A hybrid deep learning framework driven by data and reaction mechanism for predicting glycolic acid production

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Abstract

Selective oxidation at low temperatures without alkali of biomassis a promising and sustainable avenue to manufacture glycolic acid (GA), a biodegradable functional material to protect the environment. However, producing glycolic acid with high selectivity and yield using the traditional research and development approach is time-consuming and labor-intensive. To this context, a hybrid deep learning framework driven by data and reaction mechanisms for predicting sustainable glycolic acid production was proposed, considering the lack of related reaction mechanisms in the machine learning algorithms. Results showed that the fully connected residual network exhibited superior performance (average R2=0.98) for the multi-task prediction of conversion rate, GA, and by-product yields, therefore employed for the following super parameters optimization by the genetic algorithm. The L further identifies that using the optimized operating parameters, the fossil energy demand and greenhouse emissions have decreased by 2.96% and 3.00%, respectively.

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