Contribution ID: **11** Type: **not specified**

Predicting the coagulation potential of waste lubricant oils (WLO) using multiblock machine learning of NIR and MIR spectra

Thursday, 29 May 2025 15:23 (3 minutes)

Waste lubricant oil (WLO) is a hazardous residue that requires proper management. Among the options available, regeneration is the preferred approach to promote a sustainable circular economy. However, WLO regeneration is only viable if the WLO does not coagulate during processing as it can cause operational problems and possibly lead to a premature shutdown of the process for cleaning and maintenance. To mitigate this risk, a laboratory analysis using an alkaline treatment is currently used to assess the coagulation potential of the WLO before it enters the regeneration process. Nevertheless, this laboratory test is time-consuming, carries several safety risks, and its result is subjective, depending on visual interpretation by the analyst.
In this work, a rapid and robust approach to predicting the coagulation potential of WLOs using multiblock machine learning with near-infrared (NIR) and mid-infrared (MIR) spectroscopy data is proposed. Classification models were trained using interval partial least squares (iPLS) (Nørgaard et al., 2000), PLS for discriminant analysis (Barker & Rayens, 2003), and convolutional neural networks (CNN) (Yang et al., 2019). As the performance of the multiblock PLS models depends on the specific pre-processing and scaling of each spectral block, an exhaustive search over 1755 combinations of pre-processing, scaling, and modelling methods was performed automatically using the AutoML framework called SS-DAC (Rato & Reis, 2019). For reference, the single-block models, for both PLS and CNN methodologies, were also included in the study.
The single-block models indicated clear performance differences, with the MIR block exhibiting superior predictive performance than the NIR block. The best MIR single-block model using PLS achieved a classification accuracy of 0.90, while the MIR single-block CNN model attained an accuracy of 0.94. In contrast, the NIR single-block models showed significantly lower predictive performances, with the best NIR single-block model reaching a classification accuracy of only 0.47. Nevertheless, the integration of both spectral blocks led to an overall improvement in the multiblock PLS models, which attained an accuracy of 0.94. This enhancement is primarily attributed to an increase in the correct classification of WLOs that do not coagulate, which are the most critical ones for the process operation. In contrast, the multiblock CNN model had a decrease in accuracy to 0.87 compared to its single-block counterpart, suggesting that the inclusion of non-informative data negatively impacted its performance. Overall, these findings demonstrate that the combined use of NIR and MIR spectra can improve the capabilities of prediction models compared to their individual use in single-block models.
Keywords: Waste lubricating oil; Multiblock modeling; Classification; Partial Least Squares; Deep Learning

Type of presentation

Contributed Talk

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Session Classification: Poster

Track Classification: Spring Meeting