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# Comparison of Energy Profile of Waste Valorization Technologies Based on Data-driven Optimization

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## ABSTRACT

The conversion of biomass waste into bioenergy is one of the most important renewable energy production strategies. However, the energy inputs and outputs for different conversion technologies have not been fully comparatively evaluated. Herein, we developed a data-driven framework to optimize the process conditions of conversion technologies, including hydrothermal carbonization, hydrothermal liquefaction, and hydrothermal gasification, anaerobic digestion (AD), pyrolysis, and gasification. Then the predictive properties of products from conversions based on optimal conditions were employed for following life-cycle energy profiles evaluation. The results showed that the developed machine learning models performed well with most of the $R^2 > 0.80$ for all the targets from the six technologies. Energy profile evaluation indicated that the AD was the most potential one with respect to the energy return of investment by comparing with thermal conversions. The energy requirements from thermal conversions were mainly caused by the reactor heating and feedstock drying for the hydrothermal and dry-thermal conversions, respectively.

**Keywords:** waste to energy (WtE), sustainability, machine learning, optimization, biologic and thermal conversion.

## NONMENCLATURE

| *Abbreviations* | |
|---|---|
| HTC | hydrothermal carbonization |
| HTL | hydrothermal gasification |
| HTG | hydrothermal gasification |
| AD | anaerobic digestion |
| WtE | waste to energy |
| ML | machine learning |
| GBR | Gradient Boosting Regression |
| SVR | Supporting Vector Regression |
| RF | Random Forest |
| HHV | higher heating value |
| Q_reator_heat | the reactor hearting |
| Q_dring | feedstock or hydrochar drying |
| Q_oil_ext | heat for biocrude extraction |
| Q_ hexane _eq | equivalent heating of hexane as a solvent for biocrude extraction |
| E_basic | basic electricity consumption of conversion process |
| E_oil_ext | electricity consumption of biocrude extraction |

## 1. INTRODUCTION

Waste to energy (WtE) is the most attractive strategy for waste treatment and utilization due to its advantages on both environmental and energy aspects. On the one hand, the pollution from waste, including odor pollution, containments for water and soil pollution, and greenhouse emissions, can be avoided by converting the waste into valuable products [1]. On the other hand, the energy produced from waste, e.g., biogas, biocrude, biochar, and syngas, can be as alternatives for fossil fuel [2], which is also beneficial for mitigating climate change.

Therefore, it is indeed necessary to develop WtE technologies for the contribution of the Paris Agreement which is to limit the increase of global temperature far less than 2 °C or possibly 1.5 °C [3].

At present, different kinds of waste valorization technologies have been developed, including the biologic and thermal conversions [4][5][6], e.g., anaerobic digestion (AD), hydrothermal conversions (i.e., hydrothermal carbonization (HTC), hydrothermal liquification (HTL), and hydrothermal gasification (HTG)), pyrolysis, and gasification. One point should be addressed that although the products from the above technologies can be used as energy, some energy will be also consumed during the conversion process, especially in the thermal conversion. Therefore, understanding the energy production potential and consumption of each technology is vital to design the waste utilization system and make decisions for waste management.

In this work, to unveil the energy generation and consumption of waste conversion technologies, we first employed machine learning (ML) algorithms to model each conversion process. Six datasets were compiled by collecting data from literature based on six conversion technologies, including AD, HTC, HTL, HTG, pyrolysis, and gasification, as seen in Fig. 1. The feedstock composition and process conditions of these technologies as inputs and properties of products as outputs were used to develop ML models. Then, ML-based process optimization was implemented to achieve the optimal conversion conditions and maximal energy generation for comparison. Moreover, the energy requirement in each step of technologies was carefully analyzed to identify the net energy production potential.

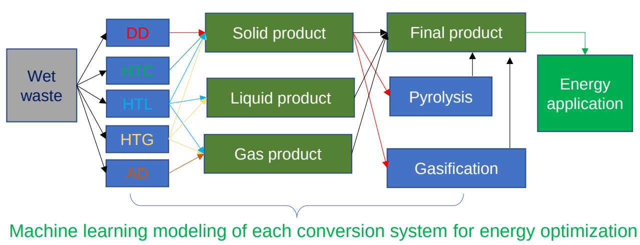


Fig. 1. The overall framework of machine learning modeling and optimization with the objectives of minimizing energy consumption and maximizing energy generation (solid product includes dry waste after dewatering and dring (DD) and hydrochar from HTC, HTL, and HTG; liquid product contains the biocrude from HTL and HTG, the gas product includes the biogas from AD and syngas from HTL and HTG ).

## 2. METHODOLOGY

### *2.1 Data collection and formation*

To model the waste conversion technologies, literature about anaerobic digestion, hydrothermal carbonization, hydrothermal liquefaction (or supercritical water gasification), and hydrothermal gasification, pyrolysis, and gasification of waste (e.g., food waste and manure) were searched and reviewed through the database of Google Scholar and Scopus. The data relating to the waste composition (i.e., C, H, N, O, and Ash contents), the process conditions, such as the reaction temperature and time, and corresponding product properties, e.g., the composition higher heating value (HHV) of char and char, combustible oil and gas from hydrothermal conversions, pyrolysis, and gasification, the biogas from AD, were collected and calculated to compile datasets for ML model development. To make the data consistent, the units for each variable were unified and all the data were normalized before ML developing the predictive models [7].

### *2.2 Machine learning models development*

To develop good models for waste conversions, the five-fold cross-validation method was employed for hyper-parameter tuning with 80% data points of each dataset and left 20% were used to test the model performance [8]. Based on the previous investigation, the Gradient Boosting Regression (GBR) model was developed to model the AD process. The composition of waste, including C and N contents, the AD process conditions, e.g., organic loading rate, hydraulic retention time, temperature, and biochar dosage, were considered as inputs. The $CH_4$ and $CO_2$ yields and HHV of biogas were identified as outputs. For the hydrothermal conversions, the Supporting Vector Regression (SVR), GBR, and Random Forest (RF) models well adapted to the HTC, HTL, and HTG, respectively. The feedstock composition (C, H, N, O, and ash), the reaction temperature, and time were considered as inputs for all the hydrothermal conversions. For HTC, the biochar yield, HHV, C, N, and H contents were identified as multi-outputs. The considered properties of the product (biocrude) from HTL were yield, C, N, and HHV. In terms of HTG, the composition (yields of $H_2$, $CH_4$, $CO_2$, and CO) and HHV of syngas were the outputs for model development. For pyrolysis and gasification systems, the SVR and GBR methods were found to be suitable for modelling. The C, H, N, O, ash, reaction temperature, and time were inputs for pyrolysis, and the C, H, N, O, ash, reaction temperature, steam-to-biomass ratio, and equivalence ratio were gasification model inputs. The yield, HHV, C, N, and H contents of pyrochar from pyrolysis were determined as outputs, and the yields of $H_2$, $CH_4$, $CO_2$, CO, and HHV of syngas were the outputs for gasification modeling. When the hyper-parameters were determined for each conversion model, the 80% data points in each dataset was used to retrain the ML model individually. To understand the prediction performance of the developed model, the $R^2$ and RMSE were used to quantify the prediction accuracy [9].

### *2.3 Optimization modeling based on input and output energy*

Although the energy can be produced by waste valorization technologies, the energy intake is not able to be avoided. Finding the optimal conversion conditions to trade off the input and output energy is significant for net energy production and conversion technology selection for specific biomass waste. Therefore, a well-known optimization method, i.e., Particle Swarm Optimization [10], was employed to cooperate with developed ML models to achieve optimal conversion conditions for maximizing the net energy production. In detail, the life-cycle energy inputs, including the reactor hearting (Q_reactor_heat), feedstock or hydrochar drying (Q_dring), the heat for biocrude extraction (Q_oil_ext), the equivalent heating of hexane as solvent for biocrude extraction (Q_hexane_eq), the basic electricity consumption of conversion process (E_basic) and biocrude extraction (E_oil_ext), were carefully considered for optimization and downstream comparison. For the output energy, the heating energy was calculated based on the HHV and the yield of products from conversions. To make the results comparable, the functional unite of 1-ton fresh waste was identified.

During the optimization, different conversion systems needed to be considered individually. For the hydrothermal conversions, three types of products, i.e., hydrochar, biocrude, and syngas, were simultaneously produced, while we only focused on the optimization of the specific process, and other products were just predicted based on the specific process optimization results. For example, when we targeted the HTL, the energy from biocrude was only identified as the objective for optimization to obtain the optimal conditions of HTL. The energy outputs from HTC and HTG were just calculated based on the optimal conditions of HTC. In the case of pyrolysis and gasification, the biochar can be separated easily, while the combustible oil vapor and gas are mixed together under high reactor temperature. Therefore, the energy from oil and gas is calculated together from the energy balance. For the AD system, the biogas yield and HHV were predicted from optimal conditions to calculate the energy output.

## 3. RESULTS AND DISCUSSION

### *3.1 Model performance*

Based on the required information for post-energy production and consumption analysis, multiple tasks were indeed necessary to be identified for each technology modeling. The ML models equipped with the optimal hyper-parameters were trained with 80% data points of datasets for different conversions.

Table 1. Multi-task prediction performance of ML models for different wet conversion technologies.

| Conversions | Prediction targets | Test $R^2$ | Test *RMSE* |
|---|---|---|---|
| AD | $CH_4$ yield (ml/g wet) | 0.89 | 20.74 |
| | $CO_2$ yield (ml/g wet) | 0.86 | 39.06 |
| | Biogas HHV (MJ/m$^3$) | 0.82 | 2.21 |
| HTC | Hydrochar yield (%) | 0.84 | 7.37 |
| | Hydrochar HHV (MJ/kg) | 0.88 | 2.18 |
| | Hydrochar C (%) | 0.90 | 4.30 |
| | Hydrochar N (%) | 0.94 | 0.52 |
| | Hydrochar H (%) | 0.82 | 0.51 |
| | Hydrochar O (%) | 0.85 | 4.07 |
| HTL | Biocrude yield (%) | 0.82 | 5.50 |
| | Biocrude HHV (MJ/kg) | 0.74 | 1.89 |
| | Biocrude C (%) | 0.71 | 2.37 |
| | Biocrude N (%) | 0.71 | 0.99 |
| HTG | Syngas _$CO_2$ yield (mol/kg) | 0.96 | 1.04 |
| | Syngas _$CH_4$ yield (mol/kg) | 0.94 | 0.57 |
| | Syngas _CO yield (mol/kg) | 0.81 | 0.57 |
| | Syngas _$H_2$ yield (mol/kg) | 0.91 | 1.67 |
| | Syngas _HHV (kJ/mol) | 0.81 | 37.66 |
| Pyrolysis | Pyrochar yield (%) | 0.92 | 5.71 |
| | Pyrochar HHV (MJ/kg) | 0.93 | 2.25 |
| | Pyrochar C (%) | 0.96 | 4.70 |
| | Pyrochar N (%) | 0.92 | 0.41 |
| | Pyrochar H (%) | 0.90 | 0.46 |
| Gasification | Syngas _$H_2$ yield (mol/kg) | 0.86 | 5.94 |
| | Syngas _$CH_4$ yield (mol/kg) | 0.86 | 0.46 |
| | Syngas _$CO_2$ yield (mol/kg) | 0.79 | 3.83 |
| | Syngas _CO yield (mol/kg) | 0.83 | 2.12 |
| | Syngas _HHV (kJ/mol) | 0.83 | 30.94 |

 

The test performance of the trained models was evaluated with the left 20% data. For the AD modeling, the test $R^2$ were 0.89, 0.86, and 0.82 for $CH_4$ yield, $CO_2$ yield, and biogas HHV predictions with corresponding RMSE of 20.74 mL/g wet waste, 39.06 mL/g wet waste, and 2.21 MJ/$m^3$ respectively. In terms of hydrothermal conversions, the $R^2$ for hydrochar property (5 targets) prediction was 0.82-0.94, for biocrude property (4 targets) was range from 0.71 to 0.82, and for HTG_syngas (5 targets) was located between 0.81-0.96. in the case of pyrolysis and gasification, the $R^2$ for the biochar and syngas property prediction was 0.82-0.96 and 0.79-0.86, respectively. The above results indicated that the prediction performances of ML models established for the waste conversion technologies were accepted to predict the property of products for downstream energy profile analysis. More details are shown in Table 1.

### *3.2 Food waste valorization as a case study for energy comparison*

Based on the optimal conditions of each waste conversion technology. The energy inputs and outputs were investigated in detail by employing food waste as an example of biomass waste for a case study. The energy consumption of the six conversion technologies was presented in Fig. 2a. The AD process consumed the lowest energy which is less than 500 MJ for treating 1 ton of food waste. However, for other thermal conversions, the energy inputs were much higher than AD due to the heating needed to heat the reactors. Among the hydrothermal conversions, it was found the energy inputs were dominated by the heating step. However, although much more heating energy was needed for HTL, the total energy consumption of HTC and HTL were close to each other, because extra energy was needed to dry the hydrochar from HTC [11]. For pyrolysis and gasification, the heat for drying of food waste was the most significant part for energy consumption owing to the high-water content in food waste.

For the energy generation (Fig.2b), the AD and HTC was the lowest, and thermal conversions achieved a similar amount of overall energy. However, by trade-off the input energy, the AD showed the highest potential with respect to the return of energy investment, while the digestate from AD may need other steps for further treatment [4]. For the thermal conversions, all the achieved products could be utilized directly. Therefore, it is indeed to consider the ultimate impacts of the conversions when we make decisions for the biomass waste treatment. Moreover, the life-cycle carbon emission should be also considered. Therefore, in our near future work, we will further investigate carbon emission and the potential of integrated technologies.

## 4. CONCLUSIONS

Six datasets were systematically complied based on the conversion of hydrothermal carbonization (HTC), hydrothermal liquefaction (HTL), and hydrothermal gasification (HTG), anaerobic digestion (AD), pyrolysis, and gasification for the ML predictive model development and post energy profile analysis. The prediction performance for all the targets from the six technologies was acceptable with $R^2 > 0.71$ and in which most of them > 0.80. The properties of energy products were predicted based on the optimal conditions achieved from ML-based optimization for downstream energy profile evaluation. It was found that the AD showed the highest potential with respect to the energy return of investment. For thermal conversions, the input energy was dominated by the reactor heating and feedstock drying for the hydrothermal and dry-thermal conversions, respectively. The integrated technology strategy will be investigated to evaluate both life-cycle energy profile and global warming potential in near

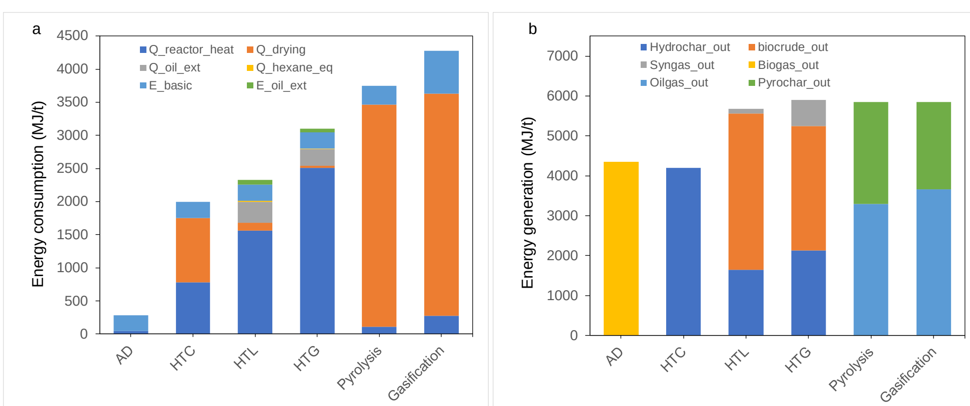


Fig. 2. Energy consumption and production of conversion technologies based on ML-optimization with food waste as feedstock.

future. Such kinds of evaluation will benefit the decision-making of treatment technologies selection and system design of biomass waste valorization.

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