Chapter 5
Net Energy Production of H_2 in Anaerobic Digestion

In this chapter the analysis of net energy production by H_2 in anaerobic digestion (AD) is considered. The net energy production has previously been defined and evaluated by using the experimental data reported in Chap. 4, taking into account the effect of temperature on H_2 production. The net energy produced was evaluated by the difference between the energy produced in the form of H_2 and the total energy used to run the plant. We take into consideration the energy balance of a batch anaerobic bioreactor, following a geometrical scale-up procedure in order to take into account the thermal as well as the electrical energy necessary to run the bioreactor.

5.1 Introduction

The important role of temperature and pH on fermentative hydrogen production was shown in Chap. 4. In particular, the increase in temperature could increase the ability of HPB to produce hydrogen during fermentation, but temperatures at higher levels (40–50 °C) cause a decrease in the hydrogen produced, shifting the biological pathways towards the production of other compounds, like lactic acid. While we have limited our considerations to improve the H_2 production by affecting the microorganisms, such as by altering temperature and pH, there is another important aspect that should be taken into consideration: the net energy production by the AD technology. The temperature is the most important parameter from an energetic point of view, because it influences not only the energy produced but also the energy necessary to run the bioreactor. Hence the temperature is the most important design parameter of a full-scale bioreactor producing energy by AD, due to its key role in the net energy balance of the technology [1]. Despite these facts, very few papers address the whole energy balance of hydrogen from AD [2]. Considering that the hydrogen bioreactor plant's purpose is to produce energy, a detailed analysis of the energy balance of the bioreactor is of the utmost important in the

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selection of the operative working conditions, in order to find the most appropriate conditions needed to maximize the net energy production of the full-scale plant.

The present chapter aims to construct a scale-up methodology using the experimental bench-scale data of an anaerobic bioreactor operated in batch mode. The energy balance of full-scale dark AD will be determined in order to evaluate the quantity of net energy produced from a carbonaceous substrate as a function of two parameters: the working temperature and the diameter of the bioreactor. The net energy produced is evaluated as the difference between the energy produced and the total energy used to run the system at the working temperature. This latter term is composed of the heat used to keep the reactor at each working temperature, the heat lost from the bioreactor walls through natural convective phenomena [3] and the electrical energy used for mixing and pumping purposes. To define the optimal working temperature, the energy balance was calculated in relation to several operating parameters such as outdoor temperature and insulation materials, while considering the bioreactor diameter as the scale-up parameter.

5.2 Maximum Obtainable Energy

In order to evaluate the maximum obtainable energy, an important issue is how to appropriately evaluate and express the H_2 production yield and conveniently convert it into a parameter representing the conversion efficiency attained by the AD. The H_2 yield may, in turn, be expressed in terms of energy units. The concept of conversion efficiency derives from the existence of biological barriers to hydrogen production from organic substances that has been elucidated by considering the conversion of a simple carbohydrate, such as glucose, in the previous chapters. It is important to recall here (Eq. 5.1) that if complete glucose conversion is taken into account, 12 mol of H_2 can theoretically be produced from 1 mol of glucose:

$$C_6H_{12}O_6 + 6H_2O \rightarrow 12H_2 + 6CO_2 \tag{5.1}$$

This direct conversion of glucose into hydrogen, unfortunately, is not feasible at the moment in the sense that microorganisms are not able to carry it out. The real conversion potential, in fact, is lower than this theoretical value. At best, the conversion of glucose into hydrogen is limited to acetate production and is therefore 4 mol H_2/mol glucose (Eq. 5.2); in practice only one third of the hydrogen production can be achieved, since part of the energy present in the original glucose remains embedded in the acetate.

$$C_6H_{12}O_6 + 2H_2O \rightarrow 4H_2 + 2CO_2 + 2CH_3COOH \tag{5.2}$$

Organic intermediate compounds act as electron acceptors, decreasing the H_2 generation yield. In the case of the butyrate fermentation pathway, the conversion efficiency is reduced to 2 mol H_2/mol glucose:

$$C_6H_{12}O_6 \rightarrow 2H_2 + 2CO_2 + CH_3CH_2CH_2COOH \tag{5.3}$$

The production of more reduced fermentation products, compared to acetate, is optimized in nature to sustain microbial growth and, conversely, not to produce H_2: it represents an energy waste from the point of view of microorganisms. This is primarily due to the fact that the electrons generated from the oxidation of substrate could be used in the metabolic pathways to produce many chemicals. Among them are propionate, butyrate, lactate, formate, ethanol, butanol, alcohols and ketones, with associated longer aliphatic acids which allow for NADH re-oxidation [4]. Taking into account the above considerations, the energy conversion efficiency may be calculated on a mass or energy basis. From an energetic perspective, the hydrogen production efficiency may be evaluated as expressed by Eq. 5.4, considering the fraction of the total energy content of the substrate recovered in the form of hydrogen:

$$\eta = \frac{\text{Energy content in produced } H_2}{\text{Energy content in the substrate}} \times 100 \tag{5.4}$$

Assuming 2,882 and 239.2 kJ/mol as lower heating values (LHVs) of glucose and hydrogen, respectively, energy conversion efficiencies of 33 and 17 % are calculated if the acetate (Eq. 5.2) or the butyrate (Eq. 5.3) fermentation pathways, respectively, are assumed to occur. These values represent the maximum energy obtainable from glucose; in practice, considering the experimentally evaluated H_2 yield from glucose, it is possible to evaluate a mean value from different literature data [5]:

$$Y = 1.76 \pm 0.85\ \text{mol}_{H_2}/\text{mol}_{\text{glucose}} \tag{5.5}$$

with a relative uncertainty value of U = 48 % considering different experimental results. Hence the energy efficiency is η = 15 ± 9.8 %: this means that butyrate fermentation is predominant and that acetate fermentation is present only in some cases, as experimentally confirmed by results reported in Chap. 4. It is important to emphasize the higher uncertainty present in the literature data. This explains why in practice energy efficiencies higher than 15 % of the original electrons present in the substrate towards H_2 can rarely to be obtained, even under optimal process conditions. The above consideration concerns glucose, which is the most easily biodegradable substrate, but it is not suitable to be used as feedstock to produce energy in full plant applications. For this purpose, organic refuse, generally called biowaste, from the alimentary chain is usually the candidate: from farm producers, from consumers and from food production firms (Chap. 6). The evaluation of the amount

Table 5.1 Units used to evaluate hydrogen production by anaerobic fermentation

mol H_2/mol_{Gl}	mol H_2/mol_{Esose}	mmol H_2/g_{Carbon}
mol H_2/$mol_{Esose\ added}$	mmol H_2/g_{COD}	mL H_2/$g_{VSadded}$
L H_2/kg_{COD}	L H_2/$L_{Reactor}$	L H_2/$g_{VSconsumed}$

of energy converted into hydrogen becomes difficult in the case of biowaste, because different authors use different units at laboratory or pilot plant scales. Table 5.1 gives a brief list of the units present in the literature. Nevertheless, the evaluation of efficiency of biohydrogen production using organic wastes is of utmost importance, both from the research point of view and for technology scale-up purposes; the following section tries to answer this question.

5.3 Energy Conversion Parameters

For the purpose of comparing different results and in order to have a useful engineering parameter, the suggestion to evaluate the energy conversion by using two energy parameters is put forward. The first parameter, efficiency (η), is used to take into account the quantity of energy produced as hydrogen that the bioreaction is able to extract, with reference to the available amount of energy embedded in the substrate. Equation 5.4 can be written in the following way:

$$\eta = E_p/E_0 \cdot 100 \tag{5.6}$$

where E_p is the total energy produced as H_2 and E_0 is the energy embedded in the substrate.

η can refer either to a mass or volume unit, but in the authors' opinion, in the present context, the use of a mass unit is preferred. The energy produced (E_p) can be evaluated through the following expression:

$$E_p = \mathrm{mol}_{H_2} * \mathrm{LHV}_{H_2} / C_{TS0} \tag{5.7}$$

where mol_{H_2} (mol/L) is the quantity of hydrogen produced per unit of fermenting broth, calculated using the experimentally evaluated volume and the ideal gas equation to take into account the working pressure and temperature; LHV_{H_2} is the lower heating value of hydrogen per mol (239.2 kJ/mol); and C_{TS0} (g_{TS0}/L) is the concentration of the fermenting broth expressed in total solids. The energy produced is thus relative to the total solids added. A good estimation of E_0 can be obtained using the LHV in kJ/g_{TS} of each substrate. Some comments on this aspect are necessary. The question of what is the "available" energy arises, and the answer is that it is the total edible energy, i.e. the energy which can be utilized by a living cell. This means that not all the C–C or C–H bonds are of the same quality; only some are utilizable by the cell machinery. As an example one can consider crude oil: it contains a large quantity of energy (with a very high LHV), but only a small

proportion of it is edible. Considering on the other hand glucose as a carbon source, all the chemical energy embedded in the glucose is edible, as generally accepted by biologists. In numerical terms the available energy of the glucose is 2,882 kJ/mol, which is the LHV of glucose. Considering organic refuse in term of chemical bonds which are able to store the chemical energy, a combination of different edible and inedible chemical energy present in the refuse can be envisaged. For instance sugar, cellulose, lignine and other combinations of C–C or C–H bonds present different degrees of edibility in terms of a macro-approach. Unfortunately, we do not at the moment have a probe able to measure the edible energy compared with the inedible, except in the case of biological tests. In other words we can evaluate the edible energy after a fermentation test, thus including in this the efficiency of the fermentation itself. Moreover, one can measure the total energy present in a refuse or a mixture of different ones by experimental determination of LHV. Hence the efficiency η, i.e. the energy produced as hydrogen from the available energy embedded in the refuse (LHV), is a parameter that can give us information relating to the ability of the biological process (microorganisms in such conditions as working parameters, bioreactor design etc.) to use the edible energy present in the organic refuse. η is global information on the technology used. Considering crude oil as a substrate, for example, the efficiency is very low using AD technology, contrary to what occurs with other technologies such as gasification or combustion. LHV is easily measured by means of a bomb calorimeter; some values for different suitable substrates are shown in Table 5.2.

The second parameter that one can use is the efficacy ζ, which takes into account the efficiency of the actual test and that obtained with glucose under the same conditions. In this way, it is possible to easily evaluate the effectiveness of the applied (or candidate) technology: the more ζ approaches glucose efficiency, the more the technology of anaerobic digestion (including microorganism consortium, working condition, type of bioreactor used etc.) is effective in the recovery of the energy embedded in the substrate. In addition, the parameter ζ permits the scoring of different working conditions for the technology and permits a fruitful comparison

Table 5.2 Experimentally evaluated LHV of several substances suitable for H_2 production

Substrate	LHV (kJ/kg_{TS})
Glucose	16,540 ± 80
Organic market waste	16,376 ± 150
Coffee seed skin	17,730 ± 45
Coffee grounds refuse	21,226 ± 150
Cooking refuse	18,350 ± 70
Rice stalk	13,710 ± 120
Sorghum	17,861 ± 65
Industrial honey refuse	11,123 ± 95
Sawdust	16,302 ± 85

for scale-up decisions. Therefore, the higher the efficacy value, the greater the effect of recovering energy in the form of hydrogen.

Lastly, considering the glucose efficiency value of Eq. 5.5 that has been experimentally evaluated, a considerable portion of carbon-reducing equivalents, and consequently the energy content of the original substrate, remains embedded in the chemicals present in the effluent from the hydrogen phase. In order to maximize the overall conversion yield and to ensure adequate substrate degradation, the biohydrogen production process should thus be thought of as part of a combined process where additional energy production and enhanced substrate conversion are attained in different process stages. These aspects will be discussed in detail in Chaps. 7 and 8.

5.4 Net Energy Balance

The net energy produced in an AD bioreactor producing H_2 corresponds to the difference between the energy contained in the gas produced per unit of bioreactor volume in a single batch run, or per unit time in the case of continuous running, under certain conditions, and the energy used to obtain and maintain the reaction conditions. To calculate the net energy balance, all the energy quantities were evaluated in energy units per unit volume of bioreactor (MJ/m^3; MJ/(m^3 day)), and thus a reference volume and a reference time period in which each term must be calculated need to be considered. In addition, as a consequence of the fact that many data are available only at laboratory scale because dark anaerobic hydrogen production has not yet reached full industrial maturity, a scale-up criterion is necessary. A geometric scale-up criterion of the bench bioreactor in order to evaluate the influence of the scale has been used. The diameter D of the bioreactor was selected as a scale-up parameter in order to evaluate the net energy, using a cylindrical digester geometry with a constant ratio of 4 between the height (L) and diameter (D) and a constant ratio of 2 between the reactor diameter and that of the mixer one (d), as in the bench-scale bioreactor used. The net energy production E_{net} may be calculated in the case of batch and continuous reactor operation modes as:

$$E_{net} = E_{H_2} - (E_h + E_l + E_m + E_p) \tag{5.8}$$

where

E_{H_2} Energy produced [MJ/m^3]; [MJ/(m^3 day)]
E_h Heating heat [MJ/m^3]; [MJ/(m^3 day)]
E_l Energy loss [MJ/m^3]; [MJ/(m^3 day)]
E_m Energy for mixing [MJ/m^3]; [MJ/(m^3 day)]
E_p Energy for pumping [MJ/m^3]; [MJ/(m^3 day)].

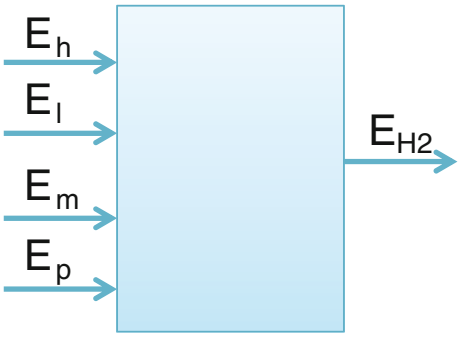

Fig. 5.1 Global view of the energies involved in the net energy balance of H_2 AD bioreactor

The evaluation of the net energy produced was performed by considering the hydrogen produced as a function of the working temperature, as well studied and recognized in the literature [6]. The calculation of the net energy production requires the evaluation of the heat demand necessary to keep the system at the working temperature. The heat required to keep the fermenting biomass at T_w is the sum of the heat used to warm the feeding biomass from the ambient outdoor temperature T_a to T_w, the heat lost from the digester walls, depending on the geography of the plant location, the seasonal variation and, obviously, the night/day oscillation, and the heat withdrawn from the out-stream in the case of continuous operation run.

Figure 5.1 is a global view of the energies involved in the energy balance of the H_2 reactor. Each energy term of Eq. (5.8) will be elucidated in the following sections, using as evidence the equations used in the scale-up procedure as a function of D.

In Table 5.3 several literature cases are reported: they show the best working temperature which maximizes the hydrogen production per unit of working volume along time necessary to reach this production in batch tests. This information is of utmost important in order to calculate the energy balance, because the time affects the energy used for agitation and that lost by natural convection across the bioreactor walls.

5.4.1 Energy Production

The energy produced per unit volume of reactor is the total energy contained in the gas produced relative to the reactor volume, i.e. the energy contained in the amount of hydrogen retrieved from a single batch run (or per unit time in the case of continuous mode); it can be calculated as:

Table 5.3 Maximum specific hydrogen production per unit of volume and working temperature for batch bioreactors

References	Substrate	Microorganisms	Initial pH	$T_{w,\max}$ (°C)	Running time (h)	Productivity (mmol H_2/L)
Wang and Wan [7]	Glucose	Mixed culture	7.0, no control	40	25	123
Zhang and Shen [8]	Sucrose	Mixed culture	8.0, no control	35	25	207
Mu et al. [9]	Glucose	Mixed culture	Control at 5.5	41	24	91
Tommasi et al. [10]	Glucose	Mixed culture	7.5, no control	25–26	50	60
Ruggeri et al. [11]	Glucose	Mixed culture	Control at 5.2	35	340	442
Gadhamshetty et al. [12]	Sucrose	Mixed culture	8.5, no control	22	466	120
		Mixed culture	8.5, no control	37	90	50
Tang et al. [13]	Cattle wastewater	Mixed culture	Control at 5.5	45	30	8
Karadag et al. [14]	Glucose	Sediments from geothermal hot spring	6.5, no control	51.7	16	625

$$E_{H_2} = F \cdot P_{H_2}(T_w) \cdot LHV_{H_2} \tag{5.9}$$

where $P_{H_2}(T_w)$ is the specific production of H_2 and represents the amount of H_2 produced in a single batch run expressed as Nm^3/m^3 (or per day for a continuous bioreactor, $Nm^3/(m^3\ day)$), which depends on the working temperature. LHV_{H2} is the lower heating value of hydrogen (10.8 MJ/Nm^3) and F is the liquid contained in the reactor, i.e., the fraction of reactor volume filled by liquid, usually assumed to be $F = 0.9$.

5.4.2 Heating Heat

The energy required to warm up the fermenting broth mainly depends on its specific heat (c_p), the difference between ambient outdoor T_a and working temperature T_w, and the efficiency of the heating system η_C. The necessary heating energy per unit volume (kJ/m^3) of the bioreactor may be calculated either as:

$$E_h = \frac{(\rho \cdot c_p \cdot \Delta T \cdot F)}{\eta_c} \tag{5.10}$$

in the case of a batch bioreactor, or as:

$$E_h = \frac{(\rho \cdot c_p \cdot \Delta T \cdot F)}{\eta_c \cdot \mathrm{HRT}} \tag{5.11}$$

in the case of a continuous bioreactor,
where:

ρ	is the biomass density [kg/m^3]
c_p	is the biomass specific heat [kJ/(kg °C)]
$\Delta T = (T_w - T_a)$	according to the season [°C]
η_C	is the global efficiency of the system to furnish the heat taking into account η_{comb} and η_{exc}
HRT	is the hydraulic retention time of the liquid in the bioreactor [day].

As sufficient assumptions, the ρ and c_p of water were used for the fermenting broth. The warming device was considered to be composed of a combustion boiler ($\eta_{\mathrm{comb}} \approx 0.8$) and a heat exchanger ($\eta_{\mathrm{exc}} \approx 0.6$); the global efficiency of the warming system was calculated as the product ($\eta_C \approx 0.48$). The outdoor ambient temperature needs to be considered for different seasonal conditions, e.g., summer and winter conditions. T_a needs to be calculated on the basis of historical data; mean night and day values over the season could be considered in order to avoid an increase in computational complexity. A heat recovery of 50 % seems a good assumption, i.e. 50 % of the heat of the broth is recovered by adequate heat exchange at the end of the batch run or of the out-flow rate. The warming of the reactor wall and insulator and that of the NaOH solution necessary to maintain the pH at low value were neglected.

5.4.3 Heat Loss

The difference between the working temperature of the broth T_w and the ambient temperature T_a outside the reactor is responsible for the heat loss from the bioreactor. The lost energy must be supplied from the heating device of the temperature control system and it depends on the insulation of the fermenting broth from the external environment and the exposed surface. The necessary energy used to replace the heat loss per unit volume of reactor may be calculated as:

$$E_l = \frac{\left(4.5 \cdot \frac{k}{s} \cdot \Delta t(T_w) \cdot \frac{\Delta T}{D}\right)}{\eta_c} \tag{5.12}$$

in the case of a batch run; while the following equation allows its evaluation in the case of a continuous reactor:

$$E = \frac{(4.5 \cdot k/s \cdot 24 \cdot \Delta T/D) + (\rho \cdot Cp \cdot F \cdot Tw/\mathrm{HRT})}{\eta_c} \tag{5.13}$$

where:

k	is the thermal conductivity of the digester walls [kJ h^{-1} m^{-1} $°C^{-1}$]
s	is the thickness of the reactor/insulator walls [m]
Δt (T_w)	is the total duration of fermentation [h]
D	is the reactor diameter [m]
4.5	is a factor according to the geometrical scale-up criterion that has been adopted.

The other terms have been introduced previously. Regarding the construction material of the bioreactor, we consider as examples two cases:

- the bioreactor walls comprise a 2.5×10^{-3} m thick steel wall as structural material and 30×10^{-3} m thick polystyrene foam as insulating material, in which also the bottom and the top of the bioreactor walls are insulated with the same thickness of insulating material;
- the bioreactor walls are completely built with 30×10^{-3} m thickness of concrete material.

As shown in Chap. 4, the total duration of fermentation Δt depends on the working temperature and is related to the bioH_2 production shut-down. The duration of fermentation and H_2 production obtained experimentally according to the working temperature are reported in Table 5.4. The total resistance, i.e. the reciprocal of the overall heat transfer coefficient U, accounts for the total insulation of the broth from the outside environment, and can be calculated as the sum of the single resistances, i.e. internal broth, steel plus insulator and the external air resistances.

Table 5.4 Total H_2 produced per unit of volume, duration of fermentation and energy production obtained by bench-scale bioreactor running at different temperatures

T_w (°C)	H_2 produced (mmol H_2/L)	Δt (days)	Energy production (kJ/L)
16	15.4	6.6	3.32
20	215.3	23.9	47.36
35	442.0	13.8	95.15
40	96.0	8.4	20.67
50	1.1	12.5	0.10

The heat flux from the bioreactor comes across the three heat resistances in series, and therefore the global thermal resistance U^{-1} is:

$$U^{-1} = h_i^{-1} + \frac{s}{k} + h_e^{-1} \tag{5.14}$$

where h_i and h_e are the internal and external convective heat transfer coefficients, respectively. A large thickness of insulator creates a higher resistance because the phenomena of heat transfer in different materials are in series [15], hence both the convective coefficients, h_i and h_e, can be disregarded. Very thick polystyrene foam (or generally higher thickness of insulator) makes the foam resistance the only relevant contribution to the total resistance. The resistance to heat transport is here only considered in the insulating material; this assumption leads to overestimating the insulator thickness for the same energy loss.

5.4.3.1 Focus on Thermal Insulator

Insulating materials are of great importance for minimizing the amount of heat exchanged between system and environment. The insulating materials are solid and usually inhomogeneous materials, characterized by a very low value of thermal conductivity λ, resulting mainly from the air enclosed in the pores of the material itself. The value of the conductivity coefficient λ (W/m K) indicates the ease with which the material transports energy via collisions at the molecular level, depending on the chemistry of the material, the phase considered (solid, liquid or gas), the crystalline structure, the temperature and the homogeneity of the materials [15]. Table 5.5 shows the thermophysical properties of some materials.

Table 5.5 Thermophysical properties of some materials

Material	T (°C)	λ (W/m K)	ρ (kg/m^3)	c_p [kJ/(kg K)]
Steel	20	52	7,800	0.44
Aluminium	20	220	2,700	0.93
Cotton	30	0.04	80	1.52
Glass wool	0	0.035	100	0.65
Expanded polystyrene	0	0.032	35	0.8
Expanded polyurethane	0	0.021	40	–
Cork sheet	0	0.04	130	–
Sheep wool	10	0.04	28	–
Straw	20	0.058	175	–
Recycled paper	20	0.07	400	–
Raw clay	20	0.132	700	–
Concrete	15	0.4–0.7	2,400	0.92

5.4.4 Electrical Energy

The electrical energy consumed to run the bioreactor is for mixing, filling up and emptying the bioreactor using a pump. In batch fermentation, the raw material and the inoculum are pumped in at the beginning of the run and the broth is pumped out at the end. The reactor is mixed throughout the run. The energy for pumping in the case of a batch reactor may be calculated as the energy necessary to lift the broth to the top of the reactor by using the following equation:

$$E_p = (q \cdot \rho \cdot Wp \cdot t_r \cdot 9.81 \times 10^{-3})/V_R \tag{5.15}$$

where q is the volumetric flow rate (m^3/h), t_r is the filling time (h), 9.81×10^{-3} is the conversion factor from kg_f.m to kJ, V_R is the reactor volume and W_p is the energy to be supplied to the fluid per unit of broth mass, in kg_f.m/kg, to transport it from the feed tank to the reactor. It can be evaluated by Eq. (5.16) under the hypothesis that the pressure in the tank is equal to that of the reactor and the fluid motion occurs in the turbulent flow regime [16]:

$$W_p = (g/g_c \cdot L + v^2/2g_c + f_f)/\eta_m \tag{5.16}$$

where g is the acceleration due to gravity, g_c is the Newton's-law proportionality factor $g_c = 1.2 \times 10^8$ (kg m h^{-2} kg_f^{-1}), L is the height of reactor, v^2 is the velocity of the fluid in the pipe, f_f represents the energy dispersed as heat generated to overcome the friction force per unit of mass of fluid occurring in the fluid along pipe between the feed tank and the reactor; finally, η_m accounts for the overall efficiency of the pump to convert mechanical energy in energy of motion. Considering a batch run of the bioreactor, it is possible to assume $E_p \sim 0$ compared with the electrical energy used for the agitation during the fermentation. This hypothesis always seems valid, because the time t_r is of the order of hours compared to the duration of a batch process, which is of the order of weeks or months. In the case of continuous operation the energy used for pumping is:

$$E_p = \rho \cdot W_p \cdot 9.81 \times 10^{-3} \cdot F/\mathrm{HRT} \tag{5.17}$$

where the terms have the same meaning as previously defined. It cannot be disregarded.

The evaluation of the energy required to mix the fermenting broth versus diameter was made by applying a turbulence scale-up criterion. The power number and the rotational Reynolds number were considered to evaluate the mixing performances of the bioreactor [17]. The rotational Reynolds number was considered to be independent of the reactor diameter, according to the turbulence scale-up criterion: $\mathrm{Re} \approx N_1 D_1^2 = N_D D_D^2$, i.e., the power number is independent of the reactor diameter [17, 18]. A geometrical similarity was assumed for the vessel and impeller scale-up, i.e., an impeller-to-reactor diameter ratio equal to 0.5 was assumed,

similar to the bench-scale bioreactor. With the above assumptions, the following equation allows the estimation of the electrical power necessary to mix the broth:

$$P_w = \left(\frac{P_n \cdot \rho}{8g\pi}\right) \cdot N_1^3 \cdot D_1^6 \cdot D_D^{-4} \cdot F \cdot 10^{-3} \tag{5.18}$$

where *1* and *D* refer to the bench scale and to the actual bioreactor, respectively, N is the rotational number (rpm) and P_n is the power number. The procedure reported in Bailey and Ollis [18] was used to calculate the power number P_n for the bench-scale bioreactor. In Eq. (5.18) P_w is the power per unit volume (kJ/m^3) of the reactor required to reach the target mixing performance, i.e. the value of the Reynolds number equal to that of the bench reactor. To evaluate the energy used for mixing it is necessary to take into account, in the case of batch mode, the running time given in Table 5.4 for each working temperature:

$$E_m = \frac{P_w \cdot \Delta t(T_w)}{\eta_{\text{el}}} \tag{5.19}$$

An efficiency of electrical energy conversion (η_{el}) into mixing energy of 0.75 was considered. In the case of continuous mode the energy can be evaluated by using 24 h/day instead of the duration of the batch Δt in Eq. (5.19). All the above Equations were implemented in an Excel sheet to perform the net energy balance for each situation; only the case of a batch reactor was considered here because the data available on hydrogen production in this case are well recognized in the literature.

5.5 Results and Comments

5.5.1 Energy Production

The energy production as H_2 achieved by the bench-scale bioreactor at each temperature investigated is reported in Table 5.4, in order to evaluate the net energy produced using the approach described in Sect. 5.4. In the present context, i.e., the net energy balance of the bioreactor, the diameter of the reactor D as scale-up parameter is able to link together all the energy terms including the energy production per unit of volume, because the energy production is linked to the third power of the diameter and the energy dispersed as heat and the energy for mixing depend on the square of the diameter. The energy production at different temperatures (from 16 to 50 °C) is shown in Fig. 5.2, the highest quantity of H_2 was obtained at 35 °C. At this temperature a peak of energy produced occurs, in accordance with several other researchers, as the optimum point in the mesophilic range for biohydrogen production, as underlined in Table 5.3.

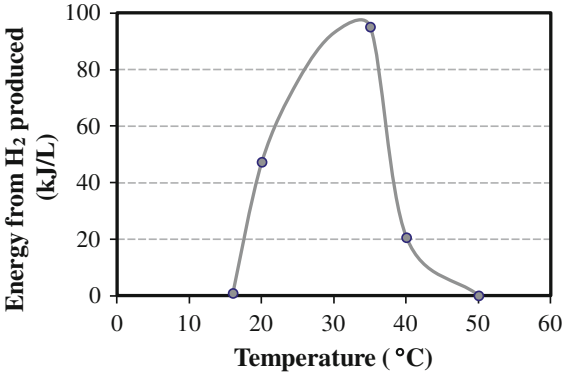

Fig. 5.2 Specific energy production as H_2 produced versus temperature

5.5.2 Net Energy Production

The net energy balance was evaluated in the following situations: winter and summer times with a mean ambient temperature of 5 and 15 °C, respectively, and for two bioreactor construction materials: concrete, and steel plus an insulator of polystyrene foam. In any case, for evaluating the effect of construction materials on net energy production, it is possible to find the thickness of insulator that maximizes the net energy, using the approach described in Sect. 5.4. In accordance with Eq. (5.8), the calculation of the net energy balance of a bioreactor producing H_2 is shown in Fig. 5.3 for concrete (30×10^{-2} m thick) and in Fig. 5.4 for steel plus polystyrene foam (2.5×10^{-3} m as structural material plus 30×10^{-2} m of insulator) versus the diameter of the bioreactor. In all the situations considered in Figs. 5.3 and 5.4, the net energy balance is never in the positive range. Figure 5.3a, b show the results of scale-up procedure evaluation for a bioreactor built with concrete walls (and without insulator) operated in winter time (a) and in summer time (b), respectively, with 50 % heat recovery as quoted in the assumptions. The results show that the net energy balance is always negative or equal to zero, except for some negligible cases for the evaluation conducted in summertime conditions with $T_w = 35$ °C and for $D > 4$ m.

Figure 5.4a, b report the evaluations of the net energy production for a H_2 bioreactor comprising steel covered with 30×10^{-2} m thick polystyrene foam as insulator in winter and summer time, with the assumption of 50 % heat recovery. Contrary to expectations, the best situation is reached by running the bioreactor not at 35 °C, which gives the maximum H_2 production, but at $T_w = 20$ °C, in which the energy production is only about 50 % of the maximum value (see Fig. 5.2). This occurs because the energy produced by working at higher temperatures is consumed to heat the reactor to higher temperatures. During winter time, the net energy is never in the positive range for all the temperatures considered. This means that

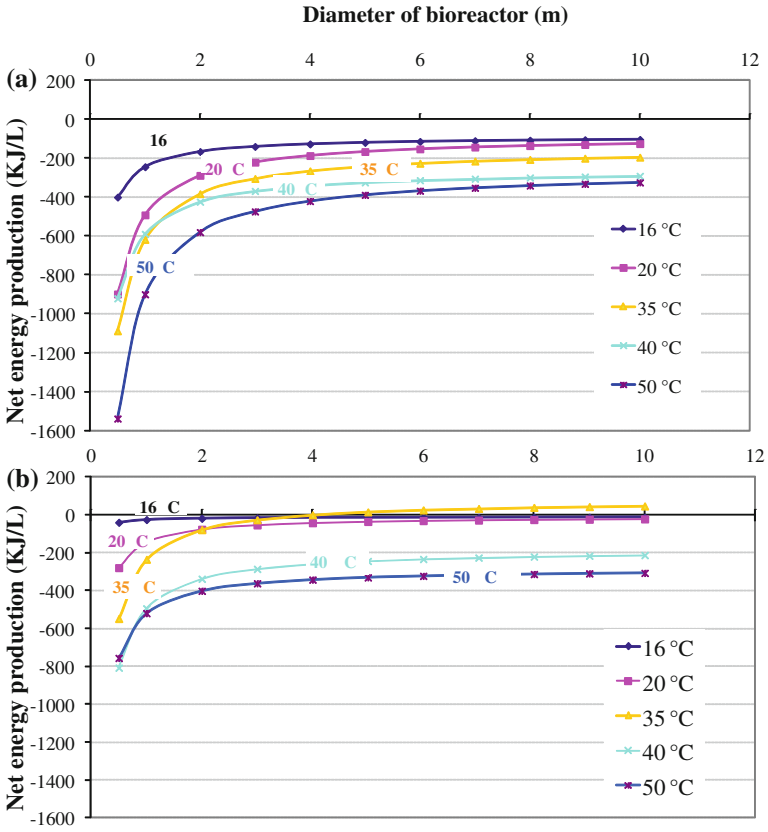

Fig. 5.3 Net energy productions versus bioreactor diameter for a concrete bioreactor with the assumption of 50 % heat recovery: **a** winter time and **b** summer time

during this period the energy produced is never able to compensate for the energy used to run the bioreactor. In addition in the summertime the net energy works out negative for diameters less than 1 m and becomes positive only for a few energy units per bioreactor volume at larger diameters, despite assuming a recovery of 50 % of the energy used to heat the fermenting broth.

On a deeper analysis of Figs. 5.3 and 5.4, the net energy production increases with the bioreactor diameter but this effect vanishes for diameters of over approximately 3 m. This fact suggests a scale-up criterion for larger diameters, which means that, for a larger quantity of feedstock to be treated in unit time, it is better to work with more than one bioreactor with smaller diameters ($\sim$3–4 m) instead of only one with a bigger diameter, for constructive reasons. Therefore, regarding the bioreactor diameter, for low diameters it is better to work at a lower temperature even if this means a lower biological activity of the microorganisms. Furthermore, without insulation it seems markedly better to choose a low reactor

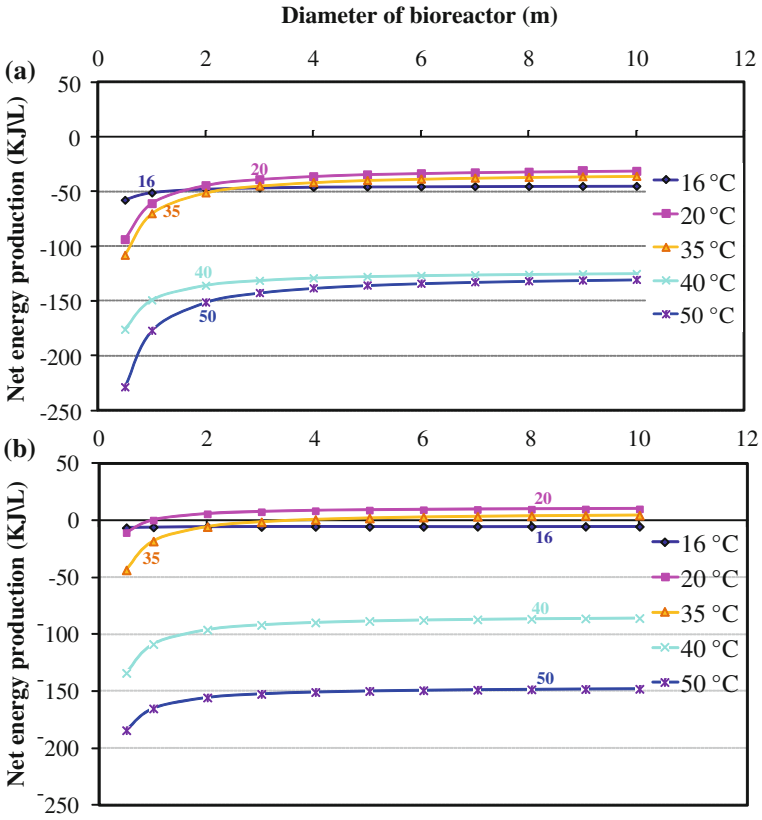

Fig. 5.4 Net energy production versus diameter for a bioreactor of steel and 30×10^{-2} m polystyrene foam insulation with the assumption of 50 % heat recovery: **a** winter time and **b** summer time

temperature as a strategy to maximize the recovery of energy. The 50 % of heat recovery results in an essential operational requirement to increase the net energy balance. Figure 5.5, where calculations are provided without taking into account the heat recovery, shows that net energy production is never in the positive range, even in the case of a reactor made of steel plus insulator.

Similar results (Fig. 5.6) are obtained using the specific hydrogen production data of other researchers, as reported in Table 5.3: in all the situations the net energy production is never in the positive range.

Figure 5.7 compares the different net energy productions under concrete and polystyrene foam in the same conditions: winter time and T_w = 35 °C. The reactor with insulation demonstrates a lower dependence on bioreactor diameter and at the

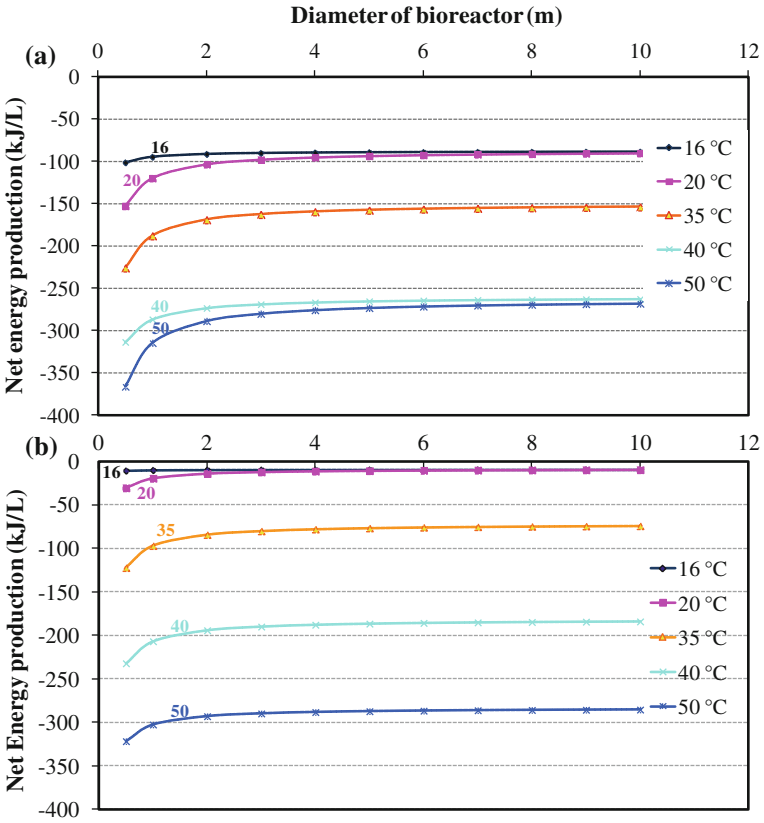

Fig. 5.5 Net energy productions versus diameter for a bioreactor of steel and 30×10^{-2} m of polystyrene foam insulation without the assumption of 50 % of heat recovery: **a** winter time and **b** summer time

same time a smaller amount of negative net energy production. Furthermore, the thermal insulation of the reactor and in general the construction material play an important role in the total energy balance because it is necessary to take into consideration the energy used to produce the materials.

The above results show the necessity, for AD hydrogen production, to obtain energy from the volatile fatty acids (VFA) and other compounds in the residue present at the end of the acidogenic fermentation step. Several approaches are candidates for this purpose [19], ranging from photobiohydrogen production [20] to the use of microbial fuel cells [21] and the methanation of the liquid residue by AD. Chapters 7 and 8 are dedicated to raising the energy value of VFA to make the net energy balance of the whole system positive.

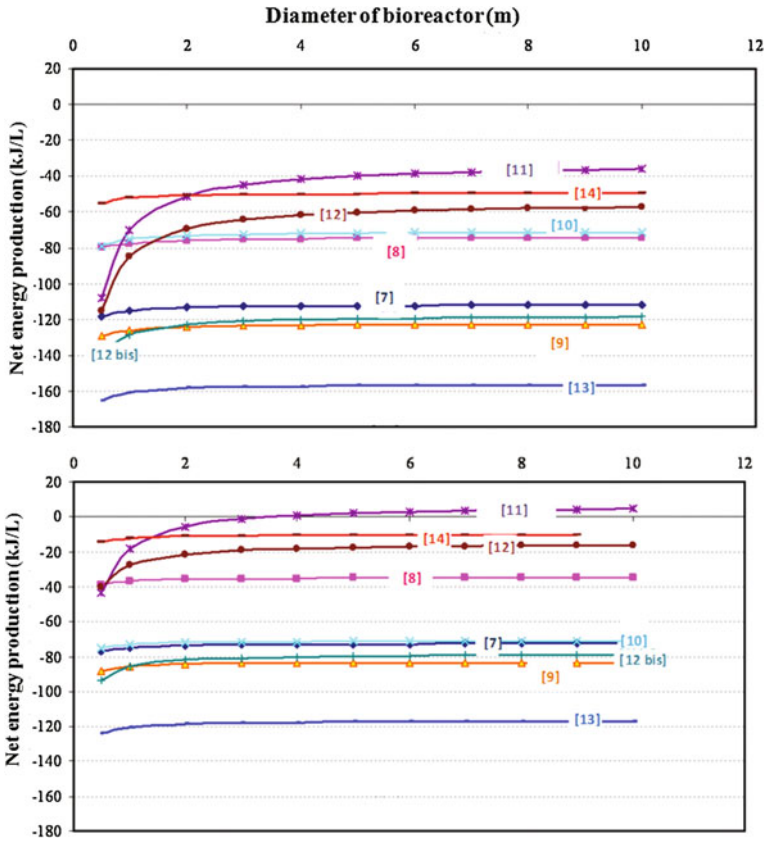

Fig. 5.6 Net energy productions versus diameter for a bioreactor of steel and 30×10^{-2} m of polystyrene foam insulation with the assumption of 50 % of heat recovery using the specific H_2 production from different authors: **a** winter time and **b** summer time

5.6 Uncertainty Evaluation

The estimation of the uncertainty is a fundamental task to be performed in the present situation. The uncertainties of net energy were evaluated accordingly to the rules given in [22]. Considering that the *Guide to Uncertainty Measurement* (GUM) defines uncertainty as a quantifiable parameter associated with the results of a measurement procedure, the suggested approach has been utilized either to evaluate the uncertainty or to estimate the parameters with the most effect. This latter approach was obtained by using the expression given in [23], known as the *law of the propagation of uncertainty*. It is based on the evaluation of the partial derivatives of the parameters in the estimation of the net energy, called *sensitivity coefficients,* which describe how the output estimate varies with changes in the value of the input estimates. Applying this procedure to Eq. 5.8, the following results were

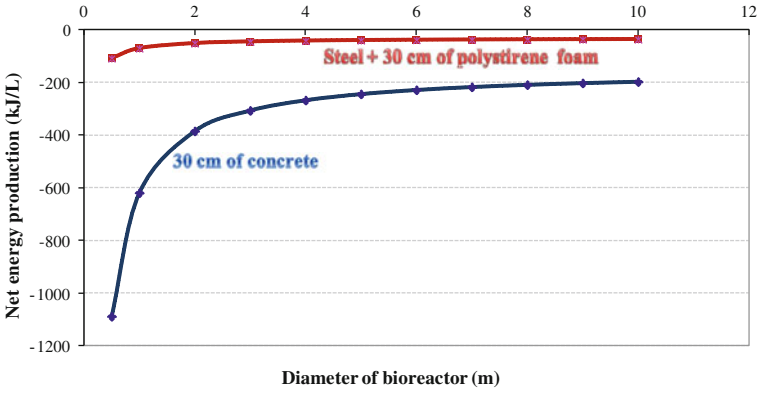

Fig. 5.7 Comparison between the net energy production versus diameter of a steel plus polystyrene foam bioreactor and a concrete one

obtained. As concerns the main parameters affecting the net energy estimation, the warming energy has the highest predominance compared to other energy terms. It reaches almost the same numerical value in both winter time and summer time: 85 and 70 %, respectively. The variability either of ambient temperature T_a or of the global thermal efficiency η_C are the main sources of the uncertainty. With a T_a variability of around 5 °C and a relative variability of η_C of around 10 % in the values used for the calculation, the uncertainty of the net energy is around 50 kJ/L; uncertainty evaluations of T_a and η_C are constant, i.e. considering only the uncertainty due to the experimental data results in a range of 5–15 kJ/L; this confirms that T_a is the main parameter affecting anaerobic digestion.

According to the value of the net energy estimation reported in Figs. 5.3 and 5.4, it is possible to consider the suggested energy balance sufficiently acceptable in the estimation of the net energy of biohydrogen production. In any case, for a specific design of a detailed plant, the uncertainty could be reduced by taking into consideration the actual variation of ambient temperature for a specific geographical situation.

5.7 Conclusion

In this chapter a scale-up procedure to evaluate the net energy production of a bioreactor producing H_2 is analyzed and applied. The main conclusions are:

- bioreactors which produce only H_2 are not energetically sustainable, apart from a few energy units per unit of volume for a bioreactor running in summer time (at least for the considered temperature) and with the hypothesis of recovering 50 % of the energy used to heat the mass to a working temperature of 35 °C;
- the net energy produced depends mainly on the seasonal temperature variations;

- other parameters with an effect are the thickness of the insulation material, the thermal conductivity and the bioreactor diameter.

Different strategies of plant running are necessary to maximize the net energy production. For example, the recovery of the heat used to warm the fermenting broth is a fundamental aspect: without recovery the net energy balance is never in the positive range. The best working temperature to maximize the net energy produced by the plant is 20 °C, whereas 35 °C is the optimal temperature for maximizing biomass activity for hydrogen production. The uncertainty analysis of the procedure shows that the main influencing parameters are the ambient temperature, because this determines the quantity of energy to be used to heat the bioreactor, and the efficiency of the heating system. Therefore, this suggests that for a full-scale application a careful estimation of T_a variation is of utmost importance. Concerning the effect of diameter, it is possible to conclude that it is better to work at a low temperature (20 °C) for diameters less than 1 m, even if the energy produced is lower, because this increases the net energy, while for values over 3 m the effect is negligible. Consequently, in order to maximize the net energy of such a process, the strategy of managing the operative conditions requires much care, without disregarding the construction material to be used.

Lastly, in order to have a net positive energy balance to sustain the biohydrogen technology, it is necessary to increase the energy production by looking to valorize the chemicals remaining in the fermenting broth at the end of acidogenesis; a great quantity of energy (>80 % of that present in the feed) is still locked up in the reaction products, which can be converted into further energy in the shape of hydrogen, methane or electricity.

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