ENERGY AND WATER OPTIMIZATION IN BIOFUEL PLANTS [♣]

Ignacio E. Grossmann[*], Mariano Martín

Center for Advanced Process Decision-making; Department of Chemical Engineering
Carnegie Mellon University, Pittsburgh, PA 15213, USA

Abstract In this paper we address the topic of energy and water optimization in the production of bioethanol from corn and switchgrass. We show that in order for these manufacturing processes to be attractive, there is a need to go beyond traditional heat integration and water recycling techniques. Thus, we propose a strategy based on mathematical programming techniques to model and optimize the structure of the processes, and perform heat integration including the use of multi-effect distillation columns and integrated water networks to show that the energy efficiency and water consumption in bioethanol plants can be significantly improved. Specifically, under some circumstances energy can even be produced and the water consumption can be reduced below the values required for the production of gasoline.

Keywords: Biothanol, water networks, energy optimization, mathematical programming,

1 INTRODUCTION

Given the forecast in the growth of energy over the next 20 years, there is a strong motivation for developing alternative energy resources that are inexpensive, renewable, without significant environmental impact and neutral in emissions so that the problems of availability and atmospheric pollution are addressed simultaneously. Therefore, attention is being placed upon a variety of energy sources including solar, wind, thermal, hydroelectric and biomass [1,2].

Mankind has used over many hundreds of years biomass as a source of energy for heating and transportation purposes. Presently biomass contributes 10–14% of the world's energy supply [3]. The worldwide raw biomass energy potential in 2050 has been estimated to be between 150 and 450 EJ/year, or 25×10^9 to 76×10^9 boe [4]. In the case of the transportation sector, which is the most challenging due to the need for high density energy sources, only biomass provides an alternative that can be implemented in the short-term [5]. Thus, bioethanol and biodiesel have become the most promising alternatives. Corn ethanol and sugar cane based

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[*] to whom correspondence should be addressed grossmann@cmu.edu

ethanol have been produced for many years. However, the high demand has raised concerns due to the consumption of raw materials that interfere with food, the high energy consumption [6-12], land required [13-17] and more recently the large amount of water consumption [18]. 2nd generation biofuels try to overcome these problems by using non-food related raw material and land, and less natural resources but no industrial production process is yet available.

Traditionally process synthesis has been addressed following two different approaches, conceptual or systematic. So far both approaches have been used for designing process flowsheets, where conceptual design is largely based on hierarchical decomposition [19], while systematic approaches consist of optimizing a superstructure of alternatives [20-21]. The conceptual approach relies on heuristics and engineering experience [22-23], in contrast to the systematic approaches that are based on mathematical programming techniques [24-28]. Regarding the simultaneous synthesis of process water and heat exchanger networks, research is not at the same level of development [29-33], and therefore, the sequential strategy is still largely used. In this paper we outline a sequential strategy for water and energy optimization, and apply it to the design of first and second generation bioethanol plants using mathematical programming techniques to develop sustainable biofuel processes by means of a two-stage approach.

2 STRATEGY FOR ENERGY AND WATER OPTIMIZATION

Water and energy are two interdependent resources; energy production requires water for cooling, hydropower, and fuel production, while water processing, treatment and reuse require energy. In the field of biofuel production, energy and water consumption are major issues that in policy and decision making. The main example is the production of corn-based ethanol for which over the years researchers have reported a broad range of values for water and energy consumption, which are shown in Tables 1 and 2 [7, 34-40]. An important question that arises for the design of sustainable production processes of biofuels is what are the minimum values for energy and water consumption that can be actually achieved in these processes. Therefore, our aim in this paper is to show how energy and water consumption can be optimized in first and second generation bioethanol processes to determine the minimum achievable values for both important resources using a strategy based on mathematical optimization techniques.

Bioprocesses present a number of challenges such as the low operating temperature of the reactors (e.g. fermentors), and the large consumption of energy in the distillation columns to separate dilute mixtures. Therefore, the energy optimization problem requires a different approach since there is commonly no source of energy at high temperature in the reactors as in most petrochemical processes, which implies that the heat recovery within the process only has a modest impact. Moreover, the low price of freshwater makes its optimization as part of the total cost to have very little effect since the economical benefit of reducing the freshwater consumption versus other utilities is currently still marginal at best. Thus, we propose a two-step optimization methodology for optimizing energy and water for the design of biofuel plants, which is as follows:

1. In the first stage, we optimize the energy consumption of the biofuel process. Due to the challenges mentioned above, we not only consider a superstructure embedding alternative technologies for the different operations [20-21], but because of the high energy demand associated with the distillation columns used in the purification of the ethanol, we also consider as alternatives the use of multieffect columns to reduce the energy consumption [41-42]. Furthermore, we design the optimal heat exchanger network for such a superstructure using the MINLP model by Yee and Grossmann [28].
2. In the second stage, we optimize the water network for the flowsheet featuring minimum energy consumption using the superstructure for water process networks developed recently by Ahmetovic and Grossmann [26], which is described in section 4. The goal is to ensure the minimun consumption of freshwater by accounting for the cost of piping, pumping and treatment units.

Although this two-stage methodology, which as is sequential in nature, is not guaranteed to provide results that are equivalent to a simultaneous optimization approach, it does provide a synergy between the minimum use of energy and water. The reason is that optimizing energy reduces the utility loads, which in turn implies lower water use for the cooling tower and lower water losses by evaporation in the tower.

In the next section we illustrate this methodology in the design of corn and lignocellulosic bioethanol plants.

Table 1.- Energy consumption in corn-based ethanol plants

Author (year)	Energy consumption (Btu/gal)
Pimentel (2001) [34]	**75,118**
Keeney and DeLuca (1992) [35]	**48,470**
Wang et al. (1999) [36]	**40,850**
Shapouri et al. (2002) [7]	**51,779**
Wang et al (2007) [37]	**38,323**

Table 2.- water consumption in corn-based ethanol plants

Author (year)	Water consumption (gal/gal)
Gallager (2005) First plants [38]	**11**
Philips (1998) [39]	**5.8**
MATP (2008) Old plants in 2006 [40]	**4.6**
MATP (2008) New plants [40]	**3.4**

3 ENERGY OPTIMIZATION OF CORN AND LIGNOCELLULOSIC BIOETHANOL

In this section we apply the first in the methodology to optimize the energy use in flowsheets for the production of ethanol from corn and lignocellulosic switchgrass, which are reported in detail in [43] and [44].

3.1 1st Generation Corn Based ethanol.

The process superstructure considered here for the dry-grain process is described in detail in [43], and consists of three different sections. The first one involves the pretreatment of the corn grain to break the physical and chemical structure of the corn making the sugars available for fermentation. The process units employed are grinding, direct contact with steam, saccharification and liquefaction. At the end of this sequence of physical and chemical treatments, sugars are obtained from the grain. The second section is the fermentation of the sugars, mainly glucose, into ethanol using yeast, *Saccharomyces cerevisiae*. The amount of water needed at the fermentor is such that the final ethanol concentration is below the toxic levels for the yeast. After fermentation, two alternatives were considered for the separation of solids from the slurry exiting the fermentor: a) mechanical separation before the beer column (BC1), or b) after the beer column. The third section comprises the technologies used for the purification and dehydration of ethanol to fuel grade. Three different options were considered: (1) a rectification column that can concentrate ethanol to the azeotropic composition, (2) adsorption of water in corn grits, and (3) molecular sieves. The superstructure was optimized in terms of energy consumption as described in [43]. The optimized flowsheet is shown in Fig. 1. The separation of the solids takes place before the beer column, while the dehydration stage consists of the rectification column together with adsorption in corn grits with final stage in the molecular sieves. In Fig. 1 neither the heat exchanger network nor structural design changes to the distillation columns (multieffect) are explicitly shown [43].

The energy consumption and cooling needs resulting from the optimized superstructure are represented by case (a) in Fig. 2. At this point it is possible to use heat integration with the software for simultaneous optimization of heat exchanger networks (HEN), *SYNHEAT* (http://newton.cheme.cmu.edu/interfaces) [28] that uses an MINLP model to determine a minimum cost heat exchanger network. Since the conversion in the reactor is high and there is no recycle, there is no advantage in performing simultaneous structural optimization and HEN design. The important feature of fermentation based processes in terms of heat integration is that the reactor is operated at low temperature, and thus it is not a source of energy as it can be in petrochemical processes. By designing the optimal HEN, case (b) in Fig. 2, we are able to reduce even further the energy and cooling water demands. However, it turns out that these are not the absolute minimum energy requirements.

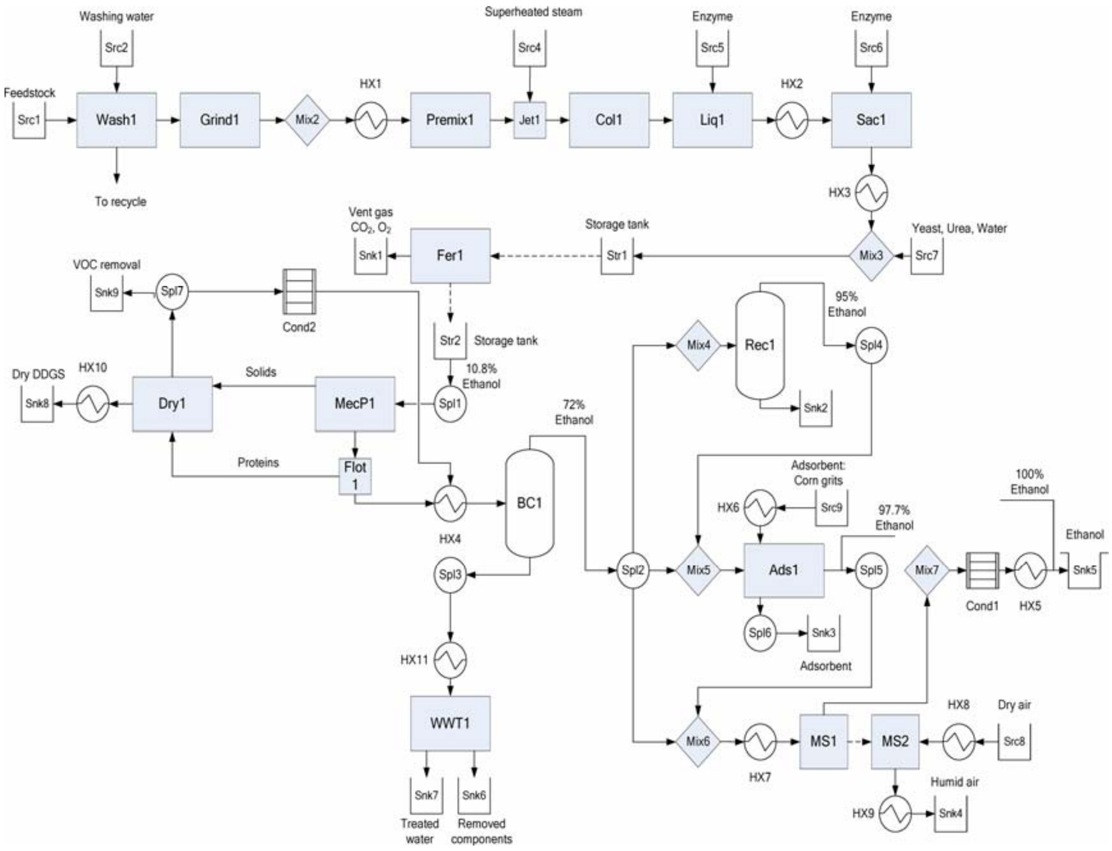

Figure 1. Optimal design of the corn-based bioethanol plant.

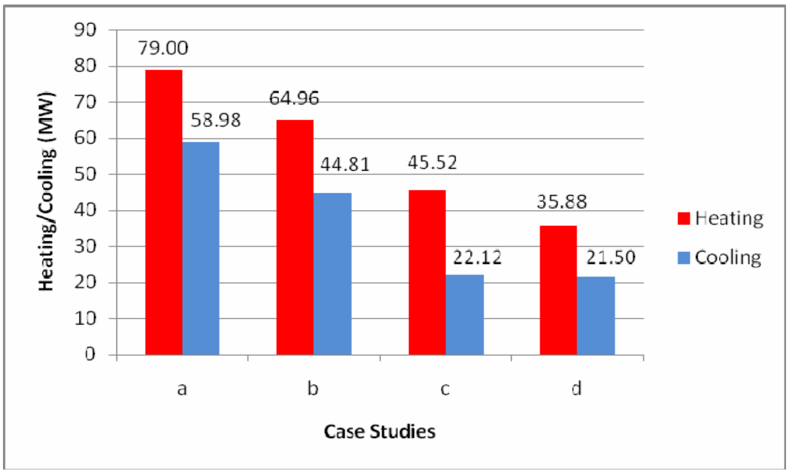

Figure 2. Energy consumption and cooling needs for the corn ethanol process.

As it is well known, distillation columns are some of the most energy intensive units in the chemical industry. Based on the studies by Larsson & Zachi [41], Haelssig et al [42], multieffect columns are very effective arrangements for reducing energy consumption in distillation systems. By operating the columns at different pressures, the condenser of the column at higher pressure serves as the reboiler of the column operating at lower pressure. The inlet feed is split roughly evenly between the columns, and their top and bottoms products are mixed together to obtain the final products with the desired flowrates and compositions. The beer column and the rectification column were replaced by multieffect columns and with them in place, the HEN was optimized to obtain further reductions, case (c) in Fig. 2. Finally, by optimizing the reflux ratio of the beer column we obtain case (d). At this point the corn-based ethanol process has a greatly reduced energy consumption and the cooling needs are adjusted accordingly yielding energy consumption values (22,000 Btu/gal including electrical energy) around half the lowest one shown in Table 1. An economic evaluation of this optimal solution yielded a production cost of 1.24USD/gal [44], which is a decrease of 20% with respect to the base case.

3.2 2nd Generation Lignocellulosic ethanol.

In order to produce ethanol from switchgrass via gasification, syngas is produced and used to obtain ethanol. The process described in [44] consists of four different parts: gasification (followed by gas cleanup), concentration adjustment, sour gases removal and synthesis. We optimized the process flowsheet by solving a superstructure embedding a number of different design alternatives (Martín and Grossmann [44]). Two alternatives are evaluated for gasification, direct or indirect. The gas obtained is cleaned up using either steam reforming or partial oxidation to remove hydrocarbons, and subsequently must be cleaned from solids as well as other compounds like NH_3. Next, the gas composition is adjusted to a CO/H_2 ratio of 1. Three technologies (bypass, membrane-PSA and water gas shift) are evaluated. Then, the removal of sour gases, CO_2 and H_2S, is required. Three alternatives, membrane separation, absorption in ethanolamines and PSA are considered for this task. Once the syngas is prepared, two synthetic paths are evaluated: (1) mixed alcohols catalytic process with two possible distillation sequences (direct and indirect), and (2) syngas fermentation followed by four possible dehydratation processes: distillation, water adsorption in corn grits, molecular sieves and pervaporation. We model this superstructure as an MINLP which is solved by partial enumeration of the integer variables in terms of gasification technologies, reforming modes and synthetic paths. We generate 8 subproblems where the clean stages and separation processes are optimized to minimize energy consumption. Subsequently, we implement multieffect columns and design the optimal HEN as in the corn based ethanol case. Finally, an economic evaluation to account for the contribution of hydrogen as byproduct, raw material consumption and utilities yields the flowsheet with highest profit that is shown in Fig. 3 [44]

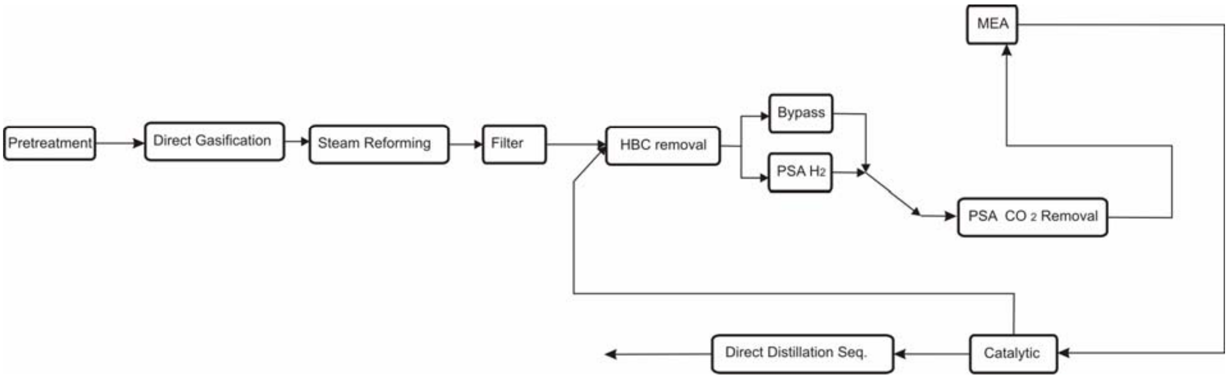

Figure 3. Thermo-chemical ethanol production from biomass

The most profitable process uses high pressure gasification, followed by steam reforming, which increases the production of hydrogen. The composition adjustment is carried out by removing the excess of hydrogen from the stream. Then sour gases are removed in two steps, PSA to remove CO_2 and MEA to get rid of H_2S. Finally, the catalytic path is selected followed by direct distillation sequence. The process produces 18 MW of energy and requires 68 MW of cooling. The production cost of this design turned out to be 0.41 USD/gal due to the large contribution of hydrogen to the income as a byproduct [44].

4 WATER OPTIMIZATION FOR CORN AND LIGNOCELLULOSIC BIOETHANOL

Bioethanol plants tend to consume rather large amounts of water, making this a major issue in the design of these plants [18]. In this section we optimize the water consumption by coupling energy optimization with the design of the optimal waster network for the bioethanol production processes described above based on mathematical programming techniques [25, 26, 45, 46].

4.1 Superstructure of the water Network.

In order to synthesize water networks for bioethanol plants we use the general superstructure of integrated process water networks which has been recently proposed by Ahmetović and Grossmann [25].

The superstructure consists of one or multiple sources of water of different quality, water-using processes, and wastewater treatment operations. The unique feature is that all feasible connections are considered between them, including water re-use, water regeneration re-use and recycle, local recycling around process and treatment units, and pre-treatment of feedwater streams. Multiple sources of water include fresh feedwater streams of different quality that can be used in the various operations, and that may be sent first for pre-treatment. The superstructure also incorporates both mass transfer and non-mass transfer operations.

The mathematical model of the generalized superstructure consists of mass balance equations for water and the contaminants for every unit in the network. The model is formulated as a nonlinear programming problem (NLP), which is nonconvex. The objective function is to minimize the total network cost consisting of the cost of freshwater, the investment cost on treatment units and the operating cost for the treatment units.

To apply the model to the bioethanol production processes, the process and treatment units, and their corresponding flow rates must be defined [47]. For all the processes under consideration we consider:

Sources: Water – ethanol distillation columns, Condensation processes.

Demand units: Gasifier, Fermentors, Dilution tanks, Boiler, Cooling tower.

Process Units: Pretreatment, Scrubbers, Boiler, Cooling tower.

The most important part, however, is the specification of the treatment units in accordance with the contaminants. Wastewater streams are generated from the boiler, cooling tower, and water-ethanol distillation columns, discharge from condensations. Three main contaminants are considered: dissolved solids, suspended solids and organics. Suspended solids are present in the water used for washing the raw material and from the scrubbers, the organics are the main contaminants in the streams coming out of the distillation columns and the scrubber, while the dissolved solids include the concentration of salts as a result of the evaporation processes in boiler and cooling tower. Furthermore, the water fed to the fermentor must have no ethanol, which is toxic for the yeast. We assume that there are three different wastewater treatment units

Solids removal: Screens are widely used for solids like straw and sand.

Organic removal: In order to purify the water from the distillation columns, a system of anaerobic and aerobic treatment is required. The anaerobic stage will remove 90% of the organics generating biogas rich in methane that can be reused to obtain energy. Subsequently, the water will be treated in an aerated lagoon to obtain relatively clean water that can be recycled to the process [48].

Total dissolved solids removal: One of the most important contaminants in the operation of boilers and cooling towers is the total dissolved solids (TDS) since they do not allow the complete recirculation on the blow downs due to the build-up of salts. In order to partially remove the total dissolved solids, a reverse osmosis system is considered. The literature reports removal of 90% at the most, better than ion exchange or nanofiltration [49]. The regulations require that the concentration of TDS in the effluent be at most 500ppm [50]

4.2 Water consumption in corn - based ethanol

Corn-based ethanol has been criticized not only for its high consumption of energy, but also because of its high water consumption. The first data available in the literature regarding water consumption in ethanol plants reveal values from 3 to 15 gal of water per gal of ethanol (see also Table 2). Acording to the literature, the best possible water consumption for corn process is 2.85 gal water per gal of ethanol, and a mean industrial value for the newest plants is 3.4 gal water per gal of ethanol [40, 51, 52]

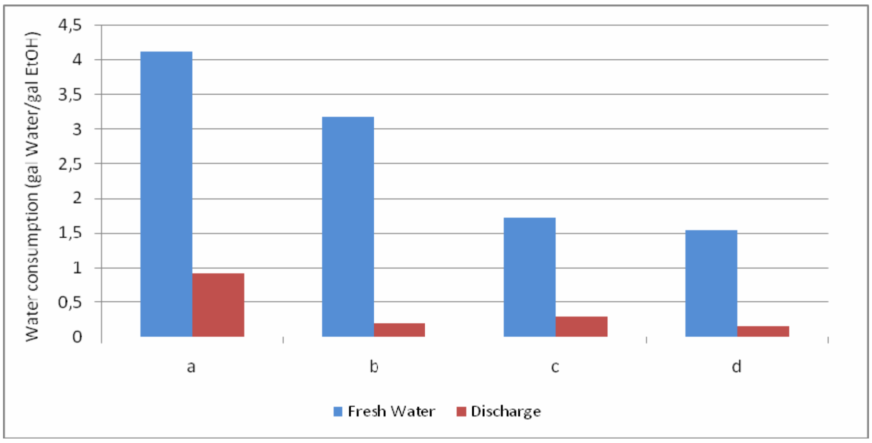

Figure 4. Water consumtion and discharge in corn ethanol process

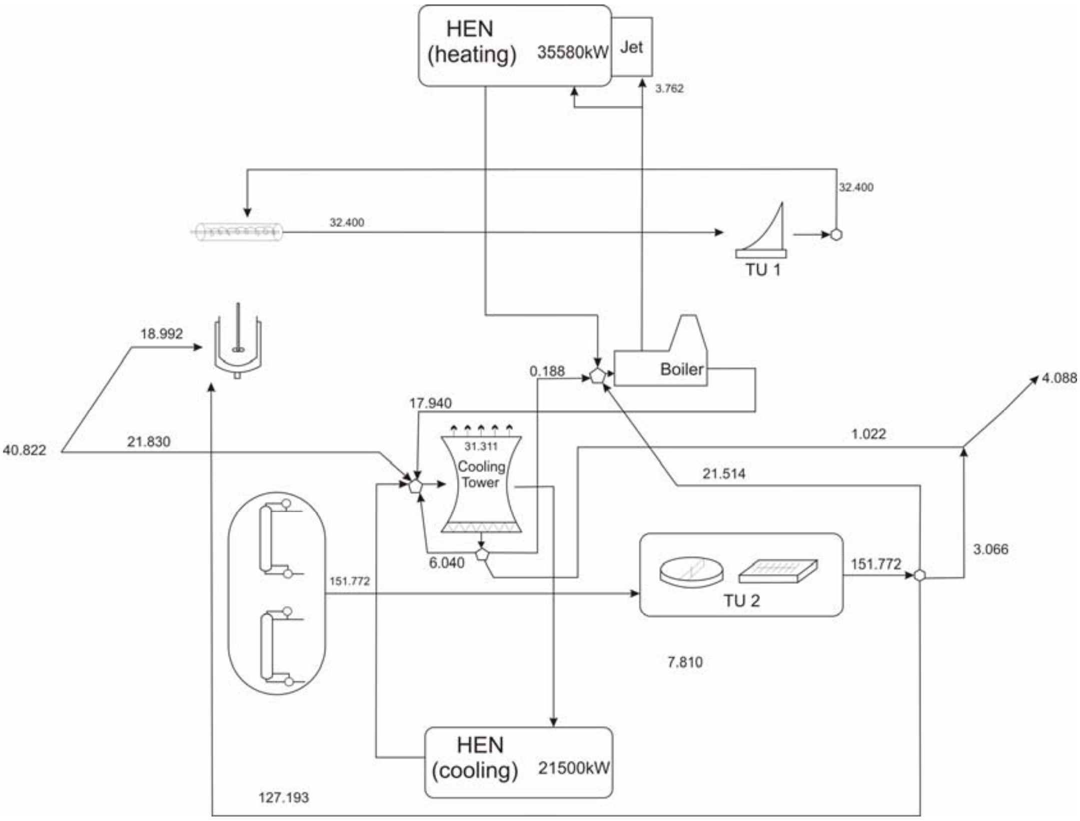

Figure 5. Optimal water network for the optimized process production of corn-based bioethanol .Case study d. TU1: Solids Removal: TU 2: Organic removal.

By developing the optimum water network for the cases in which we optimize the energy consumption (see Fig. 2), it is worth pointing out that energy optimization plays a very important role in reducing the water consumption. In this way, by coupling energy optimization and the design of optimal water networks, the water consumption in the corn-based ethanol plant can be reduced down to only 1.54 gallon of water per gallon of ethanol, which is lower than 50% from the data published in the literature (see Table 2). Furthermore, it is lower that the current goal in industry, which is 1.5 gal/gal [53] (See Fig. 4). This result is of great practical significance because it also provides a proof to those claims. Furthermore, the energy optimization and water network design also plays an important role towards zero discharge of water. However, better and cheaper wastewater technologies are needed to reach that goal. The optimal water network for the optimized corn ethanol process, case (d) in Fig. 4, can be seen in Fig. 5.

4.3 Water consumption in lignocellulosic ethanol

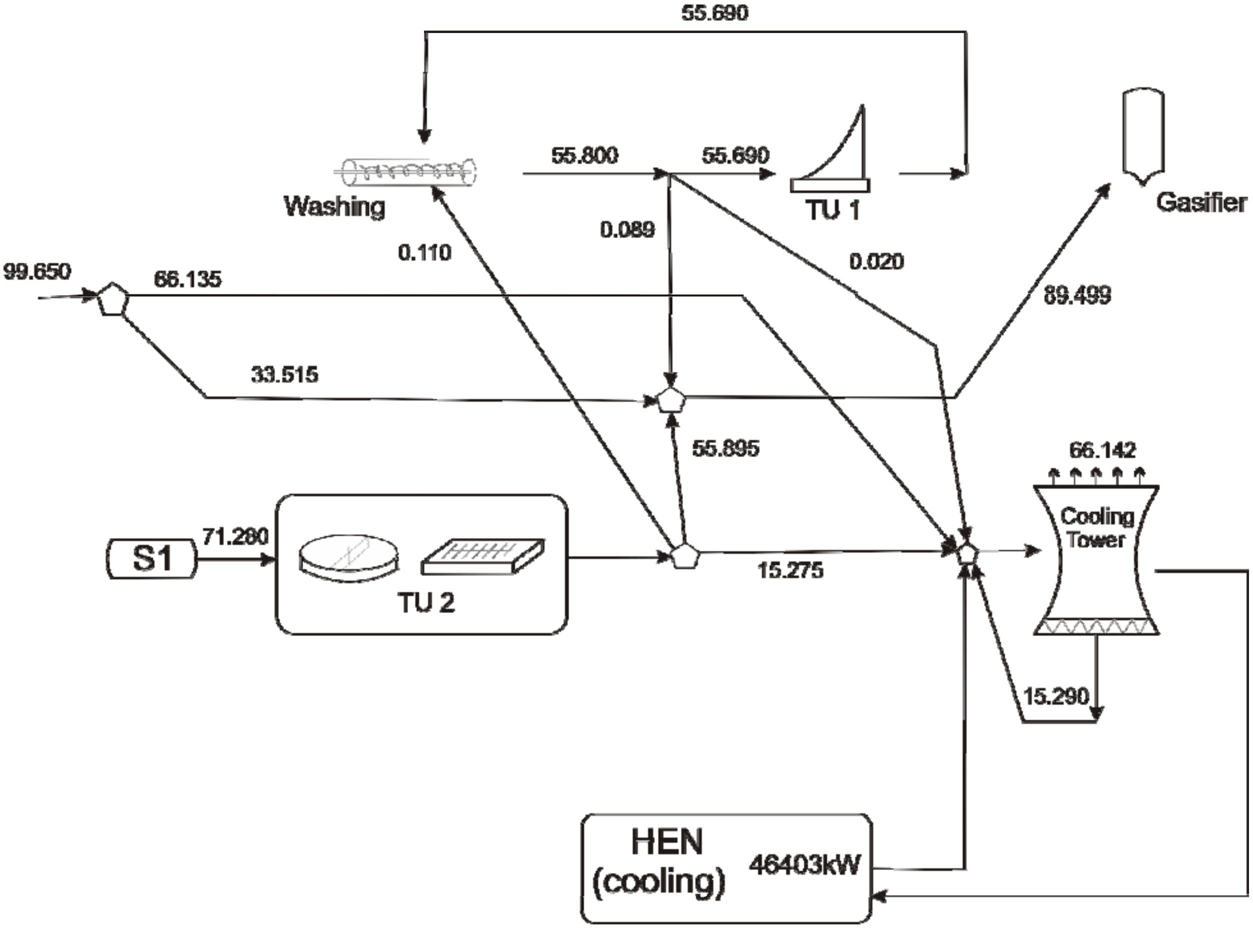

Figure 6. Water network for the Catalytic production of ethanol from syngas.
TU1: Solids Removal: TU 2: Organic removal.

The production process of ethanol from switchgrass via gasification and catalytic synthesis requires a large amount of cooling water mainly due to the high pressures and temperatures in the entire process, and to the fact that a large amount of water in the form of steam is injected into the gasifier. Due to these high cooling needs, some authors support the implementation of air cooling technologies to reduce the cooling water needs [39]. Thus, making use of this technology after energy optimization of the process presented before, it is possible to reduce the cooling water around 11%, from 114t/h to 100 t/h. Figure 6 shows the optimal water network for the thermo-chemical process when air cooling is used. Thus, the water consumed is 4 gal of water per gal of ethanol, in the range of the current corn based ethanol plants. There is no water discharge neither is the reverse osmosis used to treat TDS, mainly because the large amount of water used allows dilution of the TDS and its recycle. Thus, this process is more water intense than corn ethanol. However, a significant amount of hydrogen is also produced.

5 SUMMARY OF RESULTS

5.1.-Energy

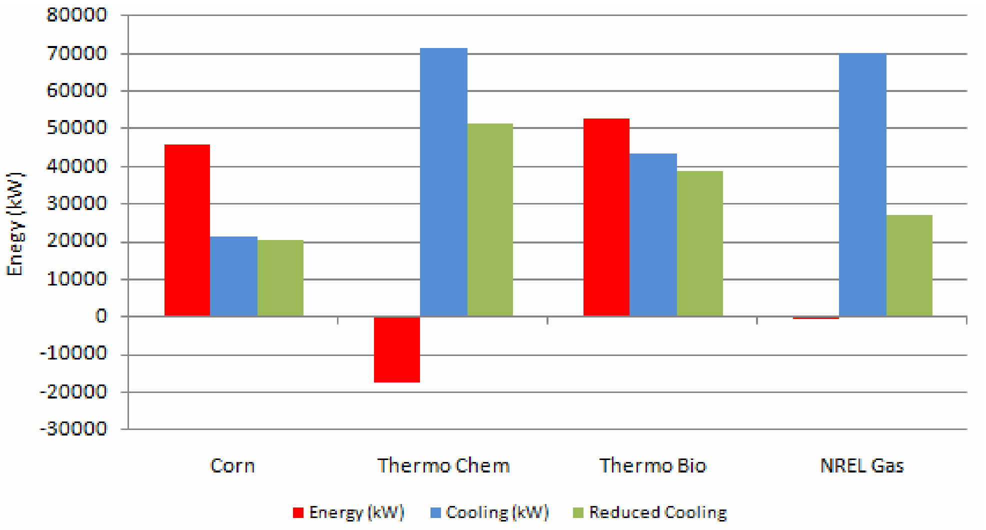

Figure 7 Summary of enery consumption and cooling needs for bioethanol production (60 Mgal/yr) (Corn includes electrical energy too)

In terms of energy consumption and cooling needs, Fig. 7 summarizes the processes presented before including an optimized process in which ethanol is obtained from fermentation of syngas instead of catalytic synthesis [44] and the results from Philips et al [39]. As it can be seen, corn-based ethanol is together with the gasified-fermentation based process, the most energy intensive. However, the weaker pretreatment needed to extract the sugars from the corn results in lower cooling water needs. Lignocellulosic ethanol obtained via gasification and catalytic reaction consumes either no energy or even produces it. On the other hand, the cooling water demands are high. Thus, designing the proper water network is clearly a key to reduce the water consumption. Philips et al [39] proposed to substitute water cooling by air cooling to reduce the losses in the cooling tower. In Fig. 7 it can be see that this technology is useful in case of the processes based on gasification and catalytic reaction since air can be used to cool down the streams in between compression stages as well as the condensers of the distillation columns (see as reduced cooling in Fig. 7). The lower operating pressures and the use of multieffect columns used in our designs for the corn based process and the gasification–fermentation process, show that the implementation or air cooling does not provide a significant advantage.

5.2.Water

In the previous section we saw that the optimization of energy results in lower cooling water use, and thus in lower freshwater consumption. In the case of the gasification based processes, there is another issue to consider, the effect that the production of hydrogen has on water consumption. Fig. 8 shows the summary of the water consumption for the different processes described before. The effect that air cooling has on the fresh water consumption as well as the effect of the production of hydrogen are also shown. Air cooling has a large impact in the catalytic processes due to the high working pressures, and thus the intercooling in the compression stages is important. When it comes to the effect of hydrogen, it turns out that for the production of ethanol only, all processes consume less freshwater than the one needed in the production of gasoline. It is important to highlight that corn ethanol is the process that requires the least amount of water consumption. However, even though corn-based ethanol consumes less freshwater than any other process, the discharge is relatively high compared to the optimized proceses for producing ethanol from switchgrass via gasification and catalytic reaction or fermentation since the low water flow rates do not allow dilution of the blowdownsto be recycled. No data on water discharge for NREL [39] nor for gasoline production is available.

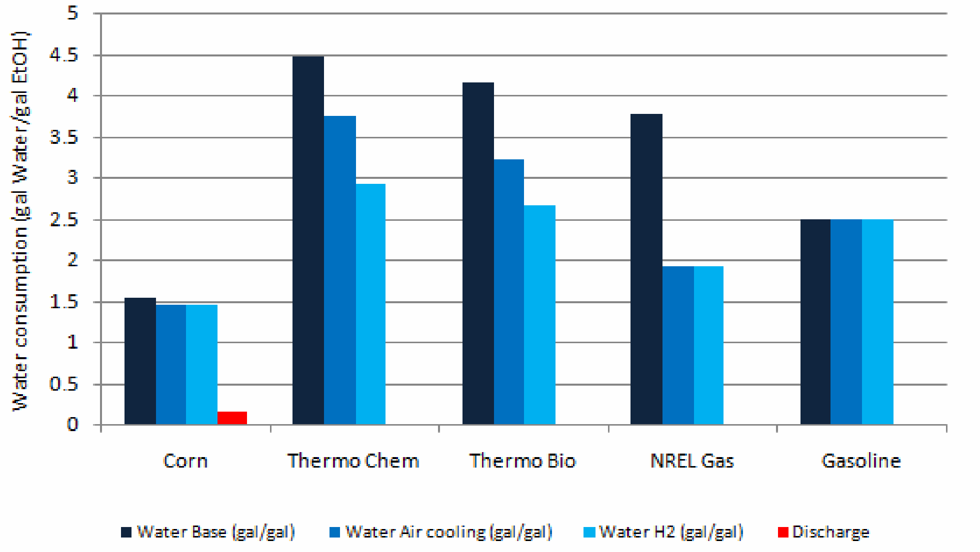

Figure 8.- Summary of water consumption for bioethanol production

6 CONCLUSIONS

This paper has shown that by the proper application of optimization techniques and process systems engineering methodologies, it is possible to design corn-ethanol plants that are not large energy consumers, nor water demanding processes as have been characterized in the literature in the past. In the case of energy we have shown it is possible to design plants that consume 22,000 Btu/gal, which are at least 50% from the ones that have been quoted in the literature (Table 1). Likewise, for water networks, we have shown that it is possible to design these so as to consume less than 50% water compared to values reported in the literature (Table 2).

Second generation ethanol requires much less energy (producing 18MW vs. the consumption of 45MW), but the more powerful pretreatments needed to break down the structure of the raw material results in higher temperatures and pressures, and thus larger cooling needs (71MW vs. 22MW). The production of hydrogen as byproduct is key for making the 2nd generation ethanol process economically attractive even though there is a trade off in terms of energy consumption and water usage. In general, producing ethanol from switchgrass does not require energy and may even produce it. Furthermore, it requires less water than gasoline.

Finally, the goal of zero discharge requires the development of more efficient and cheaper wastewater technologies even though for certain processes it can be obtain at the present degree of development.

Acknowledgments

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