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Hybrid modelling of dynamic anaerobic digestion process in full-scale with LSTM NN and BMP measurements

Alberto Meola[1,2] and Sören Weinrich[1,3]

1 - DBFZ, Deutsches Biomasseforschungszentrum gemeinnützige GmbH, Biochemical Conversion Department, Torgauer Straße 116, Leipzig, 04347, Germany

2 - Leipzig University, Faculty of Mathematics and Computer Science, Augustusplatz 10, Leipzig, 04109, Germany

3 - Münster University of Applied Sciences, Faculty of Energy · Building Services · Environmental Engineering, Stegerwaldstraße 39, Steinfurt, 48565, Germany

Abstract. Machine learning algorithms allow an accurate description of the anaerobic digestion process, but they are not applied in full-scale reactors due to the lack of physicochemical reliabilty. A hybrid model combining biomethane potential (BMP) tests data and a long short-term memory (LSTM) neural network was developed for providing previous knowledge to the neural network and improving performances. Results show that the best model configuration can predict the methane yield with a 6-hours resolution 1 day in advance with a Root Mean Square Scaled Error (RMSSE) of 36%, compared to an RMSSE of 41% obtained by the pure LSTM model configuration.

1 Introduction

Anaerobic Digestion (AD) is a biochemical process that transforms organic matter into biogas and digestate. AD plants have been commonly used for baseload power supply, but the changing conditions within the energy sector requires the development of new concepts. AD processes can potentially provide demand-oriented power and compensate for the irregularity of renewable energy conversion [1]. The Anaerobic Digestion Model No. 1 (ADM1) [2] is typically used for AD process modeling, but simplifications have been proposed due to lack of reliable measurements during regular plant operation [3]. Machine learning (ML) techniques show great potential for non-linear process prediction [4]. Deep learning algorithms such as Long Short-Term Memory (LSTM) Neural Networks (NNs) and Convolutional Neural Networks (CNN) have been recently applied to predict AD process behavior [5]. While such models perform sufficiently well for research application, they cannot be applied to industrial application due to their possible instability during reactor operation.

The current investigation demonstrates that constraining the output of a LSTM NN trained and tested on industrial-scale data provides accurate results in the prediction of methane yield. The upper and lower limits of the prediction are defined depending on the average ratio between the measured methane yield and the methane yield calculated from Biomethane Potential (BMP) tests data, only considering the training dataset.

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2 Materials and methods

For implementation of additional information based on BMP tests, the output of the last neuron of the applied LSTM NN is activated with the hyperbolic tangent (tanh) function, and then scaled between arbitrary limits (see Section 2.3). The output value of the NN represents the ratio between the actual methane ratio and the BMP-estimated methane ratio. A schematic explanation of the procedure is presented in Figure 1.

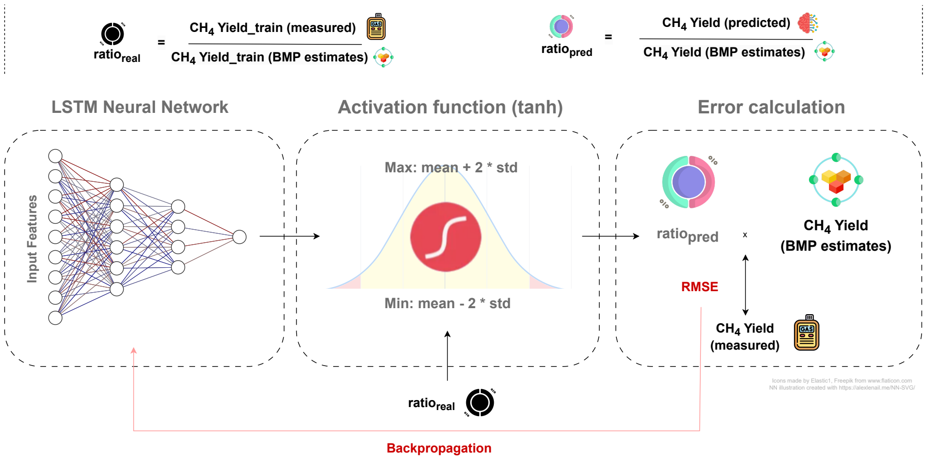

Fig. 1: Hybrid model structure

The choice of the LSTM NN was based on the succesful results of previous research [6], while the application of BMP tests is considered the state-of-art estimation of methane potential for AD of organic substrates.

2.1 Process data

For process simulation and validation of implemented optimization procedures, full-scale experiments for mesophilic AD of corn silage, grass silage, apple pomace sugar beet and cattle manure were conducted in a single primary digester (total volume of 188 m^3) at the Deutsches Biomasseforschungszentrum full-scale biogas plant for 5 months. The reactor was fed on average with 4 t of a mixture of solid and liquid substrate per day, with a highly variable liquid to solid feed ratio. The dataset consists of 14 operational features with 1-minute resolution, 70 substrate-related features with 1-minute resolution and 10 digestate-related features with 1-week resolution. The data was resampled to 6-hours resolution.

2.2 Prediction models

For prediction of methane production with a 6-hours resolution at a 24-hours observation distance, an LSTM NN was developed. The data preparation and the hyperparameters of the NN were optimized according to Meola et al. [6]. Additionally, BMP tests carried out at DBFZ on substrates of the same type were used for estimating the methane yield and limiting the output of the NN. BMP tests assess the maximum amount of methane that can be produced of a specific substrate by anaerobic digestion [7]. The model estimating the methane yield in full-scale considers the specific methane yield from the BMP tests and the Volatile Solids (VS) fed in full-scale. Equation 1 describes the model output for each timestep t.

$$\mathrm{CH_4Yield}_{BMP\_estimated,t} = \sum_{e}^{E} \mathrm{CH_4Yield}_{BMP,s}\,(t - t_{in}) \cdot VS_e \qquad (1)$$

with s being the type of substrate used within event e. A comparison between the measured methane production at 6-hours resolution and the methane production estimated from BMP tests is presented in Fig. 2. The evolution of the ratio between the two shown quantities is shown below.

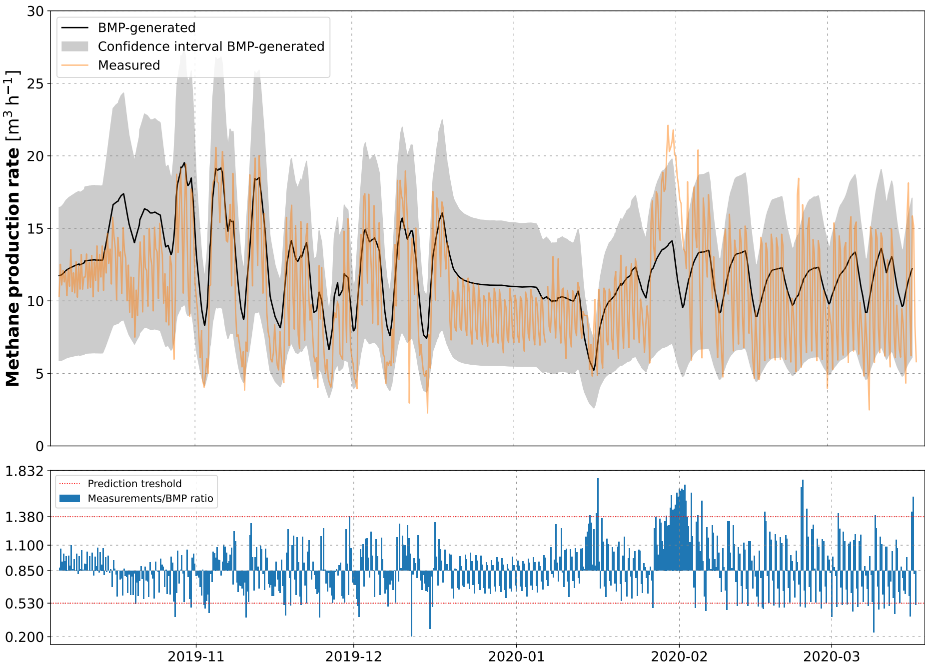

Fig. 2: Measured and BMP-based methane estimates, including ratio.

2.3 Model implementation and configurations

Six different model configurations were considered, presented in Table 1. The configurations from A to E include BMP data, while configuration 0 does not include any BMP data.

Conf. name	tanh limits	Min. delta Adam[a]	NN Epochs	Calculation of tanh limits[b]	BMP corr[c]	Extra input features[d]
A	Mean, std	0.05	400	Train data	no	no
B	1.2; 0.6	0.01	250	-	no	no
C	Mean, std	0.001	300	Train data	no	no
D	Mean, std	0.005	300	Train data from day 19	+1 day	CH4 $\text{Yield}_{BMP\_estimates}$
E	Mean, std	0.05	400	Train data	+1 day	CH4 $\text{Yield}_{BMP\_estimates}$
0	-	0.05	600	-	-	-

[a] Early stopping parameter for the Adaptive Moment Estimation (Adam) NN optimizer
[b] Which data is used for the calculation of the limits of the pseudo-tanh function
[c] Methane estimates from BMP tests can be retarded in time for a better fit
[d] Features can be added to the raw dataset as input features

Table 1: Model configurations

As introduced in Section 2, the output of the LSTM NN is limited to a pseudo-tanh function, resulting from the scaling of the tanh activation function of the last neuron of the network. While in configuration B the scaling limits are fixed to 1.2 and 0.6, in all the other scenarios including BMP data the scaling limits are calculated as per Equation 2 from the training data.

$$\begin{aligned} max_{tanh} &= \text{mean}\left(\text{ratio}_{\text{real}}\right) + 2 * \text{std}\left(\text{ratio}_{\text{real}}\right) \\ min_{\text{tanh}} &= \text{mean}\left(\text{ratio}_{\text{real}}\right) - 2 * \text{std}\left(\text{ratio}_{\text{real}}\right) \end{aligned} \tag{2}$$

with

$$\text{ratio}_{\text{ real}} = \frac{\text{CH}_4 \text{ Yield}_{\text{ measured}}}{\text{CH}_4 \text{ Yield}_{\text{ BMP\_estimated}}}$$

3 Results and discussion

The optimization pipeline [6] was run until the 2000 valid simulations were reached. Previous results show that prediction accuracy of methane yield in full-scale does not improve beyond 2000 simulations.

3.1 Optimization process results

Figure 3 shows the progression of the prediction accuracy during the optimization process. Each step involves the training and validation of the neural network for the set number of epochs (including eventually early stopping). Figure 3A represents the change in error for the validation data, and Figure 3B represents the progression of test error taking into consideration an error decrease in the test data only if corresponding to an error decrease in validation data. This allows a better evaluation of the robustness of the configurations.

While results from train and test dataset show that Configuration A outperforms the other configurations, Figure 3B demonstrates that Configuration E

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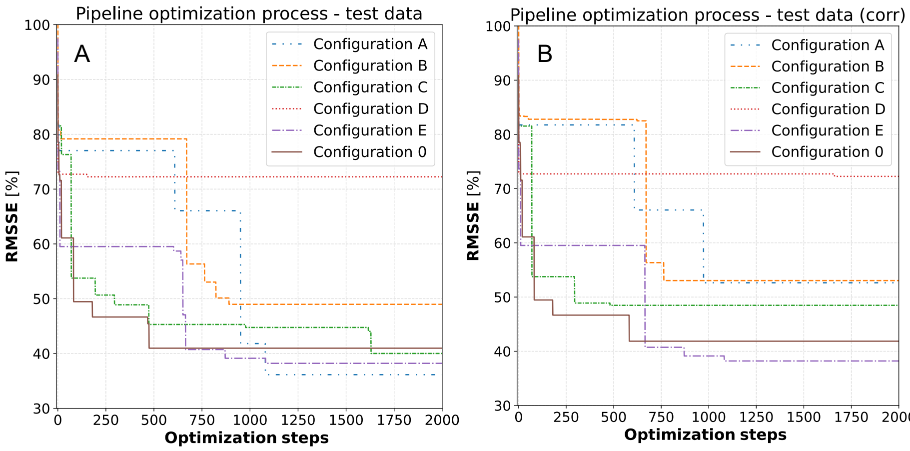

Fig. 3: Optimization process of the tested configurations

performs better when considering only validation dataset error improvements. The baseline (Configuration 0) is outperformed by both Configurations A and E, while outperforms the remaining ones. Root Mean Squared Scaled Error (RMSSE) of the optimized model configurations A, B, C, D, E and 0 are 36, 49, 40, 72, 38 and 41 %, respectively.

3.2 Optimized results of best performing configurations

Optimized results of Configurations A and E are presented in Figure 4. Configuration 0 is furthermore shown for comparison.

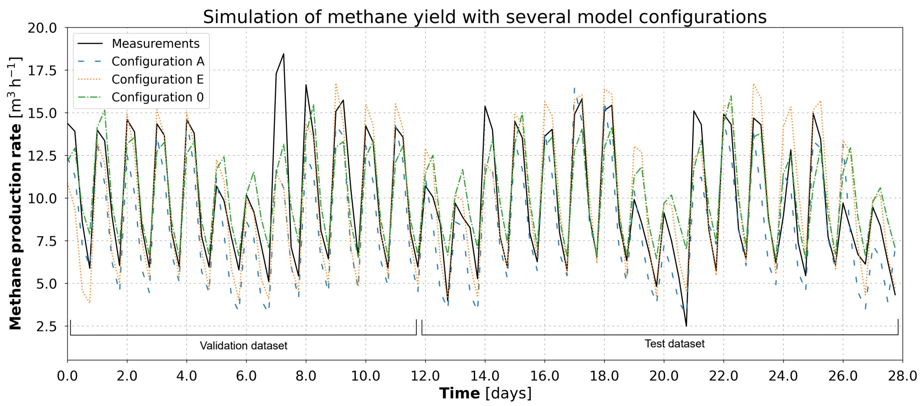

Fig. 4: Simulation results of individual model configurations

Prediction results show that all the configurations can satisfactorily predict the methane yield, with configuration A performing better than the others. While BMP-based models are not able to predict the peak on day 7, neither is the model in Configuration 0, demonstrating that the used upper limit for the pseudo-tanh activation function in the BMP-based models is adequate.

4 Conclusions

A hybrid model consisting of an LSTM NN conditioned by BMP test measurements was successfully developed and tested on full-scale AD data. Results demonstrate that BMP-based hybrid models outperform standard LSTM NNs, particularly when BMP data is used to set the output limits of the neural network. The most robust configuration includes a minimum delta of 0.05 for the NN optimizer, 400 epochs and BMP-derived methane yield as an input feature. Additionally, the model accounts for a time lag of 24 hours between BMP-derived methane yield measurements and the corresponding real-time data. The best performing model in the test dataset showed an RMSSE error of 36% for the prediction of methane yield with a resolution of 6 hours and an observation distance of 24 hours. Performances could be further improved by including individual hyperparameters (tanh limits, minimum delta of Adam optimizer, time-delay in the BMP-estimated methane production) in the numerical optimization routine and using reliable BMP data of the specific substrates that were used in the particular experiment.

References

[1] E. Mauky. *A model-based control concept for a demand-driven biogas production*, Universität of Rostock. Dissertation, 2018.

[2] D. Batstone, J. Keller, I. Angelidaki, S. Kalyuzhnyi, S. Pavlostathis, A. Rozzi, W. Sanders, H. Siegrist, V. Vavilin. Anaerobic digestion model no 1 (ADM1). *Water Science Technology*, 45, 65-73.J., 2002.

[3] S. Weinrich, M. Nelles. Systematic simplification of the Anaerobic Digestion Model No. 1 (ADM1) - Model development and stoichiometric analysis, *Bioresource Technology*, 333, 125124, 2021

[4] M. Khan, W. Chuenchart, K.C. Surendra, S.K. Khanal. Applications of artificial intelligence in anaerobic co-digestion: recent advances and prospects. *Bioresource Technology*, 307, 128501, 2023.

[5] M. McCormick, A. Villa. LSTM and 1-D Convolutional Neural Networks for Predictive Monitoring of the Anaerobic Digestion Process. In *proceedings of the* 28^{th} *International Conference on Artificial Neural Networks*, Munich (Germany), 2019.

[6] A. Meola, M. Winkler, S. Weinrich. Metaheuristic optimization of data preparation and machine learning hyperparameters for prediction of dynamic methane production. *Bioresource Technology*, 372, 128604, 2023.

[7] J. Filer, H.H. Ding, S. Chang. Biochemical Methane Potential (BMP) Assay Method for Anaerobic Digestion Research. *Water*, 11(5), 921, 2019.