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Process Analytics Technology (PAT) modeling using linear and non-linear convolutional approaches

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Waste lubricant oil (WLO) is a hazardous residual that is preferably recovered through a regeneration process, for promoting a sustainable circular economy. WLO regeneration is only viable if the WLO does not coagulate in the equipment. Thus, to prevent process shutdowns, the WLO's coagulation potential is assessed offline in a laboratory through an alkaline treatment. This procedure is time-consuming, presents several risks, and the final outcome is subjective (visual assessment).
To expedite decision-making, process analytics technology (PAT) was employed to develop a model to classify WLOs according to their coagulation protentional. To this end, three approaches were followed, spanning linear and non-linear models. The first approach (benchmark) uses partial least squares for discriminant analysis (PLS-DA) combined with standard spectral pre-processing techniques (27 model variants). The second approach uses wavelet transforms to decompose the spectra into multiple frequency components by convolution with linear filters, and PLS-DA for feature selection (10 model variants). Finally, the third approach uses convolutional neural networks (CNN) to estimate the optimal filter for feature extraction (1 model variant).
The results show that the three modelling approaches can attain high accuracy (91% on average). Thus, they can lead to a significant reduction in laboratorial burden. However, the benchmark approach requires an exhaustive search over multiple pre-processing filters since the optimal filter cannot be defined a priori. The CNN approach can streamline the estimation of an optimal filter, but has a more complex model building stage. The spectral filtering using wavelet transforms proved to be a viable option, maintaining the interpretability of linear approaches, and reducing the amount of model variants to explore.

Type of presentation

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Classification

Mainly methodology

Keywords

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