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Optimising the Water-Energy Nexus Over Process and Product Networks

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Producing renewable fuels from biomass has been proposed as a means to lower our carbon footprint and help establish sustainable industrial processes. However, key questions must be answered about these bio-based processes before they can truly be considered a promising alternative. While economics and emissions of these processes have been studied and optimised at length, the critical component of water consumption must be considered, as future water scarcity has been identified as a key challenge. This work compiles a network of hundreds of bioconversion technologies and aims to optimise them over the objectives of production cost and water consumption. The water efficiency of energy (WEE) is also calculated. Water consumption is considered from biomass cultivation to processing, providing a better glimpse into the true consumption of this resource throughout the value chain. A multiobjective MINLP model is formulated as well as an MILP-based branch and refine algorithm to boost solving efficiency. An illustrative case study using a variety of feedstocks under demand of primary fuel products (ethanol, diesel, and gasoline) is presented. The water consumption of the Pareto-optimal solutions ranged from 54.9·× 10^6 L/y to 215,121·× 10^6 L/y with corresponding production costs of 251·× 10^6 \$/y to -240.8·× 10^6 \$/y. The WEE ranged from 0.04 L/MJ to 111.3 L/MJ. The branch and refine algorithms were shown to be orders of magnitude more efficient than directly solving the original MINLP problem with general purpose solvers.

1. Introduction

Water and energy are intimately related. This relationship has held for energy technologies throughout the ages: water has powered watermills for hundreds of years, hydroelectric dams around the globe produce 19 % of the world's electricity (USGS, 2014), and modern nuclear and coal/natural gas power plants require massive quantities of cooling water. In the United States, approximately 40 % of all freshwater withdrawals are utilised to meet cooling demand for electricity production (Kenny et al., 2009). The US Department of Energy recently released a report expanding the concept of a water-energy nexus (WEN) (DOE, 2014). The report discusses key future challenges of water scarcity and increasing energy demand.

The chemical engineering community also recognizes the future challenges presented by the WEN, and the field is focusing on using water efficiently in chemical and industrial operations. Water network modelling has received significant attention. Interplant water networks with recycling techniques have been optimised with genetic algorithms (Alnouri et al., 2014). Optimisation of a wastewater network for a refinery's effluent has been investigated (Sueviriyapan, 2014). Gao and You (2015) optimised water management strategies for shale gas supply chains. The WEN has been identified as an important policy and sustainability concern, and the scientific community has responded by laying the groundwork for modelling and optimising the WEN.

However, the intersection between water and energy in biofuel and bioproduct systems has received less attention than general water management modelling. It is clear that water is intricately connected with biofuels. Water is used during both the biomass cultivation phase and the processing phase(s). Approximately 34 % of water consumption in the United States is directed towards agriculture (DOE, 2014). Thus, investigating the WEN of biofuels presents an intriguing research prospect. Given the tendency of the agricultural and the energy industries to use large quantities of water, the biofuel sector in particular must consider water consumption if the industry is to be sustainable.

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Thus, it is the goal of this work to optimise the water consumption of a large biofuel product and process network. A multiobjective MINLP model is constructed in the following section, and an MILP model and algorithm is employed to boost computational solving efficiency. A large case study is investigated to determine the trade-off between production cost and water consumption of a biofuels processing pathway, demonstrated in a Pareto-optimal curve. Finally, the water efficiency of the energy produced in the form of biofuels is calculated for a variety of cases.

2. Methods

A network of biomass to biofuels conversion technologies was constructed based on previous work (Garcia and You, 2015). Data for all technologies included a basis for the operating cost, capital cost, capacity, yields, water consumption, and energy use. Technoeconomic analyses, government reports, or other literature sources were used as the source of the data. Water consumption during cultivation of each biomass feedstock in the model was also determined from a variety of reports, such as Wu et al. (2009) for switchgrass, Mekonnen and Hoekstra for a variety of biomass types (2011), and May et al. (2012) for water consumption of a softwood plantation. If a technology is selected to be in the processing pathway via binary decision variables, there are upper and lower bounds on its capacity. An MINLP model is constructed to optimise two objectives of production cost and total water consumption of the processing pathway. The multiobjective component of the problem is tackled by the augmented epsilon constraint method (Mavrotas, 2009). Appropriate mass balance, demand, supply, and cost equations and constraints are incorporated into the model. Nonlinearities in the model arise in the capital cost scaling terms, which could result in large computation times. To avoid this potential scenario, we implement an MILP-based branch and refine algorithm with piecewise linear approximations using SOS1 variables to approximate these nonlinear terms (Garcia and You, 2015). The model is summarized below:

$$\min \left\{ \sum_j \left(foc_j + fcf_j + ccf_j \right) RX_j + \sum_j \left(ec \cdot eu_j + \frac{ioc_j}{rc_j} \right) X_j + \sum_i \left(vtc_i + ftc_i + fp_i \right) P_i - \sum_i sp_i \cdot S_i \right\} \tag{1}$$

$$\min \left\{ \sum_j pw_j \cdot \left(\frac{X_j}{rc_j} \right) + \sum_i cw_i \cdot P_i \right\} \tag{2}$$

$$s.t.\ P_i + \sum_j \eta_{ij}^{+} \cdot X_j = S_i - \sum_j \eta_{ij}^{-} \cdot X_j, \forall i \tag{3}$$

$$d_i \le S_i, \forall i \tag{4}$$

$$cp_i \le P_i \le ma_i, \forall i \tag{5}$$

$$lc_j \cdot Y_j \le X_j \le uc_j \cdot Y_j, \quad \forall j \tag{6}$$

$$X_j = \sum_n u_{j,n} \cdot W_{j,n}, \quad \forall j \tag{7}$$

$$RX_j \ge \sum_n W_{j,n} \cdot val_{j,n}, \quad \forall j \tag{8}$$

$$val_{j,n} = u_{j,n}^{sf_j}, \forall j, n \tag{9}$$

$$\sum_n W_{j,n} = 1, \forall j \tag{10}$$

$$\sum_n EX_{j,n} = 1, \forall j \tag{11}$$

$$W_{j,1} \le EX_{j,1}, \forall j \tag{12}$$

$$W_{j,n} \le EX_{j,n-1} + EX_{j,n}, \forall j, n > 1 \tag{13}$$

$$W_{j,n} \le EX_{j,n-1}, \forall j, n = N \tag{14}$$

$$X_j \in \Re_+^n, P_i \in \Re_+^m, S_i \in \Re_+^m, W_{j,n} \in \Re_+^{n \times N}, EX_{j,n} \in SOS1, Y_j \in \{0,1\}^n \tag{15}$$

where foc_j is the fixed operating cost of technology j, fcf_j is the fixed cost factor of technology j, ccf_j is the capital cost factor of technology j, RX_j is a substitute variable for the scaled capacity to calculate the capital cost of technology j, ec is the cost of electricity, eu_j is the electricity usage rate of technology j, ioc_j is the initial operating cost of technology j, rc_j is the reference capacity of technology j, X_j is the capacity of technology j, vtc_i is the variable cost of transporting feedstock i, ftc_i is the fixed transportation cost of feedstock i, fp_i is the feedstock price of feedstock i, P_i is the quantity purchased of feedstock i, sp_i is the selling price of product i, and S_i is the quantity sold of product i.

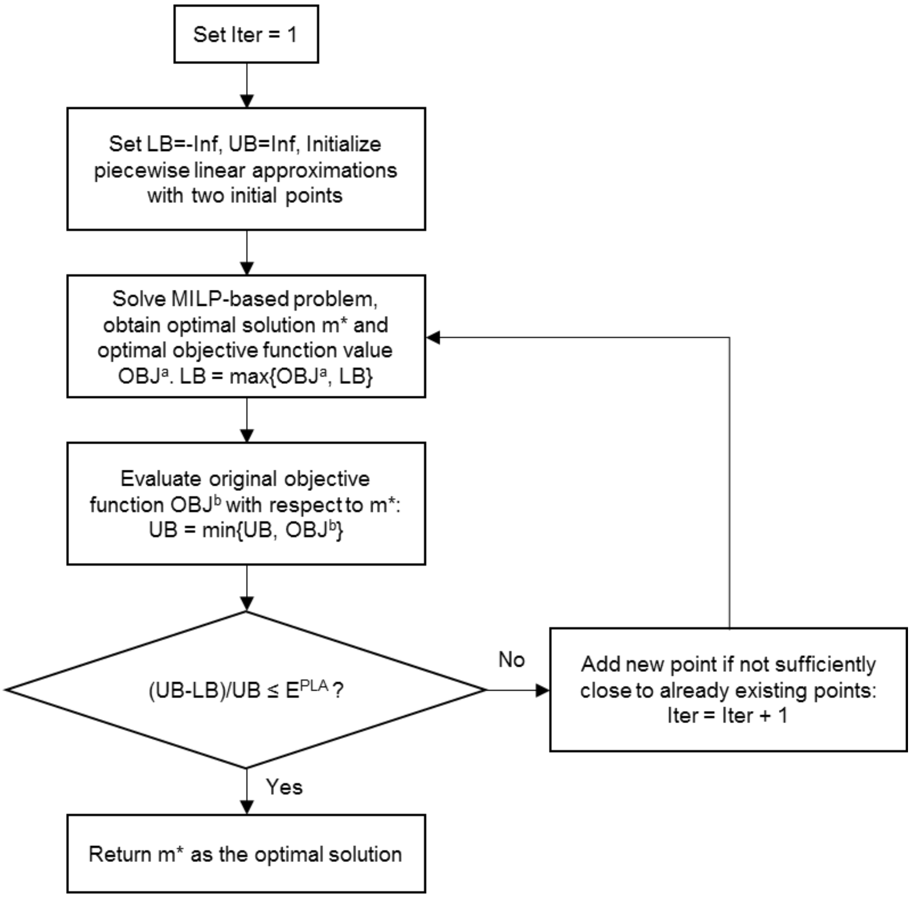

Figure 1: Flowchart for the MILP-based successive piecewise linear approximation algorithm utilized in this study.

Furthermore, pwj is the process water consumption rate of technology j, cw_i is the cultivation water consumption rate of feedstock i, $\eta_{i,j}$ is the consumptive or productive yield of compound/material i through technology j, d_i is the demand for product i, cp_i is the contracted purchase amount of feedstock i, ma_i is the maximum availability of feedstock i, lc_j is a lower bound on capacity for technology j, Y_j is a decision variable on whether to use technology j or not, and uc_j is an upper bound on capacity for technology j. For the piecewise linear approximation equations, $u_{j,n}$ is an estimator for the capacity X_j on interval at grid point n, $W_{j,n}$ are weighted variables to describe where in the interval the solution exists, $val_{j,n}$ represents the capital cost at each point $u_{j,n}$, sf_j is the capital cost scaling factor for technology j, and $EX_{j,n}$ are SOS1 variables to pinpoint in which interval the solution resides. SOS1/SOS2 variables have been successfully used to facilitate the solution of problems with nonconvexities or nonlinearities (Yue and You, 2014).
A flowchart of this algorithm is presented in Figure 1. First, initial piecewise linear approximations are established between the upper and lower bounds for each technology's operating capacity. The corresponding MILP is then solved, with the optimal objective value functioning as a valid lower bound to the original MINLP (Gong and You, 2015). Next, this solution is used to calculate the objective value with the original equation, resulting in a valid upper bound to the original MINLP problem (Gong and You, 2014). A gap is calculated between the two bounds, and successive piecewise linear approximations are added to the MILP model until this gap reaches some error tolerance.

The water efficiency of energy (WEE) is taken as the ratio of the quantity of water used in the processing pathway and the energy available in the form of the final fuel products, calculated from each fuel's higher heating value. Such an indicator could provide valuable insight into the WEN in the biofuels space.

3. Case Study, Results, and Discussion

All experiments were performed on a DELL OPTIPLEX 790 desktop PC with an Intel (R) Core (TM) i5-2,400 CPU @ 3.10 GHz and 8 GB RAM. All models and solution procedures were coded in GAMS 24.3.3 (Brooke et al., 1988). The original MINLP problem was solved with BARON 14.0.3 (Tawarmalani and Sahinidis, 2005). The MILP problem was solved using CPLEX 12.6. The results shown were obtained by solving the proposed algorithm.

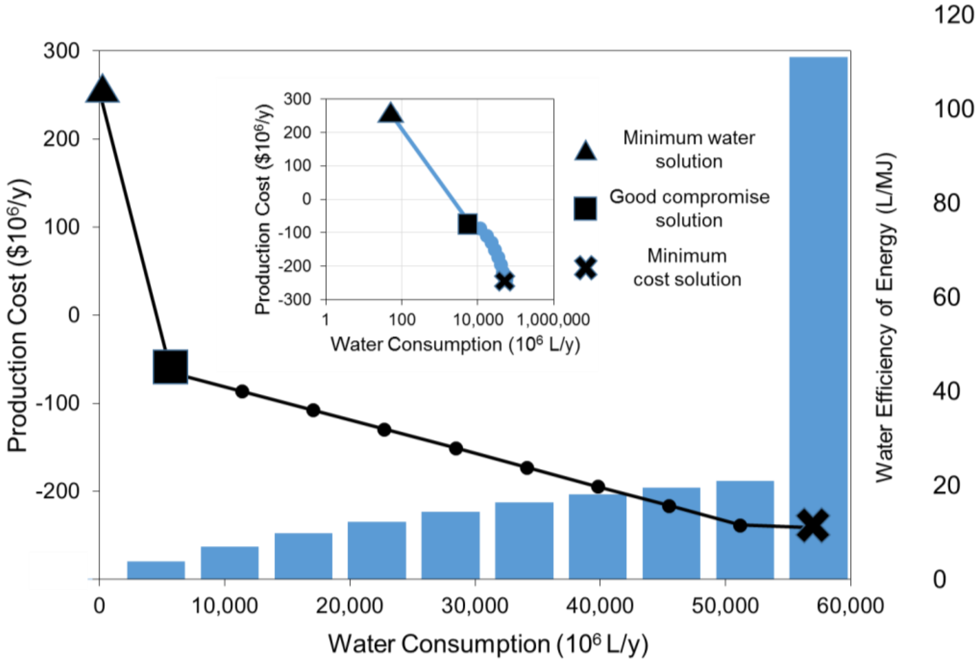

Figure 2. The Pareto-optimal curve for the case study. The line represents the production cost – water consumption relationship, and the bar graph represents the WEE on the right side of the chart.

Demands of 10.9 × 10^6 L/y of ethanol, 11.5 × 10^6 L/y of gasoline, and 10.3 × 10^6 L/y of diesel are to be met in the final processing pathway. Unlimited amounts of all varieties of biomass feedstocks were available for processing. Other byproducts and side products could also be produced. The Pareto-optimal curve for this case study is shown in Figure 2. The production cost – water consumption tradeoff is represented by the line, and the WEE for each solution is shown in the bar graph portion of the figure, with corresponding axis on the right. Water consumption and production cost have an inverse relationship. In order to minimise the water consumption of the processing pathway, a production cost, or operating loss, of approximately 250·× 10^6 $/y is incurred. When minimising the production cost, a production cost of approximately -240·× 10^6 $/y is achieved. The negative sign means the process is profitable, and the process is operated with a net operating profit. The water consumption at each of these points is approximately 54.9·× 10^6 L/y and 215,121·× 10^6 L/y. Thus, both objectives exhibit large swings in value across the Pareto curve, signaling a strong trade-off between the two objectives at the extreme points. The demand for the primary fuel products was met exactly in the minimum water consumption solution. This result is to be expected, as exceeding demand or making large amounts of secondary products or byproducts necessitates the purchase of more biomass feedstock, the cultivation of which inherently requires more water, in addition to more process water use. Furthermore, technologies were chosen that have been finely tuned in the literature to take advantage of water recycling streams, indicating that advancing water recycling technology and systems is key to minimizing the water footprint of the WEN with respect to biofuels.

However, the most important factor in minimising the water footprint was by far feedstock selection. Switchgrass was the only feedstock purchased, as this feedstock has the lowest water consumption of all possible biomass feedstocks during cultivation. Switchgrass is a hardy grass that can grow in a variety of climates, often with little to no additional water other than occasional rainfall. Some sources even assume that switchgrass requires zero additional freshwater other than natural rain to grow (Wu et al., 2009). Woody biomass also requires little additional water, and as the solutions move from left to right along the Pareto-optimal curve of Figure 2, the use of other feedstocks increases. At the minimum water consumption solution, nearly all of the non-natural (i.e. rainwater) water used throughout the process is from process water. However, at the minimum production cost solution, approximately 90 % of the water is used in the biomass cultivation stage, with only 10 % overall coming from process water consumption. These results strongly suggest that biofuels researchers, designers, and engineers consider designing and improving processes that utilize hardy biomass feedstocks, such as grasses and woody biomass, to minimise the total water footprint of the biofuels/bioproducts processing pathway.

The WEE at each point is also shown in Figure 2 as the bar chart with corresponding axis on the right-hand side. It is apparent that not only overall water consumption, but also the WEE are inversely related to the pathway's production cost. The WEE ranges from 0.04 L/MJ at the minimum water solution to 111.3 L/MJ at the minimum production cost solution, a difference of four orders of magnitude. Thus, for the case of biofuels, it appears that minimising the total water consumption (under fixed fuel demand) is tantamount to using as little water as possible for each unit of energy in the final product.

A good compromise solution is identified in Figure 2. This point demonstrates a low water consumption while still being reasonably profitable. At this solution, 21,562·× 10^6 L/y of water is consumed with a production cost of -65.3·× 10^6 \$/y, reflecting profitability. This water consumption is ten times lower than that of the minimum production cost solution. However, the operating gains are reduced by a factor of four compared to the minimum production cost solution. Thus, large decreases in water consumption can be achieved with changes that are not as large as the increase in production cost in this area of the Pareto-optimal curve. At the good compromise solution, the increase in water consumption compared to the minimum water consumption solution is largely attributed to a shift in biomass sourcing to more water-intensive crops. Approximately 98 % of all water consumption at this solution is attributed to water used during the cultivation stage, in contrast to a negligible amount at the minimum water solution and 90 % at the minimum production cost solution. There is an initial "shock" in the water consumption distribution at solutions immediately adjacent to the minimum water solution. As more water-intensive technologies are selected in solutions towards the minimum production cost solution, a trend develops of using more water in the processing stage. This phenomenon is expected, as water recycling technologies increase production costs. When technologies are employed that do not recycle water, the cost decreases, but the water consumption increases.

Table 1: Computational results to minimize production cost. 10,000 CPUs was the solving limit time

	MINLP solved with BARON 14	**Proposed algorithm with CPLEX 12.6**
Objective Value (× 10^6 \$/y)	[-240.8, -240.3]	-240.8
Continuous Variables	1,094	3,097
Integer/Binary Variables	200	400
Constraints	1,378	3,381
Solving Time (CPUs)	10,000*	2.5
Iterations	N/A	4

A minimum water consumption of 54.9·× 10^6 L/y was identified, corresponding to a production cost of 250 ×·10^6 \$/y, resulting in an unprofitable solution. The WEE was 0.04 L/MJ – attributed to using biomass that do not require large amounts of cultivation water. A minimum production cost of -240.8·× 10^6 \$/y corresponds to a water consumption of 215,121·× 10^6 L/y and a WEE of 111.3 L/MJ. The proposed algorithm was found to perform orders of magnitude faster than directly solving the original MINLP with the general purpose solve BARON (2.5 CPUs versus reaching the limit of 10,000 CPUs). Incorporating water consumption and the WEE into product and process network optimisation models produced insightful results and can help research, engineering, and management decision-makers identify promising biofuel/bioenergy projects.

shows the computational performance of directly solving the original MINLP problem with the general purpose MINLP solver BARON compared to the performance of solving the problem with the proposed algorithm with CPLEX. A maximum allowable computation time of 10,000 CPUs was set for each solving scenario with an optimality gap threshold of 10^{-5}. BARON could not find an optimal solution after 10,000 CPUs, but did manage to find upper and lower bounds, resulting in a gap of ~0.002. The proposed algorithm performed four orders of magnitude faster, finding an optimal solution of -240.8·× 10^6 \$/y in 2.5 CPUs. The algorithm took four iterations, resulting in an average iteration time of 0.625 CPUs. The proposed algorithm is efficient at solving large product and process network optimisation problems.

4. Conclusion

Investigating the WEN is critical to ensure sustainability of our water and energy systems moving forward. This work explores a preliminary analysis of the WEN of biofuels systems. Biofuels present an additional consideration of water for biomass cultivation. A bioconversion network of hundreds of technologies, feedstocks, intermediates, byproducts, side products, and biofuels was constructed. A multiobjective, MINLP model was formulated to minimise the production cost and water consumption of the biomass processing pathway under demands for ethanol, gasoline, and diesel. To boost solving efficiency and reduce computational solving times, an MILP-based piecewise linear approximation algorithm using SOS1 variables was developed. The WEE was defined as the amount of water consumed per unit of energy produced, calculated from the higher heating values of the fuels produced in the processing pathway. A minimum water consumption of $54.9 \cdot \times 10^6$ L/y was identified, corresponding to a production cost of 250 $\times \cdot 10^6$ \$/y, resulting in an unprofitable solution. The WEE was 0.04 L/MJ – attributed to using biomass that do not require large amounts of cultivation water. A minimum production cost of $-240.8 \cdot \times 10^6$ \$/y corresponds to a water consumption of $215{,}121 \cdot \times 10^6$ L/y and a WEE of 111.3 L/MJ. The proposed algorithm was found to perform orders of magnitude faster than directly solving the original MINLP with the general purpose solve BARON (2.5 CPUs versus reaching the limit of 10,000 CPUs). Incorporating water consumption and the WEE into product and process network optimisation models produced insightful results and can help research, engineering, and management decision-makers identify promising biofuel/bioenergy projects.

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