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GISCOD: General Integrated Solid Waste Co-Digestion model

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ABSTRACT

This paper views waste as a resource and anaerobic digestion (AD) as an established biological process for waste treatment, methane production and energy generation. A powerful simulation tool was developed for the optimization and the assessment of co-digestion of any combination of solid waste streams. Optimization was aimed to determine the optimal ratio between different waste streams and hydraulic retention time by changing the digester feed rates to maximize the biogas production rate. Different model nodes based on the ADM1 were integrated and implemented on the Matlab-Simulink® simulation platform. Transformer model nodes were developed to generate detailed input for ADM1, estimating the particulate waste fractions of carbohydrates, proteins, lipids and inerts. Hydrolysis nodes were modeled separately for each waste stream. The fluxes from the hydrolysis nodes were combined and generated a detailed input vector to the ADM1. The integrated model was applied to a co-digestion case study of diluted dairy manure and kitchen wastes. The integrated model demonstrated reliable results in terms of calibration and optimization of this case study. The hydrolysis kinetics were calibrated for each waste fraction, and led to accurate simulation results of the process and prediction of the biogas production. The optimization simulated 200,000 days of virtual experimental time in 8 h and determined the feedstock ratio and retention time to set the digester operation for maximum biogas production rate.

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1. Introduction

This paper presents 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 combinations of waste streams using the simulation platform Matlab-Simulink®. The Matlab® simulation platform was used for implementation of the risk assessment of gas emissions from solid waste incinerators (Kumar et al., 2009) and modeling solid waste landfills (García de Cortázar and Monzón, 2007), and suggested as a common interface model for solid waste management (bou Najm and El-Fadel, 2004).

A general co-digestion model is needed to support operation decisions at full-scale plants and to assist co-digestion research. The AD process is a widely applicable technology to treat and convert an organic waste stream to methane for green energy production. At wastewater treatment plants, trucked-in wastes are digested with wastewater sludge for renewable energy production (Wallis et al., 2008; Zupancic

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et al., 2008) as part of municipal policies for climate change mitigation and reduction of green house gas emissions. Biogas plants co-digest different solid waste feedstock to increase biogas production. However, random or heuristic decision on the ratio between waste streams or feedstock to full-scale plants often lead to process upset and significant reduction of methane production (Steyer et al., 2006). The general model would support such full-scale operation decisions. Significant research effort was devoted during the last 5 years to study the co-digestion of different combinations of municipal, industrial, agricultural and farming waste streams. A general model is needed to define optimal co-digestion experiments sparing research efforts of experimental trials, and to simulate AD improvement mechanisms that are achieved by co-digestion such as buffered pH, reduced inhibition, improved hydrolysis and/or adjusted C/N ratio. Improvement mechanisms of co-digestion can be simulated by the ADM1, International Water Association Anaerobic Digestion Model number 1, which was developed by the task group on anaerobic digestion (Batstone et al., 2002). However, the ADM1 application has practical problems related to the characterization of the digester feedstock and the associated model definition of the enzymatic disintegration and hydrolysis steps.

A generalized and separate approach is required to solve the solid waste characterization problems compared to Activated Sludge (AS) for two reasons. Firstly, ADM1 is considering constant composition of particulates with fixed fraction parameters to carbohydrates, proteins, lipids and inerts. On the contrary, solid wastes are heterogenic and dynamically changing in composition. Secondly, the lumped composite particulate model component is used as the first model input and, simultaneously, as a product from the model decay processes. This implies that the fraction parameters and hydrolysis rates of the feed substrate should match the composition and hydrolysis rates of the decaying biomass. In fact, the ADM1 was originally developed with focus on the application of AS digestion assuming similar composition of the aerobic and anaerobic bacteria. Under this assumption, there is no conflict between the feed substrate and the produced substrate from decaying bacteria. In this particular case, cell lysis (disintegration) is the limiting hydrolysis step. Such an assumption was proven to be consistent for plant-wide modeling since the AS inert fraction remains inert under anaerobic conditions (Ekama et al., 2007).

In previous applications of the ADM1, fraction parameters were estimated from experimental data (Fezzani and Cheikh, 2008a,b) or evaluated as function of VS influx (Lübken et al., 2007). Using *a priori* expert knowledge about expected wastewater characteristics and experimental measurements to estimate fraction parameters is generally applied for modeling wastewater treatment systems (Grau et al., 2007). Applying such a procedure to co-digestion is not feasible 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.

Parameter estimation problems and use of fraction parameters could be avoided 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 carbohydrates, proteins, lipids and inerts concentrations with the proximate analysis of 17 solid wastes (Zaher et al., 2009). In the research work presented in this paper, the interface procedure is generalized and implemented with GISCOD in Matlab-Simulink as a general transformer model that interface ADM1 to any combination of co-digested wastes. The influxes of the model components 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 generalized 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).

2. Methods

2.1. *Process model*

The AD process was modeled using the ADM1 (Batstone et al., 2002) as a basis with phased implementation to separate the enzymatic hydrolysis of solid wastes from the metabolic reactions utilizing soluble substrates. The ADM1 model starts with a disintegration step of composite particulate material, i.e. decomposition of feed or decaying biosolids according to their predefined fractions and composition of carbohydrates, proteins, fat (lipids) and inerts. The second step is enzymatic hydrolysis of disintegrated carbohydrates, proteins and fat (lipids), which is the start of the corresponding three pathways of anaerobic degradation. The anaerobic degradation is done in three main steps—acidogenesis, acetogenesis and methanogenesis. The degradation steps are modeled by uptake kinetics of different substrates by seven bacterial groups. The decay processes of the seven bacterial groups are also considered and the decaying particulates are sent back to the disintegration step.

The implemented GISCOD model shown in Fig. 1 is generalized to consider the degradation of any other wastes that are different in composition compared to the assumed biosolids (i.e. decaying bacteria). Each waste would have different fractions of carbohydrates, proteins, lipids and inerts that may be changing dynamically (Lübken et al., 2007). Each waste would also have different hydrolysis rates of carbohydrates, proteins and lipids (Fezzani and Cheikh, 2008a,b). Carbohydrates, proteins and lipids hydrolysis of each waste is considered in separate model nodes. The disintegration step was not considered for solid wastes assuming that enzymes can diffuse in the woven structure of wastes and hydrolysis would take place before disintegration. No cell lysis is required for solid wastes compared to AS or decaying bacteria. The hydrolysis products are combined and used as input to a single digestion node where all biological reactions of ADM1 are activated. The non-hydrolyzed fractions are fed through the digestion node as a dummy vector and hydrolysis kinetics in the digestion node are only applied to the decaying biosolids. The complete structure of ADM1 is considered in the hydrolysis nodes to allow future expansion of the co-digestion model considering more complex hydrolysis kinetics. The other biological reactions are deactivated for the hydrolysis

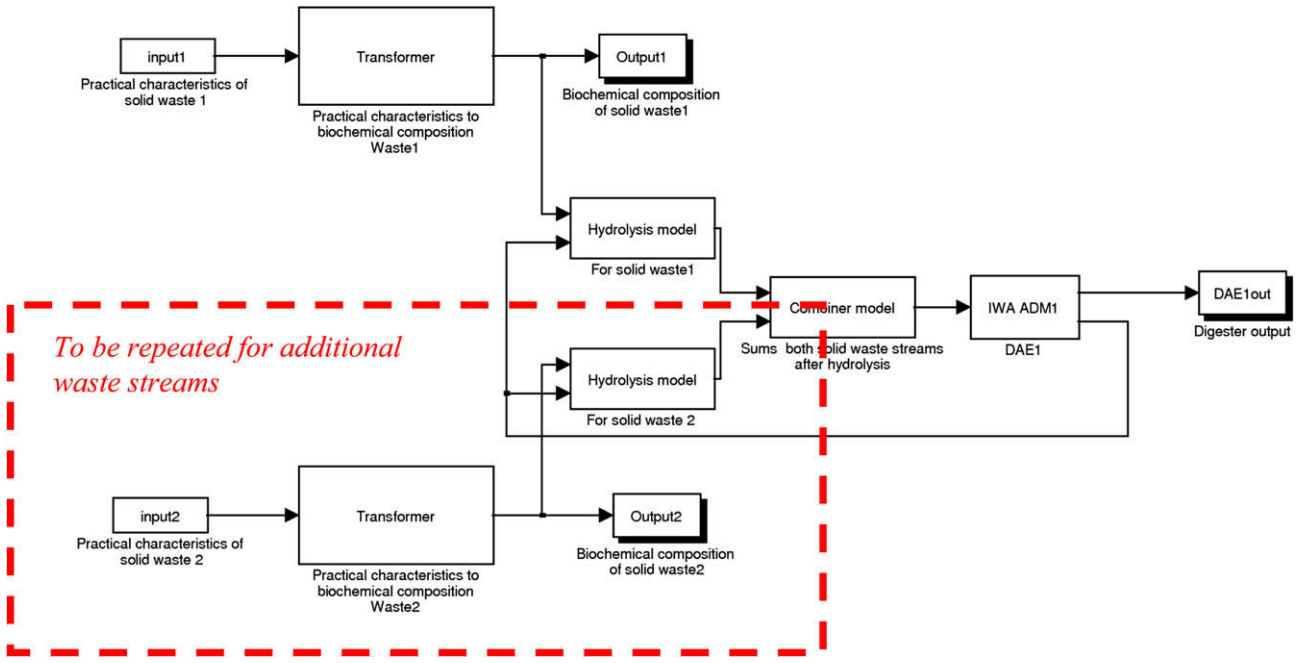

Fig. 1 – The GISCOD model in Matlab-Simulink.

nodes simply by assuming zero uptake, disintegration, decay and gas transfer rates.

In addition to the biological reactions, the ADM1 implementation considers the chemical equilibrium of all ions to evaluate the pH change. The chemical equilibrium of volatile fatty acids (VFA), the carbon and nitrogen systems is solved externally once for all hydrolysis and digestion nodes. The solution of chemical equilibrium is performed algebraically according 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 anaerobic digestion process, e.g. due to changing composition of the digester feedstock.

2.2. *Transformer model*

A general transformer model to interface ADM1 to different solid waste streams was programmed in C 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 and Chen, 2006; Zaher et al., 2009). The transformer model combines the advantages of previous interfacing methodologies applied to ADM1.

2.2.1. *Implemented interfacing advantages*

The general transformer model represents an enhancement of the Continuity Based Interfacing Methodology (CBIM) (Vanrolleghem et al., 2005). The CBIM applies Chemical Oxygen Demand (COD) balance, charge balance and elemental continuity to all macronutrient elements CHNOP to connect different models (Volcke et al., 2006; Zaher et al., 2007). The CBIM in the general transformer is applied to interface the ADM1 to practical characteristics of solid wastes. Kleerebezem and van Loosdrecht (2006) used practical characteristics such as COD, Total Kjeldahl Nitrogen (TKN), etc. 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 does not allow dynamic simulation due to changes in the feedstock composition. The 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 CHNOP elements are checked after the conversion of each component. Such an ordered maximization procedure was suggested by Copp et al. (2003) to interface Activated Sludge Model no.1 (Henze et al., 1987) ASM1 with ADM1, maintaining the COD and N balances. Most recently, Nopens et al. (in press) modified the Copp et al. (2003) ASM1–ADM1 interface. They increased the robustness of the ASM1–ADM1 conversions by changing the maximization order of ADM1 components for the co-digestion of secondary sludge (from ASM1) with primary sludge (from primary settler). The conversions from ASM1 to ADM1 were extended to include carbohydrates, proteins and lipids instead of Xc. Proteins were maximized using Total Kjeldahl Nitrogen (TKN) and the remaining particulate COD was distributed between carbohydrate and lipids using fraction parameters. Extending the balance relations in the transformer model eliminates the use of fraction parameters. The transformer model is upgraded in the implementation with GISCOD to allow the user to change the maximization order of ADM1 components without changing

the transformer model algorithm. The maximization order is implemented as a one-dimensional array parameter to the transformer S-function to increase the generality of the transformer model for the application to any solid waste.

2.2.2. *Transformer algorithm*

The transformer model transforms a set of practical measurements to the input vector of ADM1 according to the stoichiometry presented in Table 1. Table 1 consists of four panes. The lower two panes shows the assumed composition of the practical measurements on the left, components 1 to 11, and the composition of the estimated ADM1 input components on the right. The upper two panes represent the stoichiometry $\nu_{j,k}$ for the conversions j and the elements k. The stoichiometry is evaluated by mass and charge balances according to Eq. (1). The stoichiometry matrix is uploaded to the Matlab work space as a two-dimensional array parameter to transformer model S-function.

$$\sum_{k} \nu_{j,k} i_{j,\mathrm{Comp}} = 0 \text{ with Comp} = \mathrm{Thod, C, N, H, O, e} \tag{1}$$

The transformation step in CBIM was changed to include the ordered maximization procedure. The original transformation of CBIM is generated by Eqs. (2) and (3). A set of algebraic equations is generated by Eq. (2) to map the influxes to vector ρ_j, $j = 1{:}n$ where n is the number of conversions, using the stoichiometry in the left pane of the transformation matrix, i.e., for $k = 1{:}P$ where P is the number of practical measurements. Then Eq. (3) calculates the outfluxes from ρ_j using the stoichiometry in the right pane of the transformation matrix, i.e., $k = P + 1{:}P + Q$ where Q is the number of the estimated composition components.

$$\sum_{j=1}^{n} \nu_{j,k}\rho_j = \mathrm{Influx}_k \quad \text{for } k = 1 : P \tag{2}$$

$$\mathrm{Outflux}_k = \sum_{j=1}^{n} \nu_{j,k}\rho_j \quad \text{for } k = P + 1 : P + Q \tag{3}$$

In the implementation for the co-digestion model Eq. (2) is replaced by a maximization procedure according to Zaher et al. (2009) to increase the transformer robustness, to conceal (correct) possible errors in the practical measurements and to maintain the elemental mass balance during the conversions. The elements of the vector ρ_j are maximized in a predefined order to make sure that the elemental influxes sourced by the input of practical measurements are sufficient before calculating the next element of ρ_j. A predefined order of ρ_z, $z = 1{:}10$, which corresponds to $j = (10, 5{:}9, 4, 3, 1, 2)$, maximizes the conversion to inert particulates, volatile fatty acids, sugars, lipids, proteins, carbohydrates, and then inorganic components. This maximization order is uploaded before simulation to the Matlab work space as a parameter to the transformer model S-function. Thus, the maximization order can be easily changed by the user. The maximization is done according to the following steps:

1. ρ_z is calculated using Eq. (4) as a function of the influx of the most correlated measurement k, i.e., corresponding to the unique value of $\nu_{z,k} = -1$ at each conversion;
2. ρ_z is verified using the conditions imposed by Eq. (5). If shown true, the next ρ_{z+1} was calculated starting from step 1 above;
3. If shown false, ρ_z is changed and calculated according to Eq. (6), the ρ_z calculation is then terminated and other rates (ρ_i, $i = z + 1{:}n$) are assigned a value of 0;
4. Any remaining fluxes are added to the relevant inorganic components; and accordingly,
5. All practical measurements are mapped to the new vector ρ. The output flux of substrate composition is then calculated using Eq. (3).

$$\rho_z = \left(\frac{\mathrm{Influx}_k - \sum_{i=1}^{z-1} \nu_{i,k}\rho_i}{\nu_{z,k}} \right) \tag{4}$$

$$\sum_{1}^{z} \nu_{z,k}\rho_z < \mathrm{Influx}_k \quad \text{for } k = 1 : P \tag{5}$$

$$\rho_z = \min \left| \frac{\mathrm{Influx}_k - \sum_{i=1}^{z-1} \nu_{i,k}\rho_i}{\nu_{z,k}} \right| \quad \text{for } k = 1 : P \tag{6}$$

2.3. *Integrated co-digestion model*

The different models integrated in GISCOD are written in C and compiled in Matlab as MEX S-functions to run simulations and optimizations 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 to the co-digestion models are read from the Excel file into the Matlab work space using an automated Matlab script. The simulation starts from Simulink after configuring the numerical solution using any variable step solver that is available in Simulink. Fig. 1 shows the scheme of GISCOD in Matlab-Simulink. Practical characteristics and flows of each solid waste are inputs 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. 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 mixing patterns) in addition to the time of 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

Table 1 – Calculated transformation and composition matrices of the transformer model.

	k	1	2	3	4	5	6	7	8	9	10	11	12	18	21	23	24	25	33	34	35	36	37	38	39
	components	CODp	DODs-VFA	VFA	TOC	Norg	TAN	TP-orthoP	orthoP	TIC	Scat	FS	S_{su}	S_{ac}	X_{I}	X_{ch}	X_{pr}	X_{li}	S_{cat}	S_{an}	S_{ic}	S_{ip}	S_{O-h}	S_{H+}	S_{an}
		(gCOD m^{-3})	(gCOD m^{-3})	(gCOD m^{-3})	(gC m^{-3})	(gN m^{-3})	(gN m^{-3})	(gP m^{-3})	(gP m^{-3})	(mol HCO_3^- m^{-3})	(eq m^{-3})	(g m^{-3})	(kgCOD m^{-3})	(kgCOD m^{-3})	(kgCOD m^{-3})	(kgCOD m^{-3})	(kgCOD m^{-3})	(kgCOD m^{-3})	(kmole m^{-3})	(kmoleN m^{-3})	(kmoleC m^{-3})	(kmolP m^{-3})	(kmole m^{-3})	kmole	(kmole m^{-3})
j	Conversion to																								
1	ammonia						-1													7.14E-05				-5.55E-20	-4.16E-20
2	bicarbonate									-1											1.00E-03				
3	ortho phosphate								-1													3.17E-05	5.43E-07	-3.23E-05	5.43E-07
4	cations										-1								0.001						
5	VFA			-1	-0.375001									0.001							1.00E-10		-7.50E-11	-2.50E-11	-5.00E-11
6	Sugars		-1		-0.375								0.001								-1.07E-18		8.07E-19	2.80E-19	5.47E-19
7	lipids	-6.457862			-2.712302			-1										0.006458					9.75E-06	-2.86E-05	-3.83E-05
8	proteins	-6.857143			-2.57143	-1											0.006857				1.00E-10		1.79E-05	5.36E-05	3.57E-05
9	carbohydrates	-1			-0.375											0.001					1.07E-18		-8.05E-19	-2.68E-19	-5.37E-19
10	organic inerts	-0.990616			-0.40463	-0.055921		-0.006388				-1			0.000991					-1.09E-07	2.85E-07	3.71E-12	-1.01E-06	-2.09E-12	8.18E-07
composition matrix	i_ThOD (gThOD/stoich.unit)	1.000	1.000	1.0000									1000	1000.0000	1000	1000	1000	1000							
	i_C (gC/stoich.unit)				1.000					12.00			375	375.0000	403.973398	375	375	420			12000				
	i_N (gN/stoich.unit)					1.00	1.00								56.3753997		145.833333			14000					
	i_O (gO/stoich.unit)	0.417	0.500	0.5000				2.07	2.07	48.00			500	500.0000	481.150513	416.666667	250	640			48000	64000	64000		
	i_H (gH/stoich.unit)	0.052	0.063	0.0469		0.14	0.29	0.03		1.00			62.5	46.8750	61.5254609	52.0833333	62.5	60		4000	1000	1000	1000	1000	
	i_P (gP/stoich.unit)							1.00	1.00						6.44793374			154.35				31500			
	i_Ch (Ch/stoich.unit)			-0.0156			0.07	-0.03	-0.10	-1.00	1.00			-15.6250				-5	1000	1000	-1000	-2000	-1000	1000	-1000
	i_Covalent Bond (Bond/stoich.unit)	-0.125	-0.125	-0.1250	0.333	-0.07		-0.03																	
	Total mass/stoich.unit											1			1009.47271										
																			Source sink components of consequently:		N	C	P	O	H	Ch

both waste streams. In the ADM1 node, non-hydrolyzed portions are not subject again to the hydrolysis kinetics and the hydrolysis in the ADM1 node is 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. The ADM1 is solved at each time step and the output is stored in the Matlab workspace. The chemical equilibrium is solved in the ADM1 model node and the evaluated ions and pH are shared with the hydrolysis nodes. The pH calculation is linked to the hydrolysis nodes to allow future extension of the hydrolysis kinetics to reflect the pH dependency of the hydrolysis. Although the optimal pH of methanogenesis is around pH 7.0, the optimum pH of hydrolysis and acidogenesis is between pH 5.5 and 6.5 (Ward et al., 2008).

2.4. *Calibration and optimization case study*

GISCOD robustness and simulation speed were tested by running the model in 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 of digesting manure alone and manure with kitchen waste were performed to calibrate the hydrolysis parameters for each waste. Both waste average characteristics are listed in Table 2. Only the indicated 11 characteristics are needed as model inputs. It was not possible to digest food waste alone due to acidification and pH drop. 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 rates, which were varied for each experiment according to the profiles shown in Fig. 2. The reactors for both experiments were completely mixed and arranged to have a hydrolysis step of 0.6 L volume followed by a digestion step of 2 L. All reactors were kept at 35 °C. The gas production from both steps was used for calibration. First, the manure hydrolysis parameters were estimated from the manure only digestion experiment. Secondly, 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. The lipids content was determined by a Soxhlet method using petroleum ether for extraction.

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

Table 2 – 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 $\pm$ 428	153400 $\pm$ 11180
Protein		(g m^{-3})	4069 $\pm$ 367	85800 $\pm$ 8320
Lipids		(g m^{-3})	306 $\pm$ 61.2	20800 $\pm$ 2860

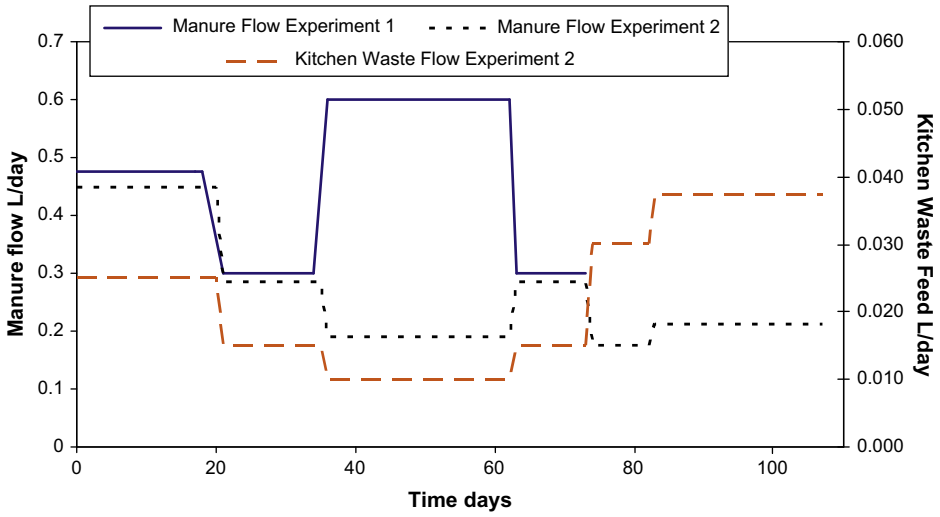

Fig. 2 – Daily feed rates implemented in the calibration experiments.

3. Results and discussion

3.1. *Transformer output*

Among other ADM1 input state variables, carbohydrates, proteins and lipids were estimated in COD units by the transformer model. The ADM1 model uses COD units for organic components and bacterial species to maintain the COD balance. The corresponding g/L concentration was evaluated according to the defined composition of ADM1 components in Table 1 and compared to the measured concentrations in Fig. 3. Generally, the estimated and measured concentrations were consistent in terms of distribution among the three main particulate components. However, some differences could be observed for each individual component when comparing the results for the manure and kitchen waste.

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, which is 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 introduced an error to the carbon balance kept within the model. Therefore, using the transformer model was necessary to keep the carbon balance.

Proteins: Measured and estimated protein contents were more consistent in the case of kitchen waste as compared to the case of 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 solids wastes is mainly sourced by the particulate proteins. The use of the transformer model maintained the nitrogen balance.

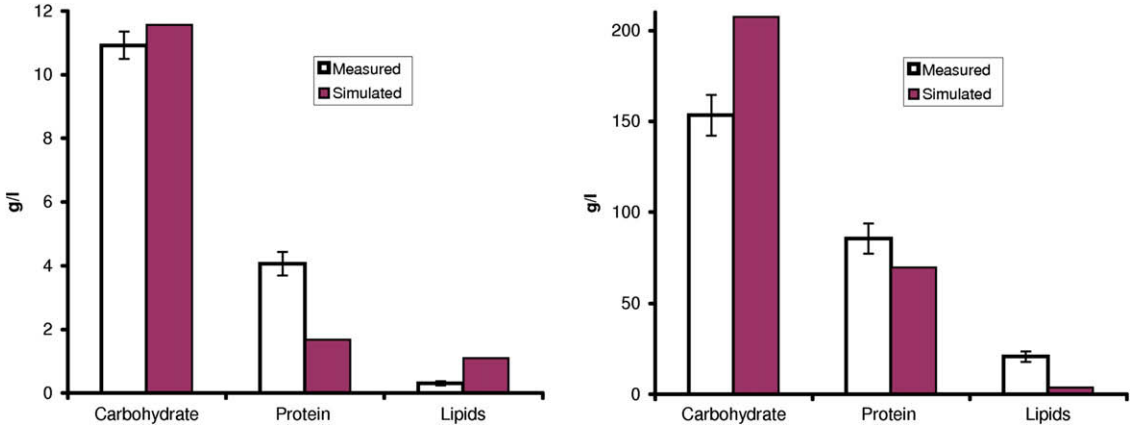

Fig. 3 – Comparison of the measured and the estimated compositions by the transformer model for diluted manure (left) and kitchen waste (right).

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 lipids composition was assumed to be in the form of phospholipids but other forms may exist in both wastes. On the other hand, Soxhlet extraction 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; Yen and Brune, 2007; Zhang et al., 2008; Shanmugam and Horan, 2009). Also, the C and N elemental continuity preserved in the GISCOD model is important when linking the AD model to other existing models of subsequent unit processes or for integrated assessment. For instance elemental continuity is the key mechanism 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 further assessment of subsequent unit processes, such as emission studies from composting (Paillat et al., 2005; Komilis and Ham, 2006), drying (Deng et al., 2009) and landfill facilities (He et al., 2006). Furthermore, estimation of the pH and NH_4^+ as well as phosphorus—evaluated from the mass balance in the transformer model—allows more integrated assessment, such as 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).

3.2. Simulation speed

The simulation speed was kept low despite the added model complexity of separate hydrolysis and transformation model nodes. The 73 days simulation of manure digestion required less than 1 min CPU-time using the ode15s solver in Simulink with 1E-7 and 1E-6 relative and absolute tolerance, respectively. The longer and more dynamic experiment no. 2 of co-digestion required 1 min 30 s CPU-time using the same simulation settings using a standard 3 GHz PC. The efficient simulation time was achieved because of the separate algebraic solution of the chemical equilibrium. The maintenance of COD and elemental mass balances using the transformer contributes to the simulation accuracy, which also contributes to improved simulation speed.

3.3. Calibration of hydrolysis kinetics

With the reliable simulation speed, it was possible to run the model using the simplex optimization algorithm for calibration purposes. Fig. 4 shows the predictions of biogas flow rate after model calibration, which are comparable to the measurements. The hydrolysis rates of carbohydrates, proteins and lipids were estimated by fitting the biogas measurements from experiment 1, digesting diluted manure only. The estimated rates were 0.019, 0.025, 0.022 d^{-1}, respectively, for diluted manure waste. These rates are considerably lower compared to the default values of ADM1 (10 d^{-1} 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 (rate $k_{dis} = 0.5$). It is noteworthy that the default hydrolysis rates presented in the ADM1 in 2002 is now considered to be at least a factor of ten too large also by the ADM1 Task Group (Batstone, 2008: personal communication). 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. When the diluted manure was co-digested with kitchen waste the biogas production was significantly increased even at periods of similar HRT in both experiments, i.e. day 0 to 38 and day 63 to 73. The higher biogas production was not only due to the higher COD load of added kitchen waste but also because the particulate fractions of the kitchen waste were easily hydrolysable. The estimated hydrolysis rates of the kitchen waste from the second experiment were 5.22, 1.86 and 1.24 d^{-1} for carbohydrates, proteins and lipids, respectively. This indicates the necessity of separating the hydrolysis of both wastes. In a similar co-digestion study of a fixed ratio 80:20 manure liquids to cow fodder (Lübken et al., 2007), the best ADM1 simulation of biogas

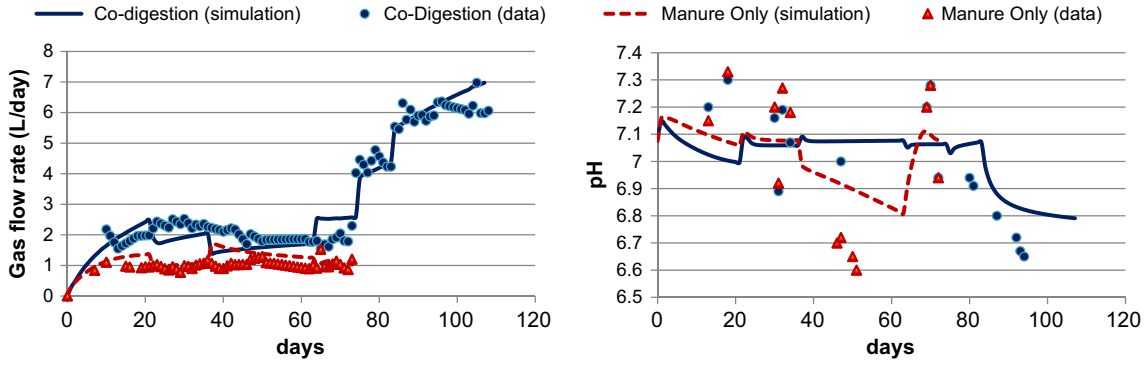

Fig. 4 – Comparison of simulated and measured biogas production (left) and pH (right) after calibration of the hydrolysis parameters.

prediction matched the experimental data at 0.3 d^{-1} 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. 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 each particulate fraction. Expanding the applicability of GISCOD to any waste combinations allows the integrated assessment of AD using different treatment scenarios. For instance, accurate evaluation of the biogas production co-digesting energy crops, agricultural residues and wastes would benefit LCA studies of alternative processes for bio-fuel production (Tan et al., 2004) adding the AD process to the complete process train.

3.4. *Simulation of chemical equilibrium*

The pH, presented in Fig. 4, was slightly higher during manure only digestion in Experiment 1 indicating that manure has higher alkalinity than kitchen waste. During overload periods, hydraulically during manure only digestion from day 34 to day 63 and organically by increasing the food waste ratio from day 84 till the end of the co-digestion experiment, the pH dropped rapidly but the biogas production increased. During process overloads, VFA's accumulate causing the pH to drop (Zaher et al., 2004). The drop of the pH is caused by stripping of alkalinity and higher CO_2 production in the biogas.

3.5. *Optimization of reactor design and operation*

The 200,000 days of virtual experimental time were simulated using GISCOD in 8 h of CPU-time to find the optimal operation for the co-digestion case study. Fig. 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 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. 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 started 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. Also, at 10 days HRT and an addition of kitchen waste >80%, pH dropped and VFA accumulated. During VFA accumulation and pH drop, methanogenesis was completely inhibited and biogas was mainly CO_2. Methane and total biogas production increased with the additional kitchen waste except at low HRT where the manure alkalinity could not maintain the pH in the optimal range.

The GISCOD simulated different feedstock and influent flow rates using two digester volumes 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 result can then be validated experimentally before full-scale implementation in a relatively short time. More generally, the model determines virtually the optimal design and operation as well as digester outputs that 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 that sometimes lead to severe problems. Steyer et al. (2006) illustrated the severe consequences of using such "heuristic" approaches to make operation decisions on full-scale biogas plants. They gave a real example of a biogas plant co-digesting pig manure and industrial wastewater in Blaabjerg, Denmark that experienced a serious accident due to an overdose of the industrial waste. The consequence of such single event was the significant reduction of bio-gas production and methane content. The process did not recover for 3 months and the biogas had to be

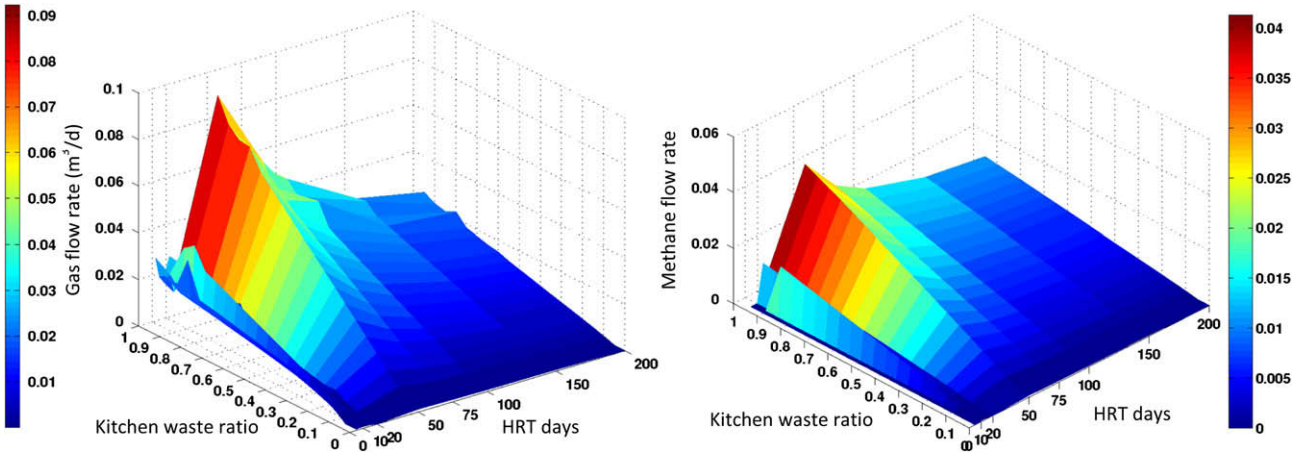

Fig. 5 – Biogas optimization results of manure and kitchen wastes co-digestion varying feedstock, flow and methanogenic volume.

flared instead of being used for power generation. The total operational loss was subsequently calculated as one million DKK (approximately US$150,000). Such example illustrates the benefit of the developed model as an optimization and decision support tool in addition to its potential application for the integrated assessment and LCA of AD applications for waste stabilization and power generation.

4. Conclusions

Feeding the digester with a combination of waste streams introduces complexities in waste characterization that requires the General Integrated Solid Waste Co-digestion (GISCOD) model to simulate improvement mechanisms of co-digestion. Maintaining the continuity of macronutrients, COD and charge during waste characterization was necessary to accurately estimate the input to the International Water Association Anaerobic Digestion Model No.1 (ADM1). In the detailed input required for ADM1, particulate components of carbohydrates, proteins and lipids vary dynamically in combined solid waste streams. Such waste heterogeneity could be resolved by applying a general transformer model to interface the ADM1 to practical characteristics of each waste stream. In co-digestion applications, it is important to consider separate hydrolysis rates for each particulate component from each waste stream. The presented case study of food waste and manure co-digestion showed that hydrolysis rates vary significantly. 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 wastes hydrolysis allowed the optimization of biogas production and defined the corresponding operation settings of the digester. Therefore, the GISCOD or a similar modeling approach would support the operation decision of digesting trucked-in wastes with wastewater sludge or, generally, optimize the feedstock and operation of biogas plants.

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