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Reducing the spectral nonlinearity error caused by varying integration time

MengQiu Zhang[a,b], Gang Li[a,b], Wenjuan Yan[c], ShaoHui Wang[d], Ling Lin[a,b,*]

[a] State Key Laboratory of Precision Measurement Technology and Instruments, Tianjin University, Tianjin 300072, China
[b] Tianjin Key Laboratory of Biomedical Detecting Techniques & Instruments, Tianjin University, Tianjin 300072, China
[c] Yangtze Normal University, Chongqing 408100, China
[d] Jinan Central Hospital Affiliated to Shandong University, Shandong 250000, China

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ABSTRACT

In the spectral analysis, it is very common to adjust the grating spectrometer's integration time to make it at the appropriate sensitivity, which can get high signal-to-noise ratio (SNR) and unsaturated spectrum. However, varying the integration time during measurement will introduce errors. The influence of varying spectrometer integration time on the spectral analysis was studied in this work, and a method was proposed to formulate a calibration model to inhibit the effect of different sensitivity spectrum due to different integration time. The strategy is to construct a model that is insensitive to the variation of integration time. This method involves the use of collected spectra under different integration time for the model establishment where the obtained model is found to satisfactorily inhibit the influence of integration time variation. An experiment was designed: Collecting the transmission spectra of Intra-lipid suspension by setting different integration time, the obtained spectral data were then processed by "Interactive-Validation method"that can evaluate the error caused by different integration, and processed by the"new modeling method". The experimental results showed that when the integration time was varied to achieve high SNR spectra acquisition, the model established via the novel modeling strategy was clearly a viable method of improving its robustness by incorporating varying integration time, and it could well inhibit the error caused by integration time variation.

1. Introduction

Spectral analysis is a non-destructive analytical technology that can measure multiple compositions simultaneously. Because it has the advantages of rapid detection, non-destructive, no consumption of any chemical reagent, low cost, etc, it is widely used in medicine [1,2], chemistry [3,4] and food science [5,6], and more. Generally, the measurement accuracy can be severely influenced by noise from both the external environment and the spectrometer. Therefore, to improve the accuracy of spectral modeling, interference factors that may occur during the process of spectral acquisition must be controlled. At present, an increasing number of researchers are focusing on errors caused by factors such as temperature [7] and humidity [8]. However, little research has been done on the spectrometer integration time.

Integration time determines the spectrometer sensitivity [9].For different analysis objects, the integration time is determined artificially to ensure that the spectrum is higher than the background noise without oversaturating [10–14], and averaging multiple measurements to reduce the random error [15–17].At present, the scientists cognition to "integration time" is usually based on its linear relationship with light intensity [18–20], in actual operation, especially for some substances with high absorbance, the integration time always be varied to obtain a high signal-to-noise ratio spectrum due to the limited measurement range of spectrometers [21]. In fact, Zhang M had illuminated that integration time and light intensity are not strictly linear, varying the integration time would results in poor model robustness, which resulting the model had a high error up to two orders of magnitude when predicting itself [22].

In this work, we study how to eliminate the influence of varying integration time on spectra analysis. A strategy is proposed to build a calibration model that is insensitive to the integration time differences. To verify the effectiveness of this strategy, an experiment is designed with different concentrations of Intralipid as the testing analyte and with different integration time. The experimental results show that this strategy can eliminate the influence of varying integration time on the spectrum.

* Corresponding author at: State Key Laboratory of Precision Measurement Technology and Instruments, Tianjin University, Tianjin 300072, China.
E-mail address: linling@tju.edu.cn (L. Lin).

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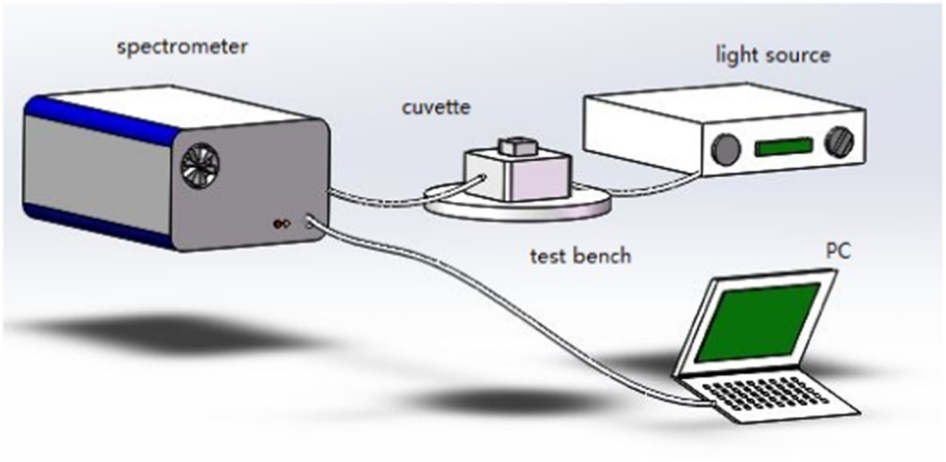

Fig. 1. Experimental setup.

2. Experiment

2.1. Samples and instruments

Intra-lipid is an emulsion of soy bean oil, egg phospholipids and glycerin. Because of its strong scattering properties and weak absorption properties, it is often used to synthesize phantom materials [23,24]. 30% intralipid suspension produced by Huarui Pharmaceutical Co. Ltd. as the stock suspension, was mixed with distilled water according to different volume ratio to obtain different intralipid concentrations. There are 16 samples with concentrations varying from 14% to 28%.

The experimental set up illustrated in Fig. 1, a super continuum laser light source (NKT Photonics, superk TM compact, Denmark) was employed as the light source (spectral range of 500–2400 nm with a 100 mW average output power); All spectra were measured from 300 nm to 1200 nm using the VIS spectrometer (spectrometer range of 300–1200 nm, 0.9 nm spectral resolution, the number of wavelengths is 945, ADC resolution: 16bit, Operating temperature: 20 °C ± 30 °C. **Spectrometer performance meets instrument manufacturer specifications for error and Spectrometer is qualified)**, the suspension is packed in an 10 mm × 10 mm × 30 mm cuvette, which is fixed in the test bench. These components are connected by optical fibers. The optical fiber coupling position of the test bench is equipped with a fiber collimator. The spectra are acquired by adjusting the integration time using the Avasoft 7.6 software. To prevent ambient light from interfering, the experiment is housed in a light-tight enclosure. Before measurements, the super continuum laser light source was turned on and preheated for at least 20 min. This experiment was performed at room temperature (26–27 °C).

2.2. Data acquisition & processing

When the integration time must be varied to achieve the measurement, there are usually two methods which are based on the linearity between integration time and signal of CCD. One way is using the spectral data multiply a factor which is the ratio of two integration time so that ensuring the data are at the same integration time; the other way is: keeping a "total sampling time (T)" constant while varying single-measurement integration time (t), the single-measurement integration time (t) and the number of measurements (Q) must adhere to Eq. (1), the sum of spectrum represents the total spectrum obtained over the total sampling time.

$$Total\text{Spectrum}_{Totalsamplingtime T} = \sum_{i=1}^{Thenumberofmeasurements Q} Spectrum_{\text{single}-\text{measurementintegrationtimet}} \quad (1)$$

Theoretically, if the total sampling time is held constant, changing the single-measurement integration time and the number of measurements will not affect the total spectral data. To determine whether the integration time will affect the measurement, we designed the following experiments: holding the total sampling time constant; changing the single-measurement integration time; and changing the number of measurement. The total sampling time, T, was set to 18,000 ms, and spectra are collected using the six integration formats shown in Table 1. The six groups of spectral data collected using the six integration formats are labeled as groups A–F, ranked by the length of the single-measurement integration time, t. Subsequent processing both takes "Total Spectrum" of each sample calculated from different integration formats as the processing object (see Fig. 2).

Groups A-F refer to a 16 × 945 matrix respectively, indicating 16 samples and 945 wavelengths of transmission light intensity values for the fixed total sampling time (18,000 ms). In order to assess the magnitude of the spectral data difference, this paper takes the total spectrum collected with the integration format A as a benchmark, the relative error between the total spectrum collected with other integration formats and the benchmark was calculated, as shown in Eq. (2):

$$\text{Relativeerror} = \frac{I_\lambda^A - I_\lambda^{BorCorD\cdots.}}{I_\lambda^A} * 100\% \quad (2)$$

Take 17% and 22% concentrations as examples. Fig. 3 (a) shows the transmission spectra at different integration formats for the 17% samples, and (b) shows the spectral data differences. Fig. 4 (a) shows the transmission spectra at different integration formats for the 22% samples, and (b) shows the spectral data differences.

Table 1
Integration formats.

	A	B	C	D	E	F
t * Q	80 ms * 225	100 ms * 180	120 ms * 150	150 ms * 120	180 ms * 100	200 ms * 90