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Improving the spectral measurement accuracy based on temperature distribution and spectra-temperature relationship

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Abstract Temperature is usually considered as a fluctuation in near-infrared spectral measurement. Chemometric methods were extensively studied to correct the effect of temperature variations. However, temperature can be considered as a constructive parameter that provides detailed chemical information when systematically changed during the measurement. Our group has researched the relationship between temperature-induced spectral variation (TSVC) and normalized squared temperature. In this study, we focused on the influence of temperature distribution in calibration set. Multi-temperature calibration set selection (MTCS) method was proposed to improve the prediction accuracy by considering the temperature distribution of calibration samples. Furthermore, double-temperature calibration set selection (DTCS) method was proposed based on MTCS method and the relationship between TSVC and normalized squared temperature. We compare the prediction performance of PLS models based on random sampling method and proposed methods. The results from experimental studies showed that the prediction performance was improved by using proposed methods. Therefore, MTCS method and DTCS method will be the alternative methods to improve prediction accuracy in near-infrared spectral measurement.

Keywords: Temperature-induced spectral variation; Calibration set selection; Temperature distribution;

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