MCBioCH4: A computational model for biogas and biomethane evaluation

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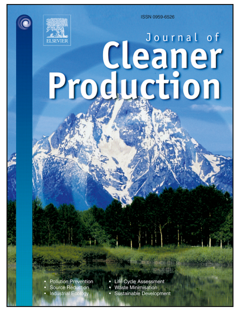

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PII: S0959-6526(19)31311-3

DOI: https://doi.org/10.1016/j.jclepro.2019.04.224

Reference: JCLP 16580

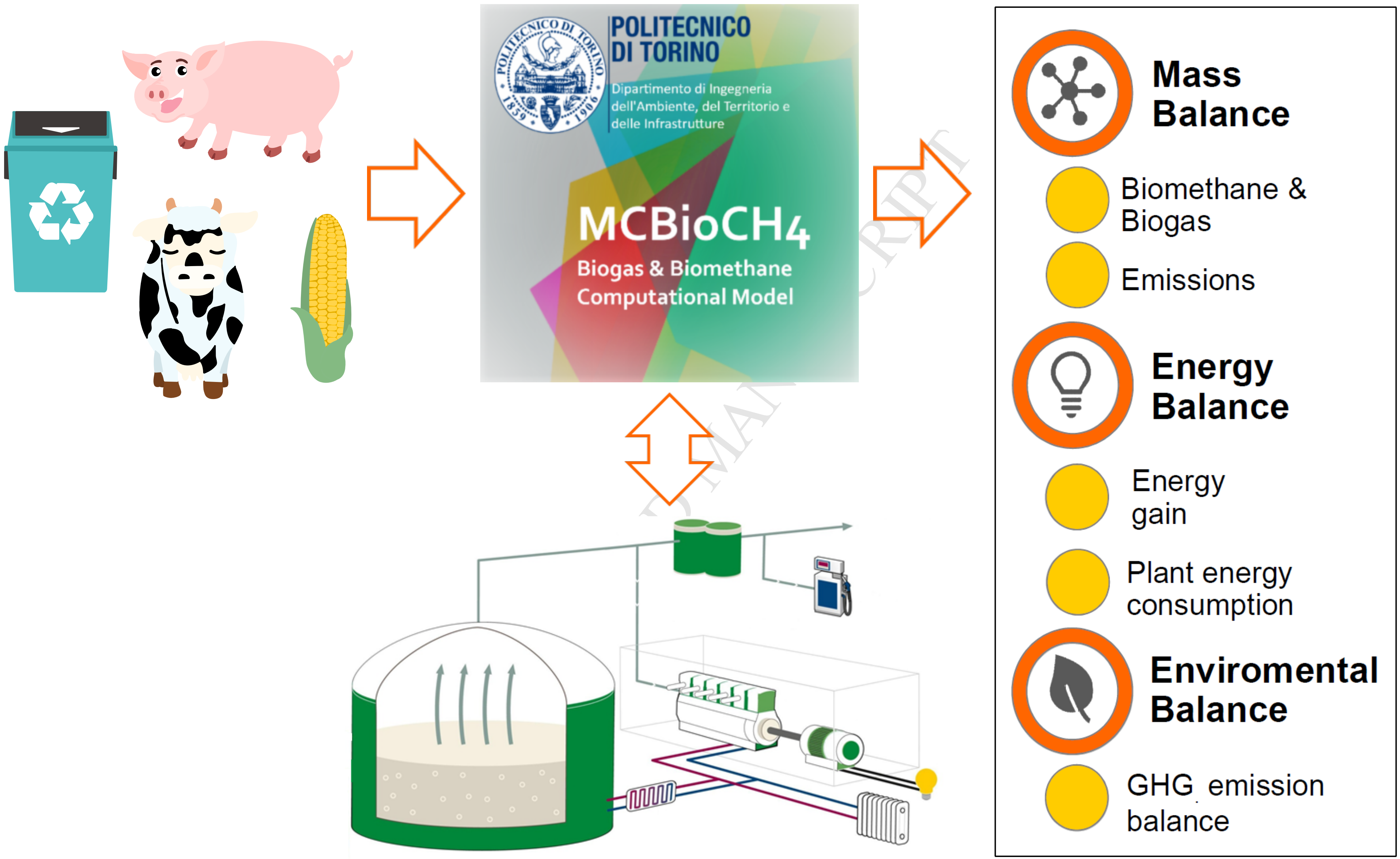
To appear in: *Journal of Cleaner Production*

Received Date: 17 December 2018

Revised Date: 15 April 2019

Accepted Date: 18 April 2019

Please cite this article as: Ravina M, Castellana C, Panepinto D, Zanetti MC, MCBioCH4: A computational model for biogas and biomethane evaluation., *Journal of Cleaner Production* (2019), doi: https://doi.org/10.1016/j.jclepro.2019.04.224.


POLITECNICO
DI TORINO
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MCBioCH4
Biogas & Biomethane
Computational Model
Mass
Balance
Biomethane &
Biogas
Emissions
Energy
Balance
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gain
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consumption
Enviromental
Balance
GHG emission
balance

ACCEPTED MANUSCRIPT

Total wordcount: 7928

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Abstract

The production and use of biogas and biomethane by anaerobic digestion is part of the critically needed energy transition, and it is achieving a growing interest in Europe. The planning and design of biogas/biomethane solutions necessitates the support of modelling tools for the calculation and evaluation of mass, energy and emission flows originated by different process and technological configurations. In the present study, a model for the preliminary evaluation of biogas and biomethane systems is presented. The model (named MCBioCH4) focuses on triple targets: i) obtaining information about the productivity of biogas/biomethane plants regarding achievable gas flow rates; ii) determining the plant energy expenditures and subsequently the economically exploitable energy flow shares; and iii) assessing the entire environmental impact of the system. The design of MCBioCH4 was specifically addressed to dual objectives: i) provide support to the preliminary assessment and comparison of different potential plant configurations and technological solutions, and ii) assist users in the complete definition of mass, energy and environmental flows, through the implementation of default datasets and assisted data input. The model is a standalone application fully equipped with graphical user interfaces. A set of default parameters was implemented in MCBioCH4, based on a detailed literature review. Alternatively, customized input parameters may be introduced by the user. If biogas scenarios are selected, the model simulates a combustion in a cogeneration unit. If biomethane scenarios are selected, the user is allowed to define the type and features of the upgrading technology. Two different options are implemented for biomethane: injection to the natural gas distribution grid, or use as a transportation fuel. The emission of carbon dioxide equivalent associated to each phase of the process is estimated by the model, based on a cradle-to-grave approach. Default emission factors are available, but these can be customized by the user. MCBioCH4 was tested on a case study in Italy. It provides a valuable support to project developers and administrations in defining the most economically and environmentally sustainable plant configurations.

Keywords: bioenergy, biogas modelling, biomethane upgrading, greenhouse gas emission, CO_2 equivalent

Abbreviations

CH_4, methane;
CHP, combined heat and power;
CO_2, carbon dioxide;
CO_{2eq}, carbon dioxide equivalent;
CRY, cryogenic separation;
DM, dry matter;
EC, European Community;
GHG, greenhouse gas;
GUI, graphical user's interface;
GWP, global warming potential;
LCA, life cycle assessment;
MB, membrane permeation;
MEA, chemical absorption with amine solutions;
MSW, municipal solid waste;
PSA, pressure swing absorption;
PWS, pressurized water scrubbing;
RED, Renewable Energy Directive;
VS, volatile solids.

1. Introduction

European policies for climate and energy have set important and challenging objectives. The main objective specified in European Union Directive 2009/28/EC is to obtain 20% of energy from renewable sources by 2020 (European Union, 2009). By 2030, the emission of greenhouse gases (GHG) is expected to be reduced by 40% compared to 1990 levels; energy use must be based on at least 27% renewables; and energy consumption must be reduced by 27% with respect to business-as-usual scenarios (European Union, 2014). Over the longer term, the EU goals establish a gradual shift toward a low-carbon economy, reducing GHG emission up to 80-95% by 2050 (European Union, 2011). The European Energy Roadmap 2050 recognizes the bioenergy sector as part of the revision of the European economy toward a sustainable, green and circular economy (European Union,

2012).
Biogas production and conversion technologies can significantly contribute to renewable energy production, especially if they are based on fully sustainable supply chains. In particular, the so-called advanced biogas production—i.e., that coming from agro-food-industry wastes and residues—provides the highest GHG emission reductions among different bioenergy supply chains (Scarlat et al., 2018). So far, the generation of electricity by biogas combustion has been favoured by the introduction of economic and financial support, such as subsidies, feed-in tariffs and investment facilities. Recently, the conversion of biogas to biomethane has been introduced and promoted, to overcome the limitations related to on-site biogas conversion (first and foremost the use of thermal energy).
Biomethane is a versatile, sustainable and economically feasible energy vector. It can be used as a substitute for transportation fuels or injected into the natural gas grid. In 2016, 459 biomethane production plants were in operation in Europe, with an energy production capacity of 17,264 GWh (European biogas Association, 2013). Biogas and biomethane potential production is high. The Green Gas Grids Project estimated a technical potential production of 48-50 billion m^3/y of biomethane by 2030 (Scarlat et al., 2015). In November 2016, a proposal for a revision of the Renewable Energy Directive (RED) was released. This proposal included modified criteria for the evaluation of biofuels' sustainability, as well as updated GHG emission accounting methods (European Union, 2016). For the mobility sector, fuel suppliers are asked to provide fuels with an increased share of renewable and low-carbon content. The objective is to reach a 3.6% share for the contribution of advanced biofuels and biogas, by 2030. The revised RED also introduces a limit of 3.8% (of the overall energy target) to the contribution of biofuels based on energy crops.
The increased use of biomethane is expected to bring positive impacts to the environmental, social and economic sectors (Rosegrant et al., 2008). Nevertheless, biomethane sustainability must be assessed over a wider evaluation scope—one that goes beyond the simple concept of bioenergy. To this end, new management models that integrate agricultural practices, residues valorisation and energy production have been recently introduced (Chinnici et al, 2018; Dale et al., 2016). These models promote the efficient use of limited resources and avoid unintended impacts on other controversial factors (such as direct and indirect land use changes and food security). In fact, in countries like Germany and Denmark, the use of energy crops for biogas/biomethane production has been recently limited by specific regulations.
The sustainability of biogas/biomethane systems strictly depends on the environmental impacts of the entire supply chain, in particular on the overall GHG emission balance (Paolini et al., 2018). Global emission balance depends, in turn, on the configuration and design of the different phases of the process, as well as on the adopted technological solutions. Project developers and administrations need efficient tools to screen and compare the GHG balance associated with different possible alternative solutions for biogas and biomethane production and use (Magaril et al., 2017).
The calculation and evaluation of the GHG emissions of biogas/biomethane systems is commonly performed by employing Life Cycle Assessment (LCA) tools (Letti et al., 2016). LCA represents a consolidated methodology for the calculation of the global warming potential of a process or material. Several studies are reported in the bibliography, in which LCA was applied to biogas or biomethane case studies. At present, the most comprehensive model for biogas and biomethane LCA is the BioValueChain (Lyng et al., 2018; Lyng et al., 2015), which was developed in SimaPro commercial software (PRé 2014) and simulates the anaerobic digestion of sewage sludge and organic waste. Other studies covering the entire biogas and biomethane production and conversion process have usually referred to single cases (Hijazi et al., 2016) or to single/multiple plant

typologies (Poeschl et al., 2012). LCA has also been widely employed to compare the GHG emissions balance of different substrates, such as single- or double-crop systems (Bacenetti et al., 2014), animal by-products (Kaparaju and Rintala, 2011) or sewage sludge (Li et al., 2017). The same methodologies have also been applied to the evaluation of biomethane upgrading solutions (Starr et al., 2012, Xu et al., 2015).
LCA tools usually cover a wide scope of applications. The database supporting simulations may, however, in some circumstances, lack detailed and complete data for the characterization of the process in terms of i) the characteristics of mass and energy flow and ii) the environmental impacts inventory. In addition, the complete set-up and definition of an LCA is usually time-consuming. For these reasons, and considering the high number of possible configurations and technological solutions currently proposed by the R&D and market sectors, the development of a dedicated model for the evaluation of biogas and biomethane solutions may be necessary.
In the present article, a model for the preliminary evaluation of biogas and biomethane solutions is presented. The model is called MCBioCH4 (an acronym for a bio-methane computational model) and focuses on triple targets: i) obtaining information about the productivity of biogas/biomethane plants in terms of achievable gas flow rates; ii) acquiring plant energy expenditures and consequently the economically exploitable energy flow shares (electrical and/or thermal energy produced, biomethane being introduced into the natural gas distribution grid, or biomethane used as a transportation fuel); and iii) accounting for the whole environmental impact of the system on a cradle-to-grave basis: i.e., from substrate production to the end-use of biogas or biomethane as alternative energy sources for fossil fuels.
The design of MCBioCH4 specifically addresses a dual objective: i) to provide support to the preliminary assessment and comparison of different potential plant configurations and technological solutions; and ii) to assist users in the complete definition of mass, energy and environmental flows, through the implementation of default datasets and an assisted data input.
The description of MCBioCH4 model design, structure and validation is reported in the following.

2. Methodology

The computing code was entirely developed using MATLAB® software (Mathworks, 1994) and the result is a stand-alone application fully equipped with graphical user interfaces (GUI). MCBioCH4 was designed with three different modules, for the calculation of mass, energy and GHG balance. Four different possible energy conversions options were implemented:

- biogas combustion with cogeneration of electrical and thermal energy (option B-H);
- biogas combustion with generation of electricity only (option B-NH);
- biomethane to be injected into the national grid at an absolute pressure of 5 atm (option M-G);
- biomethane to be used in transportation, considering a compression and storage system working at 250 bar and consuming an electrical power of around 120 kW (option M-T).

If biogas scenarios are selected, the model simulates combustion in a commercial cogeneration unit (endothermic engine). The recovery of thermal energy can also be specified. If biomethane scenarios are selected, the user is allowed to select the upgrading technology, as well as the main features of the upgrading system. The following technologies are implemented: pressurized water scrubbing (PWS), pressure swing absorption (PSA), chemical absorption with amine solutions (MEA), and membrane permeation (MB). These are considered to be the most common and mature upgrading technologies currently available (Makaruk et al., 2010). Other promising upgrading technologies, such as cryogenic separation (CRY) or those based on carbon mineralization (alkaline with regeneration or bottom ash for biogas upgrading, Starr et al., 2012) were not included, as they are not commonly diffused at present.

MCBioCH4 is structured with simple and clear dialog boxes in such a way as to ease the interaction with low-expertise users. As basic starting information, the user is asked to input the daily mass flow of substrates to be inserted into the digester. Other input parameters, specified in the next sections, can either be provided as default values, or alternatively be specified by the user. The output provided by the model is:

- the detailed mass and energy balance of the system;
- the net mass flow and energy content of the biogas / biomethane stream;
- the greenhouse gases (GHG) balance of the system, including a comparison with an equivalent system powered by traditional (fossil) fuels.

Mass and energy balance of the system may be exported in the form of a scheme in JPEG format. The complete output of the simulations may be exported into Excel® (Microsoft, 2019) format. Once the main input information is inserted, mass, energy and environmental modules may be run separately and interactively modified. The model also allows the loading of external metadata input files. The structure and main features of the modules are reported in the following.

2.1 Mass module

The mass balance module calculates the flow of biogas or biomethane produced, starting from raw substrates characterization. The parameters that define the biogas yield of each substrate are: dry matter fraction (DM), volatile solids fraction (VS) and raw biogas yield (biogas volume per mass unit of volatile solids). For the substrates coming from agriculture, the agricultural yield is also needed. Following a detailed bibliographic review, a set of default substrates, representing the most commonly used matter, was implemented in the model (Table 1). Alternatively, customized input materials may be introduced by the user, as in the case of particular agro-food wastes or municipal solid waste (MSW) organic fractions.

Table 1. Substrates implemented in MCBioCH4 and default yield values

Substrate	Dry matter fraction	Volatile solids / dry matter content	Biogas yield (m^3/t of VS)[a]	Agricultural yield (t/ha)	References
Maize	0.2200	0.9500	550	60	Oslaj et al., 2010; Dubrovskis et al.,2010
Maize silage	0.3300	0.9600	700	60	Brizio, 2012; Panepinto et al., 2013
Sorghum	0.2600	0.9600	550	72	Vindis et al., 2010; Buratti et al., 2013;
Triticale	0.3000	0.9500	625	42	Cantale et al., 2016;
Ryegrass	0.1800	0.8700	540	55	Vítěz et al., 2015
Grass	0.2100	0.8700	500	62	U.S. Environmental Protection Agency, 2013; Sustainable Energy Authority of Ireland, 2014
Cereals	0.2500	0.9500	600	50	Senghor et al., 2017;

					Sustainable Energy Authority of Ireland, 2014
Beetroot	0.2300	0.9200	675	100	Ciuffreda et al., 2010
Cattle slurry	0.0800	0.7500	375		Castelli, 2014; Centro Ricerche Produzioni Animali, 2008
Cattle manure	0.0500	0.6800	500		Castelli, 2014; Centro Ricerche Produzioni Animali, 2008
Swine slurry	0.2300	0.7800	290		Castelli, 2014; Centro Ricerche Produzioni Animali, 2008
Swine manure	0.2400	0.8300	500		Castelli, 2014; Centro Ricerche Produzioni Animali, 2008
Poultry manure	0.6000	0.6500	375		Castelli, 2014; Centro Ricerche Produzioni Animali, 2008
MSW organic fraction	0.2300	0.8700	700		Tyagi et al., 2018; Centro Ricerche Produzioni Animali,, 2008

[a] normal conditions

In this module, the digestion process is simulated. The number of digesters is defined according to the inlet mass flow. Users must then specify the temperature of the process (a mesophilic process is set by default) and the fugitive methane emissions from the digesters, as a fraction of the net biogas produced. Fugitive methane emissions from the cogeneration unit (in the case of biogas options) or from the upgrading system (in the case of biomethane options) may also be specified as a fraction of the net biogas produced.

2.2 Energy module

The energy balance module supplies a detailed picture of energy consumption based on different employed technologies and assumptions. Specific energy consumption factors are implemented in the model, based on a detailed bibliographic review. Different energy streams of the system are defined following a cradle-to-grave approach, i.e., from substrates production to the final end-use of biogas/biomethane. The selection of such an approach is useful for the definition of the environmental burden of different substrates, and is performed by the environmental module. In the case of materials coming from agricultural activities, the energy consumption of the bioenergy chain is calculated based on the use of the specific agricultural yield of the material and a specific energy consumption factor for the selected activity. Energy consumption due to the transportation of the substrates to the processing site is calculated from the following parameters: average distance to be covered (km), transportation medium capacity (t) and average fuel consumption of the transportation medium (L/km). In the case of materials coming from waste, a specific energy consumption factor is used to account for waste collection and transportation. This factor was defined according to the average capacity of organic solid waste collection media and the average distance expected to be covered from the collection point to the biogas/biomethane site.

The net energy production of the plant, i.e., the conversion of biogas/biomethane to useful energy, is simulated depending on the plant option. If biogas options are selected, the model simulates combustion in a cogeneration unit (endothermic engine). The size and features of the conversion unit are directly suggested by the model, based on a complete set of commercial models proposed by the manufacturer Jenbacher (2019). The electrical and thermal efficiency of the engine can be specified by the user. If biomethane options are selected, the useful energy is the energy content of the methane fraction of the biogas

minus the methane losses from the upgrading process.
If the biogas/biomethane scenario selected includes a production of electricity or heat, the auto-consumption terms are discounted from the gross energy production term. Otherwise, an external energy source is also simulated (electrical grid and/or auxiliary boilers) and the user can specify the conversion efficiency.
Energy auto-consumption (electricity and thermal dispersion) of the biogas section of the system (e.g., to the digester exit) can be calculated following two alternative options: i) they can be defined as a ratio of the raw energy output of the system; or ii) they can be introduced as an absolute value (MWh/y). If the first option is selected:

- electricity auto-consumption is calculated by default as 1.3% or 3% of the biogas energy content for an inlet material flow lower or higher than 20,000 t/y, respectively (Poeschl et al., 2010). This value can be customized by the user.
- thermal energy auto-consumption due to substrate pre-heating and maintenance of the temperature into the digesters is calculated by default as 12.5% or 9.6% of the biogas energy content for an inlet material flow lower or higher than 20,000 t/y, respectively (Poeschl et al., 2010). This value can be customized by the user.
- the ratio of thermal energy dispersion to the total heat auto-consumption can also be specified by the user. The default value is set to 20%. This value comes from a publication by Naddeo et al. (2016), reporting a range between 13% and 23%, depending on the characteristics of the system.

If biomethane scenarios are selected, the energy consumption of the upgrading process is calculated depending on the upgrading technology, as well as on the main features of the upgrading system. The following technologies are implemented: pressurized water scrubbing (PWS), pressure swing absorption (PSA), chemical absorption with amine solutions (MEA), or membrane permeation (MB). Consumption is introduced as specific energy (electricity or heat) per volume unit of raw biogas. The default values reported in Table 2 are proposed. Moreover, if PWS upgrading technology is selected, the energy consumption may also be calculated by introducing the main features of the system. In this case, as reported by Brizio (2012) and Ravina and Genon (2015), the main contribution to energy consumption is from biogas compression and water pumping. A partial heat recovery from the compressor may also be calculated.

Table 2. Default values of specific energy consumption of the biogas upgrading technologies implemented in MCBioCH4

Technology	Specific electricity consumption (kWh/m^3 of biogas)	Specific heat consumption (kWh/m^3 of biogas)	Heat recovery from biogas compressor (kWh/m^3 of biogas)	References
PWS	0.20	-	0.11	Khan et al. 2017; Patterson et al. 2011; Bekkering et al., 2010
MEA	0.1	0.5	0.01	Bailón Allegue and Hinge (2012); Lau et al., 2011
PSA	0.4	-	0.03	Collet et al., 2016; Götz et al., 2016; Bauer et al., 2013
MB	0.3	-	-	Meier et al., 2015; Bauer et al., 2013

2.3 Environmental module

The environmental balance module interacts with the mass and energy modules, and provides an estimation of greenhouse gases (GHG) emitted by different plant configurations. Emissions are represented in terms of CO_2 equivalent (CO_{2eq}) of the entire

complex of activities that directly or indirectly concern the biogas/biomethane plant, based on a cradle-to-grave approach, i.e., from feedstock cultivation/production to biogas/biomethane final energy conversion.
Specific customizable emission factors are assigned to the different phases of the process. The emission factor of agricultural substrates production and harvesting is calculated as the sum of three components: fuel consumption in agricultural operations; production and use of fertilizers; and N_2O emissions (direct and indirect). Emission factors associated to fuel consumption are calculated for each substrate based on the specific fuel consumption (l/ha) reported by Cropgen (2004) and Astover et al. (2015). Emission factors for fertilizer use are calculated based on average CO_{2eq} emission factors for nitrogen (N), phosphorus (P) and potassium (K) production, considering average standard N, P and K contents. Emission factors for N_2O were taken from the database of the Intergovernmental Panel on Climate Change (2013) and Astover et al. (2015). The default emission factors implemented in MCBioCH4 are given in Table 3.
Emissions generated along with the biogas/biomethane production process are then compared to the emissions reduction attributable to the replacement of fossil fuels.

Table 3. Default emission factors implemented in MCBioCH4

Phase of the process	Value	Unit	References
Methane losses (methane GWP)	28	kg of CO_{2eq}/kg of CH_4	Intergovernmental Panel on Climate Change, 2013
Substrate production (diesel fuel consumption)	Depending on substrate	L/ha	Astover et al., 2015; Cropgen, 2004
Fertilizer production (N / P / K)	2900 / 710 / 460	g of CO_{2eq} /kg of fertilizer	Intergovernmental Panel on Climate Change, 2013
N_2O emissions in agricultural activities	Depending on substrate	kg of CO_{2eq} /ha	Intergovernmental Panel on Climate Change, 2013; Astover et al., 2015; U.S. Environmental Protection Agency, 2013
Substrates temporary storage	1.74	g of CO_{2eq} /MJ of biogas	Buratti et al., 2013
Substrates transportation / handling	74.1	g of CO_{2eq} /MJ of diesel fuel	Intergovernmental Panel on Climate Change, 2013
Electricity from national grid	337.1	g of CO_{2eq} /kWh	Italian Higher Institute for Environmental Research, 2017
Natural gas combustion	206	g of CO_{2eq} /kWh	Intergovernmental Panel on Climate Change, 2013
Fossil fuel mix for transportation	256	g of CO_{2eq} /kWh	Intergovernmental Panel on Climate Change, 2013; Italian National Association of the Automotive Industry, 2017

2.4 Model calibration and case study

MCBioCH4 was tested and calibrated simulating a test case representing a biomethane production plant through anaerobic digestion of cattle manure and maize silage. This plant does not correspond to any specific existing site, but is representative of the most common commercial size and configuration in Italy (Centro Ricerche Produzioni Animali, 2008). An M-G option (biomethane injected into the national gas grid) with PWS upgrading technology was used for the base case simulation. Parallel simulations were then run considering alternative upgrading technologies (MEA, PSA, MB), and the results of the environmental balance were compared.
Unless specified otherwise, the default parameters proposed by the model were used for

the simulations. The inlet flow of material to the anaerobic digester consisted of 47.5 t/d of maize silage and 48.5 t/d of cattle slurry. The methane loss from the upgrading process was estimated to be 1.4%. The average distance coverage for substrate transportation was set to 10 km. The amount of electricity auto-consumed by the biogas section was estimated to be 400 MWh/y, according to Buratti et al. (2013). The thermal energy needed for substrates and digester heating was set to 11.2% of the raw biogas energy content. For the different upgrading technologies, the default values reported in Table 2 were used. To achieve a first model validation, the same plant (base case) was reproduced on another simulating platform, namely the SmartBiogas platform, created by Monviso Agroenergy Consortium (2019). SmartBiogas is a free on-line model for the preliminary simulation of biogas and biomethane plants. The comparison of the results was possible for mass and energy balance only, as this platform does not calculate GHG emissions. The results of the simulations are reported in the following.

3 Results

Mass and energy balances of the system, base case simulation, are reported in Figures 3 and 4. The schemes reported herein were directly generated by MCBioCH4 and exported in JPEG format. Raw biogas production of the plant amounted to 17.81 t/d. Part of the biogas was lost to the atmosphere (0.054 t/d), while the digestate production amounted to 78.08 t/d. The upgraded biomethane flow (CO_2 residual content below 3%) was 5.54 t/d. The net energy content of the biomethane amounted to 26,322 MWh/y (98.6% of the biogas energy content). Primary energy consumed for the plant auxiliary systems amounted to 2,877 MWh/y for thermal energy and 1,346 MWh/y for electricity. Of this latter term, around 65% was consumed by the biogas upgrading section and the rest by the biogas production section. A partial recovery of 343 MWh/y from the biogas compressor stage was also suggested by the model.
The comparison with the simulation of the same plant using the SmartBiogas platform is reported in Table 4. The two models present some slight differences, although the magnitude of the results is close to equality. With respect to SmartBiogas, the conversion rate of the substrates to biogas calculated by MCBioCH4 is lower (-3.3%), corresponding to a higher production of digestate (+1.8%). This difference is counterbalanced in the biogas upgrading section, where the SmartBiogas model assumes higher methane losses (+7%), meaning a less efficient upgrading process. Net biomethane production is approximately the same for both models. Other differences in the results may be attributed to minor assumptions implemented in the models (e.g., the use of water), or differences in the conversion factors (e.g., biogas and biomethane density, heating values).
The results of the environmental GHG balance are reported in Table 5, where different upgrading technologies are compared, based on the same digestion section and assuming the same amount of methane loss from the upgrading process (1.4%). Produced (positive) emissions are accounted for, and compared to the equivalent replaced (negative) emissions, generated by a process based on natural gas combustion. Thus the result depends only on the specific energy consumption of each upgrading technology. MB technologies showed the highest emission reduction (0.5014 t of CO_{2eq}/t of biogas, 2986 t of CO_{2eq}/y), followed by PWS (0.4934 t of CO_{2eq}/t of biogas, 2939 t of CO_{2eq}/y), PSA (0.4137 t of CO_{2eq}/t of biogas, 2464 t of CO_{2eq}/y) and MEA (0.4100 t of CO_{2eq}/t of biogas, 2441 t of CO_{2eq}/y).

Table 4. Results of the simulations of the test plant with MCBioCH4 and SmartBiogas models

Phase of the process	MCBioCH4	SmartBiogas	Difference %
Biogas production (t/y)	6,502	6,728	-3.3%
Digestate production (t/y)	28,498	27,992	+1.8%
Upgraded biomethane (t/y)	2,023	2,026	-0.1%
Biomethane loss from the upgrading system (t/y)	26.46	28.36	-7.1%
Raw energy content of the biogas (MWh/y)	26,695	28,312	-6.0%
Net energy content of the biomethane (MWh/y)	26,321	25,493	+3.2%

Table 5. Environmental balance of the test case simulation. Comparison of different upgrading technologies (unit: t of CO_{2eq} /t of biogas).

Process phase	PWS	MEA	PSA	MB
Substrates production	0.0575	0.0575	0.0575	0.0575
Substrates transportation/handling	0.0183	0.0183	0.0183	0.0183
Substrates temporary storage	0.0277	0.0277	0.0277	0.0277
Biogas loss from digesters	0.0244	0.0244	0.0244	0.0244
Electricity consumption (biogas section)	0.0236	0.0236	0.0236	0.0236
Thermal energy consumption (biogas section)	0.0996	0.1124	0.1124	0.1007
Methane loss from upgrading process	0.1137	0.1137	0.1137	0.1137
Electricity consumption (upgrading section)	0.0526	0.0299	0.1194	0.0435
Thermal energy consumption (upgrading section)	-	0.0933	-	-
Replacement of fossil fuels (natural gas)	-0.9107	-0.9107	-0.9107	-0.9107
Total (produced emissions)	0.4173	0.5008	0.4970	0.4093
Total (reduced emissions)	-0.9107	-0.9107	-0.9107	-0.9107
Difference	**-0.4934**	**-0.4100**	**-0.4137**	**-0.5014**

4 Discussion

The results of test case simulation confirm that, in general, biomethane production brings a significant reduction of GHG emissions compared to traditional fossil fuels. Several studies reported in the bibliography confirm this result. A study by Poeschl et al. (2012) reports a GHG saving of around 1722 t of CO_{2eq} /y for a biomethane plant. Another study by Power and Murphy (2009) reports GHG emission reduction for an M-T scenario, of between 1295 and 1524 t of CO_{2eq} /y, depending on the substrates composition. A work by Buratti et al. (2013) reports a specific emission of 0.947 t of CO_{2eq} /t of biogas produced by a biomethane production plant for transportation use. Nevertheless, the impact induced by biogas/biomethane plants on global warming largely depends on the different phases of the process, and needs to be studied case by case (Paolini et al., 2018). A number of factors have been evidenced to influence global GHG emissions of biogas/biomethane plants. The selection of the substrates (Poeschl et al., 2012), the limitation of methane fugitive emissions (Flesch et al., 2011) and the digestate management (Tufvesson et al., 2013) have been shown to contribute significantly to the GHG balance of the plant. For biomethane production, the selection of biogas upgrading technology represents the key-factor (Starr et al., 2014). The implementation of sensitivity analysis with the MCBioCH4 model could provide support toward the definition and preliminary design of environmentally sustainable bioenergy systems.

The test case reported in this study focused on the contribution of different upgrading technologies, to the total GHG balance of the process. The results provided by the

environmental module should be integrated with additional considerations on the technical and economical sustainability of each upgrading technology. MB technology yielded the highest CO_{2eq} emission reduction. Considering that this is a highly reliable and cheap process with low energy consumption (Molino et al., 2013), it is expected that MB will capture the greatest part of the market share in the future (Makaruk et al., 2010; Deng and Hägg, 2010). PWS is still the most common and well-established technology used to remove CO_2 and H_2S from biogas (Xu et al., 2015). Although it is an eco-friendly and highly efficient process with no special chemical requirements, the specific energy consumption increases if the water regeneration process is taken into account (Eze and Agbo, 2010). PSA technologies need extensive process control and require high investment and operational costs (Cavenati et al., 2005; Gomes and Yee, 2002). In addition, the eventual recovery of the off-gas plays a key role in the environmental sustainability of this process (Augelletti et al., 2017; Pertl et al., 2010). MEA is a highly efficient technology (Leonzio, 2016). The main drawback of chemical absorption processes is the high specific energy consumption, as very high temperatures, sustained over a period of time are needed to regenerate chemical solvents (Sun et al., 2015).
Besides these considerations, it must be pointed out that the results of this test case are highly dependent on the specific energy consumption assigned to each upgrading technology. As reported by Sun et al. (2015), the specific energy consumption of the upgrading technologies may present some variability depending on the operating conditions.
The comparison of test case simulations of MCBioCH4 with another evaluation model (namely the SmartBiogas platform of Monviso Agroenergy Consortium) provided a first model validation of the sections related to mass and energy flow accounting. The results of the two models vary between 0.1% and 7%, depending on the phase of the process considered. In general, the biogas production calculated by MCBioCH4 is lower, while the final energy content of the upgraded biomethane is slightly higher. Net biomethane production, however, is equal. Such differences may be attributed to minor assumptions implemented in the models, such as substrate/biogas conversion factors, fugitive methane emission rates, or external energy source conversion factors. Additional simulations should be run to clarify these details. Validation of the environmental module was not possible, as no model with similar features and scope was found in the bibliography or elsewhere.
With regard to the geographic applicability of the model, the possibility of introducing customized parameter values represents a significant advantage for the evaluation of different alternative solutions with MCBioCH4, including in the case of non-conventional plant typologies. This customization supports a wide range of plant configurations, in terms of substrate input, operating conditions, conversion technology and biogas/biomethane end use. For this reason, in principle, this model is suitable for worldwide application. Nevertheless, it is worth pointing out that the default parameter values, if possible, should be adapted to the specific country or local conditions. In addition, new biomethane production and conversion schemes are increasingly being developed worldwide, and additional efforts and integrations are therefore needed, to extend the applicability of the model. To give some examples, biomethane production and conversion processes are increasingly being adapted to extreme climates, such as colder regions (Dev et al., 2019), or to complex multi-product supply chain frameworks (e.g., Sampat et al., 2018). Similarly, input feedstock parameters should be integrated with those related to byproducts commonly considered in developing countries (Morgan et al., 2018). Avoided GHG emission rates, which depend on the assumed final use of biogas/biomethane, should also be adapted to the local or national conditions and policies under study (Ahmed et al., 2016, Kemausuor et al., 2018).

5 Conclusions

This article has presented MCBioCH4, a model for mass, energy and greenhouse gas emission flow accounting of biogas/biomethane solutions. MCBioCH4 was designed as highly flexible standalone software, to be used for a preliminary evaluation of the environmental sustainability of different process configurations and technological alternatives. The model's structure makes it appropriate for employment at the preliminary planning stage. The implementation of a clear and detailed graphical user interface makes it suitable to different levels of expertise. The definition of input data is supported by a set of default parameters obtained from a detailed bibliography review. In addition, it allows for the introduction of customized input values, representing a significant advantage for the evaluation of alternative solutions.

Compared to other existing evaluation tools, MCBioCH4 presents two main innovations. The first is the calculation of the greenhouse gas flows and balance over the entire bioenergy chain, based on a cradle-to-grave approach. This approach was inspired by life cycle assessment methodologies. It may thus be considered a simplified LCA approach, with the advantage of a more detailed and faster quantification of the impacts. Integrating the preliminary design of biogas/biomethane solutions with detailed information on the environmental burden is essential, as national and international energy planning strategies depend more and more on sustainability criteria.

Another important feature of MCBioCH4 is the detailed characterization of the material entering the digestion process. A large set of existing materials is already implemented in the model, and the possibility of a customized definition is contemplated. This provides support for the evaluation of possible alternative systems based on the production of so-called advanced biomethane, i.e., biomethane coming from agro-industrial byproducts or organic fractions of municipal solid waste. The main disadvantage detectable at present is that no action for digestate management is implemented in the model. This aspect could constitute the next step in the development of MCBioCH4.

In conclusion, the MCBioCH4 model represents a useful support for the increase in environmentally sustainable bioenergy production planned by both European and non-European countries. It thus provides valuable support to project developers and administrations in defining the most economically and environmentally sustainable plant configurations.

Conflict of interest

The authors declare no conflict of interest.

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Table 1. Substrates implemented in MCBioCH4 and default yield values

Table 2. Default values of specific energy consumption of the biogas upgrading technologies implemented in MCBioCH4

Table 3. Default emission factors implemented in MCBioCH4

Table 4. Results of the simulations of the test plant with MCBioCH4 and SmartBiogas models

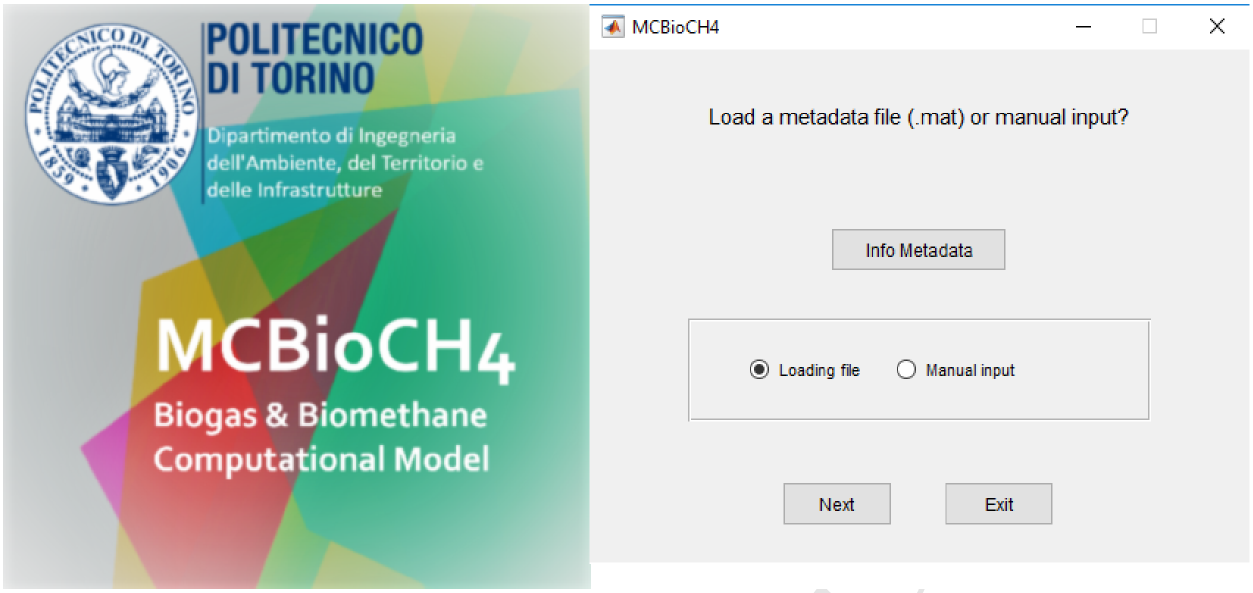
Table 5. Environmental balance of the test case simulation. Comparison of different upgrading technologies (unit: t of CO_{2eq} /t of biogas).

Figure 1. Logo and entry page of MCBioCH4 model

Figure 2. General scheme of MCBioCH4 model.

Figure 3. Mass balance of the test case simulation with PWS upgrading technology

Figure 4. Energy balance of the test case simulation with PWS upgrading technology


POLITECNICO DI TORINO
Dipartimento di Ingegneria dell'Ambiente, del Territorio e delle Infrastrutture
MCBioCH4
Biogas & Biomethane Computational Model
MCBioCH4
Load a metadata file (.mat) or manual input?
Info Metadata
Loading file
Manual input
Next
Exit

1. **Inputs**: substrates and plant technologies characterization

a. Substrates

- Energy crops
- Agricultural residues
- Organic Fraction Urban Solid Wastes

b. Plant technologies

B-H	Anaerobic digester	CHP	
B-NH	Anaerobic digester	CHP no therm	
M-G	Anaerobic digester	Upgrading *	Grid injection (5 bar)
M-T	Anaerobic digester	Upgrading *	Storage (250 bar)

2. Outputs

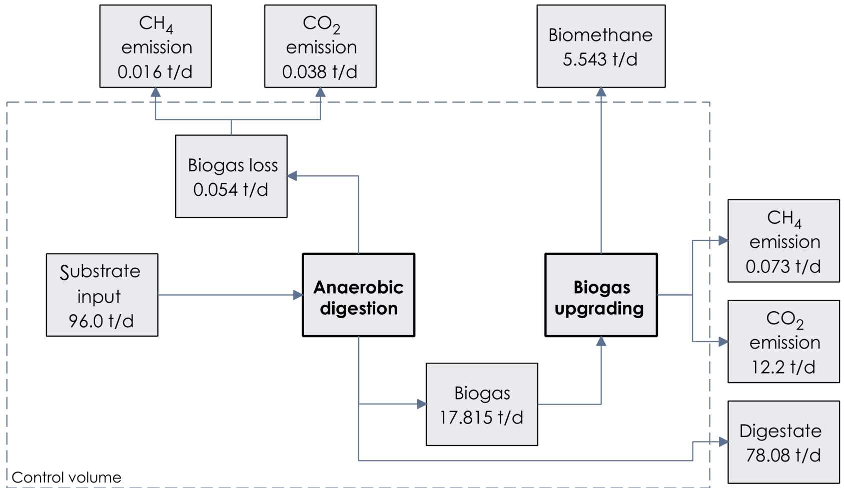
a. Tables

- Biogas & Biomethane
- CH_4 and CO_2 emissions
- Energy plant consumption
- Energy gained

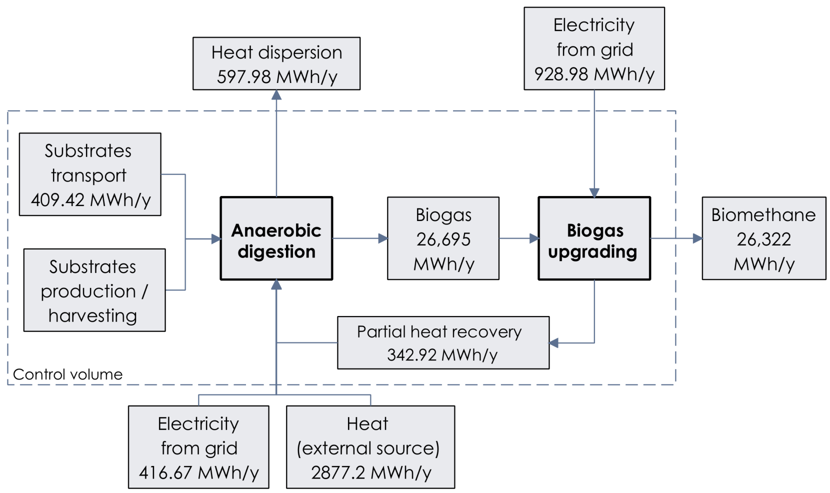
b. Plant Flowchart

c. Export data in Excel™

* Upgrading tecnologies: PWS, MEA, PSA and MB (references in scientific literature)



CH_4 emission 0.016 t/d
CO_2 emission 0.038 t/d
Biomethane 5.543 t/d
Biogas loss 0.054 t/d
CH_4 emission 0.073 t/d
Substrate input 96.0 t/d
Anaerobic digestion
Biogas upgrading
CO_2 emission 12.2 t/d
Biogas 17.815 t/d
Digestate 78.08 t/d
Control volume



Heat dispersion
597.98 MWh/y
Electricity
from grid
928.98 MWh/y
Substrates
transport
409.42 MWh/y
Substrates
production /
harvesting
Anaerobic
digestion
Biogas
26,695
MWh/y
Biogas
upgrading
Biomethane
26,322
MWh/y
Partial heat recovery
342.92 MWh/y
Control volume
Electricity
from grid
416.67 MWh/y
Heat
(external source)
2877.2 MWh/y

- MCBioCH4 model performs an evaluation of biogas and biomethane plant configurations
- It calculates the potential plant productivity and equivalent CO2 emissions
- The model is a standalone application with a user-friendly graphical interface
- Default input parameters are provided, or these may be customized by users
- The model was tested and successfully validated on a case study

Keywords:

bioenergy, biogas modelling, biomethane upgrading, greenhouse gas emission, CO2 equivalent