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On Artificial Intelligence in Sustainable and Circle Chemistry

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Abstract. In this day and age, the deficiency of resources for synthetic chemicals and massive challenges for waste carries the circular economy, including re-cycling waste, into focus. Consequently, it would provide waste a value that is one of the most essential incentives for all researchers to take better care and to avoid unnecessary waste. In fact, the researchers established how computers equipped with wide synthetic knowledge (forward-synthesis with well-known reactions in chemical industries) can help to address the chemical waste challenge. In this context, Artificial Intelligence/Machine learning (AI/ML) can spontaneously learn from data and can perform tasks such as predictions and decision-making. Combinatory studies of AI/ML with chemical health and safety have demonstrated their unparalleled advantages in identifying trend and prediction assistance, which can significantly save personnel, material resources, and financial resources. In this summary, recent research work of AI/ML in sustainable and cycle chemistry will be introduced.

At the present time, the insufficiency of resources for synthetic chemicals and increasing challenges for waste carries the circular economy, including re-cycling waste, into focus. Consequently, it would provide waste a value that is one of the most essential incentives for all researchers to take care and to avoid non-recyclable waste. In actual fact, the researchers established how computers equipped with extensive synthetic knowledge (forward-synthesis with standard reactions in chemical and related industries) can help to address the chemical waste challenge. This provides the generation of synthetic networks with around 200 commercials and new-synthetized, recycled chemicals, leading to approximately 300 important drugs and agrochemicals.[1] In this context, Artificial Intelligence/Machine learning (AI/ML) can automatically learn from data and can perform tasks such as predictions and decision-making. Interdisciplinary studies combining AI/ML with chemical health and safety have demonstrated their dual advantages in detecting trend and prediction support. This tool can significantly save personnel, material resources, and financial resources.[2] In this summary, recent research work of AI/ML in sustainable and cycle chemistry will be introduced.

Mercado-Ruiz *et al.* recently published EoL (End-of-life) data engineering framework by utilizing public database, ML algorithm, and analytic hierarchy techniques. The aim of this research was to find chemicals, assessment releases, and industrial pollution management operations. The extended approach designed pollution abatement unit (PAU) technologies. Then they assessed the efficiencies, chemical releases, exposure media, operating expenses, and capital expenditures. Some highlighted case of studies based on the food and pharmaceutical industry sectors demonstrated the use of the framework for chemical flow distribution. Furthermore, this research can study chemical of concern and the profits of incorporating and spreading the framework with ML and multi-criteria decision-making models. The authors showed how the improved framework developed and evaluated PAU technology systems for managing EoL chemical flows. It also offered release inventories and pathways for leading chemical risk evaluation and exposure assessment of potential on-site EoL scenarios.[3]

Following to this topic, Smith *et al* proposed a new framework to develop the toolbox of chemical release assessment approaches accessible for industrial processes. However, scientists and engineers usually make effort for improved accuracy. Furthermore, the progress of fit-for-purpose release estimates can speed consequences that could postpone essential decisions to protect human health and the environment. Many release estimation approaches are presented, with the most innovative using decision trees for regression and prediction. Each method was assessed in a case study for cumene production to perform the reconciliation of data quality concerns and requirements for time, resources, training, and knowledge. The evaluation of these decision support criteria and the lessons learned were used to develop a purpose-driven framework for estimating chemical releases. For example, the authors used CART (Classification and Regression Tree) model and RF (Random Forest) to predict emissions for three data sets such as train, test, and out-of-sample.[4]

Lastly, Lee *et al.* proposed ML models based on the RF algorithm. This model was used to predict the output of oxidant exposures from water quality parameters. The input variables were pH, alkalinity, dissolved organic carbon concentration, and fluorescence excitation−emission matrix (FEEM) data (to characterize organic matter). In order to build the models, they applied multiple samples of natural waters and wastewater effluents were collected and characterized. The oxidant exposures in each sample were determined at an exact O^3 dose (2.5 mg/L). Four RF models were built depending on how FEEM data were used. For example, one model free of FEEM data, and three models in FEEM data with different

resolutions. Furthermore, the regression performance and Akaike information criterion (AIC) were evaluated for each model. The models employing high-resolution FEEM data normally showed high accuracy with reasonable AIC values. It implied that organic matter features measured by FEEM can be highlight factors to recover the accuracy of the prediction model. The obtained models can be used to predict the reduction of MPs (Oxidation of micropollutants) in drinking water and wastewater ozonation processes. It also can be applied to optimize the O^3 dose for the proposed removal of target MPs.[5]

To conclude, the three research papers mentioned above, an urgent need for sustainable and circular chemistry is shown. AI/ML techniques are a validated tool to help *a priori* the recycling of chemical reagents. In the future, the use of this technology is expected to be widespread in this field, due to the low-cost analysis and less time- and resource-consuming.

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