Modeling Approaches of Biogas Production

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Biogas production is a relevant component in renewable energy systems. Model approaches of biogas production show different levels of detail. They can be classified as white, gray, and black box, or bottom-up and top-down approaches. On the one hand, biogas modeling can supply dynamic information on the anaerobic digestion process, e.g., to predict biogas yields or to optimize the anaerobic digestion process. These models are characterized by a bottom-up approach with different levels of detail: the comprehensive ADM1 (white box), simplifications and abstractions of AD models (gray box), or highly simplified process descriptions (black box). On the other hand, biogas production is included in energy system models. These models usually supply aggregated information on regional biogas potentials and greenhouse gas emissions. They are characterized by a top-down approach with a low level of detail. Most energy system models reported in literature are based on black box approaches. Considering the strengths and weaknesses of the integration of detailed and deeply investigated process models in energy system models reveals the opportunity to develop dynamic and fluctuating business models of biogas usage.

biogasmodelinganaerobic digestionenergy systemgeoinformation systemGISlife cycle assessmentLCAgreenhouse gas emissions

1. Introduction

Biogas is a relevant component of an increasingly renewable energy system in many countries. Biogas plants feature some specific properties compared to other renewable energy plants such as flexible provision of electricity and heat by gas storage, or possible contribution of energy to the transport sector.

With anaerobic digestion (AD), the main transformation process from organic matter to biogas is a biological one. The complex processes of hydrolysis, acidogenesis, acetogenesis, and methanogenesis are well known and described ^[1]. AD works with various types of organic feedstock, such as municipal sludge from wastewater treatment plants, municipal solid waste, animal waste, algae, or energy crops. Some of those are constantly available, while others are subject to regional and seasonal restrictions. Main product of the anaerobic digestion is biogas, primarily methane and carbon dioxide (CO_2). The side product is a nutrient-rich digestate. Biogas can be converted to different energy products, such as heat (by combustion), electricity and heat (combined heat and power plant: CHP), electricity (by turbines), natural gas (by the separation of CO_2), or fuels (e.g., by increasing the methane fraction or CO_2 -assisted catalytic reforming) ^[2]. A common pathway for the energetic use of biogas is electricity and heat production in a CHP. The focus in many countries lies on the production of electricity. In Germany, for instance, the privileged feed-in of renewable electricity from biogas CHPs is regulated by the Renewable Energy Act ^[3]. In comparison to other renewable energy sources, electricity production from biogas is not weather-dependent. Biogas plants can produce

electricity flexibly according to demand, by utilizing the possibility of storing feedstock and biogas ^[4]. This provides a distinguished role for biogas plants in the energy sector. Furthermore, biogas can also participate in the supply of heat and fuel where the share of renewable energies, for example, in Germany, it is much lower than for electricity. The shares of renewable energies for electricity, heat, and transport in Germany in 2019 were 37.8, 13.9, and 5.6%, respectively ^[5].

Biogas plant operation needs continuous monitoring and process control because the AD process is based on microbiological activities that require a complex biocenosis of different microorganisms. This is where process modeling comes into focus.

Biogas process modeling was originally developed for the prediction of possible biogas yields and optimization of the AD process (e.g., ^{[6][7][8]}), as well as for process control and staff training (e.g., ^{[9][10]}). Those models—often assigned to the water sector—focus on a very detailed description of microbiological transformation. Early papers on AD modeling, for instance, go back to the 1970s ^{[11][12][13]}. Since 2002, the anaerobic digestion model (ADM1) has been a commonly used tool to model physical and biological processes within biogas fermenters.

Biogas plants in energy systems are mostly investigated from an agricultural or energy economical point of view. Energy system modeling often regards biogas plants as black box models. They basically tend to be included as gas storage combined with a CHP unit (e.g., ^[14]). The modeling of biogas plants within future energy systems with high shares of renewable energies needs to look further into the biological process, though, in order to answer new questions due to the dynamic nature of energy supply and demand, such as:

-How can electricity productionbe adjusted to electricity demand profiles?

-How can biogas plants contribute to energy sector coupling?

-Which pathway of biogas exploitation is most beneficial for the energy system?

-Which pathway of biogas exploitation offers a business model for the operator?

Goal of the transition from fossil to renewable energies is the decarbonization of the energy sector, which aims to address the question of the environmental impact of biogas plants, i.e., their carbon footprint (e.g., ^[15]). Renewable energy production is often much more decentralized than fossil energy production. Biogas production is widely applied in rural areas. This also poses new questions, such as:

-What is the carbon footprint of biogas-based energy products?

-What feedstock mixture is most sustainable and are there regional limitations?

-How can biogas plants be included in regional energy systems?

Such regional aspects of substrate availability and energy-related infrastructure are commonly modeled with geoinformation systems (GIS; e.g., ^[16]).

The integration of biogas plants in energy systems thus links water or agricultural economies with the energy economy. This requires information transfer between the different sectors. Figure 1 shows possible system boundaries for different views on biogas plants from energy systems to microbiological processes in the AD process.



Figure 1. System boundaries for different views on biogas plants.

2. Biogas Plants in Renewable Energy Systems

Substantial research and development of models for biogas production was carried out in the last 18 years. Regarding biogas modeling on a process level (anaerobic digestion), these models differ substantially from modeling biogas for potential analysis, GHG emissions and in an energy system. This is reflected in Table 1 and Table 2: Table 2 (top-down) contains biogas model on process level that are not reflected in Table 1 (bottom-up) with models of potential analysis, GHG emissions and energy systems. This different modeling approach of the energy system and the AD perspective can broadly be regarded as top-down and bottom-up approaches, respectively.

Dynamic biogas models contain detailed information about AD processes, technical systems and time-dependent conditions and, thus, generate a complexity that is not to be disregarded. This bottom-up modeling approach differs from the top-down modeling approach used in energy systems, LCA and GIS models. In these models, holistic effects are modeled on a national or regional level ^[17].

Figure 2 shows the complexity of the mathematical mapping of biogas production within the discipline or view on the biogas system that the different studies represent.

		white box	gray box	black box
	ъя			[47] [14] [39]
	nerg /stei			[44] [40]
	s) ei			[46] [41]
им	ial ial			[58] [16]
-do	gion			[59] [56]
top	po			[57]
	gas			[15]
	reer		[24]	[68] [64]
	g hou			[69] [65]
	s J	[92]	[97,98] [102]	[113]
	bioga contre	[10]	[9,106,107]	[114,115]
		[91]	[100]	
dn-	y ion	[84]	[101] [100] [102]	[113]
tom	herg	[86] [10]	[97,98] [104]	
bot	eı	[91]	[99]	[114,115]
	SS	[77] [79] [81]	[8] [103]	[109]
	AD oce	[76] [80] [78] [82]	[95]	[111] [110]
	ц	[31] [75] [90]	[105]	

Figure 2. Classification of the references regarding their respective level of detail and field of application.

Table 1. Biogas top-down modeling (energy systems, regional impact, greenhouse gas (GHG) emission).

Ref.	View on Biogas Plants	Coding/Software	Biomass Modeling	Region	Additional Modeling
[<u>18</u>]	energy system	oemof ^[19]	annual chemical biogas potential	northwestern Germany	time-dependent electricity production (wind and photovoltaic) and demand
[20]	energy system	oemof ^[19]	annual chemical biogas potential	northwestern Germany	time-dependent electricity production (wind and photovoltaic) and demand
[21]	energy system	Engineering Equation Solver [22]	daily chemical biogas potential based on chicken manure and maize silage	-	electrical energy production (wind, photovoltaic), thermal energy production (photovoltaic), chemical energy production (hydrogen), electrical and thermal energy storage
[23]	energy system	Balmorel ^[24] linear optimization (CPLEX-solver)	annual energy potential (stable and increasing 1.3% per year)	Denmark, Germany, Finland, Norway, Sweden	different waste to energy technologies (e.g., gasification, co-combustion) and other technologies (e.g., heater, steam turbine), all with fixed efficiencies
[<u>14]</u>	energy system	EnergyPLAN ^[25]	annual chemical biomass potential	Denmark	electrical energy production (wind, photovoltaic, wave, CHP, power plants), biogas purification
[<u>26</u>]	energy system	Sifre	annual energy potential of manure	Danish municipality	-

Re	View on f. Biogas Plants	Coding/Software	Biomass Modeling	Region	Additional Modeling	_
			and straw			
[27	g energy system	TIMES	annual energy potential of degradable feedstock	Ireland	-	_
[<u>16</u>	j regional potential	-	electrical energy potential of manure	Northwestern Portugal	-	
[28	regional potential	-	sectoral biogas potential of manure (cattle, pigs, sheep, poultry)	Greece	chronological sequence since 1970; contemplation of regional gas grid	⊐en y system
[29] regional potential	-	time-dependent (seasons) biogas potential of agricultural residues and municipal waste	Croatia	residue-to-product ratios, sustainable removal rates	/ supply
[30] regional potential	-	methane potential of manure, grass silage, municipal waste	Finland	Maximum feasible use of regional feedstock due to 30-day HRT; optimizing GHG emissions	bruary
[<u>31</u>	j regional potential	-	municipal waste, sludge, manure, silage and crop residues	Finland	optimizing biogas plant placing	2011, 36,
[<u>15</u>] GHG emission	GaBi ^[32]	methane yield of maize	Germany	regional methane yield	essed on
[<u>33</u>	g GHG emission	GaBi [<u>32</u>]	methane yield of manure, maize silage and grass silage with different mixture ratios	-	CHP size and efficiency	100% hergy
1] GHG emission	SimaPro ^[35]	methane yield of maize, grass, rye silage, chicken manure	-	demand-oriented energy production by HRT for mass flow calculation in digester	supply Energy
[<u>36</u>	GHG emission	-	mass-specific energy of grass	-	influence of grass treatment	
[<u>37</u>	GHG emission System. Ene	Umberto ergy Policy 2013,	biogas yield of cultivated crops 53, 169–189.	-	emissions of farming, digestion, purification and upgrading to	energy

12. Silva, S.; Alçada-Almeida, L.; Dias, L.C. Multiobjective programming for sizing and locating biogas plants: A model and an application in a region of Portugal. Comput. Oper. Res. 2017, 83, 189–198.

Re	View on Biogas Plants	Coding/Software	Biomass Modeling	Region	Additional Modeling	n: A GIS
1			(maize, triticale, rye, hemp)		biomethane, transportation	sessing
[<u>38</u>]	GHG emission	SimaPro ^[35] MATLAB [®]	dynamic AD model (AMOCO)	Germany	demand-oriented energy production with dynamic AD modeling	al

15. пиорапа, т., зопу, п., којептатен, м., мізка, п. А теуюпа точеног зизгатаре рюдаз

electricity production: A case study from a Finnish province. Appl. Energy 2013, 102, 676–686.

Table 2. Biogas bottom-up modeling (process dynamics)16. Höhn, J.; Lehtonen, E.; Rasi, S.; Rintala, J. A Geographical Information System (GIS) based

Ref.	View on Biogas Plants	AD Model	Coding/Software	Feedstock	Energy Production	Region	Additional Models	'n
[<u>39]</u>	AD process	ADM1: 24 species, 19 reactions	-	-	-	-	physiochemical digester model	ſgy .11
[<u>40</u>]	AD process	ADM1	SIMBA#: C#-based	-	-	-	-	_hea
[<u>41</u>]	AD process	ADM1	SIMBA#	pig manure	-	-	-	12
[<u>42</u>]	AD process	ADM1	AQUASIM: C++-based	-	-	-	-	nei
[<u>43</u>]	AD process	ADM1	AQUASIM	sludge	-	-	-	ech
[<u>44</u>]	AD process	ADM1	AQUASIM	water thyme	-	-	-	
[<u>45]</u>	AD process	ADM1	MATLAB [®] Simulink-code: C-based S- Function	-	-	-	-	ren 1 -25
[<u>46</u>]	AD process	ADM1	ADMS 1.0: Python GUI and MATLAB [®] ADM1	-	-	-	-	ma
[<u>47</u>]	AD process	ADM1	MATLAB [®] -code	-	-	-	-	
[<u>48]</u>	AD process	ADM1	BioOptim ^[9]	bio waste	-	-	-	ität
[<u>8]</u>	AD process	modified ADM1	MATLAB [®] Simulink	pig manure & glycerin	-	-	-	lode

1 (ADM1); IWA Publishing: London, UK, 2002; ISBN 9781780403052.

26. ifak—Institut für Automation und Kommunikation. SIMBA#Biogas. Available online: (accessed on 10 February 2021).

2	Ref.	View on Biogas Plants	AD Model	Coding/Software	Feedstock	Energy Production	Region	Additional Models	ır
2	[<u>49</u>]	AD process	2 species, 2 reactions	MATLAB [®] Simulink	maize silage	-	-	-	
2	[<u>50</u>]	AD process	1 reaction	not known	manure	-	-	heat flow, thermodynamics of digester	jester 1545.
3	[<u>51</u>]	AD process	13 species, 10 reactions	MATLAB®	fictive waste composition	-	-	heat flow, thermodynamics of digester	deling o , 211,
3	[<u>52</u>]	AD process	ANN: one specific digester	MATLAB®	agricultural waste (landfill)	-	-	-	partmen
3	[<u>53]</u>	AD process	ANN: 25 digesters	NeuroSolutions [®]	manure, banana stem, sawdust	-	-	-	es:
3	[<u>54</u>]	AD process	ANN of ADM1	MATLAB [®] : ADM1 and Python: ANN	fictive (result of ADM1)	-	-	-	115. :r'S
3	[<u>55</u>]	energy production	ADM1	MATLAB [®] Simulink	manure	electricity (micro gas turbine)	-	power electronics of micro gas turbine	vailable
3	[<u>56</u>]	energy production	ADM1	MATLAB [®] Simulink	Multiple	electricity (CHP)		thermodynamics of digester	CProc.
, CJ (J)	[<u>57]</u>	energy production	4 species, 4 reactions	MATLAB [®] Simulink	manure	electricity (micro gas turbine)	-	synchronous electrical generator of micro gas turbine, gas storage, thermodynamics of digester)lant for
J								heat storage	_
3	[<u>58</u>]	energy production	1 reaction	MATLAB [®] Simulink	household garbage	electricity (CHP), heat	domestic use profile (China)	(water tank), electrical gas compressor, gas storage, battery (buffer)	cts.
4	[<u>59</u>]	energy production	1 time- dependent	MATLAB [®] Simulink	manure	electricity (CHP)	-	gas storage	from a

54, 359–363.

41. Gueguim Kana, E.B.; Oloke, J.K.; Lateef, A.; Adesiyan, M.O. Modeling and optimization of biogas production on saw dust and other co-substrates using Artificial Neural network and Genetic Algorithm. Renew. Energy 2012, 46, 276–281.

4	Ref.	View on Biogas Plants	AD Model	Coding/Software	Feedstock	Energy Production	Region	Additional Models	lles .4–15
-			function						Vienna
4	[<u>10]</u>	biogas control	ADM1	BioOptim: MATLAB [®] Simulink	-	electricity (CHP)	-	digestate storage, pumps, heating system, energy sinks and sources	f an st. Educ
4	[<u>60</u>]	biogas control	ADM1	DyBiM: MATLAB [®] Simulink	grass silage, cattle manure, agricultural substrates	electricity (CHP)	Sweden	gas storage	Energy hviron.
4	[<u>61</u>]	biogas control	ADM1	MATLAB®	maize silage, rye, triticale, sugar beets, potato pieces, potato peel	-	Germany	PI controller	em. Int.
4	[<u>9]</u> [<u>62]</u> [<u>63]</u>	biogas control	13 equations, 2 reactions	FORTRAN and WinErs for GUI and automation	-	-	-	tanks, valves, pumps	Plant of the _4
4	[<u>64]</u> [<u>65]</u>	biogas control	ADM1 simplification [66]	not known	not known	electricity (CHP)	Germany (EPEX)	gas storage	ation. In
4	[<u>67</u>]	biogas control	linear equation	HOMER®	undifferentiated	electricity (CHP, photovoltaic, fuel cell)	India (off-grid)	heat storage, energy storage (battery)	l 2011. rom
5	[<u>68]</u>	biogas control	1 species, 1 reaction	MATLAB [®] and Microsoft Excel [®]	maize silage, grass silage, manure	electricity (CHP), fuel (CNG)	Germany (EPEX)	biogas to CNG upgrade plant (black box), vehicle fleet	ol for a 19, 42,
5	[<u>69</u>]	biogas control	none	RedSim	fixed gas characteristics	electricity (CHP)	Germany (spot market)	gas storage (mass balance)	Thesis,
5	[<u>70]</u> [<u>71</u>]	biogas control	none	IPSEpro®	real data gas characteristics	electricity (CHP), fuel (methane)	-	gas storage, heat storage, tanks, gas upgrade (black box)	ration. Ir

Proceedings of the IV CMP International Conference on Monitoring & Process Control of Anaerobic Digestion Plants, Leipzig, Germany, 26–27 March 2019.

54. Mauky, E.; Weinrich, S.; Nägele, H.-J.; Jacobi, H.F.; Liebetrau, J.; Nelles, M. Model Predictive Control for Demand-Driven Biogas Production in Full Scale. Chem. Eng. Technol. 2016, 39, 652– 664. 58aN/eindids, Se Provisionable Medellierung von Piogaseriagenden genden genden genden and applied set in the setual. The setual and in the dellierung von the setual and source code, allowing great transparency of their results. In addition to complex AD process modeling, simplified AD models have been developed and applied many times. These are based partly on the setual and transmitted renewable energy system for rural electrification in india using photovoltates and use of AD models with less parameter input compared to ADM1. On a low-detail level (black box), ANNs were used for an acrobic digestion. Renew. Energy 2015, 74, 390–398. different types of problem description: Modeling the behavior of a specific plant, different feedstock conditions, or generating 57 back goz models with the dep of the behavior of a specific plant, different feedstock conditions, or generating applied for the set of the set of both highly detailed and highly abstracted models, including the thermal behavior of 589 Proceeds in terms of both highly detailed and highly abstracted models, including the thermal behavior of signification for the set of the set of

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