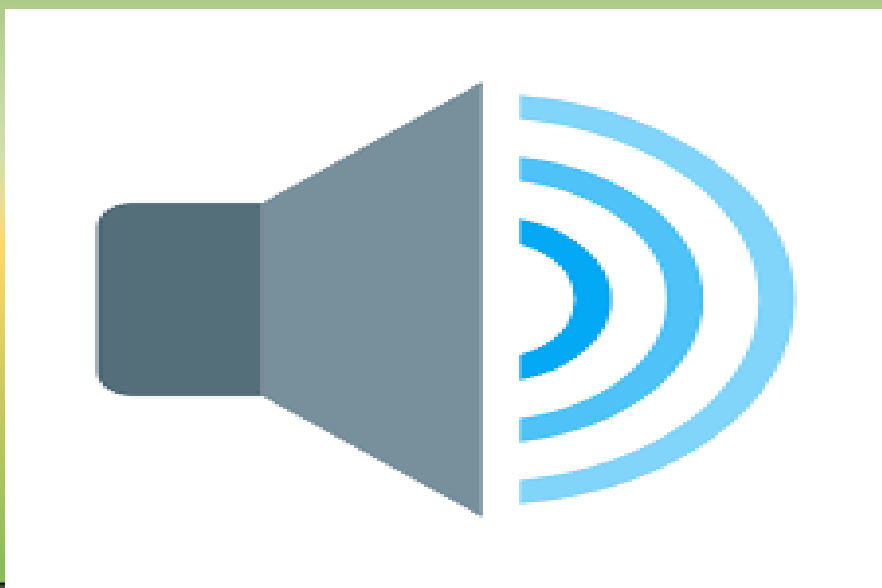




The effect of calibration transfer from a master to a slave instrument to predict water content in biodiesel

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Introduction

The near infrared (NIR) technique is applied to develop non-destructive methods for evaluating qualitative and quantitative analysis. The predicted values are calculated based on calibration models. Typically, the calibration models are developed from the NIR spectra collected instrument (master). Conversely, if these calibration models are applied to another NIR instrument (slave), the error of predicted values may be increased. Therefore, the research studies the main cause of prediction error for calibration transfer.

Materials and methods

Sample

The calibration models are developed by using 650 samples of biodiesels. and 80 samples of biodiesels for studying effects of calibration transfer from the master to the slave devices.

Spectral acquisition

NIR spectra of master and slave instruments in the wavelength of 900 nm to 1700 nm are acquired from the transmittance-mode are developed from DLP NIRscan Nano (Texas Instruments).

Data analysis

The 650 NIR spectra collected from master device are applied to develop calibration models by using “The Unscrambler 9.7”. 80 samples are measured by using master and slave devices to validate the accuracy of prediction results and analyze the effect of calibration transfer from master to slave instruments by using “MATLAB 2016a”

Reference analysis

Water content (%) of biodiesels are measured by using Karl Fisher Titration, one sample measured 2 times for calculating an average value to develop calibration models and evaluate prediction results.

Result and discussion

The statistical results for calibration models to predict water content in biodiesel (using the master's NIR spectra) in Table 1 show high determination coefficient values ($R^2 > 0.9$). This calibration models are applied directly to the master and slave instruments for the prediction of the same sample set (80 samples). The results in Table 2 demonstrate that the results of the slave instrument show significant difference between actual and predicted values at a 95% confidence level when applying the t-test. The prediction errors are caused by different characteristic responses of optical devices and sensors between the master and slave instruments as show in Figure 2. However, the error can be compensated by an appropriate constant value in order to obtain statistical equivalence of the prediction results from two devices.

Table 1. The statistical results of calibration models for determining water content (%) in biodiesel

Pretreatments	Calibration Set (650 Samples, Min: 0.0255, Max 0.1189, SD: 0.0747)				Full cross validation		
	PC	R ²	SEC	Bias	R ²	SECV	Bias
Non	6	0.966	0.010	-2.309x10 ⁻⁸	0.965	0.010	-4.604x10 ⁻⁵
SNV	6	0.956	0.012	3.407 x10 ⁻⁸	0.953	0.012	1.852x10 ⁻⁵
2D	7	0.964	0.010	6.306 x10 ⁻⁹	0.962	0.011	-1.502 x10 ⁻⁵

Conclusion

The slave device’s prediction errors when directly apply the calibration models are caused by different characteristic responses of optical devices and sensors between the master and slave instruments. However, the errors can be compensated by an appropriate constant value.

Acknowledgement

Krairuek Ngowsuwan would like to thank Kasetsart Agricultural and Agro-Industrial Product Improvement (KAPI) Institute for the financial support of the symposium attention.

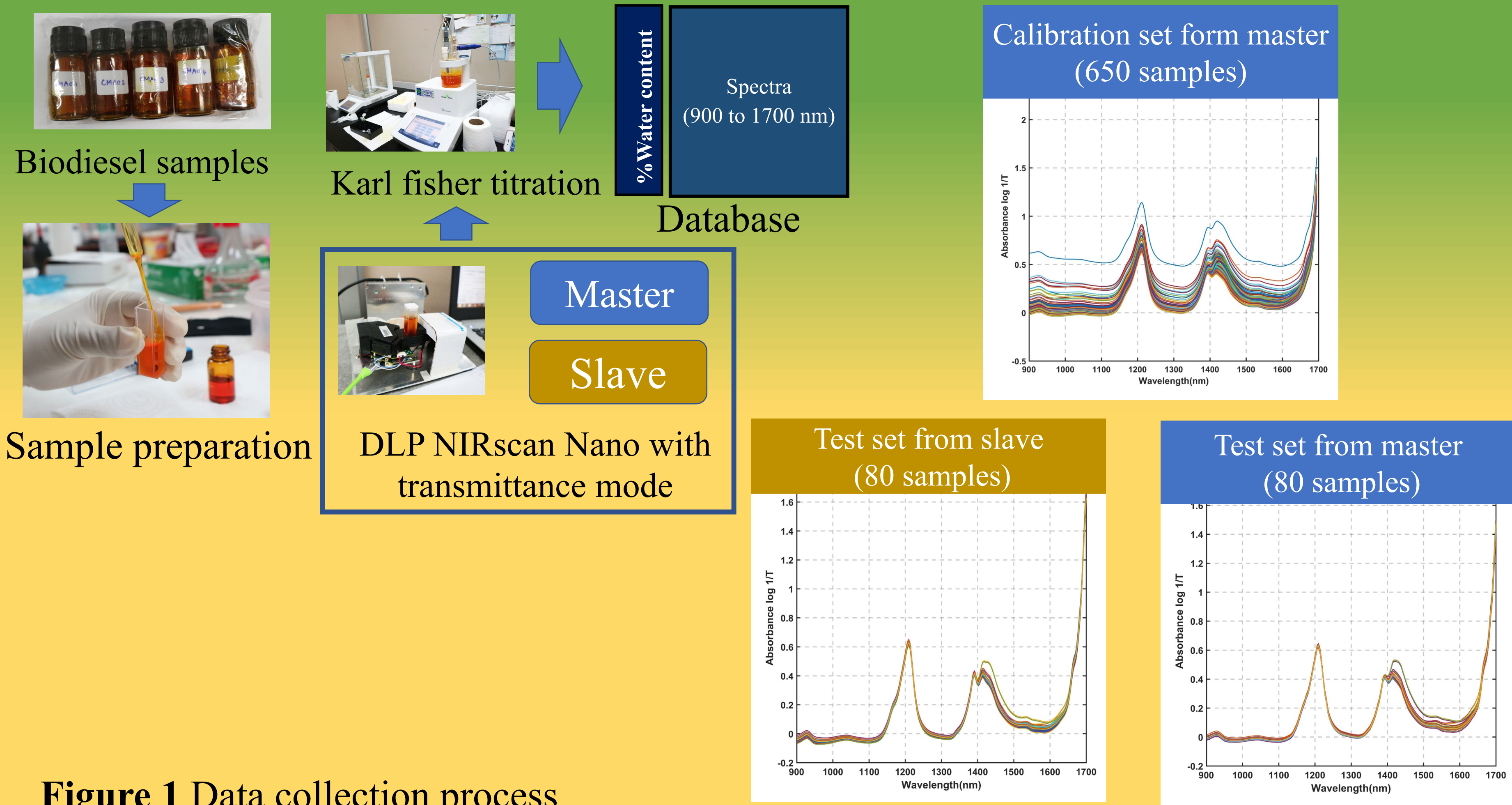


Table 2. The statistical results of both master and slave test sets

Pretreatments	Test set (80 samples, Min: 0.0390, Max: 0.2980, SD: 0.0454)							
	Spectra collected form the master instrument				Spectra collected form the slave instrument			
	R ²	SEP	Bias	t-test	R ²	SEP	Bias	t-test
Non	0.972	0.007	0.001	Non Sig.	0.996	0.005	-0.069	Sig.
SNV	0.960	0.009	0.002	Non Sig.	0.986	0.008	-0.034	Sig.
2D	0.937	0.013	0.000	Non Sig.	0.976	0.008	0.199	Sig.

