Development of Co-Digestion Software Models to Assist in Plant Design and Co-Digestion Operation

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Introduction

Co-digestion is a widely used protocol for biologically stabilizing wastewaters and waste solids that otherwise might be sent to alternative disposal sites such as landfills. The number of applications is growing, within both farm (Frear et al., 2009) and municipal digester (Wallis et al., 2008; Zupancic et al., 2008) applications. In many cases, one of the motivations for practicing co-digestion is to better exploit under-utilized digesters and to bring in added income to the facility through received tipping fees. Problems can occur, though, with co-digestion, particularly in regard to:

1. Biological inhibition and process upsets that might occur from chemical, biological and physical constituents within the waste being co-digested (Steyer et al., 2006); and
2. Proper sizing of reactors, biogas collection and engine equipment to accommodate the extra biogas being produced.

Potential co-digestion substrates are best evaluated for their biogas potential and perhaps more importantly, their potential for inhibition using laboratory-scale batch digestion studies. Although batch studies cannot completely represent the conditions that might occur under continuous flow conditions in industrial applications it can point developers to areas of concern. On the other hand, questions about proper sizing of equipment for full-scale operations decisions and project development can best be answered through development of a general mathematic model. A general model can define optimal co-digestion under a large variety of conditions, sparing research efforts of experimental trials. It can also simulate AD improvement mechanisms that are achieved by co-digestion such as buffered pH, reduced inhibition, improved hydrolysis and adjusted C:N ratio.

This paper presents General Integrated Solid Waste Co-digestion (GISCOD), a general integrated solid waste co-digestion model. The main goal of this study was to develop and test a simulation tool of the anaerobic digestion (AD) process that is applicable to any combination of organic waste streams using the simulation platform Matlab-Simulink. The Matlab simulation platform was chosen for implementation based on extensive prior use within the wastewater engineering field, including applications for risk assessment of gas emissions from solid waste incinerators (Kumar et al., 2009) and modeling of solid waste landfills (Garcia-de-Cortazar and Monzon, 2007), and use as a common interface model for solid waste management (bou-Najm and El-Fadel, 2004).

Within the Matlab-Simulink environment, the biological and physic-chemical reactions, thermodynamics and kinetics are represented using ADM1, International

Water Association Anaerobic Digestion Model number 1, which was developed by the task group on anaerobic digestion (Batstone et al., 2002). The ADM1 model starts with a disintegration step for composite particulate material, i.e. decomposition of feed or decaying biosolids according to predefined fractions and composition of carbohydrates, proteins, fats (lipids) and inert materials. The second step is enzymatic hydrolysis of disintegrated carbohydrates, proteins and fat (lipids), which is followed by the three pathways of anaerobic degradation: acidogenesis, acetogenesis and methanogenesis. The degradation steps are modeled by uptake kinetics of different substrates by seven distinct bacterial groups. The decay processes of the seven bacterial groups are also considered and the decaying particulates are sent back to the disintegration step.

Modifications to the existing ADM1 application were necessary as ADM1 has practical problems related to the characterization of the digester feedstock and the associated model definition of the enzymatic disintegration and hydrolysis steps. In previous applications of the ADM1, fraction parameters were estimated from experimental data (Fezzani and Ben Cheikh, 2008; Fezzani and Ben Cheikh, 2008) or evaluated as a function of VS influx (Lubken et al., 2007). Such estimation is not feasible for co-digestion since it is difficult to find unique parameter values that are applicable to all possible combinations and ratios of solid wastes together with decaying anaerobic biomass.

We realized that parameter estimation problems could be avoided by eliminating the use of fraction parameters, instead using a dynamic interface to ADM1 to simulate AD of animal manure and solid waste (Zaher and Chen, 2006). The interface procedure was validated by comparing the estimated carbohydrate, protein, lipid and inert material concentrations with the proximate analysis of 17 solid wastes (Zaher et al., 2009). In the research work presented in this chapter, the interface procedure is generalized and implemented. Within GISCOD, the influxes from each waste are evaluated dynamically. The hydrolysis parameters are considered separately for each waste and uncoupled from the hydrolysis of the decaying biomass. Therefore, the GISCOD modeling tool is generally applicable to study the co-digestion of any combination of different wastes and to evaluate their independent hydrolysis rates and operation settings, i.e. their optimal feed ratio and hydraulic retention time (HRT).

Methods

GISCOD Model

The different models integrated in GISCOD (Figure 5.1) are written in C and compiled in Matlab as MEX S-functions to run using the Matlab-Simulink platform and its toolboxes. The compiled version of the model works with most Matlab-Simulink (release 14) installations on Windows XP and VISTA operating systems. The practical characteristics and flows of all different solid wastes as well as all model parameters are arranged in Microsoft Excel file. All inputs, initial states and parameters for the co-digestion models are read from the Excel file into the Matlab work space using an automated Matlab script. The simulations were run in Simulink after configuring the numerical solution using any variable step solver that is available in Simulink.

Within GISCOD, each waste is assumed to have different fractions of carbohydrates, proteins, lipids and inert materials that may be changing dynamically (Lubken et al., 2007). Each waste would also have different hydrolysis rates for carbohydrates, proteins and lipids (Fezzani and Ben Cheikh, 2008; Fezzani and Ben Cheikh, 2008). Carbohydrate, protein and lipid hydrolysis of each waste is therefore considered in separate model nodes. The disintegration step was not considered for solid wastes as it was assumed that enzymes can easily diffuse and hydrolysis would take place before disintegration. Also no cell lysis is required for solid wastes (as opposed to decaying bacteria). Practical characteristics and flows of each solid waste are input from the workspace to the transformer model nodes. The practical characteristics are converted to the complex composition of the ADM1 input state vector and assigned to the input of separate hydrolysis nodes. The hydrolysis output signals are rearranged by the combiner model, which generates the input to the ADM1 node.

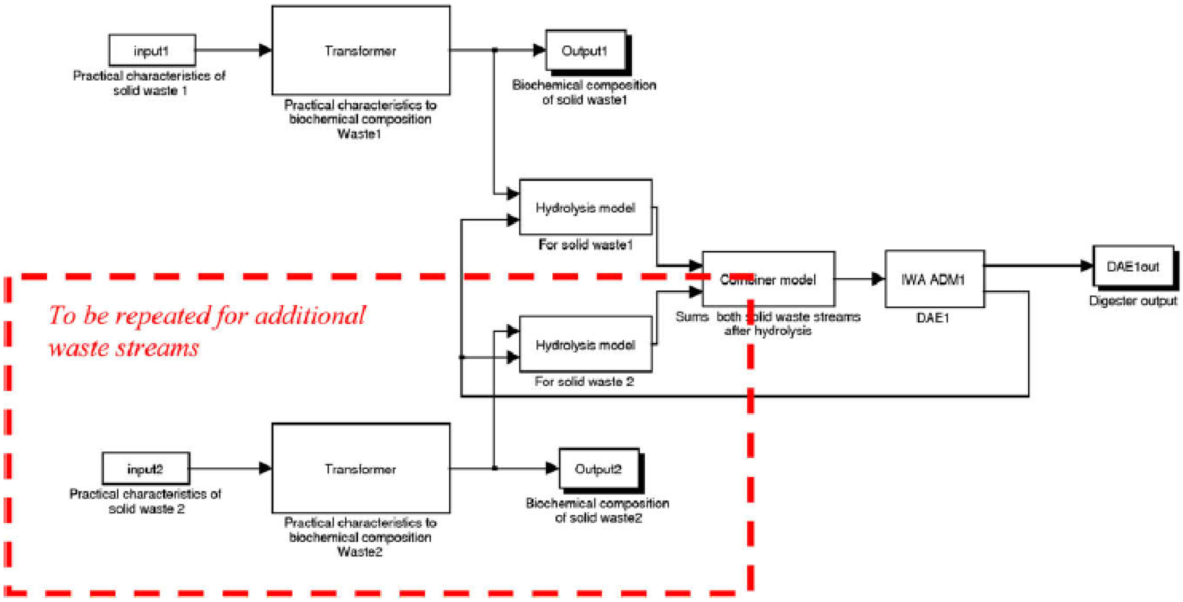


Figure 5.1: The GISCOD model in Matlab-Simulink

The combiner model divides the solid wastes AD process into an enzymatic hydrolysis phase in the hydrolysis nodes only and an uptake phase of the hydrolysis products in the ADM1 node. Thus, Solids Residence Time (SRT) of each waste is considered separately for each hydrolysis node according to the time its particulate components are allowed to stay in the digester (i.e., according to mixing patterns) plus the time used for any pre-hydrolysis steps. The combiner node passes the non-hydrolyzed particulates as dummy variables to the ADM1 and sums other variables on the basis of fluxes from both waste streams.

In the ADM1 node, non-hydrolyzed portions are again not subject to the hydrolysis kinetics and the hydrolysis in the ADM1 node is therefore only considered for particulate fractions of the decaying biosolids (bacteria). Thus, the digester out-flux contains non-hydrolyzed carbohydrates, proteins and lipids originating from the solid wastes in addition to the corresponding components resulting from decaying biosolids. Thus the mass balance is maintained. In addition to the biological reactions, the ADM1 implementation considers the chemical equilibrium of all ions to evaluate the pH change. The pH calculation is linked to the hydrolysis nodes to allow ongoing hydrolysis kinetics to reflect the pH dependency of the hydrolysis. The chemical equilibrium of volatile fatty acids (VFA) and the carbon and nitrogen systems are solved externally once for all hydrolysis and digestion nodes. The solution of chemical equilibrium is performed algebraically according to the ADM1–DAE implementation (Rosen et al., 2006). The ADM1–DAE implementation removes stiffness from the original ADM1 Ordinary Differential Equations (ODE) system to simulate rapid dynamic changes in the AD process, e.g. due to changing composition of the digester feedstock.

Transformer Model

The general transformer model used to interface ADM1 to different solid waste streams was programmed in C code and incorporated in the GISCOD Matlab-Simulink model as a C-MEX S-Function. The general transformer model is based on the ADM1 interface to solid wastes (Zaher et al., 2009; Zaher and Chen, 2006). The transformer model combines the advantages of previous interfacing methodologies applied to ADM1.

The developed general transformer model represents an enhancement over the Continuity Based Interfacing Methodology (CBIM) developed by Vanrolleghem et al. (2005). The CBIM applies Chemical Oxygen Demand (COD) balance, charge balance and elemental continuity to all macronutrient elements (C, H, N, O and P) (Volcke Eveline et al., 2006; Zaher et al., 2007) and can interface with ADM1 regarding practical characteristics of solid wastes via the general transformer model. Kleerebezem and van Loosdrecht (2006) used practical characteristics such as COD and Total Kjeldahl Nitrogen (TKN) to characterize the ADM1 influent. They assumed the digester's feedstock as a single composite particulate (Xc) with constant composition and used the practical characteristics to estimate ADM1 fraction parameters that distribute Xc after disintegration to particulate components of carbohydrates, proteins and lipids. The use of the fraction parameters however does not allow dynamic simulation due to changes in the feedstock composition. In contrast, the developed transformer model applies CBIM to estimate the influxes to ADM1 and avoids the overuse of fraction parameters to allow dynamic simulation. The transformer model robustness is increased by updating the CBIM procedure to maximize the conversions to ADM1 components in a predefined order. COD and charge balances, and the continuity of all macronutrient elements are checked after the conversion of each component.

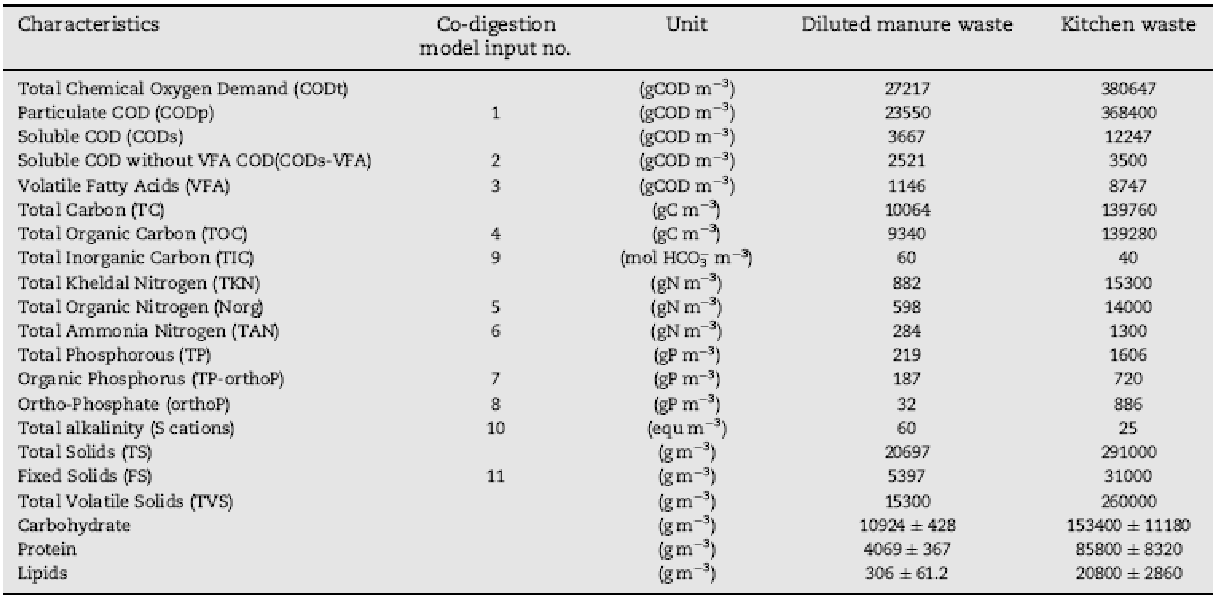
Calibration and Optimization Case Study

The robustness and simulation speed of GISCOD were tested by running the model through parameter estimation and optimization algorithms. Parameter estimation was done using Simulink Parameter Estimation software and the simplex optimization algorithm (Nelder and Mead, 1965). Two experiments were performed to calibrate the hydrolysis parameters (one involving digesting manure alone and one involving manure with kitchen waste). An experiment with food waste alone was not possible due to acidification and pH drop. The average characteristics for each waste stream are shown in Table 5.1. Only the indicated 11 characteristics are needed as model inputs. Both wastes were homogenized and kept frozen in batches that were only thawed before feeding. The only degree of freedom used during the experiment was the daily feed rate, which was varied for each experiment according to the profiles shown in Figure 5.2. For both experiments, reactors were mixed, with a hydrolysis step of 0.6 L volume followed by a digestion step of 2 L. Reactors were kept at 35^{o}C. The gas production from both steps was used for calibration. First, the manure hydrolysis parameters were estimated from the manure only digestion experiment. Second, the kitchen waste hydrolysis parameters were estimated from the co-digestion experiment.

Carbohydrates, proteins and lipids were analyzed for each waste to validate the transformer predictions. Carbohydrates were quantified by sequential extraction using neutral and acid detergent, followed by strong acid extraction. Proteins were analyzed by the Lowry colorimetric method calibrated on bovine serum albumin. Lipid content was determined by a Soxhlet method using petroleum ether for extraction.

Optimization of the solid waste ratio and HRT was done by comparing the steady state biogas flow rate from several virtual experiments using the calibrated model. The ratio of kitchen waste, flow and methanogenic reactor volume was varied for each simulation, for a total of 200 cases. The kitchen waste ratio was varied from 5% to 100% in 5% increments. Ten retention times were considered: 5, 7.5, 10, 15, 20, 50, 75, 100, 150, and 200 days. Two methanogenic volumes were considered: 2 L for HRT ≤20 days and 20 L for HRT >20 days. The hydrolysis volume was 2 L for all the simulated cases. Each case was simulated until the gas flow rate reached a steady state after 1000 days of simulation time, for a total virtual experimental time of 200,000 days.

Table 5.1: Characteristics of diluted manure and kitchen waste



Characteristics	Co-digestion model input no.	Unit	Diluted manure waste	Kitchen waste
Total Chemical Oxygen Demand (CODt)		(gCOD m^{-3})	27217	380647
Particulate COD (CODp)	1	(gCOD m^{-3})	23550	368400
Soluble COD (CODs)		(gCOD m^{-3})	3667	12247
Soluble COD without VFA COD(CODs-VFA)	2	(gCOD m^{-3})	2521	3500
Volatile Fatty Acids (VFA)	3	(gCOD m^{-3})	1146	8747
Total Carbon (TC)		(gC m^{-3})	10064	139760
Total Organic Carbon (TOC)	4	(gC m^{-3})	9340	139280
Total Inorganic Carbon (TIC)	9	(mol HCO_3^- m^{-3})	60	40
Total Kheldal Nitrogen (TKN)		(gN m^{-3})	882	15300
Total Organic Nitrogen (Norg)	5	(gN m^{-3})	598	14000
Total Ammonia Nitrogen (TAN)	6	(gN m^{-3})	284	1300
Total Phosphorous (TP)		(gP m^{-3})	219	1606
Organic Phosphorus (TP-orthoP)	7	(gP m^{-3})	187	720
Ortho-Phosphate (orthoP)	8	(gP m^{-3})	32	886
Total alkalinity (S cations)	10	(equ m^{-3})	60	25
Total Solids (TS)		(g m^{-3})	20697	291000
Fixed Solids (FS)	11	(g m^{-3})	5397	31000
Total Volatile Solids (TVS)		(g m^{-3})	15300	260000
Carbohydrate		(g m^{-3})	10924 ± 428	153400 ± 11180
Protein		(g m^{-3})	4069 ± 367	85800 ± 8320
Lipids		(g m^{-3})	306 ± 61.2	20800 ± 2860

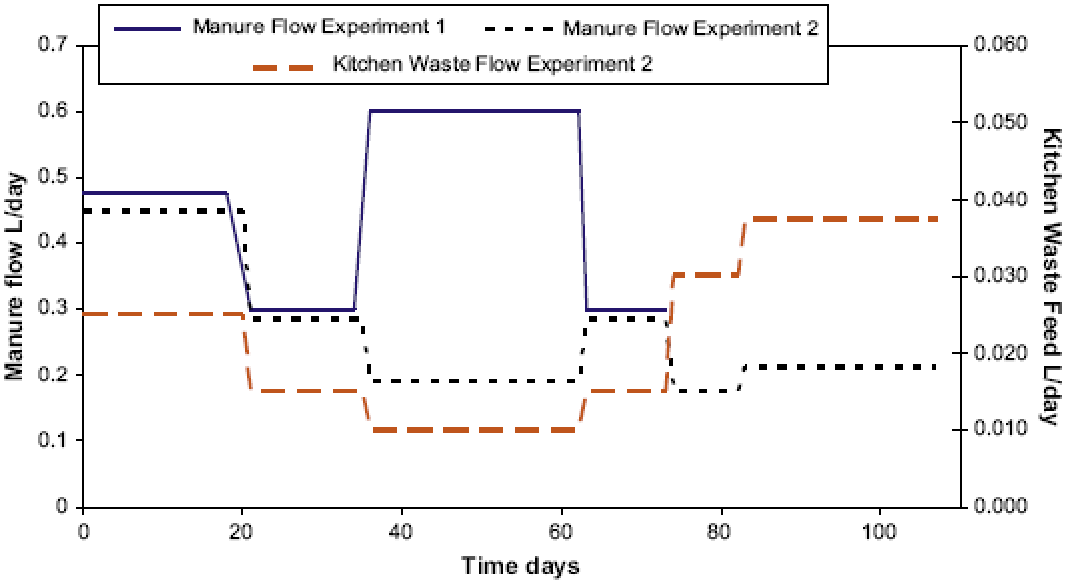


Figure 5.2: Manure and kitchen waste experimental design.

Results and Discussion

Transformer Output

Among other ADM1 input variables, carbohydrates, proteins and lipids were estimated in COD units by the transformer model. This was done to allow the ADM1 model to maintain the COD balance. The corresponding g/L concentration was evaluated according to the defined composition of ADM1 components and compared to the measured concentrations (Figure 5.3). Generally, the estimated and measured concentrations for each of the three main particulate components were consistent. However, some differences could be observed for individual components.

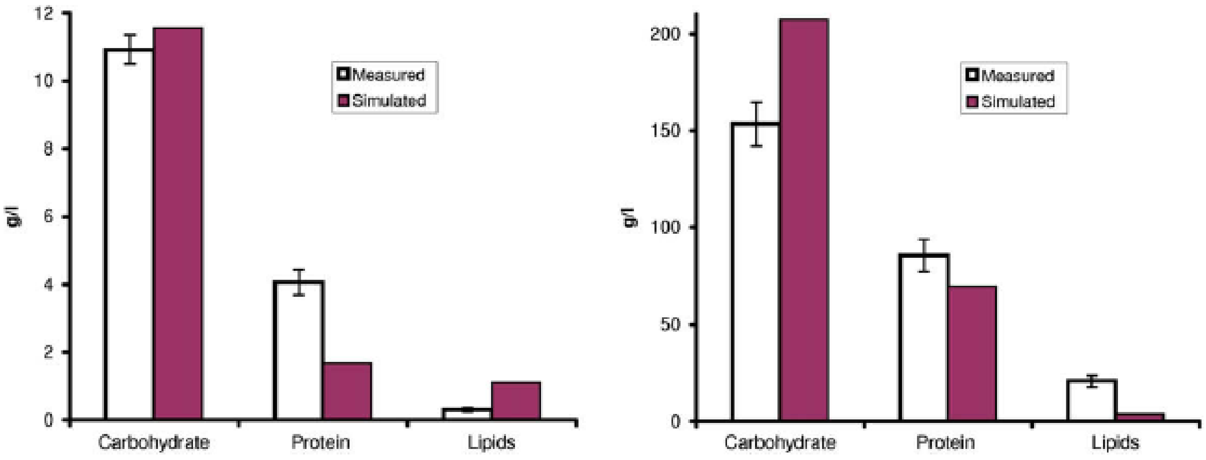


Figure 5.3: Comparison of measured and simulated values for waste components in manure and kitchen waste, respectively.

Carbohydrates

Estimated carbohydrates content was consistent with measured data in the case of manure but it was higher in the case of kitchen waste. The detergent extraction method is an accurate standard method to break the crystal structure of fiber, the main form of carbohydrates in manure. The starch content is high in kitchen waste but would not be quantified as accurately as fiber with the same extraction method. Using the carbohydrate measurements as a direct input to the ADM1 model would have therefore introduced an error to the carbon balance within the model. Thus, the transformer model was used to keep the carbon balance.

Proteins

Measured and estimated protein contents were more consistent for kitchen waste than for manure. The measuring method was calibrated using bovine serum albumin, which is more relevant to the kind of proteins that normally exist in kitchen wastes, such as beef or whey. Using the protein measurements for manure as a direct input to ADM1 model would have introduced errors to the nitrogen balance. Nitrogen in solid wastes such as manure is mainly sourced by the particulate proteins. The use of the transformer model was therefore used to maintain the nitrogen balance.

Lipids

Lipids were the smallest fraction of particulates in both wastes. The estimated and measured lipids contents were relatively inconsistent. On one hand, the estimated lipid composition was assumed to be in the form of phospholipids but other forms may exist in both wastes. In addition, Soxhlet extraction, the method we used, is highly biased if the sample matrix is mainly non-lipids (Manirakiza et al., 2001).

Generally, the use of the transformer model within GISCOD maintains the continuity of COD and elemental mass that are essential to guarantee accurate and reliable simulation. Direct measurements of the waste particulate fractions would not achieve the same reliability. The analytical methods are dependent on the types of the particulate fractions, which are unknown for wastes and are often different from the types defined in the model stoichiometry. Maintaining accurate carbon and nitrogen balances during the simulation is necessary since the C:N ratio is a key factor affecting the co-digestion of different waste streams (Hartmann and Ahring, 2005; Shanmugam and Horan, 2009; Yen and Brune David, 2007; Zhang et al., 2008).

In addition, the C and N elemental continuity preserved in the GISCOD model is important for linking the AD model to subsequent model unit processes and for integrated assessment. For instance, elemental continuity is the key mechanism needed to evaluate pH and chemical equilibrium variables, such as CO_2/HCO_3^- and NH_4^+/NH_3 in the AD process out-flux. The evaluation of CO_2 and NH_3 emissions allows assessment of subsequent unit processes, such as emission studies from composting (Komilis Dimitris and Ham Robert, 2006; Paillat et al., 2005), drying (Deng et al., 2009) and landfill facilities (He et al., 2006). Furthermore, estimation of the pH and NH_4^+ as well as phosphorus devaluated from the mass balance in the transformer model allows for more integrated assessment, such as in studies evaluating added fertility to soils from waste application (Alvarenga et al., 2007; Kang et al., 2008) or evaluating leachate pollution to water bodies (Singh et al., 2005).

Calibration of Hydrolysis Kinetics

Models were calibrated using the simplex optimization algorithm. Figure 5.4 (left) shows that predictions of biogas flow rate after model calibration were comparable to the measurements. The hydrolysis rates of carbohydrates, proteins and lipids were estimated by fitting the biogas measurements against digested diluted manure-only data. The estimated hydrolysis rates were 0.019, 0.025, 0.022/day, respectively, for diluted manure waste. These rates are considerably lower compared to the default values of ADM1 (10/day for each particulate component) that were originally designated for the hydrolysis of activated aerobic sludge and are still used in GISCOD for the hydrolysis of the decaying anaerobic bacteria after a disintegration step. It is noteworthy that the default hydrolysis rates presented in the ADM1 in 2002 are now considered to be at least a factor of ten too large also by the ADM1 Task Group (Batstone et al., 2002). The low rates indicate that the digestion of the manure waste was limited by hydrolysis and that the amount of methane produced was mainly from soluble COD digestion.

In a similar co-digestion study of a fixed ratio waste stream of 80:20 manure liquids to cow fodder (Lubken et al., 2007), the best ADM1 simulation of biogas prediction matched the experimental data at 0.3/day hydrolysis rate for the three particulate fractions. The slightly higher hydrolysis rate compared to digesting manure is due to the addition of the cow fodder. Cow fodder hydrolysis rate is higher compared to manure that has already been passed through hydrolysis and digestion in the rumen.

When the diluted manure was co-digested with kitchen waste, the biogas production was significantly increased, as indicated by comparing biogas production at periods of similar HRT in both experiments, (i.e. day 0 to 38 and day 63 to 73) (Figure 5.4). The higher biogas production was not only due to the higher COD load of added kitchen waste but also because the kitchen-waste particulate fractions were easily hydrolyzed. The experimentally derived hydrolysis rates of the kitchen waste were 5.22, 1.86 and 1.24/day for carbohydrates, proteins and lipids, respectively. The difference between these values and the manure-only values indicates the necessity of separating the hydrolysis of these two wastes when modeling.

Thus, for reliable simulation and prediction of the biogas production at variable ratios of co-digested wastes, accurate hydrolysis rates should be estimated for each waste and particulate fraction. Expanding the applicability of GISCOD to other waste combinations allows the integrated assessment of AD using different treatment scenarios. For instance, accurate estimations of the biogas production for co-digesting energy crops, agricultural residues and wastes would benefit Lifecycle Assessment (LCA) studies of alternative processes for biofuel production (Tan et al., 2004) by allowing for the inclusion of the AD process to the analysis.

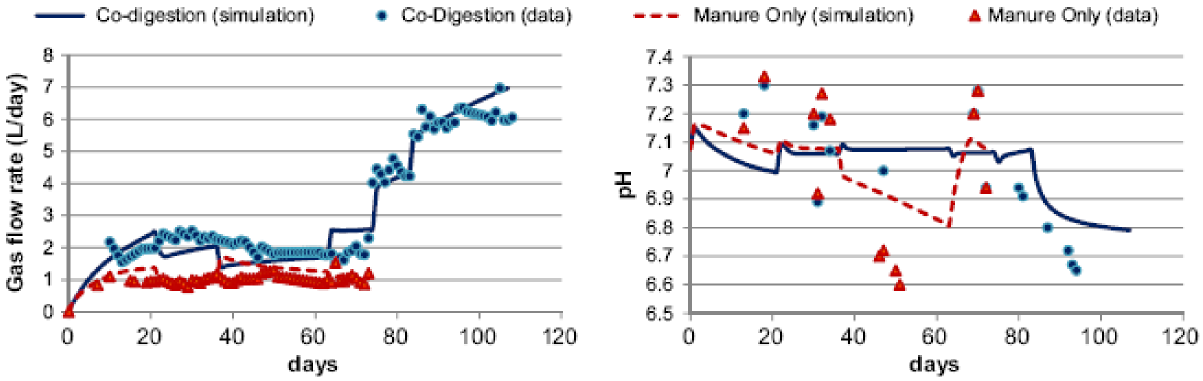


Figure 5.4: Calibration of hydrolysis kinetics.

Simulation of Chemical Equilibrium

Both the simulated and measured pH, presented in Figure 5.4, were slightly higher during manure only digestion, indicating that manure has higher alkalinity than kitchen waste. To further explore the pH dynamics, we induced overload in each system. For manure-only digestion, overload was hydraulically-induced from day 34 to day 63. For the co-digestion scenario, overload was organically-induced by increasing the food waste ratio from day 84 through the end of the experiment. During each of these overload phases, the pH dropped rapidly but the biogas production increased for kitchen waste. During process overloads, VFAs accumulate, causing the pH to drop. The drop of the pH is also caused by stripping of alkalinity and higher CO_2 production in the biogas.

Optimization of Reactor Design and Operation

Using GISCOD, the 200,000 days of virtual experimental time were simulated to find the optimal operation for the co-digestion case study in 8 h of CPU-time. Figure 5.5 shows the predicted gas flow rates of the model for the 200 virtual experiments of the optimization procedure after filtering for a few anomalies due to numerical errors and the high level of non-linearity of the model. The optimal biogas and methane production was found at a HRT of 50 days using a pre-hydrolysis step of 2 L and a digester volume of 20 L. Increasing the HRT more than 50 days did not produce any increase in the daily gas production since the process was rate-limited by the COD loading rate. Meanwhile, at HRT <20 days the process was limited by the methanogenesis step since 2 L volume was assigned to both hydrolysis and methanogenesis steps. There was another local optimum of biogas production at HRT of 10 days that was mainly related to soluble substrates and not the particulate substrate. Inhibition due to VFA accumulation and pH occurred at HRT less than 20 days. However, the addition of diluted manure buffered the pH near the optimum range except for HRT <10 days. Simulations showed VFA accumulation and pH drop at HRT <10 days. During VFA accumulation and pH drop, methanogenesis was completely inhibited and biogas was mainly CO_2, with little methane. Both methane and total biogas production increased with the additional kitchen waste except at low HRT where the alkaline manure could not maintain the pH in the optimal range.

The GISCOD simulated different feedstock and influent flow rates to determine the optimum design and operation of an AD application to the co-digestion of two different waste streams. The simulation saved excessive experimental time, which would be needed to determine the optimum for such co-digestion applications. The determined optimal conditions can then be validated experimentally before full-scale implementation in a relatively short time.

More generally, the design and operation parameters and digester outputs determined by GISCOD would benefit environmental and economic studies of AD applications. Such model-based optimization of design and operation settings is of a great practical advantage compared to ‘‘random’’ or ‘‘heuristic’’ approaches. (Steyer et al., 2006) illustrated the severe consequences of using such ‘‘heuristic’’ approaches to make operation decisions on full-scale biogas plants. For example, a biogas plant co-digesting pig manure and industrial wastewater in Blaabjerg, Denmark experienced a serious accident due to overloading of the industrial waste. The single event caused significant reductions in bio-gas production and methane content over the next three months, and the biogas had to be flared instead of being used for power generation. The total operational loss was subsequently calculated as one million DKK (approximately US $150,000). This example illustrates the practical benefit of the model for optimization and decision support, in addition to its potential application for the integrated assessment and LCA of AD applications for waste stabilization and power generation.

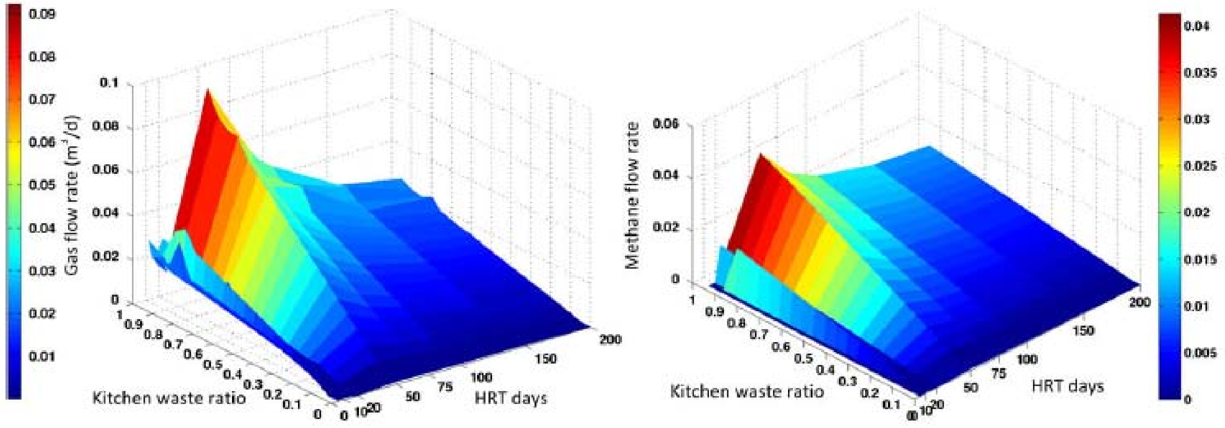


Figure 5.5: Simulation scenario optimizations showing gas flow rate (left) and methane flow rate (right) as a function of kitchen waste ration and hydraulic retention time.

Conclusions

Feeding the digester with a combination of waste streams introduces complexities in waste characterization that requires a model to simulate optimal parameters for co-digestion. The General Integrated Solid Waste Co-Digestion (GISCOD) model has been developed and tested for this purpose.

Model development overcame several challenges to achieve reliable, precise simulations. Accurate characterization of macronutrients, COD and charge for waste streams was necessary input to the International Water Association Anaerobic Digestion Model No.1 (ADM1). Particulate components of carbohydrates, proteins and lipids vary dynamically in combined solid waste streams, making it difficult to define the waste streams for accurate input. Such waste heterogeneity could be resolved by applying a general transformer model to interface the ADM1 to practical characteristics of each waste stream. In addition, our research showed that hydrolysis rates for manure only varied considerably from hydrolysis rates for food waste-manure co-digestion. Thus, for co-digestion applications, it is important to consider separate hydrolysis rates for each particulate component from each waste stream. Also, hydrolysis rates of solid wastes differ from that of decaying biomass which is mainly limited by a disintegration step for cell lysis. The separate characterization and phasing of the co-digested waste hydrolysis allowed the optimization of biogas production and defined the corresponding operation settings of the digester.

As currently designed, GISCOD can support the operational decisions necessary for digesting trucked-in wastes with wastewater sludge or, generally, optimize the feedstock and operation of biogas plants. Further refinement of the developed GISCOD model is required and on-going. In particular, the model is undergoing iterative improvements resulting from validation and re-calibration through testing against available commercial co-digestion data. Ultimately, a user-friendly software package is envisioned to make GISCOD available to digestion engineering firms, wastewater treatment plants and farm digesters.

Key Project References Related to Chapter

The majority of the work presented in this chapter has been previously published as:

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