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# Machine Learning Prediction of Syngas Composition of Hydrothermal Gasification from Wet Organic Wastes

Jie Li[1], Lanjia Pan[2], Manu Suvarna[1], Yen Wah Tong[1], Xiaonan Wang[1*]
1 Department of Chemical and Biomolecular Engineering, National University of Singapore, Singapore 117585, Singapore
2 Key Laboratory of Urban Pollutant Conversion, Institute of Urban Environment, Chinese Academy of Sciences, Xiamen 361021, China
* Corresponding Author: Xiaonan Wang; Phone: (+65) 66016221; E-mail: chewxia@nus.edu.sg

**ABSTRACT**

Hydrothermal gasification is an effective and economic technology for production of combustible gases and valuable chemicals from wet wastes. In the present work, machine learning (ML), a data-driven approach, is employed to predict the composition of syngas in terms of $H_2$, $CH_4$, $CO_2$, and CO). A gradient boosting regression (GBR) model with optimal hyper-parameters was developed for the prediction of syngas composition with a test $R^2$ of 0.92, 0.90, 0.95, and 0.92 for $H_2$, $CH_4$, $CO_2$, and CO prediction, respectively. This ML framework provides useful model inference, to identify the correlation and causal analytics between the inputs (feedstock compositions and operational conditions of HTG) and outputs (syngas compositions) essential for our future work, and it lays a concrete foundation to devise ML-based process optimization or inverse design for experiments.

**Keywords:** Gasification, Hydrogen, Data driven, Waste to energy, Sustainability

**NONMENCLATURE**

| *Abbreviations* | |
|---|---|
| HTG | Hydrothermal gasification |
| ML | Machine learning |
| GBR | Gradient boosting regression |
| SD | Solid content |
| T | Temperature |
| P | Pressure |

## 1. INTRODUCTION

Energy depletion and environmental pollution are two of the primary global challenges of the current generation. There is an urgent need to develop technologies for clean and renewable energy production to reduce the dependence from the traditional fossil fuel. Hydrothermal gasification (HTG) is one of the renewable energy production technologies, which can convert biomass or organic waste into syngas, a combustible gas containing $H_2$, $CH_4$, $CO_2$, and CO [1]. HTG is a thermal conversion process involving the presence of water in a near critical temperature and pressure (374.3 °C and 22.1 MPa) [2]. The temperature and pressure of HTG over critical point of water is called supercritical water gasification (SCWG) [3]. In the HTG process, the near-critical or supercritical water can be an effective solvent to accelerate the decomposition of organic matter, which benefits the generation of syngas [4].

In this work, we mainly focus on the wet organic wastes (i.e. sewage sludge, food waste, and manure) as feedstocks for HTG due to following two reasons. Firstly, wet organic wastes are non-negligible culprits of environmental pollution. Various containments, including heavy metal, antibiotics, and micro-plastics, are included in these wet wastes, especially in sewage sludge and manure [5][6][7]. Moreover, the cacosmia and greenhouse gas emission during the collection, transportation, and storage process also poses a serious problem to the environment [8]. Second, these wet wastes can be directly introduced into the HTG reaction for syngas production without any prior dewatering and drying. This in return avoids the need for extra energy for pre-treatment, which is the unique feature and positive attribute of hydrothermal conversion compared to other thermal conversions, such pyrolysis and dry gasification. Therefore, significant efforts have been made in this direction primarily through experimental investigation of HTG from various wet wastes for valuable syngas and

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chemicals production [1][9]. The large amount of related experimental publications inspires us to conduct a data-driven investigation on this topic to find valuable insights from big data analysis.

Machine learning (ML) is a one of the most popular data analysis methodology in the domain of artificial intelligences. ML can be broadly categorized into three types, i.e. supervised learning, unsupervised learning and reinforcement learning. In the present work, we can employ the supervised learning methods to develop ML models based on the labelled data collected from the literatures. The ML model can be well trained based on a historical dataset and then used to predict the target variable of interest when it encounters a new datapoint [10]. In this work, the dataset for hydrothermal gasification of wet organic wastes was complied with the feedstock properties and operational conditions as input features, and the syngas composition ($H_2$, $CH_4$, $CO_2$, and CO) as output targets. Then a machine learning algorithm called gradient boosting regression (GBR) was employed to predict the syngas composition based on the set of input features as discussed above. The hyper-parameters in GBR were well optimized in training process with five-fold cross validation.

## 2. METHODOLOGY

### *2.1 Dataset compiling and pre-processing*

In order to compile a dataset for HTG of wet wastes, a systematic literature review was conducted in the databases of Scopus, Google scholar, and Web of Science with the keywords of hydrothermal, gasification, supercritical water gasification/SCWG, sludge, food waste, and manure. The related literatures were carefully read to find the desired data with the information on feedstock properties, i.e. C, H, N, O and ash contents, the operational conditions, including solid content (SD), temperature (T), pressure (P), and time, with corresponding yield and composition of syngas ($H_2$, $CH_4$, $CO_2$, and CO, with units of mol/kg). Finally, 295 pieces of data were collected from 35 peer-reviewed papers on HTG of sludge, food waste, and manure.

The data pre-processing was conducted for the dataset to unify the units and the calculation for O content. Furthermore, the dataset was normalized to aid in a fast convergence in the ML training process, as reported in our previous work [10]. The O content was calculated according to formulation (1), with unit of percentage.

$$O(\%) = 100 - C - H - N - O - ash \quad (1)$$

Before modelling, the dataset was divided into two parts, 90% random dataset was used to train the ML models, and the left 10% of the dataset was employed to validate the prediction performance of the developed model. Moreover, during the training process, the ten-fold cross validation was used based on the 90% training dataset.

### *2.2 Model development*

Recent literatures have cited the application of ML for prediction of fuel properties, derived from thermochemical waste conversion, especially the random forest algorithm [11][12][13]. Random forest algorithm is an ensemble model with many decision trees, and it is developed by employing the bagging strategy with bootstrap aggregating. Apart from random forest algorithm, another machine learning algorithm called gradient boosting is also an ensemble decision tree [14]. However, there is a dearth of its application in literature for the waste conversion system. Therefore, the gradient boosting regression (GBR) algorithm was employed in present work to validate whether it is capable in the gasification of wet wastes. The MultiOutputRegressor in *scikit-learn* library was applied for multi-task prediction of syngas composition ($H_2$, $CH_4$, $CO_2$, and CO) simultaneously.

The GBR model is trained using boosting strategy which is one of the ensemble learning algorithms [15]. The typical conception of boosting is to integrate a series of weak prediction models to a final strong model with good prediction performance [14][16]. In detail, a leaf will be obtained by averaging the observed values of output as an initial value, it is also the first prediction of the model, and then gradient boost builds the first tree to predict residuals of observed values and initial value. The new prediction values are based on the previous prediction values and the predicted residuals of new tree times learning rate. The learning rate is between zero and one, with a smaller learning rate benefiting to reducing the effect of each tree on the finial prediction to improve the prediction accuracy in the long run. Next tree will be further developed based on the new residual of prediction values from previous tree and observed values. The number of trees (or the number of boost stages) and the maximum depth of the trees can be tuned in the model training process. Therefore, the gradient boost continues to build tree until it reaches this number of trees we set, or if more trees fail to decrease the residuals.

## 3. RESULTS AND DISCUSSION

### 3.1 Model optimization and evaluation

The training data was used for the optimization of Gradient boosting regression (GBR) model by tuning its hyper-parameters for the multi-prediction of syngas composition. The 5-fold cross validation was used in the optimization process to avoid the overfitting problem. As depicted in Fig. 1, four main hyper-parameters (i.e. number of boosting stages or number of decision trees, learning rate, subsample ratio and maximum depth of trees) were tuned and optimized to improve the prediction performance based on average 5-fold cross validation RMSE. The RMSE decreased with increase in both boosting stages, and learning rate, while the RMSE began to increase for the learning rate over 0.1 with boosting stage of 32 (Fig. 1a). Therefore, the optimal learning rate and boosting stage were identified as 0.1 and 32. Based on above two optimal hyper-parameters, the impact of subsample ratio and maximum depth of trees on average RMSE was future investigated, as seen in Fig. 1b. According to the contour plot of subsample ratio vs. maximum depth, three minimum areas were achieved in the left and upper parts. This indicated that smaller subsample ratio (=0.5-0.65) and smaller maximum depth (=7) are enough to achieve a smaller RMSE. Finally, the optimal subsample ratio and maximum depth were identified at 0.5 and 7. Other hyper-parameters of GBR model were the kept at default values.

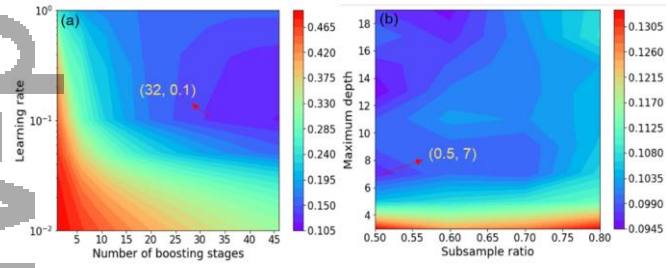


Fig 1 Hyper-paramters tuning of Gradient boosting regression (GBR) model for improving the prediciton performance of syngas composiston.

To evaluate whether the trained GBR model can be applied to give accurate prediction for new experimental data, the remainder 10% testing data were used for validation for syngas composition prediction. Both $R^2$ and RMSE were employed to identify the prediction of optimal model based on training and testing datasets, and the plots of experimental values vs. predicted values for syngas compositions, including $H_2$, $CH_4$, $CO_2$, and CO, are shown in Fig. 2. The line of y=x is shown as a standard line to evaluate the predicated values, and the points closer to the line are associated with a higher prediction accuracy. The prediction of syngas exhibited outstanding performance for the training dataset, and the $R^2$ for the four gases prediction was more than 0.97. Compared to the performance of training data points, the prediction accuracy of test points slightly decreased with lower $R^2$

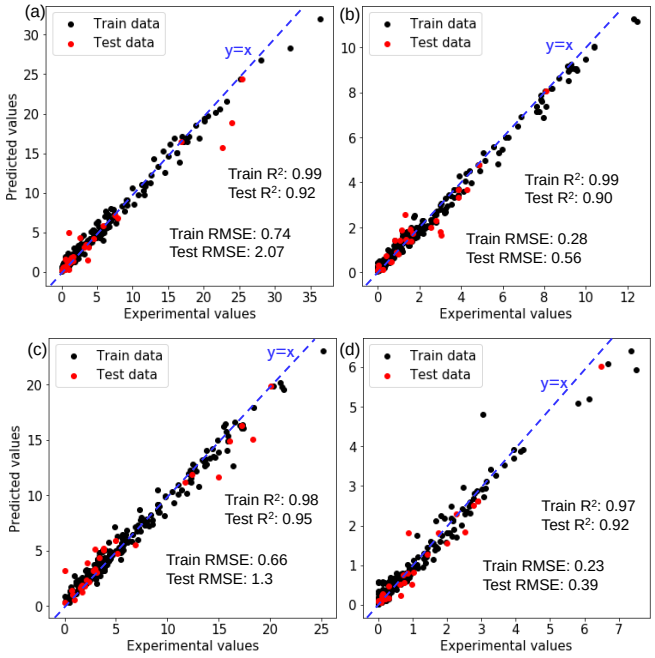


Fig 2 Performance of GBR model for the (a)$H_2$, (b) $CH_4$, (c) $CO_2$, and (d) CO yield prediction.

(0.92, 0.90, 0.95, and 0.92) for $H_2$, $CH_4$, $CO_2$, and CO prediction. However, the prediction performance was still acceptable because of their lower RMSE. The above results indicate that GBR algorithm is capable to be employed to develop ML model for the syngas composition prediction. Moreover, this developed GBR model also provides us with the opportunity to determine the influence of input features (feedstock properties of wet wastes and operational conditions of hydrothermal gasification) to the output targets (syngas yield: $H_2$, $CH_4$, $CO_2$, and CO).

## 4. CONCLUSIONS AND FUTURE WORK

A GBR model with optimal hyper-parameters was developed for the prediction of syngas composition. The testing $R^2$ for the prediction of $H_2$, $CH_4$, $CO_2$, and CO composition the in syngas were 0.92, 0.90, 0.95, and 0.92, respectively. The developed model provided a bridge between input features and output targets, which promoted the investigation of the importance and correlation of feedstock and operational conditions to the syngas composition. More work will be done based on this model in the future, including feature analysis

and engineering, ML-based optimization or inverse design, to provide detailed experimental design schemes and accelerate the experiment procedure. It should be mentioned that the present work only investigates the non-catalyst hydrothermal gasification system, and the catalyst-aided system will further be explored due to its higher yield of $H_2$ and $CH_4$ generation.

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**REFERENCE**

[1] He C, Chen CL, Giannis A, Yang Y, Wang JY. Hydrothermal gasification of sewage sludge and model compounds for renewable hydrogen production: A review. Renew Sustain Energy Rev 2014;39:1127–42. https://doi.org/10.1016/j.rser.2014.07.141.

[2] Peterson AA, Vogel F, Lachance RP, Fröling M, Antal MJ, Tester JW. Thermochemical biofuel production in hydrothermal media: A review of sub- and supercritical water technologies. Energy Environ Sci 2008;1:32–65. https://doi.org/10.1039/b810100k.

[3] Kruse A. Supercritical water gasification. Biofuels, Bioprod Biorefining 2008;2:415–37. https://doi.org/10.1002/bbb.93.

[4] Savage PE. A perspective on catalysis in sub- and supercritical water. J Supercrit Fluids 2009;47:407–14. https://doi.org/10.1016/j.supflu.2008.09.007.

[5] Cao DQ, Yang WY, Wang Z, Hao X Di. Role of extracellular polymeric substance in adsorption of quinolone antibiotics by microbial cells in excess sludge. Chem Eng J 2019;370:684–94. https://doi.org/10.1016/j.cej.2019.03.230.

[6] Akyol Ç, Aydin S, Ince O, Ince B. A comprehensive microbial insight into single-stage and two-stage anaerobic digestion of oxytetracycline-medicated cattle manure. Chem Eng J 2016;303:675–84. https://doi.org/10.1016/j.cej.2016.06.006.

[7] Djekic I, Miloradovic Z, Djekic S, Tomasevic I. Household food waste in Serbia–Attitudes, quantities and global warming potential. J Clean Prod 2019;229:44–52.

[8] Zheng L, Zhang Q, Zhang A, Hussain HA, Liu X, Yang Z. Spatiotemporal characteristics of the bearing capacity of cropland based on manure nitrogen and phosphorus load in mainland China. J Clean Prod 2019;233:601–10. https://doi.org/10.1016/j.jclepro.2019.06.049.

[9] Qian L, Wang S, Xu D, Guo Y, Tang X, Wang L. Treatment of municipal sewage sludge in supercritical water: A review. Water Res 2016;89:118–31. https://doi.org/10.1016/j.watres.2015.11.047.

[10] Li J, Pan L, Suvarna M, Tong YW, Wang X. Fuel properties of hydrochar and pyrochar: Prediction and exploration with machine learning. Appl Energy 2020;269. https://doi.org/10.1016/j.apenergy.2020.115166.

[11] Li L, Flora JRV, Berge ND. Predictions of energy recovery from hydrochar generated from the hydrothermal carbonization of organic wastes. Renew Energy 2020;145:1883–9. https://doi.org/10.1016/j.renene.2019.07.103.

[12] Zhu X, Li Y, Wang X. Machine learning prediction of biochar yield and carbon contents in biochar based on biomass characteristics and pyrolysis conditions. Bioresour Technol 2019;288. https://doi.org/10.1016/j.biortech.2019.121527.

[13] Li J, Zhu X, Li Y, Tong YW, Wang X. Multi-task prediction of fuel properties of hydrochar from wet municipal wastes with random forest, Energy Proceedings; 2019.

[14] Cai J, Xu K, Zhu Y, Hu F, Li L. Prediction and analysis of net ecosystem carbon exchange based on gradient boosting regression and random forest. Appl Energy 2020;262:114566. https://doi.org/10.1016/j.apenergy.2020.114566.

[15] Polikar R. Ensemble learning. Ensemble Mach. Learn., Springer US; 2012, p. 1–34. https://doi.org/10.1007/978-1-4419-9326-7_1.

[16] Rzychoń M, Żogała A, Minerals LR. An interpretable extreme gradient boosting model to predict ash fusion temperature. MDIP 2020. https://doi.org/10.3390/min10060487.