Flexigas theme A-WPA2

Hanze Research Centre – Energy / University of Groningen – Centre for energy and environmental sciences

An integrated approach for the validation of Energy and Environmental system analysis models: Used in the validation of the Flexigas Excel BioGas model

F. Pierie^{a,b}, C. van Someren^a, W. Liu^a, J. Bekkering^{a,b}, E.J. Hengeveld^{a,b}, J. Holstein^c, R.M.J. Benders^b, G. Laughs^b, W.J.T. van Gemert^a, H.C Moll^b

^A Hanze University of applied science – HanzeResearch - Energy, Zernikeplein 11, 7947 AS Groningen, The Netherlands.

^b University of Groningen - Centre for Energy and Environmental Sciences, Nijenborgh 4, 9747 AG Groningen, The Netherlands.

^c DNVGL - Energy - Energieweg 17, 9743 AN, Groningen, the Nederland

INFO

Date publication: 2016-05-10

Keywords:

Validation, Modeling, Biogas, Energy and Environmental System Analysis

Correspondance:

Hanze University of applied science, Hanze Research Centre – Energy P.O. box 3037, 9701 DA Groningen, The Netherlands: Visiting address: Zernikelaan 17, 9747 AA Groningen, T: +31 (0)50 595 4640, M: +31 (0)6 510 67 674, E: <u>f.pierie@pl.hanze.nl</u>, W: www.hanzegroningen.eu

ABSTRACT

A review has been completed for a verification and validation (V&V) of the (Excel) BioGas simulator or EBS model. The EBS model calculates the environmental impact of biogas production pathways using Material and Energy Flow Analysis, time dependent dynamics, geographic information, and Life Cycle analysis. Within this article a V&V method is researched, selected and applied to validate the EBS model. Through the use of the method described within this article: mistakes in the model are resolved, the strengths and weaknesses of the model are found, and the concept of the model is tested and strengthened. The validation process does not only improve the model but also helps the modelers in widening their focus and scope. This article can, therefore, also be used in the validation process of similar models. The main result from the V&V process indicates that the EBS model is valid; however, it should be considered as an expert model and should only be used by expert users.

(c) 2016 Hanze Research - Energy Ltd. All rights reserved.

Nomenclat	Nomenclature				
AD	Anaerobic Digestion	(P)EROI	Process Energy Returned On Invested		
V&V	Verification and Validation	GWP100	Global Warming Potential 100 year scale		
oDM	Organic Dry Matter	Pt	Environmental impact in EcoPoint		
FM	Fresh matter	LCI	Life Cycle Inventory		
GJ	Giga Joule	LCA	Life Cycle Analysis		
MJ	Mega Joule	aLCA	Attributed Life Cycle Analysis		
Mg	Mega gram (equivalent to metric tonne)	MFA	Material Flow Analysis		
EBS	(Excel) Biogas Simulator	MEFA	Material and Energy Flow Analysis		
Nm ³	Normal cubic meter	kgCO₂eq	Kilograms of Carbon dioxide equivalent		

1. Introduction

The Flexigas project researches the integration of biogas produced from anaerobic digestion within decentralized smart energy systems [1]. One goal of the project is the development of "a BioGas Simulator" a tool which can be used for measuring the sustainability of complex energy production pathways. For this purpose a specific model was created for the environmental system analysis of biogas production pathways, called the (Excel) Biogas Simulator or EBS.

Within exact science models are often used for complex calculations. Variables in the model are changed for different scenarios to observe the effect on the results, thereby opening the way for scientific analysis. However, before results from a model can be deemed trustworthy (or not) the model must first be verified and validated (V&V). The process helps in: strengthening the model by resolving mistakes in the model; and bringing to light strengths and weaknesses of the model. Furthermore, V&V also helps to test and strengthen the conceptual model and research goals behind the model. Therefore, Verification and Validation of a newly created model is a vital part of the process towards a trustworthy model. However, validation in itself is not a solid science. "Validity, in its generic form, refers to measuring what we think we are measuring or, in the case of models, representing what we think we are representing" [2]. Within literature the definition of Validation and Verification is not settled as differences are still present between researches [3-9]. Within this article, verification confirms that the realized system satisfies stakeholder needs, providing the correct solution to the customer's problem (e.g. the right model was built). Computerized model verification is defined as assuring that the computer programming and implementation of the conceptual model are correct [4]. Validation confirms that all elements of the system perform their intended functions and meet technical (performance and operational context) and interface requirements and constraints (e.g. the model was built correctly). Operational validation of a computer model is defined as determining that the model's output behavior has a satisfactory range of accuracy for the model's intended purpose over the domain of the model's intended applicability [4].

Overall, a model is considered valid for a set of experimental conditions if its accuracy is within an acceptable range, which is the amount of accuracy required for the model's intended purpose. Within this context it is important to remember that: "A model should be developed for a specific purpose (or application) and its validity determined with respect to that purpose" [4]. Theoretically a model should represent exactly the physical system it models. "In the V&V of physical systems, there is "ground truth" against which the as-built system can be measured – it can either fly so far or it can't, it weighs less than X or it doesn't, and so on" [2]. However, "it is often too costly and time consuming to determine that the model is absolutely valid over the complete domain of its intended applicability or describes the ground truth. Instead tests and evaluations are conducted until sufficient confidence is obtained that a model can be considered valid for its intended application" [4]. There is an abundance of literature available which describes the process of validation and tests and evaluations for validating models [3-9]. However, the abundance of literature and the variety of options make it difficult to select a specific V&V method for the Excel based model. To achieve a preferable result for the V&V of the model, a good balance must be found between model confidence cost, time invested, and value of the model to the user. This leads to the main question: How to verify and validate the EBS model, such that the accuracy of the models intended purpose is within an acceptable range?

Within this article a review was performed on validation research in literature [3-9] to select the most viable V&V method for the EBS model. The review concluded that most articles had notions and ideas of how to perform a verification and validation; however, they lacked a clear method to follow, with exception of Balci et al. and Sargent. Balci et al. described a list of golden rules helpful in the validation process, and Sargent described a list of topics or focus points to use within the validation of simulation models. The latter is specifically of interest for the validation of the EBS model, due to the detailed description which Sargent 2013 gives per focus point. The validation process can indicate the value and accuracy of the EBS model and therefore add to scientific understanding regarding the sustainability of biogas production. Therefore, the developed V&V method described within this article is derived from Sargent, 2013. The V&V method is discussed in the method section; the results from the V&V method performed on the EBS model are discussed in the results are reviewed and summarized in the discussion and conclusion sections.

2. METHODOLOGY

The model will be validated through the use of a question list containing focus points, retrieved from Sargent, 2013 [4], selected specifically for the validation of the EBS model. The focus points are separated into two main sections: First, the verification will focus on the goal of the model, in order to find out if the correct model was built for answering the main research questions; second, the model itself will be validated, through a testing structure, to estimate transparency, correctness etc. The verification and validation process will be performed with the help of multiple focus points addressing the concept, the overall model, or a particular area of the model. The focus points aforementioned will be elaborated in the following section.

2.1. Verification of concept: did I build the right thing?

The first step in the overall verification and validation process will be focusing on the problem entity (Fig. 1) and the conceptual model. When building a model it is important to keep in mind that most models have the purpose of providing

answers to complex issues. From this perspective it is important to start with the right question, and verify your question. The main question stated: Did I build the right model? To verify this, the concept must comply with the following statements. Does/is the model:

- 1) Ad to scientific understanding or add to societal benefit?
- 2) Refer to clear answers which can be provided through modeling?
- 3) Reviewed (e.g. literature review etc.) and verified by experts in the field (e.g. professors, researchers)?



Fig. 1. Main list of subjects used in the validation process [4]

2.2. Model validation: Did I build the thing right?

Within this section the validation techniques selected for the EBS model are discussed. Most of the techniques described here are found in literature, although some may be described slightly differently. They can be used either subjectively or objectively. By subjectively; we mean common reasoning by modeler and experts in the field and by objectively; "we mean using some type of mathematical procedure or statistical test, e.g., hypothesis tests or confidence intervals" [4]. A combination of techniques is generally used. These techniques can be used for validating individual components or submodels within the model and the complete model. The following list of validation techniques is retrieved from Sargent, 2013 [4] for use in this article and in the verification and validation process of the BioGas simulator.

(A) Comparison to other models: Various results (e.g. outputs) of the simulation model being validated are compared to results of other (valid) models. For example simple cases of a simulation model are compared to known results of analytic models, and the simulation model is compared to other validated simulation models.

(B) Data relationship correctness: Data relationship correctness requires data to have the proper values regarding relationships that occur within a type of data, and between and among different types of data. For example, are the values of data collected on a system or model correct for some known relationship within some type of data such as an inventory balance relationship or a dollar relationship?

(C) Event validity: The 'events' of occurrences of the simulation model are compared to those of the real system to determine whether they are similar. For example, compare the number of fires in a fire department simulation to the actual number of fires.

(E) Extreme condition test: The model structure and outputs should be plausible for any extreme and unlikely combination of levels of factors in the system. For example, if in-process inventories are zero, production output should usually be zero.

(F) Face validity: Individuals knowledgeable about the system are asked whether the model and/or its behavior are reasonable. For example, is the logic in the conceptual model correct and are the model's input–output relationships reasonable?

(G) Internal validity: Several replications (runs) of a stochastic model are made to determine the amount of (internal) stochastic variability in the model. A large amount of variability among the replications may cause the model's results to be questionable, and if typical of the problem entity may question the appropriateness of the policy or system being studied.

(H) Parameter variability-sensitivity analysis: This technique consists of changing parameters in the model to determine the effect upon the model's behavior or output. The same relationships should occur in the model as in the real system. This technique can be used qualitatively—directions only of outputs—and quantitatively—both directions and (precise) magnitudes of outputs. Those parameters which are deemed sensitive because of significant changes in the model's behavior or output should be made sufficiently accurate prior to using the model. (This may require iterations in model development.)

(I) Structured walkthrough: The model under review is formally presented usually by the developer to a peer group to determine the entity's correctness. An example is a formal review of computer code by the code developer explaining the code line by line to a set of peers to determine the code's correctness.

(J) Trace: The behavior of a specific type of entity in a model is traced (followed) through the model to determine whether the model's logic is correct and if the necessary accuracy is obtained. (Most current simulation software provides for trace capability making the use of traces relatively simple.)

2.3 Expected accuracy of the model.

Most models can be placed along a "continuum of objectivity" (Fig. 2), where physical models are often more objective and theoretical models more abstract. According to the position of the model within this "continuum of objectivity" the validation process and techniques can be determined. When considering V&V of theory-based models, however, the option of validating against ground truth (i.e., historic data collected from a real system) is often not available to modelers. Within the aforementioned context, the EBS model, being a physical model, can be compared on many aspects ranging from the factual aspects (e.g. compared to the ground truth Fig. 2), to the conceptual aspects (e.g. opinion by experts or face Fig. 2).



Fig. 2. The ground truth principle within V&V [2]

There is a link between accuracy and development time required. Within this context the goal is to retain the highest accuracy with the lowest time requirements (Fig. 3). Therefore, for the fact based comparison the preferred accuracy of the EBS model should be at least 80% for the basic calculations and around 80% for the economic calculations (Fig. 3). However, for primary calculation (e.g. biogas, green gas, heat and power production) accuracy is expected to be in the range of 95 to 99% accurate. Accuracy levels will be mainly expressed in the difference between the reference models and the EBS model in percentages. These should then not exceed 20% for the model to maintain its 80% accuracy. For the conceptual validation, however, the accuracy of 80% is very difficult to quantify. Therefore, additional theoretical explanations are required.



3. RESULTS

The list of validation techniques mentioned in the method (section 2.1 A to J) will be used to validate the EBS model. The results from the validation process will be discussed in the following section.

3.1. Model verification; did I build the right thing?

To indicate if the right model was built the Verification of concept method is applied (described in section 2.1) to the EBS model. The overall results indicate that the validated model adds to scientific understanding and helps to answer the main questions stated in the line of research for which the model is constructed. Both literature and experts from the field addressed for the V&V of the model agree that the right model was built. In the following section this result is explained in more detail.

3.1.1. Adding to scientific understanding or to social benefit

The EBS model combines energy and environmental system analysis, geographic modeling, and temporal dynamic load modeling, in order to gain more insight into biogas production pathways, which can operate as a load balancer in decentralized smart energy systems. The discussed model in this article can expand current knowledge on the efficiency and sustainability of biogas production pathways operating within a decentralized smart energy system. This knowledge can help in designing a tailor-made biogas production chain for a specific geographic location, increasing the efficiency and sustainability of biogas as a renewable resource. Furthermore, a full life cycle-based understanding of the absolute energy and environmental impact of biogas and green gas production pathways can help governments form proper policies which effectively support the European Union in achieving renewable energy and emission reduction goals, as described in the EU energy directive and the EU roadmap 2050 [10, 11].

3.1.2. Refer to clear answers which can be provided through modeling

The EBS model is based on the industrial metabolism concept, and is expanded with three known methods: the Material Flow Analysis (MFA) method is used to simulate the decentralized energy system; the Material and Energy Flow Analysis (MEFA) method is used to determine the direct energy and material requirements; and the Life Cycle Analysis (LCA) is used to calculate the indirect material and energy requirements, including the embodied energy of the components and required maintenance. The resulting efficiency and environmental impact calculated in the EBS model will be expressed in three known indicators which correlate with the definition of "strong sustainability" [12], wherein environmental quality precedes social prosperity which precedes economic prosperity [12, 13]. The indicators used are: The (Process) Energy returned on Invested or (P)EROI, indicating the efficiency of the chosen scenario in energy invested in the process divided by energy produced by the same process [14]; The carbon footprint (GWP100), indicating global warming potential in kgCO2-equivelant per GJ of produced energy [15]; And the Eco Indicator 99, indicating the overall environmental impact to the ecology, nature and human health using the Recipe indictor [16] given in Pt per GJ of produced energy. Taken together, these indicators will give a clear overall impression of the efficiency and sustainability of biogas production pathways functioning within dynamic systems, and can help answer the main question and main goal stated, namely: How to measure the sustainability of complex energy production pathways.

3.1.3. Review by experts

A group of reviewers was selected, made up by specialists in the field of modeling, biogas systems, and specialists in the field of energy transition. To receive feedback on a wide range of subjects regarding the model, a mixed review group is chosen on all aspects (Table 1).

The participating reviewers for the I	EBS model	
Name	Organization	Position
Wim van Gemert PhD. MSc.	HanzeResearch - Energy	Leading lector HanzeResearch - Energy
Jan Bekkering MSc.	HanzeResearch - Energy	PhD. Researcher on the topic of modeling biogas
Evert Jan Hengeveld MSc.	HanzeResearch - Energy	PhD. Researcher on the topic of modeling biogas
Wen Liu PhD. MSc.	HanzeResearch - Energy	Researcher and specialist in EnergyPlan model
Henk Moll Prof. PhD. MSc.	RuG - IVEM	Professor on subject Energy and Environmental Sciences
Rene Benders PhD. MSc.	RuG - IVEM	Researcher and designer of several energy models
Gideon Laugs MSc.	RuG - IVEM	PhD. Researcher of decentralized storage modeling

Johan Holstein MSc.	DNVGL	Safety expert in the field of gas

The reviewing process started off with an opening session. During the opening workshop the EBS model was explained to the reviewers. The inner workings, the formulas and the used variables were explained through the use of a walk-through of the model. At the end of the workshop the reviewers were sent home with a version of the model and an assignment containing explanatory documents and a questionnaire. Within this questionnaire the reviewer was asked to grade the model sufficient or insufficient for use. After the reviewing process, the group reconvened in a final walk-through session, where feedback, remarks and improvement options were discussed.

The group of reviewers concluded that the right model was built for answering the research questions stated (see introduction). Furthermore, according to the reviewers the model will add to scientific understanding when used correctly. However, the model layout and use is too complex for non-expert users and therefore should only be used under supervision of one of the creators of the model until a sufficient level of expertise is reached. Overall, the review session helped strengthen the model. During both session many adaptions where devised and put in place, including a more transparent interface. The classification of the model "as only usable by experts" was kept due to the overall complexity of the variables and outcomes of the model.

3.2. Model validation: Did I build the thing right?

To indicate if the model was built correctly the validation method (described in section 2.2) is applied to the EBS model. Overall the results indicate that the validated model and the used database were built correctly. Statistical validation, verification tests, and experts from the field indicated that the right model was built and is within the accuracy level set (at 80% accuracy of the model). In the following section this result is explained in more detail.

3.2.1. Comparison to other models

Table 2

During this validation phase the EBS model is compared to the Bekkering et al. model [17], which focusses on biogas production and economic calculation but also includes efficiency and carbon footprint results. The Bekkering et al. model has been validated against the Weidenaar model [18] and the calculation for subsidization schemes in the Netherlands [19] and has produced several articles [20-23]. The Bekkering et al. model and EBS model have common outputs in biogas and green gas production, cost per Nm3 of green gas, energy efficiency of green gas production, and carbon footprint of green gas production. However the Bekkering et al. model does not produce results in the field of environmental impacts. The validation comparison scenario is based on a co-digestion system of manure (50% fresh matter) and maize (50% fresh matter). The main variables for biogas production are kept the same (Table 2). Within both models losses of biomass and biogas are switched off, excluding the biogas loss from the digester. However, professional settings between the models differ (e.g. losses of biomass during processing). Also, for the efficiency and carbon footprint calculations the variables and data differ between the models.

Main inputs comparison scenario models			
Main variables	Value	Unit	
Economic depreciation period	12	Years	
Technical lifespan installation	25	Years	
Electricity price	0.14	€/kWh	
Operating hours per year	8760	h/a	
Total transport distances	0	km	
Losses of biogas from digester	1	%	
Manure input	9000	Mg/year FM	
Organic dry matter manure	8	%	
Biogas potential of manure	310	Nm ³ /Mg.oDM	
Methane potential of manure	180	Nm ³ /Mg.oDM	
Cost of the manure	-15	€/Mg	
Maize input	9000	Mg/year FM	
Organic dry matter maize	31.5	%	
Biogas potential of maize	620	Nm ³ /Mg.oDM	
Methane potential of maize	330	Nm ³ /Mg.oDM	
Cost of the maize	35	€/Mg	

*Transport was not indicated in the scenarios. The price for the biomass is the same in both models

The same scenario (Table 2) is run in both models and the results are compared based on: the biogas and methane production of both models; the cost of green gas production; the efficiency and carbon footprint in GWP100. The

comparison of the two models indicates that the EBS model performs sufficiently when looking to the primary calculations of biogas production and costs of green gas production. The difference in biogas production between the models is around 0.74%, which can be found in the professional settings and margins or rounding of numbers (Table 3). The costs differ by 3.58%, which is also within an acceptable level. However, when looking to the efficiency and environmental impact, values differ significantly (Table 3). This can be explained by the focus of the models: The Jan Bekkering et al. model focusses mainly on the economics of biogas production; whereas the EBS model focusses mainly on efficiency and environmental impact. The boundaries of the EBS model takes into account more energy and environmental impacts (e.g. indirect energy production, embodied energy,). This can be seen in the energy efficiency outcomes of both models where the difference is over 32%. Again, when comparing the carbon footprint results the difference is around 39%. Within this context the Jan Bekkering et al. model cannot be used for validation of environmental indicators.

Table 3

Outcomes both models

Outcomes both models				
Outcome	Unit	Bekkering et al, model	EBS model	
Biogas production	Nm3/h	226	223.9 °	
Green gas production	Nm3/h	135.0	134.0 ^ª	
Costs	€ct/Nm ³ green gas	75.3	78.0 ^a	
Efficiency	(P)EROI	3.9	2.6	
Carbon footprint	kgCO2eq/GJ (GWP100)	29.6	41.1 ^b	
^a The use of the internal biogas	s boiler for besting the digester is not includ	hod		_

The use of the internal biogas boiler for heating the digester is not included

^b Emissions when using biogas boiler for heating the digester

3.2.2. Data relationship correctness

Within this section the database of the EBS model will be compared to peer-reviewed literature. Most of the values and variables (around 90%) used in the EBS model are based on either peer reviewed literature, reports or practical data [24]. However, there is still a large variation between values and variables used in literature. Within the model most of the values and variables, when multiple sources are available, are based on averages of the total range. However, there are cases when only one source from literature is present; the use of this number depends on the quality of the source. The model itself is constructed in such a way that all important variables can be altered, for instance when new and better data presents itself. Within the model all values used are also fitted with a source.

Besides the data itself the correlation between the data, namely the calculations, are all performed through a standard modeling methodology, as described in Pierie et al., 2016 [25]. The structure of modeling is based on modules and sub-modules. Within each sub-module, one main physical process of the biogas production pathway is described. Every sub-module will be capable of determining three environmental impact indicators; the efficiency in (Process) Energy Return on Investment or (P)EROI; the Carbon Footprint in carbon dioxide equivalents; and the Environmental impact in EcoPoints. The summation of impact factors from the sub-modules used in the scenario will determine the total efficiency and environmental impact of the biogas production chain. To determine the aforementioned factors, each sub-module is separated into four levels: level one, the primary (mass) flow level; level two, the direct energy and material level; level three, the indirect energy and material level; and level four, the embodied energy level. Each level will be described through the use of an existing method and will perform its own specific calculations. Additionally, the first three levels in the sub-module will be linked together functioning as a cascade. Level one will deliver the input, through primary functional flows, for level two; and level two will provide input, through direct functional flows, for level three. This will allow dynamics in the higher level to influence the following levels, hence transmitting the dynamic element downstream. Level four will work independently [25].

3.2.3. Event validity

In this section the EBS model will be validated against an actual biogas facility situated at the Dairy Campus near the city of Leeuwarden, the Netherlands, which consists of two digester units and two CHP units. The digesters were owned by the University of Wageningen. During operation the biomass inputs and electricity production was recorded. The outcomes of the EBS model will be compared in two instances with data from the WUR digesters: (a), the primary biogas production calculated by the WUR digesters input will be validated against the biogas production of the model; and (b), the measured power output of the CHP units from the WUR digesters will be compared to the main EBS model.

(A) The WUR biogas input sheet comparison: In this validation comparison the theoretical biogas potential calculated by the employees of the WUR digesters in Leeuwarden for the year 2011 will be compared to the EBS model, programmed with the same values (Table 4).

Table 4 Main variables WUR digester and EBS model

Wall valiables work digester and LDS	mouer			
Main variables	Value	Unit		
Average methane content	58.07	%		
Theoretical efficiency CHP unit	35	%		
Loss of biogas	0	%		
	Biomass input	Organic fraction	Biogas potential	Biogas potential
Feedstocks digester	Mg/a	oDM (% of FM)	m3/Mg.FM	m3/Mg.oDM
Dairy cow manure	7107.4	6.00%	20	333.3
Solid manure	2442.7	33.00%	70	212.1
Maize field	1917.3	34.00%	175	514.7
Organic waste flows	531.9	62.00%	700	1129.0
Maize source	433.2	45.00%	300	666.7
Unions and onion peels	550.7	20.00%	60	300.0
Ecofrit	3179.5	20.00%	500	500.0
Digestate reuse	505.4	20.00%	5	25.0

The theoretical output of the calculation sheet is comparable with the outcome of the model using the same input parameters, with a difference of 0.35% (Table 5). However, when looking to the actually measured power production of the CHP unit of the WUR digester the production is 31.03% less than that of the EBS model (Table 5). Therefore, the use of theoretical values in the input sheet might not reflect the actual process taking place in the biogas production pathway.

Table 5

Main outputs from th	e comparison scenario
----------------------	-----------------------

Outcome	Unit	WUR data sheet	EBS model
Biogas production	Nm³/hr	171.7	171.1
Methane	Nm³/hr	99.7	99.4
Electricity production total	MJ/hr	862.0	1249.9
Electricity exported	MJ/hr	746.2	1155.7

(B) The WUR CHP comparison: In this validation comparison the measured output of the biogas CHP unit located at the WUR Dairy Campus Biogas plant will be compared to the output of the CHP in the EBS model. From the previous validation it became clear that the theoretical production of the biogas plants as calculated by Dairy Campus does not fully comply with the measured outcome of the CHP units (Table 5). The overall efficiency of the CHP unit given by Dairy Campus is 35%; however, the biogas production calculated in the previous validation implies that the efficiency of the CHP unit only reaches 25%. This discrepancy might be found in the losses of the system during the biogas production process. Losses might include: losses of biomass during transport, storage and loading; losses of biogas during storage or transport to the engine; and a lower efficiency of the engine due to less than optimal operation. To test the EBS model on accuracy the same case is programmed back into the model, this time also including the aforementioned losses and using the preset values present in the model (which include internal use, losses, etc.), (Table 5).

When looking to the results (Table 6), the EBS model is on the difference between the EBS model and the measured values when looking to electricity production lays at around 14.66%, which is within the 20% accuracy range of the model. The difference between the real case scenario of the WUR and the EBS model can result from many factors (e.g. internal electricity consumption, lower CHP unit efficiency, more internal losses). If for instance the CHP efficiency is set to 31% in the EBS model the net electricity production becomes similar to the output of the WUR digester.

Table 6

Main outputs WUR CHP comparison

Outcome	Unit	WUR data sheet	EBS model
Net production CHP unit	MJ/hr	746.24	855.7
Efficiency CHP unit	%	?	35.0
Biogas production	Nm3/hr	?	119.0
Methane production	Nm3/hr	?	68.4

3.2.4. Extreme condition test

During the zero tests all the inputs within the EBS model are set to zero. All the main outputs of the EBS model indicate zero (0) or divided by zero during the zero tests. Also when individual sub-modules are turned to zero they will not influence the outcome of the model. There is an exception; machinery installed in the digester which is not used can still have an embodied impact. Within this concept, the impact of construction of the machine is evenly spread out over the

lifetime of the total installation, which will still be the case when the machinery is not used. Within the model there is the possibility of turning the embodied energy off if the machinery is not installed in the scenario. Furthermore, there are some cases where the model indicates divide by zero fault, this can be expected as all values, including e.g. efficiency of the CHP unit or all biomass flows, are zero as well.

3.2.5. Face validity

During the face validity phase a group of experts in the field of modeling, biogas production, and energy transition was selected (Table 1) and given the task of reviewing the model. The reviewers followed a program that resulted in a written review report and a final remark which is either 'inadequate' or 'adequate'. The reviewers concluded that: The model can fulfil its intended purpose of analysing the environmental impact of biogas production chains. The structure used in the model is logical and transparent, strengthening the trustworthiness of the model. The model can also help in creating a better scientific understanding in the sustainability of biogas production. However, the calculations are still numerous and not always transparent, making validation difficult. The complexity of the topic and multiple level inputs needed in the model make it only usable by experts. The outputs are understandable and logical, but the EcoPoint system will need better explanation. The reviewers advised to integrate a Net Present Value cost calculation into the model for a more complete and comparable outcome. Finally all reviewers agreed on the fact that the model can be used for its intended purpose.

3.2.6. Internal validity

Table 7

Internal validity is analyzed through the use of two different techniques: (a) internal comparison of calculation, and (b), sensitivity analysis of the main parameters.

(A) Internal comparison of scenarios: Within the EBS model there are multiple calculation pathways which use the same variables and inputs and calculate the same outputs. This property can be used for internal validation. Therefore, for validation purposes the pathways are pre-set to calculate the same scenario. Two biomass inputs scenarios chosen for this comparison are; cow manure with energy maize, and cow manure with grass (Table 7). The results from these pathways using the same biomass inputs can be compared with each other as the outcome should be exactly the. This approach also covers the validation step called trace. For every scenario made the calculation pathway is traced when compared to other scenarios. Furthermore, discrepancies between scenarios are mostly solved using trace.

The method of comparison together with trace proved very useful for the validation process of the model and brought to light several programming mistakes. Overall, the calculation pathways within the model are aligned through the use of internal comparison of scenarios (Fig. 4). However, transport in result 1 and 2 (Fig. 4) where not similar, which was traced back to the programed transport distance in the model and the type of transport (e.g. tractor or truck).





(B) Output sensitivity analysis: Within the EBS model the outputs (e.g. efficiency, emissions and environmental impact) are given per unit of produced energy, e.g. GJ, which could be in the shape of electricity and heat or green gas injected into the grid. Therefore, the outputs from the model, e.g. the (P)EROI factor, over the projected range of biomass input are expected to be relatively similar per GJ of produced energy. Within this context, the main input, biomass, will be varied from a minimum 250 Mg per year up to a maximum 50000 Mg per year with steps of 250 Mg. During the analysis all other variables are kept constant and the biomass mix will be fixed at 50% manure and 50% maize. When looking to the outputs indicator, (P)EROI, similar results with only a very gradually incremental increase or decrease are expected over the biomass input range.



Fig 5. (P)EROI outputs of the model over a projected biomass input range of 50% manure and 50% maize

As expected the model is very stable in a large part of the biomass input range, with a small incline starting from an input of 10000 Mg/a, which is mainly caused by the indirect and embodied energy values (Fig. 5). An explanation for this small incremental increase might lay in the economy of scale, where larger installations become more efficient. However, when looking to the biomass input below 2000 Mg per year, the indirect and embodied impacts have a very large impact on the end result e.g. (P)EROI. Therefore the accuracy of the model cannot be guaranteed below a yearly biomass input of 2000 Mg/a. Beyond the 2000 Mg/a input rage upwards the factors increases very gently and within that range the model is trustworthy. However, beyond the range of 50000 Mg/a of biomass input per year the behavior is not measured making this the maximum value for the model, which is beyond the scale of a farm size digester system.

3.2.7. Parameter variability (sensitivity analysis)

Within the EBS model the most sensitive parameters where indicated empirically, through the use of a sensitivity analysis. By keeping all variables constant except one, sensitivity of that specific variable can be determined. The sensitivity analysis performed on the EBS indicates great sensitivity in: biogas potential, organic dry matter content in biomass, and biomass yields from fields. These parameters are highly variable and depend greatly on local conditions, specific type of biomass, etc. The most dominant variables in the model are depicted in table 8, which are often linked to the biomass source. Unfortunately, biomass quality and quantity varies per growing season, location, field quality, harvest date and time, etc., making biomass already sensitive by itself. Often averages are used, which include many samples; however, even these vary within literature [24].

Table 8

Most dominant variables in EBS model	
Biomass variables	Impact in model
Yield of biomass from a curtain area	Medium to Low ^a
Organic matter ratio	High
Biogas content of the biomass type	High
Methane content within the produced biogas	High
Costs of the biomass	High
Biogas production process	Impact in model
Energy use digester (heat and electricity)	High
Lifergy use digester (near and electricity)	
Efficiency upgrader	High
Efficiency upgrader Efficiency CHP unit	High High
Efficiency upgrader Efficiency CHP unit Remainder	High High Impact in model
Efficiency upgrader Efficiency CHP unit Remainder Total biomass input in model	High High Impact in model Low to high ^b

^a Depends on use of own fields in model.

^b Below a threshold yearly input of biomass per year (2000 Mg/year) the model becomes inaccurate

3.2.8. Structured walkthrough

During the final session of the review process a walkthrough session was organized with the reviewers (Table 1), where the model was discussed. During this session improvement points are noted as well as limitations of the model. From the session resulted that this model can be a good tool in the hand of experienced professionals. The model is built correctly and can add to scientific understanding, however, to do so it must be used professionally and responsibly.

3.2.9. Trace

During the internal validity phase (discussed in section 3.2.6) a trace of biomass inputs was performed. As already discussed, the model contains several calculation pathways capable of calculating the same scenarios. When the comparison scenarios where programmed into the model per calculation pathway the results were traced and also compared to other calculation pathways in the model. At every control point during the trace the intermittent results were checked and also compared with the other calculation pathways.

4. Discussion

Within this article the review process of the EBS model was discussed. To ensure a correct and trustworthy model, several validation techniques were used. During this phase many mistakes and errors were detected and corrected in the model. The internal validation method aligned with several calculation pathways in the model such that the outcomes were similar. The comparison with external models (which are already validated themselves) and a case study of a biogas system showed that the main mass flow calculations of biomass and biogas production are in the same range. Furthermore, the economic calculations in the model (not being the primary goal) are in the same range as well. The aforementioned also confirms the usability of the validation method proposed in this article. However, the discussed validation process in this article cannot guarantee a 100% accurate model. The complexity of the model makes it very difficult to remove all mistakes. Through the comparison with other models and their results, an accuracy of a projected 80% can be expected. Within this article the model with its current calculations and dataset has been validated; however, the model also depends heavily on information retrieved from literature and as explained in the sensitivity analysis, some values have great influence on the final result. Most of the literature-based values used in the EBS model are programed as changeable parameters. However, this shifts the responsibility of selecting these values to the user. When doing so the user is expected to be an expert capable of determining which values are trustworthy and which ones are not. Hence, there is a principle difference between the validation of the model and the data used in the model. Additionally, the accuracy of the model can only be guaranteed for a specific range of yearly biomass inputs; below this range it is shown that indirect and embodied values have too much influence on the final outcome. Additionally, the model also contains new and untested methods and calculations focused on the sustainability of biogas production, which is hard to validate due to lack of comparable literature and models. The calculations are validated using the internal validation method but the methodology and chosen formulas can only be validated partly by literature. Furthermore the core data used in the model is based on a well-known scientific database of environmental impacts (e.g. Ecolnvent database [26]). Overall, the validation process, used for validating the EBS model, indicated no discrepancies in its intended purpose, namely: Analyzing the sustainability and efficiency of farm scale biogas installations. From the results in this article the model is classified as adequate for use through both validation techniques and through expert review. The results coming from the model can now be used to improve the scientific understanding regarding the sustainability of biogas production through anaerobic digestion in farm scale biogas installations.

5. Conclusion

The V&V method constructed and applied to validate an Excel based model, based on a simple model development process [4], is a useful tool for improving the quality of physical calculation models. Through the use of the V&V method: mistakes in the model were resolved, the strengths and weaknesses of the model were found, and the concept of the model was tested and strengthened. Going through the process not only helps the model but also the researchers in widening their focus and scope, helping them perform a correct validation and verification and re-evaluate the function and goal of their model. Besides the use of common sense when interpreting results, validation of a model is of the utmost importance. A model which has not been validated can potentially give inaccurate or even incorrect results, which could have been prevented by a V&V process. The V&V method researched, constructed and applied within this article can be a guide for the validation of models with a similar goal and context. The main results from the V&V process in this article indicate that the EBS model is valid and is ready for use in determining the energy efficiency, carbon footprint and sustainability of farm-scale biogas production pathways based on anaerobic digestion. The validation method described in this article resolved several problems in the model and strengthened the concept. The results presented in this article classify the EBS model as adequate for use through both verification and validation techniques and through expert review. The model, however, is considered an expert model and the outputs can only be trusted when the model is used by expert users. When used by experts in a proper and responsible manner the model can be capable of adding to scientific understanding regarding the sustainability of biogas production.

SOURCES

[1] Flexigas. Official website of the Flexigas project 2013; 2013.

[2] Hahn HA. The Conundrum of Verification and Validation of Social Science-based Models. Procedia Computer Science 2013; 16: 878-87.

[3] G. Sargent R. A New Statistical Procedure for Validation of Simulation and Stochastic Models. Electrical Engineering and Computer Science 2010.

[4] R. G. Sargent. Verification and validation of simulation models. Journal of Sim 2013; 7: 12-24.

[5] O. Balci O. Golden Rules of Verification, Validation, Testing, and Certification
of Modeling and Simulation Applications. SCS M&S Magazine – 2010 / n4 (Oct) 2010; October: 1-7.

[6] K. Pace D. Modeling and Simulation Verifi cation and Validation Challenges. JOHNS HOPKINS APL TECHNICAL DIGEST, VOLUME 25, NUMBER 2 (2004) 2004; 25.

[7] S. Robinson S, R.J. Brooks R. Independent Verification and Validation of an Industrial Simulation Model. Society for Modeling and Simulation International (SCS) 2009; SIMULATION 2010 86: 405 originally published online 17 July 2009.

[8] P.C. Kleijnen J. Case Study: Statistical validation of simulation models. European Journal of Operational Research 87 (1995) 21-34 1995: 21-13.

[9] P.C. Kleijnen J. Verification and validation of simulation models. European Journal of Operational Research 82 (1995) 145-162 1995.

[10] EUROPEAN PARLIAMENT. DIRECTIVE 2009/28/EC OF THE EUROPEAN PARLIAMENT AND OF THE COUNCIL of 23 April 2009 on the promotion of the use of energy from renewable sources and amending and subsequently repealing Directives 2001/77/EC and 2003/30/EC 2009; DIRECTIVE 2009/28/EC OF THE EUROPEAN PARLIAMENT AND OF THE COUNCIL of 23 April 2009.

[11] EUROPEAN COMMISSION. COMMUNICATION FROM THE COMMISSION TO THE EUROPEAN
br />PARLIAMENT, THE COUNCIL, THE EUROPEAN ECONOMIC AND SOCIAL
br />COMMITTEE AND THE COMMITTEE OF THE REGIONS. Energy Roadmap 2050. 2011; Brussels, 15.12.2011. COM(2011) 885 final.

[12] Mori K, Christodoulou A. Review of sustainability indices and indicators: Towards a new City Sustainability Index (CSI). Environ Impact Assess Rev 2012; 32: 94-106.

[13] Elkington J. Cannibals with forks – The triple bottom line of 21st century business: Capstone Publishing Ltd, Oxford; 1999.

[14] Hall ASC, Balogh S, Murphy JRD. What is the Minimum EROI that a Sustainable
Society Must Have?. Energies 2009; Energies 2009, 2, 25-47;: 25-47.

[15] Intergovernmental Panel on Climate Change. Climate Change 2007, Working Group I: The Physical Science Basis 2007; 2012.

[16] Goedkoop M, Spriensma R. SimaPro Database manual. The Eco-indicator 99 A damage oriented method for Life Cycle Impact Assesment. 2001; 22 June 2001.

[17] Bekkering J, Hengeveld EJ. Calculation Model Description Basis of Gas Suply Chains 2013; 2.0.

[18] Weidenaar T. Dutch gas distribution grid goes green: Decision support tool for local biogas utalization 2011.

[19] Lensink SN, Zuijlen van CL. Eindadvies basisbedragen SDE+ 2015 2014; ECN-E--14-035.

[20] Bekkering J, Broekhuis AA, van Gemert WJT, Hengeveld EJ. Balancing gas supply and demand with a sustainable gas supply chain – A study based on field data. Appl Energy 2013; 111: 842-52.

[21] Bekkering J, Hengeveld EJ, van Gemert WJT, Broekhuis AA. Designing a green gas supply to meet regional seasonal demand – An operations research case study. Appl Energy 2015; 143: 348-58.

[22] Bekkering J, Broekhuis AA, van Gemert WJT. Optimisation of a green gas supply chain – A review. Bioresour Technol 2010; 101: 450-6.

[23] Bekkering J, Hengeveld EJ, van Gemert WJT, Broekhuis AA. Will implementation of green gas into the gas supply be feasible in the future?. Appl Energy 2015; 140: 409-17.

[24] Pierie F, van Someren CEJ, Benders RMJ, Bekkering J, van Gemert WJT, Moll HC. Environmental and energy system analysis of bio-methane production pathways: A comparison between feedstocks and process optimizations. Appl Energy 2015; 160: 456-66.

[25] Pierie F, Bekkering J, Benders RMJ, van Gemert WJT, Moll HC. A new approach for measuring the environmental sustainability of renewable energy production systems: Focused on the modelling of green gas production pathways. Appl Energy 2016; 162: 131-8.

[26] Ecoinvent. Ecoinvent: Database of consistent, transparent, and up-to-date Life Cycle Inventory (LCI) data 2014.