Abstract

Chemom. Intell. Lab. Syst., **101**, 14-22 (2010)

Felkel Y., Dörr N., Glatz F., Varmuza K.:

Determination of the total acid number (TAN) of used gas engine oils by IR and chemometrics applying a combined strategy for variable selection

The most common analyses carried out to assess gas engine oil quality include determination of viscosity, total base number (TBN), and total acid number (TAN). TAN has been considered to be an important indicator of oil quality, specifically in terms of defining oxidation and the extent of acidic contamination of used oils.

TAN can be determined by potentiometric titration, and typical values for used oils can reach up to 4 mg KOH/g. A more convenient approach for the determination of TAN is based on infrared (IR) spectral data and multivariate regression models.

We developed partial least-squares (PLS) models for the determination of TAN using IR data measured from monograde mineral gas engine oils (SAE 40, medium ash) that have been used in sewer and wood gas engines run with gaseous fuels from a sewage plant and a wood gasification plant, respectively. The final model performance was 0.07 mg KOH/g for the standard error of prediction (SEP).

Essential for the development of powerful empirical models was an appropriate variable selection by combining expert knowledge, biPLS or dyn-biPLS, and a genetic algorithm. The optimum complexities of the models (the number of PLS components) and their prediction performances have been estimated by repeated double cross validation (rdCV).