identified substrates in Sweden, in terms of wet weight, are sewage sludge, manure, industrial waste from the food industry, and food waste [22]. For these, except for manure, anaerobic digestion is more than just a way of producing biogas, it is also a treatment method. Digestion of the food waste instead of land-filling reduces the amount of methane that will be released from landfills.

Food waste can either be directly removed at the source (restaurant or households) or be sorted mechanically from the municipal waste. It is part of the organic fraction of municipal solid waste (OFMSW). In the EU, the definition of OFMSW, in addition to food waste, includes waste from gardens and parks [23]. The composition of the OFMSW is dependent on the region from which it is collected (due to different food preferences) and how it is separated [23]. The methane potential can vary but is generally high. The range found in the literature is 61 - 675 NmL CH\textsubscript{4} g\textsuperscript{-1} VS (for 37 samples, the average is 420 NmL CH\textsubscript{4} g\textsuperscript{-1} VS) [23, 24]. One challenge with OFMSW is the presence of undesirable and indigestible material, such as bones, glass, porcelain, plastic, etc. [25]. Mechanically sorted OFMSW generally has a higher percentage of the undesirable material as well as a lower methane yield compared to source-sorted OFMSW [26]. Some of these materials can increase the wear on equipment, and some can prevent the use of the digestate on farm land [4, 25]. Another challenge is the accumulation of VFAs [4, 18]. Other drawbacks with OFMSW include high solids content, high C:N ratio, deficiency in macro and micronutrients, and content of toxic compounds [26].

Anaerobic digestion at WWTPs helps to reduce the solids of the sewage sludge lowering the cost for final disposal of the sludge as well as producing biogas that benefits the WWTP energy balance [27]. One drawback with the sewage sludge as a substrate is low biodegradability, especially waste activated sludge (WAS) that has low biodegradability [27, 28]. One study found that, for a number of mixed sewage sludges, the COD removal rate was in the range of 58% to 66% [29]. Another study found that the biodegradability of WAS was 47% and that it could be increased to 56% with thermal pre-treatment [28]. The biogas potential of mixed sludge (primary sludge (PS)+ WAS), according to literature, is about 310- 390 mL CH\textsubscript{4} g\textsuperscript{-1} VS (for 9 samples, the average is 351 mL CH\textsubscript{4} g\textsuperscript{-1} VS, assuming VS and volatile suspended solids (VSS) to be about the same) depending on the ratio between PS and WAS and other factors [29, 17, 30]. The biogas potential for WAS was found to be about 212 - 300 mL CH\textsubscript{4} g\textsuperscript{-1} VS (for 3 samples, the average is 271 CH\textsubscript{4} g\textsuperscript{-1} VS) [27] or about 165 mL CH\textsubscript{4} g\textsuperscript{-1} COD\textsubscript{in} [28].

Ley crop is one example of crops that can be cultivated for biogas production. Ley crop constitutes of a mixture of leguminous plants and grass. The ley crop can be stored using ensilaging, where the ley crop is packed into plastic or is otherwise separated from air and fermentation. One study estimates the biogas yield of ley crop, from literature values, to be 147-362 CH\textsubscript{4} dry g\textsuperscript{-1} with a best estimate of 287 CH\textsubscript{4} dry g\textsuperscript{-1} (recalculated from GJ using an assumed en-
ergy content of biomethane of 9.97 kWh m\(^{-3}\)) [31]. The biogas yield of grass silage is about 200-460 CH\(_4\) g\(^{-1}\) VS (for 8 samples, the average is 200 CH\(_4\) g\(^{-1}\) VS) [32, 33]. The LCA of a number of different substrates for anaerobic digestion shows that for ley crop as much as 40% of the energy needed goes to the handling of the substrate (cultivation, harvesting, etc.) [31].

Microalgae can be cultivated in a wide range of different media, for example in sea water or wastewater. The biogas potential of microalgae depends on the strain of microalgae, pre-treatments, and other conditions [14]. The range of methane yield found in the literature is 17.5 - 557 mL CH\(_4\) g\(^{-1}\) VS (for about 69 samples, the average is 268 mL CH\(_4\) g\(^{-1}\) VS) [14, 34, 35]. The co-digestion of microalgae with a number of different substrates has been considered, including energy crops [7], swine manure [36] and sewage sludge [6, 37]. Co-digesting microalgae with sewage sludge has the potential to enhance biogas production and process stability, but the variation in results between studies is large [38].

2.1.3 Co-digestion

Co-digestion is one way to improve methane yield and process stability. Co-digestion can avoid a number of the difficulties encountered when using mono-digestion. In section 2.1.1, a number of important factors for anaerobic digestion are listed. Through co-digestion, some of these factors can be improved or optimised. Using co-digestion, an optimal C:N ratio can be achieved [4]. Co-digestion can dilute incoming inhibitory compounds, such as heavy metals, and avoid accumulation of formed inhibitory compounds, such as VFAs [4]. The availability of trace elements can also be improved through co-digestion. This can be especially valuable for a substrate, such as OFMSW, that has a number of challenges as described in section 2.1.2.

There are drawbacks to co-digestion as well. Co-digestion means extra storage and handling is needed for the additional substrate(s) [25]. Extra monitoring and control of the co-substrates can also be necessary [25]. In addition, depending on the co-substrate(s), the co-substrate(s) can introduce new challenges to a plant, such as an increase in wear and tear on equipment [25]. There is also the risk that the addition of co-substrates lowers the digestate quality [4].

2.2 Modelling and Simulation

Models can be classified according to a number of different criteria, such as static vs. dynamic or 0-, 1-, 2-, or 3-dimensional. Furthermore, a model can be a mechanistic (white box) or an empirical model (black box). A mechanistic model is based on the underlying phenomena of the system. An empirical model is developed by experimentally investigating the correlation between
the input and output. An empirical model is, therefore, only valid for the particular system for which it was developed [39]. The benefit of empirical models is that it is not necessary to fully understand the studied system. They can also be useful for cases where data needed for a mechanistic model is missing.

2.2.1 Anaerobic Digestion Model No.1 (ADM1)

The very first dynamic model for anaerobic digestion was developed by Andrews in 1969 [40]. The model only considered one single process step: the acetoclastic methanogenesis. It was based on the idea of a rate-limiting step, that is, that there is one process stage that is always the slowest and that the total rate of the whole process is dependent on that step [40]. Many other models that followed were also of the rate-limiting step type. The rate-limiting step models are simple and easy to use, but do not describe the process very well [41].

The models continued to develop and become more complex by including inhibition and additional process steps. There were many different models developed and very little reuse of models between researchers. In 1998, the International Water Association (IWA) formed a task group called the IWA Task Group for Mathematical Modelling of Anaerobic Digestion Processes to create a common platform for anaerobic process modelling and simulation. The model was first presented in 2001 and was called the Anaerobic Digestion Model No. 1 (ADM1). The ADM1 contains 19 biochemical kinetic processes, including disintegration, hydrolysis, acidogenesis, acetogenesis, and methanogenesis. ADM1 also includes equations for a number of inhibitions as well as gas-liquid transfer equations [42].

The ADM1 has been used for a number of different applications, both mono-digestion and co-digestion. Example of applications include grass silage [43], OFMSW with sewage sludge [44], agro-waste [45], microalgae [46], olive mill wastewater with olive mill solid waste [47], and co-digestion of cattle manure and energy crops [48]. It has also been used for full-scale plants treating sewage sludge [49, 50] and the full-scale co-digestion of sewage sludge and organic waste [51], cattle-manure and food waste [52], and mixtures of vegetable waste and process wastewater from food factories [53].

The ADM1 has 27 possible parameters for the input of the model. Deciding which parameters to use and their value are challenges when using the model. The base unit of measurement for the ADM1 is chemical oxygen demand (COD). At a WWTP, it is common to measure COD. For sewage sludge, it is possible to have the input of the model as the concentration of composite material in COD. However, for other substrates, it is not as common to measure COD, and the measurement of COD can even be very difficult [43, 54]. This is typical of solid materials, such as food waste or grass silage.
Many studies have found ways around this problem by analysing the substrates for other properties and then converting these measurements into COD. One way is measuring the substrate composition (mainly carbohydrates, proteins, and lipids) in terms of weight and then converting the weight measured into COD using the theoretical oxygen demand (ThOD) as a conversion factor [43, 46, 55]. Another way is converting a set of measurements to the wanted COD inputs based on the balance of elements (C, hydrogen, N, oxygen, and phosphorus (P)) [56]. A third method is to fractionate the incoming COD using the methane production curve received when doing bio-methane potential (BMP) tests [57]. It is also possible to combine methods [58].

There have been a number of different extensions and adaptations suggested for the ADM1 to make it more applicable for different studied scenarios. Ramirez et al. [28] suggested using Contois kinetics for the disintegration and hydrolysis step and also include dependence on the amount of biomass. It has also been suggested to include the dependence on particle size for the rate of disintegration [44] or dependence of the total solids (TS) concentration on the hydrolysis rate for substrates with a high TS level [43]. Most studies use first-order kinetics for the hydrolysis rate [4]. Another suggestion is to divide the composite matter state (XC) into two states: slowly hydrolysable composite matter and readily hydrolysable composite matter [59]. The most suitable adaptations are dependent on the studied system. Mata-Alvarez et al. [60] suggest that, for co-digestion, it is not suitable to use the composite component in the input, but to instead give the input directly as carbohydrates, proteins, and lipids.

The ADM1 is built for one influent stream with one set of characteristics. This is something that also needs to be addressed when dealing with co-digestion. Either the two substrates need to be characterised together as if they were one substrate [51], or the combined characteristics be calculated and a common hydrolysis rate can be estimated [61]. Alternatively, the hydrolysis step can be separated into two hydrolysis steps, one for each substrate [62], or two disintegration steps, one for each substrate [45].

Regarding three previous full-scale co-digestion simulations, two of them, one by Rönner-Holm et al. [53] and the other by Derbal et al. [51], seem to characterise the two incoming substrates as one. In the study by Rönner-Holm et al. [53], the influent is characterised using assumptions for the composition and later calibrated using measurements. In the study by Derbal et al. [51], the measurements are reserved for parameter estimation. In the third study, by Biernacki et al. [52], it is unclear how the co-digestion is modelled. However, since different hydrolysis rate are suggested depending on substrate, it is likely that a structure supporting two different hydrolysis rates were used. Biernacki et al. [52] also suggest using a common kinetic constant for the disintegration and hydrolysis of proteins, carbohydrates, and lipids to simplify model calibration.
2.2.2 Empirical Models for Anaerobic Digestion

There is little work published concerning empirical/statistical models of anaerobic digestion compared to mechanistic models. This is perhaps because empirical models can only be expected to be valid for the process(es) and conditions related to the model data. There are different kinds of empirical models, including fuzzy-logic models, artificial neural network models, and linear and non-linear regression-models.

Artificial neural networks (ANNs) are mathematical models that have drawn their inspiration from the structure of the human brain. They are built up by a number of interconnected nodes. An illustration of a general node in an ANN can be seen in Figure 2.2.

\[ p 
\]
\[ w \]
\[ \sum \]
\[ n \]
\[ f \]
\[ a \]
\[ b \]

*Figure 2.2. General neuron as found in a general artificial neural network adapted from [63]*

In Figure 2.2, \( p \) is the scalar input received by the individual node. This input is multiplied by the weight \( w \) and, to this value, the bias or offset \( b \) is added. The sum is then entered into the function \( f \). The output from the node is the equation, \( a = f(wp+b) \) [63]. The function \( f \) is some predefined function, such as a sigmoid or hyperbolic tangent function [64]. ANN is adapted to the process through training in which the weight and bias of each node is adjusted to fit some known given output. There are several different algorithms that can be used for training; one of the most common is backpropagation training, which is used in several studies [64, 65, 66].

Examples of the application of ANN to anaerobic digestion cases are applications of ANN together with genetic algorithms to predict biogas production from the co-digestion of rice bran, banana stem, paper waste, cow dung, and saw dust [66], the prediction of biogas rate in thermophilic digestion of molasses [67], the prediction of methane flow and volatile solids (VS) from anaerobic digestion of sludge [64], and the prediction of the percentage of methane in biogas from a full-scale anaerobic digestion reactor digesting food waste [65].

The model discussed in section 2.2.1 predicted several output parameters. Unlike the model in section 2.2.1, the models mentioned above predict one [65, 66, 67] or two parameters [64] each. Examples of the use of ANN include prediction and control [68]. Other examples of the types of empirical models for anaerobic digestion are fuzzy-logic [69] and linear regression [70].
2.3 Microalgae in Wastewater Treatment

Wastewater treatment using the conventional activated sludge process is energy demanding, using more energy than it produces [9, 71]. However, there is a large potential in the incoming wastewater in terms of chemical energy [9]. A large part of the energy used for wastewater treatment is for aeration in the biological treatment, and it is not usual for aeration to use half of the total energy [9, 71].

Concepts for lowering or eliminating net energy use at WWTPs include increasing the efficiency of primary settling [72], autotrophic nitrogen removal as tertiary treatment [72], anaerobic digestion in combination with nitritation-anammox [71], co-digesting the sludge with external substrates [73], and inclusion of microalgae in the wastewater treatment process [74].

Using microalgae in wastewater treatment has several possible benefits. They produce oxygen which can reduce the aeration cost in the biological treatment [74]. They can also reduce nutrients, use inorganic nitrogen and phosphorus for their growth, and remove heavy metals [75]. The microalgae biomass will contain both the internal energy from the wastewater but also solar energy (from the photosynthesis) [10]. One study found that the energy balance of the WWTP could be improved by cultivating microalgae for biofuel in the effluent stream [76]. Another study looked at using the microalgae as part of WWTPs in the Netherlands during May through October [77], considering using the microalgae for both post-treatment and total integration. The study found the area requirement to be considerable, 0.32-2.1 m$^2$ PE, and achieving both the N- and P-targets simultaneously was not possible.

The cultivation of microalgae can be done in a number of different ways, including in open ponds, closed photobioreactors (PBRs), and immobilized cell systems/biofilms [74, 75]. Closed PBRs can be designed in a number of different ways, including as tubular PBRs which offer a high ratio between illuminated surface and volume [74, 75] and as flat-plate PBRs [78]. However, enclosed PBRs can be expensive [74]. During a LCA of microalgae cultivated for biofuel in raceway ponds, a comparison of flat-plate PBR and tubular PBR found that cultivation in tubular PBRs is too unfavourable regarding the energy balance, producing less energy than that required for operations and construction [79]. The other cultivation methods had positive energy balances [79].
3. Materials and Methods

In papers I, II, and III, the simulations focused solely on the digester. The ADM1 was used for simulations in papers I and III, and in paper II an ANN was used. In paper IV and paper V, calculations are made on the whole biogas plant and WWTP to evaluate how the energy balance and carbon dioxide balance change with the inclusion of microalgae in the systems. In paper IV, the annual change in energy balance and carbon dioxide is calculated for different surface areas. In paper V, a partial life-cycle assessment is used to evaluate the energy use and carbon dioxide emission. This section describes the models and calculation methods used. Further details can be found in the appended papers.

3.1 Case Study of a Biogas Plant (Papers I, II, and V)

The data for the full-scale digester in papers I and II and the data for the existing biogas plant in paper V come from the VafabMiljö biogas plant (formerly known as Växktraft) in Västerås. The biogas plant has a digester of 4000 m³ operating under mesophilic conditions. The layout of the plant can be seen in Figure 3.1. During 2011, the plant digested 15 300 tonnes of source-sorted municipal solid waste (OFMSW) (entering the plant at point 1 in Figure 3.1), 3100 tonnes of grease trap sludge (entering at point 2 in Figure 3.1), and 1100 tonnes of ley crop silage (entering at point 4 in Figure 3.1).

3.2 Semi-continuous Lab-scale Digesters (Paper III)

The data that were used for paper III were collected from a semi-continuous lab-scale experiment. Two digesters of 5 litres each were used. In the first reactor (RK1), PS and WAS were digested with a VS-ratio of 60:40. In the second reactor (RK2), PS, WAS, and microalgae were digested together in a VS-ratio of 41:22:37. Inoculum for the digesters came from the Mälarenergi WWTP digester in Västerås, digesting PS and WAS under mesophilic conditions. Two different organic loading rates (OLRs) were used. During the first 46 days, an OLR of 2.4 kg VS m⁻³ d⁻¹ was used with a hydraulic retention time (HRT) of 15 days. During the second period, lasting 30 days, the OLR was 3.5 kg VS m⁻³ d⁻¹ and the HRT was 10 days. The reactors were fed once every day, seven days a week. To get the right OLR, the substrates were diluted. More details on the experiment can be found in the master’s thesis by Forkman [80].
3.3 ADM1

The kinetic model used for the modelling anaerobic digester in papers I and III was the ADM1 (the model is described in detail in section 2.2.1). For the ADM1, the modifications suggested by Rosén et al. [81] were used regarding the closing of nitrogen (N) balances and implementing the inhibition functions as switch functions. Matlab/Simulink was used to simulate the model.

3.3.1 Modelling Co-digestion

Co-digestion is studied in both papers but has been implemented in different ways in the model.

For the simulation of the full-scale digester (paper I), the setup for the co-digestion suggested by Zaher et al. [62] is used. Two substrates are considered: a mixed substrate (OFMSW + grease trap sludge) and ley crop silage. A total of three ADM1-blocks are used to build the model, one for the hydrolysis of each of the two substrates and one for the rest of the reactions. In the hydrolysis block, only the equations related to the hydrolysis are active. Temperature dependence was also included.

In the simulation of the lab-scale digester (paper III), the approach to the modelling of the co-digestion was different. Only one ADM1-block was used, and the two streams were combined using Matlab-code outside of Simulink. Different hydrolysis rates were used for the two substrates in this approach as
well. To accommodate this, the Peterson matrix was changed. Separate states were introduced for the proteins, lipids, and carbohydrates of the second substrate (microalgae). For details, see the supplement to paper III. An illustration of the two approaches and their differences can be seen in Figure 3.2. In theory, these two substrates should lead to the same result since the only different is in the hydrolysis rate for the two substrates. The second approach (paper III) can be expected to be faster since the extra equations are entered directly into the main ADM1 block, making the Simulink model less complex.

![Figure 3.2](image_url)

**Figure 3.2.** Illustration of the two different approaches used in papers I and III for modelling the co-digestion

### 3.3.2 Characterisation of Substrates

The ADM1 requires extensive characterisation of the substrate(s). As described in section 2.2.1, there are many ways that the inlet substrate(s) can and has been characterised to fulfil model requirements. For characterisation of both the substrates in paper I and paper III, there were issues that needed to be overcome. COD was not measured continuously in either scenario during the operation of the digester. Instead, VS was the more common measurement. It was, therefore, assumed that COD was fixed with VS, as has been shown in previous studies [82, 83].
Three different methods were used for the characterisation of the sewage sludge and two for the microalgae (paper III). The first one was using the measured value for the particulate COD (CODp) and the other two included using the ThOD-values to calculate the particulate CODp. Both the ThOD-values for proteins, lipids, and carbohydrates suggested by Mairet et al. [46] and by Koch et al. [43], were used to determine how the final result would be affected by different ThOD-values. In the results section, the two sets of ThOD-values are referred to as "ThOD1" (for ThOD-values from Koch et al. [43]) and "ThOD2" (for ThOD-values from Mairet et al. [46]). The measured CODp was found to be low in comparison to literature. For comparison, it was used as a third alternative for the characterisation of sewage sludge, using the calculation method suggested by Arnell et al. [55]. The use of the measured CODp is called "COD" in the results sections. It was not possible to use the measured CODp for the microalgae with the calculation method suggested by Arnell et al. [55], since it gave a negative result for the concentration of carbohydrates.

The following steps were taken for the characterisation of the sewage sludge and microalgae:

- Particulate COD (CODp) was first determined using measurement or using ThOD-values for proteins, lipids, and carbohydrates.
- Measured soluble COD (CODs) was used.
- The biodegradability extent, $f_d$, was determined using the BMP tests.
- Protein and lipids in terms of COD were calculated using ThOD-values and subtracting the amount assumed to be non-biodegradable as determined by $f_d$.
- The remainder of the biodegradable part of the CODp was allocated to carbohydrates. The concentration of individual VFAs was determined by converting the measured VFAs in mass to units of COD using the conversion of 1.07 gCOD per g of acetate and 1.51 gCOD per g propionate (the concentration of butyrate and valerate was so low that it was assumed to be zero).
- Monosaccharides, amino acids, and long-chain fatty acids (LCFA) were determined from CODs after the VFAs and the non-biodegradable portions (1 - $f_d$) had been subtracted as in the study by Arnell et al. [55].
- Inorganic N was directly measured and then converted to moles (unit for inorganic N and carbon in the ADM1) using the molar mass of N.

There were no analyses available of protein, fats, and carbohydrates for the OFMSW, grease trap sludge, and ley crop silage (paper I). Another difficulty was that it was hard to find a good point in the process to characterise the streams. The point chosen for the mixed substrate was at the inlet 3 in Figure 3.1, and for the ley crop silage, the silage inlet was at 4 in Figure 3.1. The correlation used between COD and VS was 1.91 COD/VS for the mixed sub-
strate (OFMSW + grease trap sludge + recirculated process water) and 1.73 COD/VS for the ley crop. The assumptions were:

- The relationship between COD and VS, as well as the COD fractions of OFMSW, recirculated process water, and grease trap sludge, was fixed and did not vary with the season.
- The recirculated process water only consisted of non-degradable material (since it had already passed through the digester).
- 85% of the grease trap COD was degradable lipids and the rest of the COD contained inert materials. According to an extensive evaluation of the plant [84], 85% of the VS of the grease trap sludge was degradable.

The proteins, lipids, carbohydrates, and inert materials in the remaining fraction, OFMSW, was calculated using data from the extensive evaluation [84, 85] according to the following steps:

- The non-biodegradable fraction was assigned to inert COD.
- The fraction of proteins was calculated by multiplying organic N (total N - total ammonium nitrogen (NH₄-N)) with 6.25 [45, 86] and then it was adjusted using ThOD to get the correct fraction in terms of COD.
- The percentage of lipids was set to 6% in accordance with the literature [24].
- The carbohydrate fraction of VS was calculated by subtracting the amount of lipids and proteins from VS before being converted to COD using ThOD.

For the inorganic nitrogen, measurements at the digester inlet were used. The ley crop silage was fractioned in the same way as the OFMSW apart from the lipid content. The lipid content was assumed to be zero for the ley crop silage. For grass silage, another study found the lipid content to be 3% of TS [43].

3.3.3 Comparison to Artificial Neural Network

The prediction for biogas and CH₄ content made by the ADM1 (paper I) was compared with the predictions made by an ANN (paper II). The set-up of the ANN is described in more detail in section 3.4. To be able to make the comparison, the ADM1 was also used to simulate the Växtkraft digester in the period 7 April to 25 May 2011 (the testing period for the ANN). The model structure and method remained the same. Only the input was changed to include, in addition to the original period, the time until 25 May 2011.

3.4 Artificial Neural Network (Paper II)

In paper II, an empirical approach was used to simulate the VafabMiljö digester. The empirical model used was an ANN. It was created using the Mat-
lab Neural Toolbox. It was a nonlinear autoregressive neural network with external input (NARX) with defining equation 3.1.

\[
\hat{y}(t) = f(\hat{y}(t-1), \hat{y}(t-2), ..., \hat{y}(t-n_y), x(t-1), x(t-2), ..., x(t-n_x)) \quad (3.1)
\]

The variable \( \hat{y}(t) \) is the value(s) predicted by the NARX, \( x(t) \) is an independent input signal, and \( n_y \) and \( n_x \) are the time-delays for each signal [87]. The ANN had one level of hidden neurons and was trained using Levenberg-Marquardt backpropagation training. The ANN included a closed loop where the output of the network was fed back to the network. During training, this loop was open and real output values were fed to the network. Data were gathered from the biogas plant, described in section 3.1, for the time period of January 2006 to May 2011. The available data measured with sufficient frequency were selected for use as inputs and outputs. The selected input parameters were set to mixed substrate inflow, silage inflow, effluent flow (differentiated from inflow), incoming mixed substrate VS (mixed substrate inflow * mixed substrate VS), incoming ley crop TS (ley crop silage inflow * ley crop silage TS), and digester temperature. The output parameters were set to raw biogas outflow and CH\(_4\) content of the biogas. The measurements used are found in Table 3.1.

The VS values for the ley crop were not available for the whole data series, and, instead, TS values were used for the ley crop. A linear relationship between TS and VS was also observed. TS and VS values were only available on a weekly basis, so they were interpolated to provide daily values. After interpolation and removal of faulty data, 1890 data points for each variable remained. Of this data, two months (61 data points) were reserved for testing of the final closed loop ANN. The rest of the data was divided into training (80 %), validating (15 %), and testing of the open loop (5 %). Since the system is time-dependent, the chronological order was kept for the data points. The training used the very first part of the data in the time series, and the testing used the very last.

### 3.5 Quantitative Measures of Fit

To evaluate the fit between simulated values and measurements, the fit was also quantified using the Index of Agreement (IoA), see Eq. 3.2 [88]. This function was used in papers I, II and III. The IoA gives a value between 0 and 1, where 0 indicates no agreement and 1 indicates perfect agreement.

\[
IoA = 1 - \frac{\sum_i^n (y_i - x_i)^2}{\sum_i^n (|y_i - \bar{x}_i| + |x_i - \bar{x}_i|)^2} \quad (3.2)
\]
Table 3.1. Measurements from the biogas plant used in the ANN

<table>
<thead>
<tr>
<th>Measurement</th>
<th>Measurement frequency</th>
<th>Number of data points</th>
<th>Mean</th>
<th>Max</th>
<th>Min</th>
<th>Stdev</th>
</tr>
</thead>
<tbody>
<tr>
<td>MS inflow (tons)</td>
<td>Online</td>
<td>1976</td>
<td>164</td>
<td>735</td>
<td>0</td>
<td>93</td>
</tr>
<tr>
<td>MS VS (%)</td>
<td>Weekly</td>
<td>225</td>
<td>5.6</td>
<td>8.3</td>
<td>2.4</td>
<td>0.9</td>
</tr>
<tr>
<td>LCS inflow (tons)</td>
<td>Online</td>
<td>1976</td>
<td>8.1</td>
<td>65.0</td>
<td>0</td>
<td>9.6</td>
</tr>
<tr>
<td>LCS TS (%)</td>
<td>Weekly</td>
<td>232</td>
<td>36.7</td>
<td>60.3</td>
<td>23.8</td>
<td>7.4</td>
</tr>
<tr>
<td>Digester temp.(°C)</td>
<td>Online</td>
<td>1976</td>
<td>41.0</td>
<td>45.0</td>
<td>31.0</td>
<td>2.0</td>
</tr>
<tr>
<td>Gas flow (Nm³)</td>
<td>Online</td>
<td>1976</td>
<td>6714</td>
<td>15970</td>
<td>0</td>
<td>2497</td>
</tr>
<tr>
<td>CH₄ content</td>
<td>Online</td>
<td>1976</td>
<td>63.0</td>
<td>85.0</td>
<td>43.0</td>
<td>4.5</td>
</tr>
</tbody>
</table>

MS = mixed substrate, LCS = ley crop silage

where \( x \) is the measured value, \( \bar{x} \) is the mean of the measured values, \( y \) are the simulated values, \( \bar{y} \) is the mean of the simulated values, and \( n \) is the total number of measurements.

In paper II, the Pearson correlation coefficient, \( R \), was also presented, see Eq. 3.3 [64]. It is also estimated for [66] using the plot presented in the study.

\[
R = \frac{\sum_{i=1}^{n} (x_i - \bar{x})(y_i - \bar{y})}{\sqrt{\sum_{i=1}^{n}(x_i - \bar{x})^2 \sum_{i=1}^{n}(y_i - \bar{y})^2}}
\]  
(3.3)

Another measurement, the normalised root mean squared deviation (NRMSD), was used to evaluate the fit when doing the parameter estimation in paper I.

\[
NRMSD = \frac{\sqrt{\sum_{i=1}^{n}(x_i - y_i)^2}}{x_{max} - x_{min}}
\]  
(3.4)

where \( x \) is the measured value, \( y \) denotes the simulated values, \( n \) is the total number of measurements, \( x_{max} \) is the maximum observed value, and \( x_{min} \) is the minimum observed value.

3.6 Inclusion of Microalgae at the WWTP

In wastewater treatment, the inclusion of microalgae in biological treatment (see Figure 3.3) was investigated using a system model. The aim was to see how the energy use and carbon dioxide emissions of the plant as a whole would be affected. Including microalgae can reduce or eliminate the need for aeration [74] and contribute to the reduction of nutrients from the incoming wastewater. The calculations were based on data from three WWTPs in Sweden as well as from previous studies (to obtain data on microalgae properties). The three WWTPs were located in the cities of Västerås, Uppsala, and Eskilstuna. The
Figure 3.3. The general overview of wastewater treatment plants and the point where the microalgae were included.

connected Population Equivalents (PE) was on the order of 82 000-149 000 depending on the plant.

Except for Västerås, the plants had primary, secondary, and tertiary treatment. Västerås only had primary and secondary treatment. All three plants utilise the activated sludge process for the secondary treatment.

For each month and WWTP, the following were calculated:
1. Amount of P, biological oxygen demand (BOD), and NH₄-N that is reduced in the biological step in the present WWTP. Assuming that the biological treatment can be made as effective with microalgae, it is assumed that this is the amount to be reduced in the microalgae biological treatment as well,
2. The amount of oxygen produced by the microalgae using solar irradiance data from the database STRÅNG (using literature values for the amount of photons needed for the release of O₂) and the amount of microalgae biomass produced,
3. The amount of P and NH₄-N reduced by the microalgae, using data from the literature (it is assumed based on the literature that the microalgae does not reduce any BOD, and the rest of the BOD, P, and NH₄-N is reduced by bacteria biomass),
4. The amount of bacteria biomass formed (based on literature data on the performance and growth of bacteria biomass),
5. The oxygen needed by the bacteria, as well as the portion of the oxygen need covered by the microalgae,
6. The reduction of electricity consumption for the aeration, assuming that it will decrease linearly with oxygen consumption,
7. The amount of extra biogas due to microalgae, assuming that microalgae has the same biogas potential as biosludge,
8. Additional electricity consumed for sludge handling, using the data from the Uppsala WWTP regarding electricity consumption per m³ of sludge,
9. The extra heat and electricity required for the digestion of the additional microalgae sludge,
10. The extra heat and electricity that can be generated by the extra microalgae biogas,
11. The net CO₂ emission and absorption,
12. The change in heat and electricity consumption compared to the base case, and
13. The biomass concentration in the basin (using a solid retention time of 12 days and a microalgae VS of 62 % TS [6] and current basin volumes).

A sensitivity analysis was also conducted. The parameters related to the microalgae, CO₂ absorption by microalgae, NH₄-N reduced by microalgae, P reduced by microalgae, O₂ yield per microalgae, quanta of light needed to liberate O₂, and the observed bacterial biomass yield (Yobs), were individually changed by +/- 50 % of the original value. For the sensitivity analysis, the largest surface factor studied was used so that the impact of the parameters would be as large as possible.

3.7 Inclusion of Microalgae at the Biogas Plant

The microalgae was compared to the ley crop silage, and the replacement of ley crop silage with microalgae was investigated (the case study plant described in section 3.1). The microalgae would be cultivated in flat-plate PBRs inside a greenhouse and then co-digested with OFMSW and grease trap sludge. Three scenarios were investigated using partial LCA (cradle to gate) [89]: 1) cultivating microalgae for 180 days annually without greenhouse heating (case I), 2) cultivating microalgae for 330 days annually with greenhouse heating (case II), and 3) the base case, operating the plant with ley crop (case III). The stages that were considered were cultivation, concentration, biogas production, biogas upgrading, transportation, and infrastructure construction for the PBR and greenhouse. Using literature values and information from the biogas plant, a number of assumptions were made as given in Table 3.2. For several of the parameters, there is not a single value that is valid under all conditions. However, a single value needed to be selected for each parameter from the range of values found in the literature. A life cycle energy (Eₜₐₜ) is calculated, which is the sum of energy use associated with each input at each stage. In the same way the life-cycle GHG emission (GHGLC) is the GHG due to each input at each stage.

To compare the energy efficiency between the different cases and to allow for comparison with other fuels, the net energy ratio (NER) [79] was calculated, according to Eq. 3.5.
\[
NER = \frac{E_p}{E_{LC}}
\]  

(3.5)

where \( E_p \) is the amount of energy in the product, in this case \( \text{CH}_4 \), and \( E_{LC} \) is the life-cycle energy use.

**Table 3.2. Assumptions used for the LCA for inclusion of microalgae at the biogas plant**

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
<th>Unit</th>
<th>Reference</th>
</tr>
</thead>
<tbody>
<tr>
<td>Ley crop silage, productivity</td>
<td>5.83</td>
<td>t DM ha(^{-1})</td>
<td>[90, 91]</td>
</tr>
<tr>
<td>Ley crop silage, ( \text{CH}_4 ) potential</td>
<td>9.7(^a)</td>
<td>GJ</td>
<td>[92]</td>
</tr>
<tr>
<td>GHG emission - silage cultivation</td>
<td>250</td>
<td>kg CO(_2)e</td>
<td>[93]</td>
</tr>
<tr>
<td>Energy use - silage cultivation</td>
<td>1.4</td>
<td>MJ kg(^{-1}) silage</td>
<td>[93]</td>
</tr>
<tr>
<td>Average transportation distance - silage &amp; digestate</td>
<td>17</td>
<td>km</td>
<td>[91]</td>
</tr>
<tr>
<td>Microalgae, volumetric productivity</td>
<td>1</td>
<td>kg m(^{-3}) d(^{-1})</td>
<td>[94, 95, 96]</td>
</tr>
<tr>
<td>Microalgae, ( \text{CH}_4 ) potential</td>
<td>9.4(^a)</td>
<td>GJ</td>
<td>[35, 97, 98, 99]</td>
</tr>
<tr>
<td>Height of PBR unit</td>
<td>1.45</td>
<td>m</td>
<td>[78, 79]</td>
</tr>
<tr>
<td>Working height of PBR unit</td>
<td>1.25</td>
<td>m</td>
<td>[78, 79]</td>
</tr>
<tr>
<td>Width of PBR unit</td>
<td>0.1</td>
<td>m</td>
<td>[78, 79]</td>
</tr>
<tr>
<td>No. of PBR unit vertically stacked</td>
<td>2</td>
<td>-</td>
<td>[78, 79]</td>
</tr>
<tr>
<td>Annual consumption of district heating</td>
<td>62</td>
<td>kWh m(^{-2})</td>
<td>[100, 101]</td>
</tr>
<tr>
<td>Energy use transportation</td>
<td>0.7</td>
<td>MJ diesel t(^{-1}) km(^{-1})</td>
<td>[31]</td>
</tr>
<tr>
<td>Glass requirement for PBR and greenhouse construction</td>
<td>15</td>
<td>kg m(^{-2})</td>
<td>[102]</td>
</tr>
<tr>
<td>Lifespan of the greenhouse &amp; PBR</td>
<td>30</td>
<td>yr</td>
<td>[97, 102, 103]</td>
</tr>
<tr>
<td>Electricity requirements - CO(_2) injection</td>
<td>53</td>
<td>W m(^{-3})</td>
<td>[78]</td>
</tr>
<tr>
<td>Electricity requirements - settling</td>
<td>15.3</td>
<td>kWh</td>
<td>[97]</td>
</tr>
<tr>
<td>Electricity requirements - centrifugation</td>
<td>42</td>
<td>kWh</td>
<td>[97]</td>
</tr>
</tbody>
</table>

The references either give the value used or a value was selected using the range found in the references, \( a = \) calculated assuming the energy content of biomethane to be 9.97 kWh m\(^{-3}\).
4. Results and Discussion

In this section, the results from the different studies are presented and discussed.

4.1 Simulation of the Växtkraft Biogas Plant

The digester at the Växtkraft biogas plant was simulated using two different modelling approaches, ADM1 (mechanistic model) and an ANN (empirical model).

4.1.1 Simulation using ADM1 (Paper I)

Six parameters were calibrated for the model, Monod maximum specific uptake rate for acetate and hydrogen ($k_{m,ac}$ and $k_{m,h2}$), half-saturation value for acetate and for hydrogen ($K_{S,ac}$ and $K_{S,h2}$), and the hydrolysis first rate coefficient for the mixed substrate and for the ley crop silage ($k_{hyd,ms}$ and $k_{hyd,lcs}$). The result of the parameter estimation can be seen in Table 4.1.

**Table 4.1. Results from the parameter estimation for the co-digestion of microalgae and sewage sludge**

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Units</th>
<th>ADM1 standard value</th>
<th>Calibrated value</th>
</tr>
</thead>
<tbody>
<tr>
<td>$k_{m,ac}$</td>
<td>kgCOD kg^{-1}COD d^{-1}</td>
<td>8</td>
<td>8</td>
</tr>
<tr>
<td>$K_{S,ac}$</td>
<td>kgCOD m^{-3}</td>
<td>0.15</td>
<td>0.21</td>
</tr>
<tr>
<td>$k_{m,h2}$</td>
<td>kgCOD kg^{-1}COD d^{-1}</td>
<td>35</td>
<td>21</td>
</tr>
<tr>
<td>$K_{S,h2}$</td>
<td>kgCOD m^{-3}</td>
<td>7*10^{-6}</td>
<td>9.8*10^{-6}</td>
</tr>
<tr>
<td>$k_{hyd,ms}$</td>
<td>d^{-1}</td>
<td>10</td>
<td>3</td>
</tr>
<tr>
<td>$k_{hyd,lcs}$</td>
<td>d^{-1}</td>
<td>10</td>
<td>3</td>
</tr>
</tbody>
</table>

The most influential of these parameters was $k_{m,ac}$, however, calibration left it at its standard value. The two second most influential parameters regarding total NRMSD were $K_{S,ac}$ and $k_{hyd,ms}$, while the others had only a minor influence. The effect of the parameters on the fit of individual outputs was also studied. In general the same pattern repeated itself as for the total NRMSD, with $k_{m,ac}$, $K_{S,ac}$ and $k_{hyd,ms}$ showing the greatest influence. However, $k_{hyd,ms}$ only had a significant influence on the NH$_4$-N and the biogas outflow, while $k_{hyd,lcs}$ did not seem to influence CH$_4$ content.
The feeding of the digester was uneven, and it had a large effect on the output, especially biogas outflow, as shown in Figure 4.1. The measured values for some of the output parameters appeared to vary less than the simulated values. However, the values were only measured once per week, on same day and at the same time each week, which might hide some of the variation. If the simulated values for these times are selected (marked as matched simulated values in the figures), the variations between them seem less than the variations between the continuous values as shown in Figure 4.2.

The model predicts, in general, a lower CH$_4$ content of the biogas than what is measured as shown in Figure 4.1. On average, this deviation is 3.7 percentage points. This can be compared to the uncertainty of the gas composition measurement which is about 1 % of the span with daily calibration and up to 3 % with a week of no calibrations. The mean of the simulated biogas production is close to the mean of the measured biogas production. However, the simulated biogas production fluctuates more. According to the manufacturer, the measurement error should be about 1-2 % for the biogas measurement which makes the deviation between simulated and measured biogas outflow larger than what is explained by the measurement error. The quantified fit between simulated and measured values can be seen in Table 4.2.

The positive influence of the silage on the production of biogas and CH$_4$ might have been overestimated by the simulated values. During the period of day 244 to day 258, the silage inflow was zero and the model estimated much less CH$_4$ than what was actually produced (see Figure 4.2).
Figure 4.2. Simulated and measured values from the simulation of the Växtkraft digester using ADM1

There are a number of factors that could have an impact on the results. First, the inflow of grease trap sludge into the digester is not measured on a daily basis. Only the amount of grease trap sludge received per month is known. A large portion of grease trap sludge entering the digester on a certain day can make the composition for that day different than what has been assumed in this study.

Table 4.2. Quantified fit between simulated and measured values for implementation of ADM1 at the biogas plant

<table>
<thead>
<tr>
<th>Parameter</th>
<th>IoA</th>
</tr>
</thead>
<tbody>
<tr>
<td>Biogas</td>
<td>0.78</td>
</tr>
<tr>
<td>CH₄ content</td>
<td>0.61</td>
</tr>
<tr>
<td>CH₄ flow</td>
<td>0.77</td>
</tr>
<tr>
<td>NH₄-N</td>
<td>0.68</td>
</tr>
<tr>
<td>pH</td>
<td>0.28</td>
</tr>
<tr>
<td>VFA</td>
<td>0.36</td>
</tr>
</tbody>
</table>

The steps previous to the digester, especially the suspension buffer tank and the sanitation step, can also have an influence on the results. The degradation of the substrate can already begin in or before the suspension buffer tank. In the sanitation step, the substrate is heated to 70 °C, and this pre-treatment can speed up the degradation of the material. An increased value of the hydrolysis rate for the mixed substrate (k_{hyd,ms}) can lead to a better fit with biogas pro-
duction, while a decreased value can lead to a better fit with NH4-N. If part of the substrate was already hydrolysed, it could be expected that the substrate as a whole would degrade faster into biogas. In addition, if parts of the protein of the mixed substrate had already been hydrolysed, it would have added to soluble inorganic N (SIN). Part of the SIN measured at the digester inlet could be degraded proteins from the OFMSW. Therefore, the hydrolysis rate estimated in this study could be too low, to compensate for the degraded portion of the proteins. However, a large part of the NH4-N in the mixed substrate came with the process water.

In addition, the ADM1 assumes that the digester is perfectly mixed. In fact, a computational fluid dynamics model, made of the digester in this study, suggests that are zones that are mixed very little or not at all [104]. As mentioned in section 2.1.1, mixing affects a number of different areas such as distribution of temperature, microalgae and nutrients. Imperfect mixing can, therefore, have a large impact on simulation results and affect everything from degradation rate to inhibition to liquid volume. A number of different of methods have been presented for including the effect of mixing in the digestion simulation [16]. However, inclusion of mixing will add to the complexity of the model and can be difficult to validate.

4.1.2 Simulation Using ANN (Paper II)

The ANN biogas outflow and CH4 content are predicted quite well and even follow the drop in biogas outflow exhibited in the middle of the validation period, as shown in Figure 4.3. R (see Eq. 3.3) was 0.76 for biogas and 0.57 for CH4 content. The ANN could predict raw biogas with a higher accuracy than CH4 content. The CH4 could not be fully predicted over the whole span of CH4 content even though it followed the general fluctuations. Reviewing other studies using empirical models, the results seemed to be in a similar range. For example, R was found to be in the range of 0.63-0.71 for the CH4 flow [64] and about 0.76 for biogas flow (estimated from a graph in the study by Guegium Kana et al. [66]). Another study [65] estimated the CH4 content and found the model fit in terms of $R^2$ to be 0.87. Unlike this study, none of the other studies predicted more than one output.
4.1.3 Comparison of the Two Models (Papers I and II)

For the studied period, the ANN had a better fit than the ADM1 as indicated in Table 4.3. The ADM1 predicted higher variations in the biogas output and especially in the CH$_4$ content than what was measured and what the ANN predicted, as shown in Figure 4.4. For both systems, it would have been easier to evaluate the extent of the fit if there had been some large change in the system or if there had been more instability, for example, a large drop in pH. The system contained natural fluctuations and noise. Both models would show a better response if more of the measurements could be made online, especially, daily measurement of incoming grease trap sludge which is missing today. Online measurement would also provide more measurements for the ANN to be used for training and could increase the accuracy since some of the input parameters in this study were interpolated. In addition, for the ADM1, one difficulty was the characterisation of the incoming substrate.

Table 4.3. Comparison of the quantified fit between simulated and measured values for ADM1 and ANN

<table>
<thead>
<tr>
<th>Model</th>
<th>Parameter</th>
<th>IoA</th>
</tr>
</thead>
<tbody>
<tr>
<td>ADM1</td>
<td>Biogas</td>
<td>0.70</td>
</tr>
<tr>
<td></td>
<td>CH$_4$ content</td>
<td>0.63</td>
</tr>
<tr>
<td>ANN</td>
<td>Biogas</td>
<td>0.86</td>
</tr>
<tr>
<td></td>
<td>CH$_4$ content</td>
<td>0.68</td>
</tr>
</tbody>
</table>

Figure 4.3. Simulation result for the ANN network for the period of 7 to 25 May 2011
4.2 Simulation of Co-digestion of Microalgae and Sewage Sludge (Paper III)

In the simulation of the two semi-continuous lab-scale reactors using ADM1, the separate hydrolysis rate coefficients were estimated for the sewage sludge as well as the microalgae. The sludge hydrolysis rate coefficients were estimated using values from RK1. The hydrolysis rate coefficients using "COD" (measured particulate COD) had the best fit and are the ones that are presented in Table 4.4 for sludge.

The hydrolysis rate coefficient for carbohydrates (\(k_{\text{hyd,ch}}\)) had a definite range for the sum of fit of all parameters, unlike the hydrolysis rate coefficient for lipids (\(k_{\text{hyd,li}}\)). The hydrolysis rate coefficient rate for proteins (\(k_{\text{hyd,pr}}\)) seemed to have a peak close to 1 d\(^{-1}\). For microalgae the hydrolysis rate coefficient with the strongest pattern was \(k_{\text{hyd,pr}}\) (better fit, the higher the \(k_{\text{hyd,pr}}\)), determined using data from RK2. The hydrolysis rate coefficients determined using "ThOD2" for the microalgae had the best fit, and are the ones presented in Table 4.4. The calibration results are shown in Table 4.4.

As described in section 3.3.2, the characteristics of substrates were calculated using two different sets of ThOD-values (in addition, measured CODp was also used for sewage sludge in RK1). These are marked as "ThOD1", "ThOD2", and "COD" in the Figure 4.5 and Figure 4.6.

Evaluating the method characterising of the substrate, it also seemed that the characterisation had the greatest effect on the fit for the NH\(_4\)-N and bi-
Table 4.4. Results from the parameter estimation for the co-digestion of microalgae (using characterisation method “ThOD2”) and sewage sludge (using characterisation method “COD”)

<table>
<thead>
<tr>
<th>Estimated parameter</th>
<th>Unit</th>
<th>ADM1 standard value</th>
<th>Calibrated value</th>
</tr>
</thead>
<tbody>
<tr>
<td>$k_{hyd,ch,sludge}$</td>
<td>d$^{-1}$</td>
<td>10</td>
<td>0.16</td>
</tr>
<tr>
<td>$k_{hyd,pr,sludge}$</td>
<td>d$^{-1}$</td>
<td>10</td>
<td>0.69</td>
</tr>
<tr>
<td>$k_{hyd,li,sludge}$</td>
<td>d$^{-1}$</td>
<td>10</td>
<td>1.78</td>
</tr>
<tr>
<td>$k_{hyd,ch,microalgae}$</td>
<td>d$^{-1}$</td>
<td>10</td>
<td>7.49</td>
</tr>
<tr>
<td>$k_{hyd,pr,microalgae}$</td>
<td>d$^{-1}$</td>
<td>10</td>
<td>7.61</td>
</tr>
<tr>
<td>$k_{hyd,li,microalgae}$</td>
<td>d$^{-1}$</td>
<td>10</td>
<td>6.36</td>
</tr>
</tbody>
</table>

Additional parameters for the other characterisation methods can be found in paper III.

Figure 4.5. Simulation results for RK1, from upper right to lower left: raw biogas flow, CH$_4$, pH, HCO$_3$/alkalinity, NH$_4$-N and VFA.
carbonate (HCO₃)/alkalinity. Furthermore, a better fit for either NH₄-N or HCO₃/alkalinity resulted in a worse fit for the other. The characterisation called "ThOD2" included more incoming protein compared to "ThOD1". More protein means the release of more NH₄-N. Changing the input characteristics also change the amount of inorganic carbon in the system. There is also a charge balance, and the ammonium ions (NH₄⁺) and HCO₃ ions (HCO₃⁻) are on opposite sides. For RK2, the pattern of the NH₄-N and HCO₃/alkalinity also seem to differ from the measured values. The NH₄-N is overestimated especially for the beginning of the experiment. The starting value is dependent on the simulation of the start-up period. The start-up period/inoculum was simulated using the average values for the full-scale digester which provides the inoculum. Both the HCO₃/alkalinity and NH₄-N seemed sensitive to the HRT and OLR of the starting period. As with the hydrolysis rate coefficient, there seemed to be a trade-off between the fit of NH₄-N and HCO₃/alkalinity.

![Graphs showing various parameters over time](images)

Figure 4.6. Simulation results for RK2, from upper right to lower left: raw biogas flow, CH₄, pH, HCO₃/alkalinity, NH₄-N and VFA

The output parameters that visually show the best fit between measured and simulated data are gas production, CH₄ content, and VFAs for both RK1 and RK2. The inorganic N also seems to be in the same range (apart for ThOD2 for RK1). All measurements were made once every day (gas volume was read as accumulated gas volume). The measurements for VFA are visible in the figures (Figure 4.5 and Figure 4.6). The reason that the measurement is at the
bottom of the simulated values is that the VFA are at their lowest just before feeding. A mistake was made in the measurements on day 22 when the VFA for RK1 was measured after feeding. The measured value for day 22 for RK1 matched a peak in the simulated values (as the VFAs are highest after feeding).

The strategy for the experiment was to always feed the reactors and take the measurements at the same time each day. However, there were days when the feeding was made at a different time, and no data on time for each feeding were available. Therefore, some of the variations between simulated and measured can be explained knowing that the simulated values assumed that the feeding was carried out exactly at 10:00 each day and the measurements at 09:00. The gas flow and CH₄ content also followed the trend of each measurement, even though for RK1, the measured CH₄ content was a bit higher than the simulated values for the first period.

According to the simulation, the pH should remain stable during both the first period (46 days and OLR of 2.4 kg VS m⁻³d⁻¹) and the second period (30 days and OLR of 3.5 kg VS m⁻³d⁻¹). However, measurements shows that the pH is higher in the first period (around 7.6 for RK1 and 7.5 for RK2) and lower for the second period (around 7.1 for RK1 and 7.0 for RK2). The difference is too consistent for it to be only measurement error. The model does not seem to be able to predict the pH in the current configuration. The calculation of pH in the model is complex and is dependent on a number of ions. The ion states are in their turn dependent on the balance between acids and bases for several of the intermediate products.

The output parameters that visually had the greatest difference between simulated and measured values are HCO₃ and the alkalinity. However, it should be noted that they are dependent on each other. The greatest contributor to alkalinity for this case is HCO₃. For both RK1 and RK2, the HCO₃ and the alkalinity are underestimated as shown in Figures 4.5 and Figure 4.6. The NH₄-N is, in contrast to HCO₃ and alkalinity, overestimated as shown in Figures 4.5 and Figure 4.6.

4.2.1 Steady-state Simulation of the Full-scale System

Using the result from the simulation of the lab-scale semi-continuous system, an imagined full-scale system was also simulated using ADM1. The model gave a good prediction of the gas flow and CH₄ content of the two lab-scale reactors, and it is should predict the performance of a full-scale system. Four different characteristics were used for the microalgae to represent different findings. One set of data were from a study by Mairet et al. [46], two sets (summer and winter) were from a study by Passos et al. [105], and the characteristics of the microalgae in this study were also used. Only the microalgae described in Mairet et al. [46] increased the CH₄ production compared to the
base case. The microalgae differ in composition and in biodegradability (see Table 4.5).

Table 4.5. Comparison of the different microalgae

<table>
<thead>
<tr>
<th>Species</th>
<th>Source</th>
<th>COD/VS-ratio</th>
<th>f_d</th>
<th>Lipid-fraction of degradable</th>
</tr>
</thead>
<tbody>
<tr>
<td>Chlorella vulgaris</td>
<td>[46]</td>
<td>1.84</td>
<td>0.7</td>
<td>0.31</td>
</tr>
<tr>
<td>Mixed-summer</td>
<td>[105]</td>
<td>1.4</td>
<td>0.36</td>
<td>0.19</td>
</tr>
<tr>
<td>Mixed- winter</td>
<td>[105]</td>
<td>1.4</td>
<td>0.41</td>
<td>0.19</td>
</tr>
<tr>
<td>Mixed</td>
<td>This study</td>
<td>1.87</td>
<td>0.2</td>
<td>0.09&lt;sup&gt;a&lt;/sup&gt;-0.11&lt;sup&gt;b&lt;/sup&gt;</td>
</tr>
</tbody>
</table>

a) using "ThOD2"  b) using "ThOD1"

The Chlorella vulgaris described by Mairet et al. [46] stands apart from the others since it is more degradable and also contains a higher content of fat (Figure 4.7).

![Figure 4.7. Comparison of the daily biogas and CH₄ production for the different microalgae characteristics from literature, the mixed microalgae from this study (average result for ThOD1 and ThOD2), and the base case](image)

The data in Table 4.5 shows a comparison of the different microalgae species based on their COD/VS-ratio, f_d fraction, and lipid-fraction of degradable components. The Chlorella vulgaris species stands out due to its higher degradability and higher lipid content compared to the other species listed. The figure illustrates the biogas and methane production for various studies and the current study's results.
To produce the same amount of raw biogas when replacing part of the WAS with the mixed microalgae, the $f_d$ of the microalgae need to be increased to 0.47. The $f_d$ of the microalgae needs to be increased to 0.52 if the CH$_4$ production is to be matched. In comparison, the mixed microalgae-species described by Passos et al. [105] needs to increase its $f_d$ to 0.61 to match raw biogas production and to 0.63-64 to match CH$_4$ production. The microalgae described by Mairet et al. [46] contains more fat than the other microalgae, which could be a contributing factor to the greater potential of the microalgae. Lipids have a higher gas potential than carbohydrates and proteins. The lipid content of microalgae can vary depending on the species. Becker et al. [106] studied a large number of different microalgae species and found that lipid content for the studied species ranged from 2% to 22%. Growing conditions are also a factor that decide the composition of the microalgae. N-starved Chlorella vulgaris contain more lipids than non-limited Chlorella vulgaris [46].

If the microalgae are integrated into the wastewater treatment and are grown in wastewater, the wastewater will most likely be N rich and it will not be possible to N-starve the microalgae. In wastewater treatment, it is most common to use open high-rate algae ponds making contamination likely and limiting the possibility of using a specific species. The total amount of sludge might increase with microalgae [77] which could lead to additional CH$_4$. Pre-treatment could also be investigated to improve the biodegradability of the microalgae, since biodegradability seems to be a limiting factor for the anaerobic digestion of the microalgae.

4.3 Introduction of Microalgae in WWTP (Paper IV)

Introducing the microalgae in the biological treatment step and using the current basin area for the biological treatment will only lead to a small reduction in heat and power consumption and CO$_2$ emission (less than 10%), as shown in Figures 4.8 and 4.9.

If the surface area is increased, the reduction will increase as well, as the sunlight and growth of microalgae increases. The plant that shows the largest potential for change, in percentage, is the Uppsala C-block. This is because the heat consumption related to the C-block is the smallest of the three plants. However, the Uppsala C-block is only one of the Uppsala WWTP’s three separate lines. The C-block treats 52% of the incoming wastewater. Therefore, it was assumed that the C-block also uses 52% of the heat consumption of the plant.

The largest reduction in heat and electricity, as well as CO$_2$ emissions, can be achieved during the three summer months (May to August) when the solar irradiance is at its highest. As the surface area increases, the basin also becomes shallower. At the largest surface area investigated in this study, 12 times the current basin surface, the depth of the basin becomes 0.3 - 0.4 m
Figure 4.8. The effect on energy use in the WWTPs by changing the surface size of the microalgae-bacteria basin

Figure 4.9. The effect on the carbon dioxide emissions in the WWTPs by changing the surface size of the microalgae-bacteria basin
for the WWTPs studied. This depth (0.3 m) is common for high-rate algae ponds (HRAPs) [74]. The drawback is, as has been discussed in previous studies [74, 77], the large land requirement. For two of the plants, Västerås and Uppsala, the land requirement for the algae pond using the largest surface size is almost equal to current total land use for the WWTPs. However, the Eskilstuna WWTP has a large wetland (about 430 000 m²) as a tertiary treatment step. In comparison, the large algae treatment basin would require about 29 000 m². In locations where land use is not an issue, this could still be a viable option. There are also WWTPs that have more people connected to them in summer (typically tourist locations). They could also benefit from a microalgal system. Examples of WWTPs in Sweden with a greater load in summer are the Visby WWTP (double connected PE in summer) [107] and Omholmen’s WWTP (quadruple connected PE in summer) [108].

There are alternatives that could be used to reduce the required surface area. Using stacked tubular PBRs [109] requires less land than HRAPs. Another possibility is using internal illumination of the PBR, either using natural light [110, 111] or artificial light [112]. However, both of these alternatives can carry high costs. For artificial light, the lighting can also consume a lot of electricity. The efficiency of commercial horticultural LED lighting, photosynthetic photon flux (PPF) efficacy, ranges from 2.00 µmol J⁻¹ to 3.05 µmol J⁻¹ (depending on wavelength) [113, 114]. With a PPF efficacy of 2.7 µmol J⁻¹ and photon requirement of 20 photons per O₂, the aeration efficiency becomes 0.016 kg O₂ kWh⁻¹ (doubled if the minimum photon requirement of 10 photons per O₂ is used). If this is compared to the aeration efficiency of mechanical and air-blowing aeration, which are in the range of 1.5 to 5.9 kg O₂ kWh⁻¹, it can be seen that the aeration efficiency of using artificial light is much lower. Artificial light could, however, have other benefits not listed here.

4.3.1 Sensitivity Analysis
The two parameters with the largest impact on the results are the oxygen yield per microalgae and the quanta of light needed to liberate O₂, as shown Figure 4.10c and d. The quanta needed to liberate O₂ can be difficult to determine since it will be affected by the operating conditions. If the biomass concentration would be too high or if there is not enough stirring, the amount of sunlight needed can increase since more of the sunlight will be lost. As the quanta needed increases, the amount of microalgae and their impact on the system decreases as shown in in Figure 4.10d.

In this study, according to calculations, the biomass concentrations in the basins are of the same order of magnitude as found in many PBRs [115]. The amount of CO₂ that the microalgae can absorb also has a large impact on emissions of CO₂ from the plant (Figure 4.10b). The observed yield of the
Figure 4.10. Sensitivity analysis for energy balance, CO\textsubscript{2} emissions, and biomass concentration for the inclusion of microalgae in the WWTPs
biomass, $Y_{obs}$, have an impact on the biomass concentration in the basins, but otherwise have a very small impact on the result (Figure 4.10a). The P and N reduced by the microalgae have only a small impact on the result. The impact of the P on the output was less than $\pm 0.075\%$ and the impact of N less than $\pm 4\%$

The bacteria biomass is much larger than the microalgae biomass and therefore reduces much more of the total P and N. Therefore, increasing the bacteria biomass is more significant than increasing the microalgae biomass and reduces much more of the total P and N. Therefore, increasing the reduction by the microalgae has only a small impact on the results.

4.4 Introduction of Microalgae in a Biogas Plant (Paper V)

The energy used and the GHG emissions to produce 1 GJ of CH$_4$ from microalgae and from ley crop can be seen in Figure 4.11. According to the results, both cases of microalgae cultivation would use more energy from a life-cycle perspective than the current ley crop cultivation. The majority of the energy is used in the cultivation and in the biogas production. In the case of GHG emissions, cultivating microalgae for 180 days yields somewhat lower GHG emissions than the other two alternatives. The GHG emissions of this alternative can be compared to the GHG emissions of one GJ of diesel which is 89 kg of CO$_2$e [116].

As for the energy use, the cultivation as well as biogas production leads to the largest amount of GHG emissions. It should be noted that a lot of the GHG emissions follow the use of heat and electricity, since the production of the heat and electricity is one source of GHG emissions. The cultivation of microalgae needs less land than the ley crop. The ley crop land requirements are 68 times that of the microalgae.

Another alternative would be to cultivate the microalgae in a high-rate algal pond (HRAP). The power used for cultivation is likely to be less than for a flat-plate PBR. Using the average productivity, depth, and power consumption given for a HRAP by Alcantara et al. [74], the cultivation energy use for a HRAP operating under 180 days becomes ca 175 MJ. Assuming that the infrastructure energy use would be zero and the other energy use would be the same as the flat-plate PBR, the NER (see Eq. 3.5) would be around 1.7 which is close to the ley crop NER of 1.78 (there would be some energy use for the construction of the HRAP, however). Assuming the same productivity as for the flat-plate PBR, the HRAP would require 2.3 times the land area required by the flat-plate PBR, which is still less than what is required by the ley crop. A study comparing the life-cycle assessment of HRAP, flat-plate PBRs, and tubular PBRs for cultivation of microalgae for biofuel production found the HRAP to have the lowest NER [79].
Figure 4.11. Energy use and GHG emissions for the life-cycle assessment of introduction of microalgae at the biogas plant; Case I is cultivation of microalgae for 180 days annually without greenhouse heating; Case II is cultivation of microalgae for 330 days annually with greenhouse heating, and Case III is cultivation of ley crop
4.4.1 Sensitivity Analysis

For the case of microalgae cultivation without greenhouse heating, the algal growth rate and the CH$_4$ potential of the microalgae became the two most important parameters in the sensitivity analysis (Figure 4.12). For microalgae cultivation with greenhouse heating, the greenhouse heating also is an equally important factor (Figure 4.12). The actual CH$_4$ potential of the microalgae can vary depending on the final characteristics of the microalgae. Other studies have reported a range of results for the mono-digestion of microalgae. In a study by Olsson et al. [6], two different mixes of microalgae were found to have a potential of 367 Ncm$^3$CH$_4$ gVS$^{-1}$ for one and 178 Ncm$^3$CH$_4$ gVS$^{-1}$ for the other. As described in section 2.1.2, the range found for CH$_4$ yield in the literature was 17.5 - 557 mL CH$_4$ g$^{-1}$ VS with an average of 268 mL CH$_4$ g$^{-1}$ VS) [14, 34, 35]. The microalgae studied in the analysis was *Spirulina* sp., and the CH$_4$ yield found for the genus *Spirulina* was 113 - 481 mL CH$_4$ g$^{-1}$ VS (average 277 CH$_4$ g$^{-1}$ VS) [14, 35, 117].

The worst case of 113 mL$^3$CH$_4$ gVS$^{-1}$ corresponds to a decrease in CH$_4$ potential of the microalgae with 57%; while the best case of 481 mL$^3$CH$_4$ gVS$^{-1}$ correspond to an 84% increase. For the scenario without greenhouse heating, the best case would give a slightly higher NER for microalgae cultivation than for ley crop cultivation, assuming that everything else stays the same. However, for the scenario with greenhouse heating, NER would be lower even for the best case.

The microalgae growth rate is difficult to estimate. A wide range of different values can be found in the literature, and it is also dependent on location and season. Using the data for the Photosynthetic Photon Flux Density (PPFD) for Västerås in 2014 and microalgae productivity per photon used in paper IV, the expected production was roughly estimated. A horizontal surface was used in the calculations, while the flat-based PBR consisted of two vertical surfaces. Using the horizontal surface should still yield a rough estimate of the amount of production. For the 180 days with the highest irradiance (April to September), the estimated growth is 60% of the one used in the paper IV. For the whole year, it is 35%. To compare with the literature, a decrease to 60% of the estimate growth in paper V leads to a productivity of 30.4 g microalgae m$^{-2}$ d$^{-1}$. A decrease of the estimated growth to 35% leads to a productivity of 17.7 g microalgae m$^{-2}$ d$^{-1}$. Alcantara et al. [74] suggests that the typical productivity for a tubular PBR is 15-27 g microalgae m$^{-2}$d$^{-1}$ and 10-25 g microalgae m$^{-2}$d$^{-1}$ for high-rate algal ponds. A productivity of 25 g microalgae m$^{-2}$d$^{-1}$ would correspond to 50% of the growth assumed in this study. The NER for then be 1.12 for case I and 0.64 for case II. Due to the low irradiance in winter time, case II does not seem to be a viable option.

A loss factor could also be considered for the cultivation of silage, during fermentation when some of the sugars will degrade into water and CO$_2$ [93]. If the losses for the cultivation of silage are considered, using the results by
Strid & Flynso [93], the total energy use for case III increases from 561 MJ to 582 MJ. The total GHG emissions increase from 49 to 54 kg CO₂e. Case III will still use the least amount of energy (NER would be 1.72), but it have GHG emissions at the same level as Case II.

4.4.2 Comparison with the Inclusion of Microalgae at the WWTP (Paper IV and V)

The two studies introducing microalgae in the WWTPs (paper IV) and introducing microalgae into the biogas plant (paper V) have quite different perspectives. Different PBRs are considered, with a comparison of an open PBR versus a flat-plate PBR. Furthermore, the microalgae in the WWTP are not mainly an alternative substrate for the anaerobic digestion but a part of the biological treatment, making the microalgae more integrated into the wastewater treatment process. The system boundaries are also different. The lifecycle assessment of the biogas plant included the up-take of carbon dioxide of the substrates that will later be released during anaerobic digestion and combustion of the CH₄. This means that some or all of the carbon dioxide emissions of the WWTP that are reduced by using microalgae can be released during later upgrading and/or burning of the biogas. To avoid the emissions
of carbon dioxide, capture and storage techniques need to be used [118], or the biogas should be stored indefinitely. One study [119] argues for the use of microalgae as a biological way of capturing CO$_2$ from power plants and other CO$_2$ sources. However, the same study also sees the microalgae being used for biofuel production, meaning that total reduction of CO$_2$ only occurs when the biofuel replaces a fossil fuel and prevents the emission of CO$_2$ from the fossil fuel.

The result for the use of land area is different in the two studies. This is partly due to the use of different PBRs but mainly because of comparison used for the microalgae. At the three WWTPs, the current basins are deep and, therefore, are not suited for using only incoming natural sunlight. Increasing the surface area requires the land requirement for the basins and the whole WWTP to also increase. In the biogas plant, the microalgae is compared with ley crop silage, and ley crop silage requires much larger areas of land for cultivation.
5. Conclusions

The results in this thesis show that ADM1 and the ANN are both suitable for replicating the dynamics of a full-scale co-digestion plant. Both models could predict raw biogas flow and methane content at the full-scale co-digestion plant with reasonably high accuracy. For the tested 49 day period, the ANN showed a better fit for biogas (IoA of 0.86 compared IoA of 0.7) and methane content (IoA 0.68 compared to 0.63). The extensive analysis needed for substrate characterization for the ADM1 is a hindrance for utilization of the simulation in industrial applications.

Simulations showed that co-digesting microalgae with primary and waste activated sludge yielded less methane than co-digesting only primary and waste activated sludge. The methane yield is dependent on the species of microalgae used. Simulating co-digestion using microalgae (from another study) with higher biodegradability yielded more methane than only primary and waste activated sludge.

It was also shown that inclusion of microalgae could decrease the energy demand of the studied WWTPs and decrease CO₂ emissions in both the studied biogas plant and the studied WWTPs. In the WWTPs, the size of the decrease of energy demand and CO₂ emissions depended on surface volume. The largest reduction in energy use achieved was 35 %, considering the whole year, and 68 % from May to August. The reduction in CO₂ emissions was 54 % for the whole year and 103 % from May to August. In the biogas plant, inclusion of microalgae led to a lower net energy ratio (NER) for the methane than when using ley crop, a 1.54 ratio for six months of cultivation/1.01 for a whole year was compared to a ratio of 1.78. However, the land use of ley crop cultivation was approximately 68 times that of microalgae cultivation. Both studies showed that in the northern climate, microalgae cultivation was best suited for the summer period.
6. Future Work

It is concluded in this thesis that both ADM1 and an ANN are suitable for replicating the dynamics of a full-scale co-digestion plant. However, more work should be done to see how this can be made more practical. One way of doing that is by evaluating sensors to see if more of the current measurements can be made online. One interesting pathway is near-infrared spectroscopy (NIRS) that could be directly connected to model inputs. Using NIRS for some substrate characterisation and prediction of biogas yield has already been demonstrated [120]. Work is needed to connect the result from NIRS to existing models. In addition to NIRS, there are also many other methods for online monitoring that could also be considered for model connection, such as other types of spectroscopy and titrimetric methods [121].

One interesting application for the ADM1 and ANN would be testing different control strategies. The ADM1 has already been used for control for WWTPs as part of the Benchmark Simulation Model No. 2 [122]. For this application, the ADM1 will be better suited since it predicts a number of different interesting parameters, such as pH, while the ANN only predicts raw biogas and methane content.

More work is necessary in improving the prediction of microalgae growth under known light conditions, as well as further mapping the capability of microalgae to reduce N, P, and other nutrients depending on species and growth conditions. It has also been suggested that microalgae can reduce pharmaceutical residues and heavy metals in the waste streams. It would be interesting if this can be quantified to better estimate the value of microalgae within wastewater treatment.

Microalgae could also be of interest for other applications, such as the production of liquid biofuels. Another LCA-study [97] found biogas production from microalgae to be worse than biodiesel production in several categories. It would be interesting to compare biogas production in the case study plant by integrating biodiesel. The residual mass from the production of biofuels could still be used for anaerobic digestion.
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4. RESULTS AND DISCUSSION

It was found that the best result for the network was obtained for the open loop network with 10 neurons in the hidden layer and a time-delay of six. The first network set-up using ammonia and pH as additional parameters gave a slightly less accurate prediction of methane content and biogas outflow than the second. Since the pH and ammonia had to be interpolated a lot of data points were created that might not match the actual fluctuations of these two parameters. Having these two parameters as output nodes could therefore have had a negative rather than a positive impact on the accuracy of the network. In addition, it is better to keep models as simple as possible with consideration of the accuracy of the modeling compared to the real plant data therefore ammonia and pH as output nodes were not considered further.

Table 2 Statistical analysis of the model results, IoA have a value between 0 and 1, the closer to 1 the more accurate the model is.

<table>
<thead>
<tr>
<th></th>
<th>Methane content</th>
<th>Gas flow</th>
</tr>
</thead>
<tbody>
<tr>
<td>Pearson correlation coefficient R</td>
<td>0.573</td>
<td>0.758</td>
</tr>
<tr>
<td>Rot mean squared error (RMSE)</td>
<td>2.2</td>
<td>888.1</td>
</tr>
<tr>
<td>Mean absolute percentage error (MAPE) (%)</td>
<td>2.7%</td>
<td>10.4%</td>
</tr>
<tr>
<td>Index of Agreement (IoA)</td>
<td>0.564</td>
<td>0.748</td>
</tr>
</tbody>
</table>

The resulting network was better at predicting biogas outflow (R = 0.76) than methane content (R=0.57), see Figure 4 and Table 2.

![Figure 4](image_url)

Figure 4 Target vs output for the gas flow (to the right) and the methane content (to the left).

The prediction for the biogas outflow follows the pattern of the actual biogas outflow quite well even when the biogas outflow drops in the middle of the period, see Figure 5.

\[
MAPE = \frac{1}{n} \sum_{i=1}^{n} \left| \frac{x_i - y_i}{x_i} \right| \times 100
\]

\[
IoA = 1 - \frac{\sum_{i=1}^{n} (y_i - x_i)}{\sum_{i=1}^{n} (|y_i - \bar{x}| + |x_i - \bar{x}|)^2}
\]
Figure 5 Output response of gas flow for the period April 2011 and May 2011, the unit for the gas flow is Nm$^3$.

The prediction of the methane content followed the general fluctuations of the methane but did not fully predict the span of the methane content. The actual methane content drops to lower levels and increases to higher peaks than the network is able to follow, see Figure 6. Since a NARX uses a feedback loop for the results the time period for which the network can predict ahead is generally limited. A larger error could therefore be expected the further into the future that the network is predicting. However, for the time period tested, the accuracy of the prediction does not seem to decrease toward the end of the period which means that the network seems to be able to predict more than two months ahead of time.

There are many articles published on modeling of AD, at least if also AD of wastewater and other liquid waste streams is considered. However, it is challenging to compare the result between different models since few include quantitative evaluation of the result. Güclü et al. (2011) evaluated different neural networks for AD of sludge with regards to R, MSE and mean absolute error. Their network outputs were VS and methane flow. For methane flow Güclü et al. (2011) reported R in the range of 0.63-0.71. Gueguim Kana et al. (2012) predicted biogas production from co-digestion AD using various substrates, the neural network was never quantitatively evaluated but the graph depicted is quite easily read. Approximately R = 0.76 and MAPE = 56%. The network created by Abu Qdais et al. (2010) has some similarities to the neural network in this study. It also considers pH, temperature, VS and TS as inputs (but not flows). In contrast, two hidden layers are used instead of one (each with 25 nodes). Abu Qdais et al. (2010) only predicted methane content but achieved a higher degree of accuracy ($R^2 = 0.87$). They have 177 data points for each variable over one year, it suggest that if the interval between measurements could decrease at Växtkraft, the accuracy of a model such as the one suggested in this study could be increased. In the best scenario VS and pH could be measured online. Other biogas plant might measure these parameters more often or even online, for these biogas plants it is possible that a neural network could achieve a higher degree of accuracy than in this study.

If non-empirical models are also included, Esposito et al. (2011) models AD of synthetic organic...
waste and reports an IoA of 0.999. Derbal et al. (2009) reports a unique application of ADM1 to a full-scale plant co-digesting organic waste and waste activated sludge. Unfortunately no quantitative evaluation is reported. However if R and MAPE is roughly estimated from the graphs, then R = 0.41 and MAPE = 6% for methane content. The values for biogas production is roughly R = -0.06 and MAPE = 23%. It should be noted however that these are estimates from the graph and that the model predicts more parameters than these.

This study was made only using data that was available from the plant and the result are still reasonably accurate which means that neural network could be a tool for biogas plant to consider.

![Response of Output Methane Content](image)

Figure 6 Output response of methane content for the period April 2011 and May 2011, the unit for the methane content is %.

Since the data for training, validation and testing has not been randomized, to keep the time series intact, there is the possibility that especially the testing data set are not representative and that might affect the accuracy of the network. It should also be noted that the weights and biases are given random values at the initialization of the network (before training) so even though the training and validation set is fixed there could be a difference in result when retraining the same network with the same training data.

This model (and similar models) could be utilized to find the optimum operation parameters for the plant. It could also be used for forecasting. In comparison to theoretical, non-empirical models it is easier to apply since it does not require any substrate characterization or estimation of kinetic parameters. On the down side, it is only valued in the range in which it has been tested. If the process should undergo large alterations it might no longer be valid while theoretical model might still be valid. Furthermore a theoretical model is more useful when studying processes not yet in existence.

5. CONCLUSIONS
A NARX network was created and trained using backpropagation training. The model developed in this paper can predict both the biogas outflow ($R = 0.76$) and methane content ($R = 0.55$) at reasonable accuracy even with limited and large-fluctuated data available from the real biogas plant. The accuracy of the network could be further improved with a higher frequency of measurement (for example measuring more parameters online). If applying a NARX (or similar neural network) to another plant with more frequent measurements or more online measurements it is also possible that the accuracy will be higher. The neural network could be used to find a suggested optimal point for the operation settings (of digester temperature, inflows and substrate VS).

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