

Supporting Information for A Review of Anaerobic Digestion Process Models for Organic Solid Waste Treatment with a Focus on C, N, and P Fates

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Table S1. Code List of target variables related to modeling objects

No.	Target variables related to modeling objects	Description
1	CH ₄	Methane
2	NH ₄ ⁺ – N	Ammonium Nitrogen
3	TAN	Total Ammonium Nitrogen
4	COD	Chemical Oxygen Demand
5	NH ₃	Ammonia
6	CO ₂	Carbon Dioxide
7	ON	Organic Nitrogen
8	TOC	Total Organic Carbon
9	TP	Total phosphorus

Table S2. Code List of Mechanistic Model types

NO.	Mechanistic model types	Description
1	ADM1	Anaerobic Digestion Model No.1
2	CMB	Carbon Mass Balance
3	FOK	First-order Kinetic Model
4	M-ADM1	Modified Anaerobic Digestion Model No.1
5	MB	Mass Balance Model

Table S3. Code List of Emperical Model types

NO.	Emperical model types	Description
1	FOK	First-order Kinetic Model
2	MFOK	Modified First-order Kinetic Model
	GM	Gompertz Model
3	MGM	Modified Gompertz Model
4	MRG	Modified product generation model of Romero Garc ía Model
5	KD	Koch and Drewes Model
6	NC	Numerical Calculations
7	ETK	Exponential Two-phase Kinetic Model
8	LN	Log-normal Model
9	LL	Log-logistic Model
10	WM	Weibull Model
11	CHM	Chen & Hashimoto Model
12	LM	Logistic Model
13	VTD	Variable Time Dependency Model
14	TCFO	Two Combined First Order Model
15	MT	Monod Type Model
16	QMT	Quadratic Monod Type Model

Table S4. Code List of Statistical Models model types

NO.	Statistical model types	Description
1	LR	Line Regression Model
2	FR	Fuzzy network model Regression Model
3	MR	Multiple Regression Model
4	PLS	Partial Least Squares Regression Model
5	QR	Quadratic Regression Models
6	RSM	Response Surface Methodology
7	ANN	Artificial Neural Networks Model
8	GA-ANN	Genetic Algorithm Artificial Neural Networks
9	PC-ANN	Principal Component Analysis Artificial Neural Networks
10	ANFIS	An Adaptive Neuro-fuzzy Interference System
11	MLR	Multiple Linear Regression
12	FNN	Fuzzy Neural Networks Model
13	RF	Random Forest
14	GLMNET	Logistic Regression Multiclass
15	SVM	Support Vector Machines
16	KNN	K-nearest Neighbors
17	EN	Elastic Net
18	CEF	Critical exponential function
19	RHF	Rectangular hyperbola function
20	FF	Fourier function
21	BN	Bayesian network model
22	RM	Regression model
23	RBNN	Radial basis functional neural network model
24	BPNN	Backpropagation neural network model

Table S5. Code List of applied scales types

NO.	Applied environment types	Description
1	LS	Lab scale
2	IpS	Industrial plant scale
3	FmS	Farm scale

Table S6. Summary of 52 models

No.	Types	Applied/modeling Environment	Characteristics and Features	Target variables related to modeling objects	References
1	ADM1	LS	The aim of this study was to implement ADM1xp model to simulate behavior of anaerobic co-digestion of maize silage and cattle manure. The accuracy of ADM1xp has been assessed against experimental data of anaerobic digestion.	CH ₄	Bułkowska et al., 2015; Klimiuk et al., 2015
2	CMB	IpS	Simulation of methane and NH ₄ ⁺ -N during AD of seaweed, vegetable waste and fishery	CH ₄ and NH ₄ ⁺ – N	Kuroda et al., 2014
3	ADM1, Angelida ki, DBFZ, and FOK	LS	Depending on the type and number of the required components, it can be shown that in comparison to the complex Anaerobic Digestion Model No. 1 (ADM1) different simplified model structures can describe the gas production rate, ammonia nitrogen and acetate concentration or pH value equally well.	CH ₄ and TAN	Weinrich and Nelles, 2015
4	M-ADM1	LS	In this study, a novel ADM1-based model was developed to simulate the solids and reactor mass/volume dynamics of a homogeneous High-solids reactor.	CH ₄ and NH ₄ ⁺ – N	Pastor-Poquet et al., 2018
5	M-ADM1	LS	In this study a mathematical model which has been improved by adding inorganic components and integrating the inhibition of high TS and liquid-solids processes was developed to simulate the performance and fate of carbon (C), nitrogen (N) and phosphorus (P) in wet and high total solids (TS) anaerobic digestion (AD) processes.	CH ₄ , COD and NH ₄ ⁺ – N	Li et al., 2020
6	M-ADM1	LS	The ADM1 was modified by improving the biochemical framework and integrating a more detailed physicochemical framework. Inorganic carbon and nitrogen balance terminology was introduced to address the discrepancy between carbon and nitrogen content in degradants and	CH ₄ , NH ₄ ⁺ – N and NH ₃	Zhang et al., 2015

			substrates in the original biochemical framework.		
7	ADM1	LS and IpS	New parameters were determined for each substrate evaluated and tested against experimental cumulative biogas production results and evaluated against default values of disintegration and hydrolysis kinetic constants for ADM1, where ADM1 values were used for medium temperature high rates and ADM1 values were used for solids. The optimised results lead to accurate predictions of anaerobic degradation kinetics for complex matrices.	CH ₄	Biernacki et al., 2013a; Biernacki et al., 2013b
8	M-ADM1	LS	The modified ADM1 model proposed in this study allowed us to accurately simulate more than 80% of the experimental data for both configurations, including methane production, pH and lactate production.	CH ₄	Parra-Orobio et al., 2020
9	ADM1	IpS	This study shows that the ADM1 model shows a good fit for the plant scale production between the simulated values of biogas, methane effluent and NH ₄ -N	NH ₄ ⁺ – N and CH ₄	Nordlander et al., 2017
10	M-ADM1	FS	An anaerobic digestion model was set up based on Simplified ADM1 and applied to estimate desired methane production in the form of biogas as well as unwanted methane emissions associated with farm-scale digestion of manure.	CH ₄	L.I. Vergote et al., 2019
11	M-ADM1	IpS	The modified ADM1 including lactic acid was applied to a large biogas plant. It was shown that the model could reliably simulate the biogas production and methane content.	CH ₄	Satpathy et al., 2016
12	M-ADM1	IpS	ADM1 was extended to simulate syngas biomethanation from laboratory scale to pilot scale. Data from the pilot-scale reactor were then used for model validation, and the methane yield predictions were in excellent agreement with the measured data.	CH ₄	Sun et al., 2021

13	M-ADM1	LS	In this study, the modified ADM1 simulated methane production in the anaerobic digestion of food waste, and the results showed that the modified ADM1 could predict methane production well.	CH ₄	Zhao et al., 2019
14	DL	LS	This study proposed that mass diffusion limitation due to high TS content may be responsible for the observed decrease in methane production. Based on this hypothesis, a new SS-AD model was developed taking into account mass diffusion limitation and hydrolysis inhibition.	CH ₄	Xu et al., 2014
15	MB	LS	This study presented a novel mathematical model that predicted the output per unit volume of a continuous batch AD process during the start-up phase as well as at steady state.	CH ₄	Keener and Xu, 2019
16	FOK and MFOK	LS	Kinetic models were developed that represent the behavior of hydrolysis and biogas generation more accurately than conventional models. The developed model was evaluated based on experimental data from six intermittent reactors.	CH ₄ and CO ₂	Pham Van et al., 2018a
17	GM	LS	A new kinetic model for biogas production with meaningful constants was developed, and the kinetic constants of the model were determined by applying the least squares fitting method to experimental data.	CH ₄	Pham Van et al., 2018b
18	FOK	LS	Anaerobic digestion of sugarcane straw co-digested with sugarcane filter cake was investigated and intermittent and semi-continuous experiments were performed for kinetic evaluation.	CH ₄	Janke et al., 2017
19	FOK	LS	This study investigated the recovery of ammonia from pig excreta by dry anaerobic digestion (AD) and ammonia vapor extraction. The results showed an extremely strong negative linear	ON	Huang et al., 2016

20	GM	LS	The Gompertz model was used to simulate the volume distribution of methane during co-digestion of poultry litter and wheat straw.	CH ₄	Shen and Zhu, 2016
21	MGM	FmS	The anaerobic digestion characteristics of swine manure at different growth stages were studied and the methane yield was simulated using a modified Gompertz model with errors ranging from 1.1% to 29.6%.	CH ₄	Zhang et al., 2014
22	MG	LS	The kinetic parameters of the biodegradation reaction were calculated during rice straw digestion and showed reasonably good agreement between the experimental and predicted values of the modified gompertz model ($R^2 > 0.98$)	CH ₄	Kainthola et al., 2019
23	MG	LS	The modified Gompertz model was tested to fit the methane production kinetic experimental results of anaerobic digestion of corn stover on biogas production.	CH ₄	Yao et al., 2017
24	MG	LS	Kinetic parameters of leachate and glycerol generation in industrial landfills were simulated using a modified Gompertz model.	CH ₄	Castro et al., 2020
25	MRG	LS	This study presented a modification of an extensively validated kinetic model for product generation. The results obtained from the modified model parameters in the steady indicated that the characteristics of the feedstock significantly influence the kinetics of the process.	CH ₄	Fdez-G üelfo et al., 2012
26	MG, CM, and FOK	LS	Fitting error between measured and predicted total biogas yield from <i>Salvinia molesta</i> and rice straw for 30 days fermentation by using modified Gompertz, Cone, First Order model was 0.96–6.45%, 0.14–3.52%, and 1.97–15.25% respectively.	CH ₄	Syaichurrozi, 2018
27	KD and MGM	LS	The Koch and Drewes model and the modified Gompertz model were applied to evaluate the effects of PDs on	CH ₄	Li et al., 2016

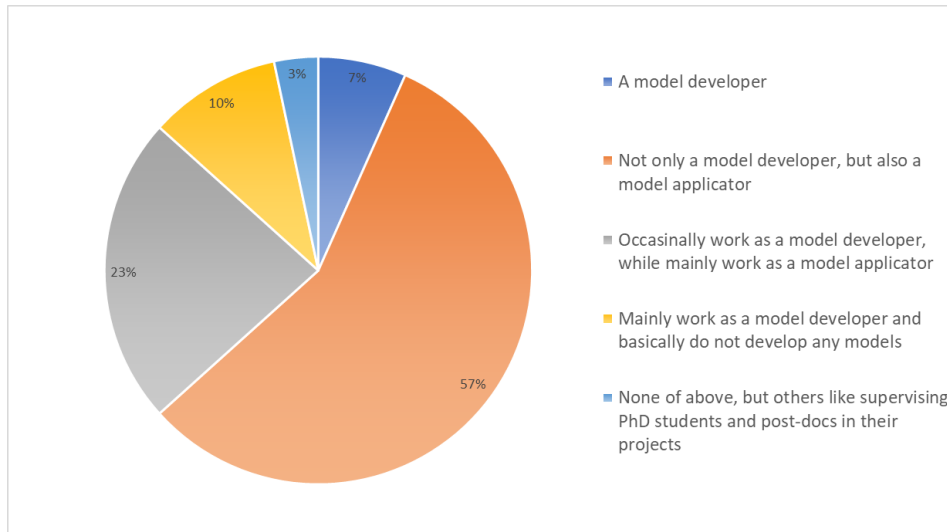
			hydrolysis rate constants, biomethane yield and lag time. The results showed that the methane yield, kitchen waste's organic matter degradation efficiency and hydrolysis rate decreased with increasing pungency degree, while pH and total and free ammonia nitrogen concentrations increased.		
28	MGM and NC	LS	AD experiments for pre-treated wheat straw and pre-digested cow dung were conducted and numerical calculations by using the improved model and the modified Gompertz model have been in full agreement with the experimental observations.	CH ₄	Baitha and Kaushal, 2019
29	MGM and ETK	LS	Methane production from coffee husks was simulated using the Gompertz model and the exponential two-phase kinetic model.	CH ₄	Santos et al., 2018
30	LN, LL,WM and GM	LS	Proportional probability distributions were used to approximate the obtained cumulative methane production curves. The results show that the Gompertz distribution best fit the process.	CH ₄	Piątek et al., 2016
31	FOK, GM AND CHM	LS	Biomethane production was systematically evaluated using bagasse pretreated with liquid hot water , dilute acid and KOH solution. The kinetics of methane production was evaluated with several models, and the Chen & Hashimoto model simulated the biomethane production with the highest accuracy.	CH ₄	Ketsub et al., 2021
32	MGM and LM	LS	In this study, the effects of different substrate mixing ratios of pig manure and rice straw on the AD reaction process were calculated and simulated by a modified Gompertz model and a logistic model.	CH ₄	Zhang et al., 2021
33	FOK, VTD, TCFO, MT,	LS	This study evaluated the ability of several different models to predict final BMP and required degradation time based on data	CH ₄	Strömberg et al., 2015

	QMT, and MGM		from 138 different substrate types tested for BMP.		
34	LR	IpS	C / N and OLR regression optimization models were developed for the AD process of goose manure and wheat straw.	CH ₄	Hassan et al. 2017
35	LR	LS	The methods used in this paper to measure C, N and P distributions and mass balances may be useful in assessing the efficiency of the AD process, optimising methane production and establishing mechanisms for the reuse of digestate. The linear models derived can be used to predict methane production as well as COD, TOC, NH ₄ ⁺ -N and TP concentrations in the supernatant.	CH ₄ , NH ₄ ⁺ - N, COD, TOC and TP	Li et al. 2016b
36	FR	LS	Biogas production during AD of cow manure with co-digested Spent Tea waste was modeled using fuzzy regression and good agreement was found between experimental and predicted data with a coefficient of determination of 0.994.	CH ₄	Khayum et al. 2019
37	MR	IpS	In this study, eight model equations including different combinations of input parameters were analyzed. Based on the results of the regression analysis, the optimal coefficients of the model equations were determined.	CH ₄	Akkaya et al. 2015
38	PLS	LS	In order to be able to make predictions on all substrates, partial least squares (PLS) regression was performed to relate organic nitrogen bioaccessibility indicators to biodegradability. The model successfully predicted the biodegradability of organic nitrogen with a maximum prediction error of 10%.	ON	Bareha et al. 2018

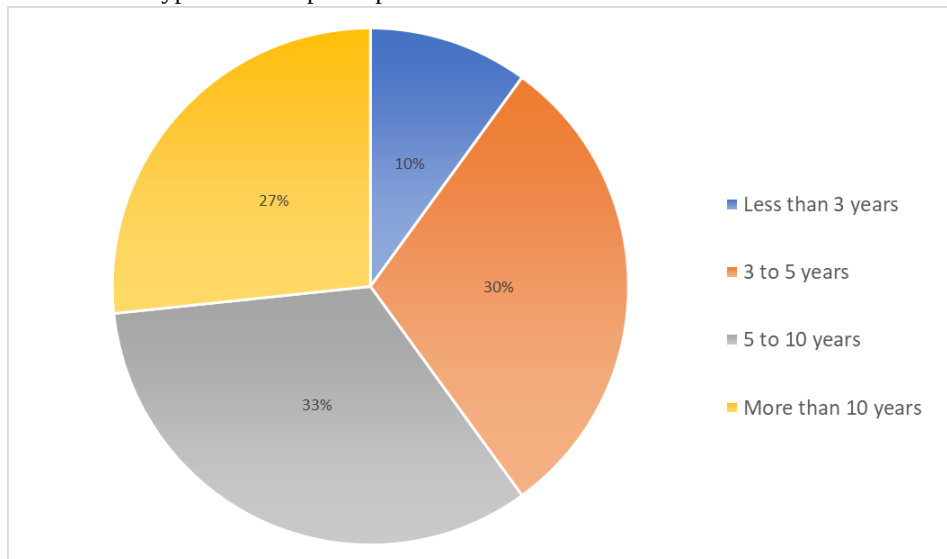
39	QR and RSM	LS	Anaerobic digestion of peanut shells and swine manure was investigated. The interaction effects of total solids percentage (TS%), carbon to nitrogen ratio (C/N ratio) and inoculum percentage (I%) on total biogas production and methane content were evaluated using quadratic regression models and response surface methodology.	CH ₄	Deng et al. 2019
40	ANN	LS	In this study, the performance of a laboratory-scale anaerobic bioreactor was investigated to determine the methane content in biogas production during the digestion of organic matter in municipal solid waste. The experimental results were statistically optimized through the application of an ANN model using free forward-backward propagation in the MATLAB environment.	CH ₄	Nair et al. 2016
41	ANN	IpS	The ANN model developed in this study can satisfactorily predict the volatile solids concentration and methane yield.	CH ₄	Güdü et al. 2011
42	ANN	LS	In this study, an artificial neural network was used as a model for estimating biogas production from a laboratory-scale upflow anaerobic sludge bed (reactor treating cattle manure and simultaneously digesting different organic wastes.	CH ₄	Tufaner et al. 2017
43	GA-ANN	LS	Modeling of the AD process using ANN and GA for the cake of Karanja and cow dung mixture to predict and optimize biogas production.	CH ₄	Barik and Murugan 2015
44	RSM and GA-ANN	LS	A CCD-RSM and ANN coupled with a GA model were used to optimize the process parameters of anaerobic codigestion of potato waste and aquatic weed. After comparing these two optimization techniques, the ANN-GA model obtained by the feed-forward back propagation method was found to be effective.	CH ₄	Jacob and Banerjee 2016

45	ANN and PC-ANN	LS	ANN models based on principal component analysis (PC-ANN) were developed for estimating the fate of C (CH ₄ yields and COD concentrations in the supernatant), showing higher prediction accuracies than the original ANN models. The fate of N (NH ₄ ⁺ -N concentrations in the supernatant) was well predicted by the ANN model with two inputs, namely, total Kjeldahl nitrogen (TKN) and total ammonium nitrogen (TAN) in the substrates.	CH ₄ , NH ₄ ⁺ – N, COD	Li et al. 2016a
46	ANFIS, ANN, and LM	LS	Logistic, ANFIS, and ANN models were employed in modeling the production process of biogas of spent mushroom. ANFIS network accurately predicted the output values of the both thermophilic and mesophilic situations.	CH ₄	Najafi and Faizollahzadeh Ardabili 2018
47	ANN, MLR	LS	In this study, multiple linear regression (MLR) and artificial neural network (ANN) models were explored and validated to predict methane production from lignocellulosic biomass in medium temperature solid state anaerobic digestion (SS-AD) based on feedstock characteristics and process parameters. The ANN model obtained the lowest standard error of prediction	CH ₄	Xu et al. 2014
48	FNN	IpS	This paper presents the development and evaluation of a FNN model for a full-scale anaerobic digestion system to treat paper mill wastewater. From the results, the FNN model can be applied in an anaerobic reactor to predict the biodegradation and biogas production of paper mill wastewater.	CH ₄	Ruan et al. 2017
49	ANFIS	LS	This study focused on the prediction and optimization of biogas production from corn stover cow manure at various total solids (TS), carbon to nitrogen ratio (C/N) and agitation intensity. The ratio between the observed and	CH ₄	Zareei and Khodaei 2017

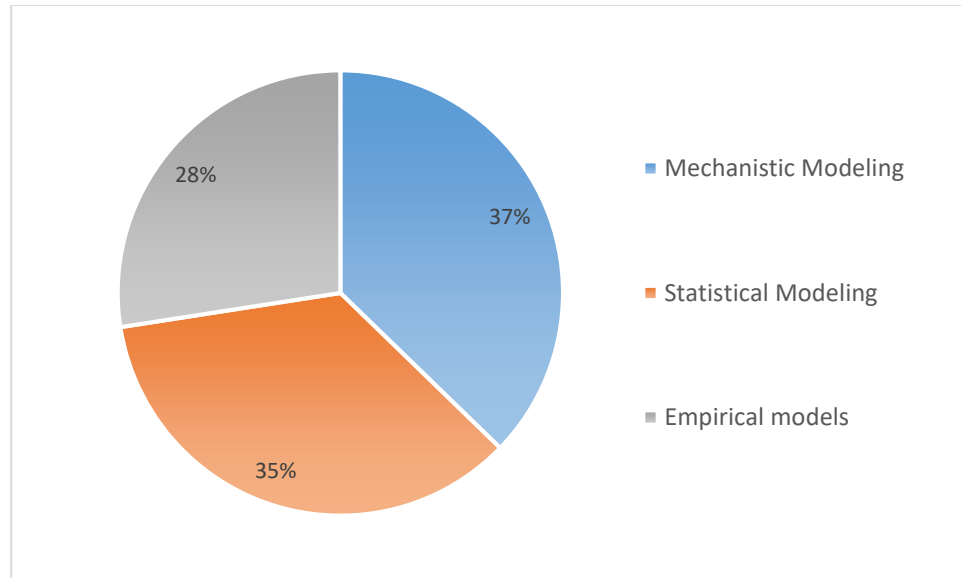
			predicted values of the coefficient of determination (R ²) was 0.99, which indicates that the model has a good fit and accuracy.		
50	RF, GLMNET, SVM and KNN	LS	In this study, several machine learning algorithms were applied to regression and classification models of digestion performance to determine the decisive operational parameters and predict methane production. KNN was tested to be the algorithm with the best prediction accuracy.	CH ₄	Wang et al. 2020
51	SVM	LS	Experimental data from AD of poultry manure were used. The relative mean error of the SVM-based model in TAN prediction was 15.2%.	TAN	Alejo et al. 2018
52	EN, RF, and XGBoost	IpS	The objective of this study was to apply a machine learning model to accurately predict daily biomethane production in an industrial-scale co-digestion facility. The results show that the elastic net (a model with linear assumptions) significantly outperforms random forest and extreme gradient enhancement.	CH ₄	Clercq et al. 2020



a. the main types of work participants have been involved in



b. the main types of work participants have been involved in



c . Categories in which participants are primarily involved in modeling

Figure S1. Research background of the participating researchers

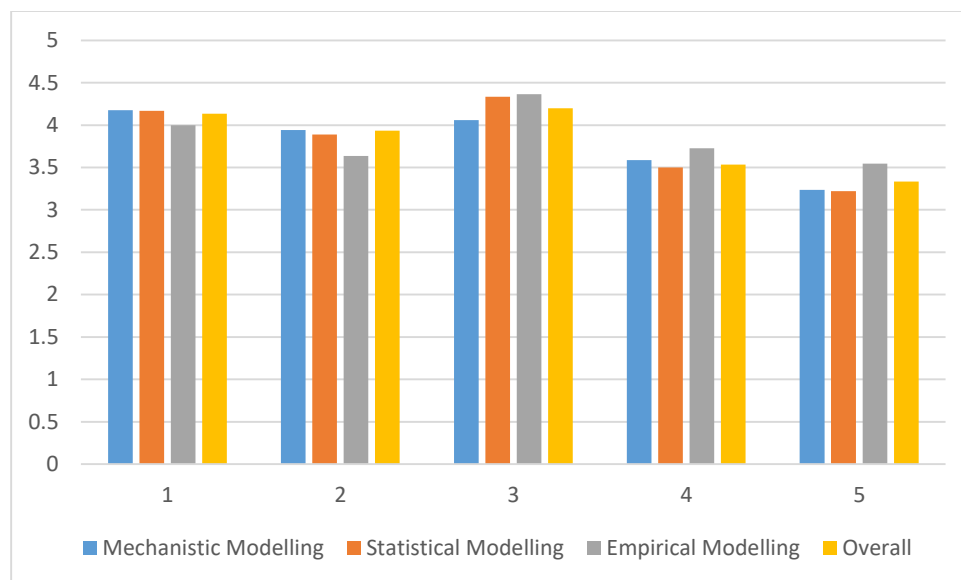


Figure S2. Average scores of the importance evaluation of the five statements in the process of developing the AD model classified according to model category

The survey on important factors during the process of anaerobic digestion modelling

1. In the field of AD modeling, what kind of work are you mainly involved in?

- A. I am a model developer.
- B. I do not only develop models, but also apply the models developed by myself or others to carry out research work. Anyway, I mainly focus on developing models.
- C. I occasionally develop models or even perform secondary development on existing models, but I mainly focus on model applications.
- D. I mainly focus on model applications and basically do not develop any models.
- E. None of above, but others like: _____

2. Generally, there are three categories of AD modelling, which are mechanistic, statistical and empirical models. Which category of modelling do you mainly work on?

- A. Mechanistic Modelling
- B. Statistical Modelling
- C. Empirical Modelling
- D. None of above, but others like: _____

3. How many years of working experience you have regarding the field you have answered in question 1?

- A. Less than 3 years
- B. 3 to 5 years
- C. 5 to 10 years
- D. More than 10 years
- E. No answer

4. There are a number of factors that have to be considered when developing models. The factor/s I would focus on most during the AD modeling process is/are (multiple answers possible):

- A. Modeling approaches (e.g. the biochemical reaction process on which the model is based or the algorithm used in the model, etc)
- B. Modeling parameters (e.g. parameter variables for model inputs, etc.)
- C. Modeling results (e.g. accuracy of model output results, etc.)
- D. Modeling applications (e.g. the application environment and the potential for expansion of the model)
- E. Other factors, such as _____

How do you evaluate the importance of the following statements (Q5.1-Q5.5) in the actual process of developing AD models?

(Scored on a scale of importance from 1 to 5: a 5-star means very important and 1-star means not important at all)

5.1 During the developmental process of modelling (mechanistic, statistical and empirical models), the variables, algorithm, and the computational rules in the modelling should follow the rules of the actual reaction process of the real AD as much as possible.

★ ★ ★ ★ ★

5.2 To support running the model, the parameters and variables used in the model should have a wide-range of multi-channels and reliable sources, that is to say, the parameters and variables of the model should have good identifiability and availability to support the successful operation of the model.

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5.3 The output of the model has been verified by some real experiments or tests, and its results should meet the corresponding confidence interval (or should be verified by other relevant approaches).

★ ★ ★ ★ ★

5.4 The model should have a module-interface or possibility for the secondary or further development.

★ ★ ★ ★ ★

5.5 The model should have universal applicability to users, e.g. the model should be easy to understand and the platform or software on which the model based should be commonly used.

★ ★ ★ ★ ★

6. Apart from theses statements, I also think that the following aspect is important when developing anaerobic digestion models:

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