Remote Sensing of Nitric Acid and Temperature via Design of Experiments, Chemometrics, and Raman Spectroscopy

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Abstract:

This study presents an effective method for the quantification of nitric acid (0.1–9 M) and the temperature (20–60 °C) through optimal experimental design, chemometrics, and Raman spectroscopy. Raman spectroscopy can be deployed using fiber-optic cables in hot cell environments to support processing operations in the nuclear field and industry. Chemical operations frequently use nitric acid and operate at nonambient temperatures either by design or by circumstance. Examples of Raman spectroscopy for the quantification of nitric acid with applications in the industrial field are profuse. However, the effect of temperature on quantification is often ignored and should be considered in real-world scenarios. Statistical design of experiments was used to build training sets for partial least-squares regression and support vector regression (SVR) models. The SVR model with a nonlinear kernel outperformed the top partial least-squares models with respect to temperature and resulted in percent root-mean-square error of prediction of 1.8% and 2.3% for nitric acid and temperature, respectively. The D-optimal design strategy decreased the sampling time by 75% compared to a more traditional seven-level full factorial option. The new method advances chemometric applications within and beyond the nuclear field and industry.