Handling batch-to-batch variability in portable spectroscopy of fresh fruit with minimal parameter adjustment

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HIGHLIGHTS

- A parameter free calibration update approach is demonstrated on fruit.
- Fresh fruit quality models were updated in a parameter free way.
- Transferred model was also updated for fresh fruit quality prediction.
- An online model was locally updated and used for fruit quality prediction.

GRAPHICAL ABSTRACT
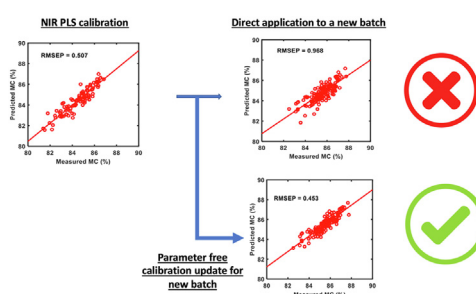
ARTICLE INFO

ABSTRACT

Near-infrared (NIR) spectroscopy models for fresh fruit quality prediction often fail when used on a new batch or scenario having new variability which was absent in the primary calibration. To handle the new variability often model updating is required. In this study, to solve the challenge of updating NIR models related to fresh fruit quality properties, the use of a semi-supervised parameter-free calibration enhancement (PFCE) approach was proposed. Model updating with PFCE was shown in two ways: first where the model on the primary batch was updated individually for each new fruit batch, and second where the model was sequentially updated for the next batches. Furthermore, for the first time, a case of updating an instrument transferred model was also presented. The PFCE approach was shown in two real cases related to moisture and total soluble solids prediction in pear and kiwi fruit. In the case of pear, the model was later updated for 3 new measurement batches, while, for kiwi, a commercial model was updated to incorporate the variability of a new experiment carried out with a new instrument in the laboratory environment. For each modelling demonstration, the performance was benchmarked with the partial least-square (PLS) regression analysis on the primary batch. The results showed that the models updated with a semi-supervised approach kept a high predictive performance on new measurement batches, without any extra parameter optimization. An instrument transferred model was also updated to maintain its performance on different batches. Further, the sequential updating approach was found to be performing better than the update for individual batches, as the models were able to learn from multiple batches. Model updating with a semi-supervised approach can allow the NIR spectroscopy of fresh fruit to be scalable, where models can be shared between scientific or application community.

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1. Introduction

Near-infrared (NIR) spectroscopy has proved itself as one of the main tools for rapid and non-destructive analysis of fresh fruit in the post-harvest domain [1,2]. Two main fruit quality traits i.e., moisture content (MC) and total soluble solids (TSS) can be precisely predicted with NIR spectroscopy [3,4]. Although, at first, the NIR spectrometers require calibration concerning the property of interest [5]. Calibration is needed as NIR is a low-selective technique and unlike the mid-infrared spectra captures only the overtones and combination bond vibrations of the functional bonds such as CH, OH, NH and SH [5−7]. In the NIR signal, these overtones appear as highly overlapped peaks and require extensive chemometric calibration algorithms to extract back the signal related to the property of interest [5].

Once the NIR spectrometers are calibrated, they can be deployed for daily use but requires routine checks to confirm their predictive ability or any changes due to failure of the mechanical systems such as sensor, light source, or reference module [8]. In the case of fresh fruit analysis, the implementation of NIR is not as straightforward and very often the NIR calibration does not precisely predict the property of interest when the models are used on a new batch of fruit [1,2,5,9]. The term 'new batch' is broad but can be related to measurements performed on e.g., the samples measured at a different moment in time [4], different seasons [10], different cultivars/varieties [11], different geographic location [10] or different ripeness levels [10]. In addition, models may need adjustments if measurements are performed at different temperature conditions [10] or if components in the instrument are changed, such as the light source. From a chemometrics perspective, there are two main reasons for model failure [12]. The first is the absence of the new variability in the calibration model related to the property of interest in the new batch [12]. The second is the presence of some variability due to the external influences in the new batch which is not related to the property of interest but masks the variability related to the property of interest [12,13]. The examples of the new variability can be related to a new cultivar or a harvest season, and variability not related to the property of interest may be a different measurement temperature. To make it more complex, sometimes the new variability and the variability due to external influences are mixed such as for a batch where a new cultivar of fruit was measured at a different temperature and with a new light source. Hence, to achieve NIR models that work well on a new batch, it is important to both incorporate the new variability and remove/reduce the influences of external factors from the data wherever possible [12−14].

The failure of NIR models in the domain of fresh fruit analysis is widely recognised and several solutions to incorporate new variability and remove external influences are available. A common approach to incorporate new variability is to update the model by incorporating some new measurements [4] or by combining models of different cultivars and seasons [10,15]. The external influences can be removed with advanced chemometric techniques such as dynamic orthogonal projections and domain adaption (DA) [12,14]. The removal of external effects can be performed with only the NIR data (with DA techniques) [12,13]. However, to incorporate the new variability there is also no other solution having some new reference measurements [4]. Hence, based on the understanding of the case, either the model updating or external effects correction should be explored.

Most of the model updating and external effects removal methods require several parameters to be optimized [12,13,16]. For example, the simplest model updating approach i.e., recalibration of PLS models by incorporating new samples also requires optimization of latent variables (LVs) from scratch [4]. Similarly, in the case of external influence correcting methods such as dynamic orthogonal projections (DOP), several parameters such as dimension of external parameter orthogonalization, optimal LVs need to be reoptimized to build the calibration [12,14]. The more parameters a method requires to optimise, the more it becomes difficult for routine usage [16]. Recently, to reduce the need for several parameters for model updating, a new parameter-free framework for calibration enhancement (PFCE) of NIR data was proposed [16]. The PFCE framework allows model updating and calibration transfer (CT) by implementing a correlation constraint on the regression coefficients [16]. The PFCE framework was recently tested and compared with classical approaches to model updating/CT and was found to be of either equal performance or better [16].

This study aims to present a recently developed semi-supervised PFCE approach utilising a correlation constraint to update NIR models related to fresh fruit. Model updating with PFCE was shown in two ways, first when the model on the primary batch was updated individually for each new fruit batch, and second when the primary model was continuously updated for the next batches. Further, for the first time, a case of updating a transferred calibration model was also presented. In the chemometrics domain, CT between instruments is widely performed, however, most of the studies end with the transfer of calibrations and the performance of the model on the new batches of samples is never followed. This work was novel in the sense as a transferred calibration model performance was evaluated on multiple new batches, and later, the transferred model was updated with the PFCE approach.

2. Materials and method

2.1. Data sets

2.1.1. Pear fruit data

The pear fruit data consist of NIR and corresponding MC and TSS content of four batches of 'Conference' pear fruit. All fruits were sourced from a local fruit distributor in The Netherlands. The four batches were measured along the period of 14 months from September 2019 to November 2020. Based on the chronology of measurements the batches were termed as batch 1 (~September 2019), 2 (~May 2020), 3 (~September 2020) and 4 (~November 2020). Batch 1, 2, 3 and 4 have 239, 232, 80 and 230 fruit, respectively. In all the cases, the spectral measurements were performed with a portable spectrometer (Felix F-750, Camas, WA, USA). The spectrometer acquired spectra in the range of 310−1135 nm with a spectral resolution of 8−13 nm with spectral sampling at every 3 nm. In this study, only the NIR spectral range (720−997 nm) of the data was used for modelling purpose. The spectrometer uses a Xenon Tungsten Lamp for illumination and a built-in white painted reference standard for estimating the reflectance. The data acquisition was performed at the center belly part of the fruit [3,4]. In addition to the Felix spectrometer, for batch 1, extra spectral measurements in the range of 400−2500 nm were performed with the Hi-res ASD LabSpec spectrometer, Malvern Panalytical, United Kingdom. The spectral resolution of the ASD LabSpec spectrometer was 6 nm with a spectral sampling of 1 nm. The measurements with ASD spectrometer were performed at the same spot as the Felix spectrometer using the hi-Brite contact probe with an integrated light source. The extra measurements with a new spectrometer were performed to show the CT model update case for the pear fruit. For all batches, after spectral measurements, a 1 cm thick slice was cut from the equator of the fruit and divided into four equal parts. Two of these parts without peel were used to determine MC and TSS. MC was determined by recording the weight of the parts before and after drying in a hot-air oven (FP 720, Binder GmbH, Tuttlingen, Germany) at 80 C for 96 h. From the two other

parts, TSS of extracted pear fruit juice was determined using a handheld refractometer (HI 96801, Hanna Instruments Inc, Woonsocket, RI, USA).

The data for batch 1 were partitioned into calibration (60%) and test set (40%) with the Kennard-Stone (KS) algorithm [17]. Further, the data of batch 2, 3 and 4 were divided into model updating (40%) and test sets (60%) with the KS algorithm. A summary of the MC and TSS for all four batches after the partition is shown in Table 1. A summary of total samples in each batch after KS partition are shown in Table 2.

2.1.2. Kiwi fruit data set

The Kiwi experiment consisted of updating an already calibrated model provided by the portable spectrometer manufacture (Felix F-750, Camas, WA, USA). The kiwi model can be downloaded from the official website of Felix instruments i.e. https://felixinstruments.com/support/F-751-Kiwi/software/. The raw spectra were extracted using the model builder app from the Felix instruments. In total, 524 spectra and corresponding TSS measurements were extracted corresponding to cultivar Gold and Hayward. A key point to note was that a PLS calibration was developed in the local computer prior to the model update. A local model was needed as the format of the model made available by the portable spectrometer manufacture was not readable in the MATLAB software. In addition to that, a local experiment was carried out with 80 new kiwi fruit of cultivar Hayward obtained from a local distributor in The Netherlands. For each kiwi fruit, the spectral measurements were performed at the central belly part of the kiwi with a portable spectrometer (Felix F-750, Camas, WA, USA). The spectral range was limited to the NIR part i.e., 750–999 nm. After the spectral measurement, a 1 cm thick slice was cut from the equator of the fruit, the juice was squeezed out and used to determine the TSS with a handheld refractometer (HI 96801, Hanna Instruments Inc, Woonsocket, RI, USA). The data extracted from the model downloaded from the website of Felix instrument was divided into calibration (60%) and test (40%) set using the KS algorithm. Further, the locally acquired data was divided into model updating (40%) and test (60%) set using the KS algorithm. A summary of the TSS content in the different batches of kiwi fruit is shown in Table 3.

2.2. Data analysis

There were two types of analysis performed in this study. The first was the PLS analysis where the calibration model for batch 1 was developed. In the following part of the study, the model made on batch 1 was referred to as primary batch model. Later, the regression coefficient of the primary model was updated using the semi-supervised PFCE framework [16]. Further, the model update was performed in two ways, in the first way, the primary model was updated independently for each batch. In a second way, the primary model was sequentially updated for the next batch. Furthermore, a case of updating the transferred calibration model was also presented. In that case, at first, the model was transferred using the fully supervised framework of PFCE [16], later the transferred

Table 2
A summary of total samples in each batch after Kennard-stone partition.

Samples	Batch 1	Batch 2	Batch 3	Batch 4
Calibration/Model updating	123	92	32	92
Test	96	140	48	138

Table 3
A summary of total soluble solids (TSS %) range for calibration/model updating and test set for the online model and the local experiment.

Sample set	Online model		Batch 1 measured locally in lab	
	TSS (%)	Samples	TSS (%)	Samples
Calibration/model updating	10 ± 4.39	314	12.44 ± 1.20	30
Test	12.89 ± 4.32	210	12.22 ± 1.16	45

model was updated in two ways i.e., the primary model was updated independently and sequentially. Performances of all models were compared based on the root mean squared error of prediction (RMSEP) of the independent test set. A summary of the PLS and semi-supervised PFCE method was outlined below.

2.2.1. PLS analysis

PLS regression analysis [18,19] was performed to develop the primary models. Later, the regression coefficients of the batch 1 PLS models were updated. The PLS was implemented using the non-linear iterative partial least squares (NIPALS) algorithm. In this work, 10-fold cross-validation was used to determine the optimal number of LVs for the final PLS model. The PLS analysis was carried out using the 'plsregress' function in MATALB's 'machine learning and statistics' toolbox.

2.2.2. Semi-supervised parameter free framework for calibration enhancement

The semi-supervised approach to calibration enhancement was a sub-method of the parameter-free calibration enhancement methods (PFCE) [16]. The PFCE approach for semi-supervised calibration enhancement was based on the minimization of the difference between the property of interest and the estimated response, subject to the correlation constraints. The objective function of the semi-supervised PFCE is as Eq. (1).

$$\min_{b_{0,s}, b_s} \left(y - [1\ X_s]\begin{bmatrix} b_{0,s} \\ b_s \end{bmatrix} \right)^2 \tag{1}$$

s.t. $\cdot corr(b_s, b_m) > r$

where, X_s was the spectra from the new batch, a key point to note was that X_s are the spectra chosen as the model updating set in Tables 1–3, $b_{0,s}$ are the intercept and b_m and b_s are the coefficients of the model from the primary and new batch. r was the correlation which was predefined as 0.98 [16]. b_m for the primary model can be

Table 1
A summary of moisture content (MC %) and total soluble solids (TSS %) range for calibration/model updating and test sets for four batches of pear fruit. Batch 4 does not have TSS measurements.

Sample set	Batch 1		Batch 2		Batch 3		Batch 4	
	MC (%)	TSS (%)	MC (%)	TSS (%)	MC (%)	TSS (%)	MC (%)	TSS (%)
Calibration/model updating	84.66 ± 1.42	12.74 ± 1.37	84.35 ± 1.39	12.68 ± 1.21	86.88 ± 1.48	11.68 ± 1.18	85.56 ± 1.04	[a]
Test	84.53 ± 1.29	12.88 ± 1.22	84.19 ± 1.38	12.79 ± 1.14	87.29 ± 1.76	11.38 ± 1.41	85.55 ± 1.01	[a]

[a] Batch 3 lacks the total soluble solid content measurement.

obtained with the PLS regression analysis. The objective function in Eq. (1) was optimized with sequential quadratic programming [16] using the 'fmincon' optimization routines in MATLAB 2018b, MathWorks, Natick, MA, USA. To update the model, the semi-supervised PFCE approach requires the regression coefficient of the primary model and some new spectra and corresponding property measurements from the new batch. Here the new spectra mean only the model updating set, which was a small set of spectra and reference property measurements. Finally, the updated model was independently tested on the test set of the new batch for which the model was updated. Model performance was reported as root mean squared error of prediction (RMSEP) and was estimated on the independent test set as mentioned in Tables 1–3.

3. Results

3.1. Pear data set

At first, to benchmark, the performance of the PLS model calibrated on batch 1 (primary model) was tested on the next batches for MC and TSS prediction. A summary of primary model performance for different batches was shown in Fig. 1. The primary model for predicting MC (12 LVs) has a RMSEP of 0.507 but was higher for batch 2, 3 and 4, similarly, for TSS, the PLS model (13 LVs) performed well for batch 2 but reached high RMSEP for batch 3. Such an increase in the RMSEP indicates that there was a need to update the primary PLS model, so it can be effectively used on the next batches. The performance of the primary model was better on batch 2 compared to batch 3 and 4. A reason was that the batch 1 and 2 were from the same harvest season and same orchards, and were just measured in separate experiments, while the batch 3 and 4 were from a different harvest season. Hence, the season variability could be the cause of the inferior performance of the primary model on batch 3 and 4.

A summary of the PLS model for predicting MC (%) updated with the semi-supervised PFCE was shown in Fig. 2. The model was updated independently (first-row Fig. 2) and sequentially (second-row Fig. 2). After the independent update for each batch, the RMSEP

for batch 2, 3 and 4 were reduced to 0.473%, 0.402% and 0.453% from 0.61%, 2.532% and 0.968%, respectively. Similarly, for the sequential update, the RMSEP for batch 2, 3 and 4 were also reduced. However, the main benefit of the sequential update approach was related to a further reduction of RMSEP for batch 4 i.e., 0.449% compared to the 0.453% reached by updating the model independently for batch 4. The reduction in RMSEP with the sequential approach shows that the model might have enhanced by learnings from all the earlier batches.

The model update with either the independent or sequential update bring adjustment in the regression coefficients. Further, these adjustments were specific to the new batches and the variability present in the batches. To have more insights into the batch-specific adjustment in regression coefficients, the evolution of regression coefficients for the model updated independently and sequentially were shown in Fig. 3A and B, respectively. The first main difference in the regression coefficients of the batch 1 model and the regression coefficients of the next models was the overall decrease in the regression weights. Further, this decrease was more in the spectral range >850 nm compared to the <850 nm. The differences in the regression coefficients were unique to the batches, however, it was difficult to extract chemically relevant information to conclude about the cause of variability.

A summary of the PLS model for predicting TSS updated with the semi-supervised PFCE was shown in Fig. 4. The model was updated independently (first-row Fig. 4) and sequentially (second-row Fig. 4). After the independent update for each batch, the RMSEP for batch 2 and 3 were reduced to 0.436% and 0.462% from 0.583% to 1.245%, respectively. Similarly, for the sequential update, the RMSEP for batch 2 and 3 were reduced. However, the main benefit of the sequential update approach was related to a further reduction of RMSEP for batch 3 i.e., 0.432% compared to the 0.462% reached by updating the model independently for batch 3. Like the sequential updating for MC, the reduction in RMSEP of TSS with the sequential approach shows that the model was enhanced due to learnings from earlier batches. One key point to note was that the RMSEP for the sequential modelling were decreased numerically, however, considering higher uncertainty with NIR prediction
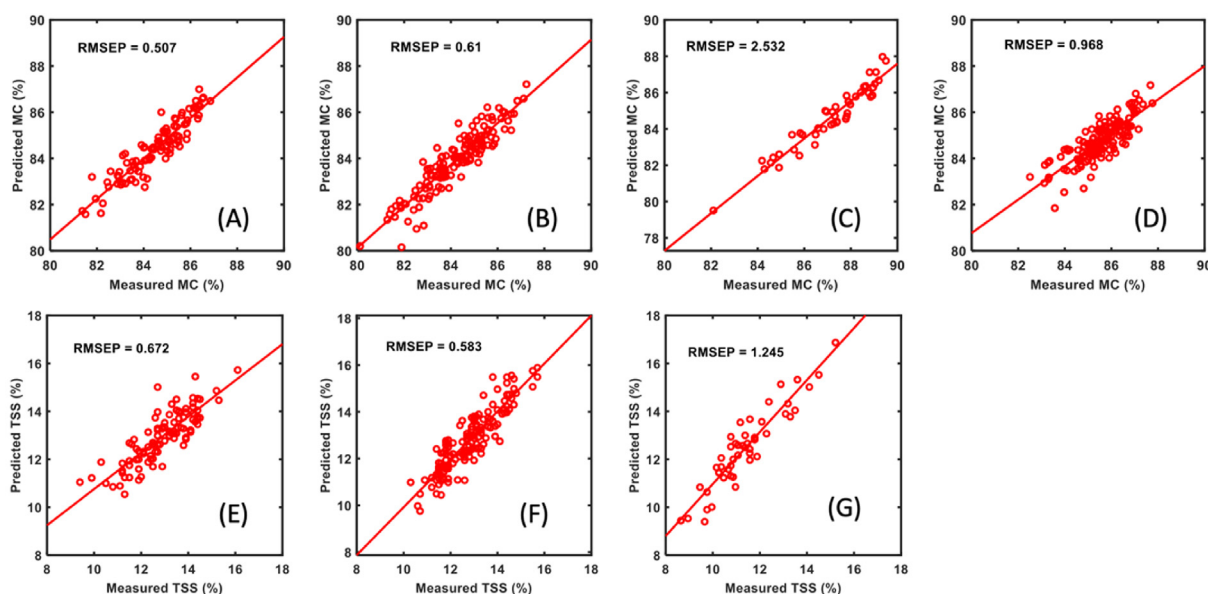

Fig. 1. Summary of partial least-square models for moisture content (MC %) and total soluble solids (TSS %) prediction without update. PLS model for MC made on batch 1 and tested on (A) batch 1, (B) batch 2, (C) batch 3, and (D) batch 4. PLS model for TSS made on batch 1 and tested on (A) batch 1, (B) batch 2, and (C) batch 3. RMSEP = the root mean squared error of prediction.
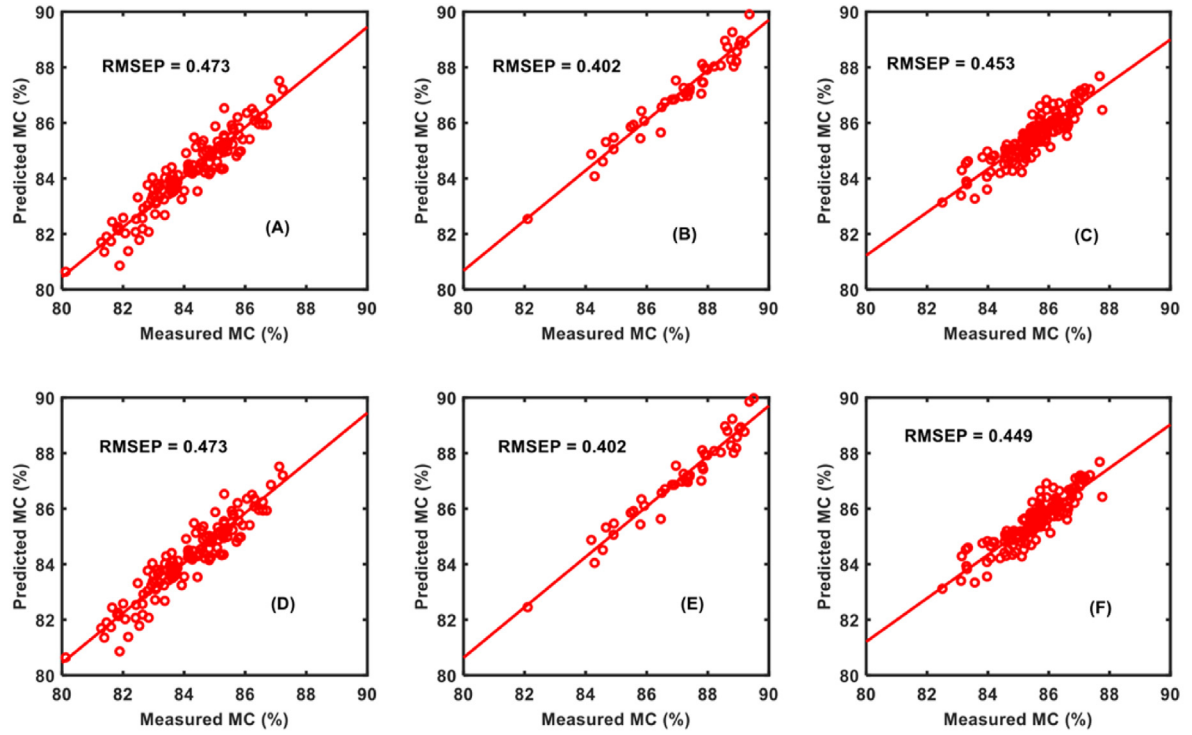
Fig. 2. Moisture content predictions for different batches based on two different model updating approaches. The first update approach in which the primary model was updated independently for each batch (first row) and tested on (A) batch 2, (B) batch 3, and (C) batch 4. The second update approaches involved sequential update (2nd row) and tested on (D) batch 2, (E) batch 3, and (F) batch 4.
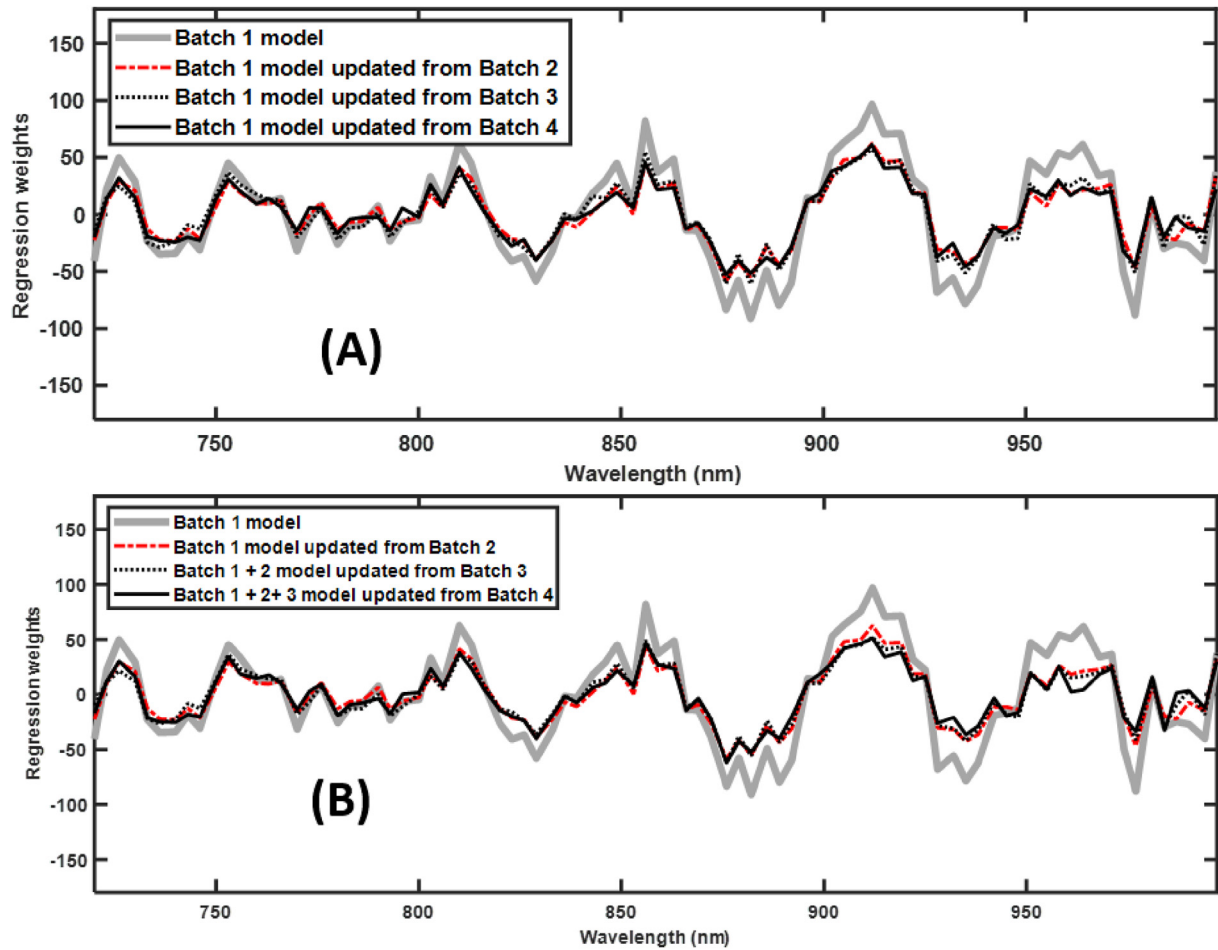

Fig. 3. The effect of model update on the regression coefficients of moisture content prediction in pear fruit. (A) Primary model updated independently for each batch, and (B) primary model was updated sequentially for each batch.
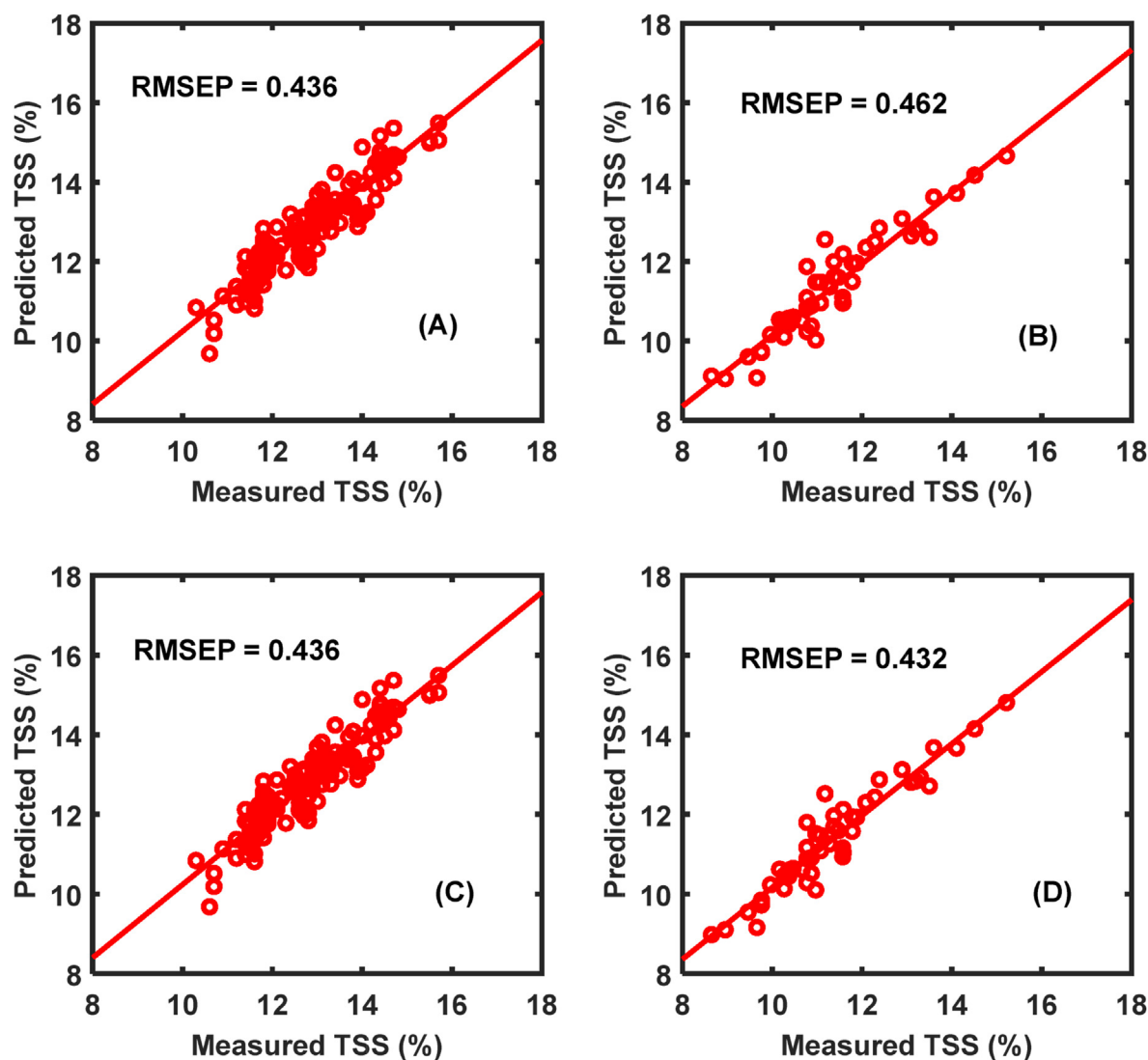
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Fig. 4. Total soluble solids predictions for different batches based on two different model updating approaches. The first update approach in which the primary model was updated independently for each batch (first row) and tested on (A) batch 2, and (B) batch 3. The second update approaches involved sequential update (2nd row) and tested on (C) batch 2, and (D) batch 3.

models, the current study lacks proving if the improvements were significant. The evolution of regression coefficients for the model updated independently and sequentially were shown in Fig. 5A and B, respectively. The main difference in the regression coefficients of the batch 1 model and the regression coefficients of the subsequent updated models is the overall decrease in the regression weights.

The results from PFCE analysis showed that both the independent and sequential modelling approaches were able to keep the predictive performance of models made on Batch 1 when used on the next batches. As a comparison to PFCE, the performance of the PLS recalibration model independently for each batch and sequential were also explored, furthermore, the offset correction approach was also used as a comparison and the results were summarised in Table 4. The model made independently for each batch showed better performance (lower RMSEP) compared to the model made on batch 1 and test on the next batches without any recalibration. Furthermore, recalibrating the PLS model made on batch 1 sequentially showed better performance compared to using the PLS model made on batch 1 without any recalibration. However, the performances of the recalibrated PLS models were far from the performance of the PFCE approach. Offset correction

showed better performance than the recalibration of the PLS model, however, the PFCE outperformed the offset correction, as the RMSEP obtained with PFCE were the lowest. Due to the excellent performance of the PFCE, in the following part of the manuscript, analysis was solely based on the PFCE modelling.

3.2. Kiwi dataset

A summary of the PLS model before and after updating for predicting TSS in kiwi fruit was shown in Fig. 6. The PLS model on the data extracted from the online model had a RMSEP of 0.752% (Fig. 6A). The PLS model when applied on the local batch reached a higher RMSEP of 6.38% (Fig. 6B), showing the need to update the model. Finally, after updating the primary model (with the data of the local batch), the RMSEP for the local batch was reduced to 0.584% (Fig. 6C). Further, the regression coefficients of the online model and the updated model were shown in Fig. 7. The main difference between the regression coefficients was a slight adjustment in the weights over the complete spectral range. However, from the regression coefficient, it was difficult to report anything on the background cause of variability in the new batch, but it was
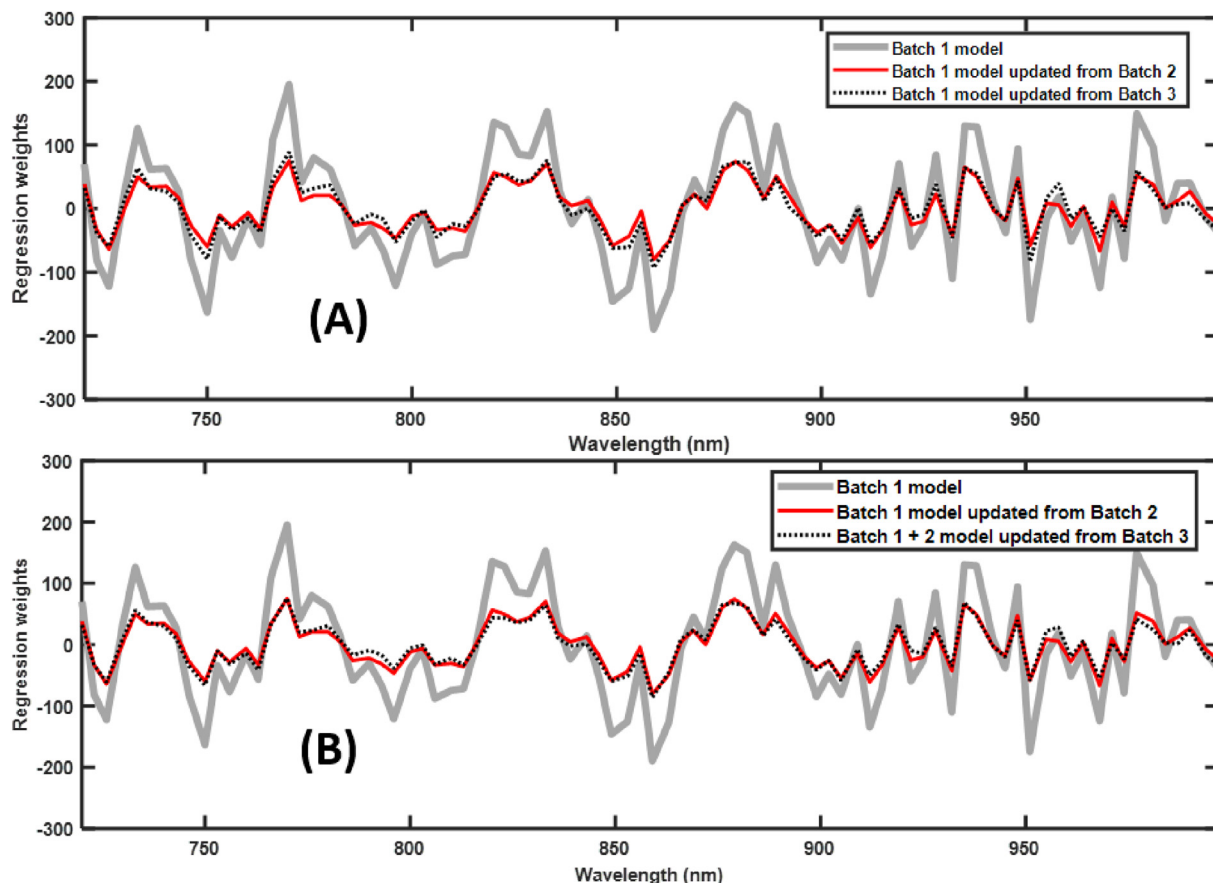
Fig. 5. The effect of model update on the regression coefficients of total soluble solids prediction in pear fruit. (A) Primary model updated independently for each batch, and (B) primary model was updated sequentially for each batch.

Table 4
A summary of root mean square error of prediction (RMSEP %) different approaches to update PLS model (12 LVs) as well as offset correction.

|	Applying the PLS model built on batch 1 on subsequent batches			
	Batch 1 Model applied to Batch 1	Batch 1 Model applied to Batch 2	Batch 1 Model applied to Batch 3	Batch 1 Model applied to Batch 4
Moisture	0.507	0.61	2.532	0.968
SSC	0.672	0.583	1.245	
	Individual PLS models for each batch			
	Batch 1 Model applied to Batch 1	Batch 2 Model applied to Batch 2	Batch 3 Model applied to Batch 3	Batch 4 Model applied to Batch 4
Moisture	0.507	0.501	0.601	0.513
SSC	0.672	0.49	0.535	
	Sequentially recalibrating a PLS model and applying on a new batch			
	Batch 1 Model applied to Batch 1	Batch 1 + 2 Model applied to Batch 2	Batch 1 + 2+3 Model applied to Batch 3	Batch 1 + 2+3 + 4 Model applied to Batch 4
Moisture	0.507	0.49	0.752	0.581
SSC	0.643	0.467	0.523	
	Offset correction			
	Batch 1 Model applied to Batch 1	Batch 1 Model applied to Batch 2 after offset correction	Batch 1 Model applied to Batch 3 after offset correction	Batch 1 Model applied to Batch 4 after offset correction
Moisture	0.507	0.54	0.46	0.59
SSC	0.643	0.554	0.523	
	Performance of PFCE approach (independent update)			
	Batch 1 Model applied to Batch 1	Batch 1 Model updated & applied to Batch 2	Batch 1 Model updated & applied to Batch 3	Batch 1 Model updated & applied to Batch 4
Moisture	0.507	0.473	0.402	0.453
SSC	0.672	0.436	0.462	
	Performance of PFCE approach (sequential update)			
	Batch 1 Model applied to Batch 1	Batch 1 Model updated & applied to Batch 2	Updated batch 1 model updated & applied to Batch 3	Updated batch 1 model updated & applied to Batch 4
Moisture	0.507	0.473	0.402	0.449
SSC	0.643	0.436	0.432	
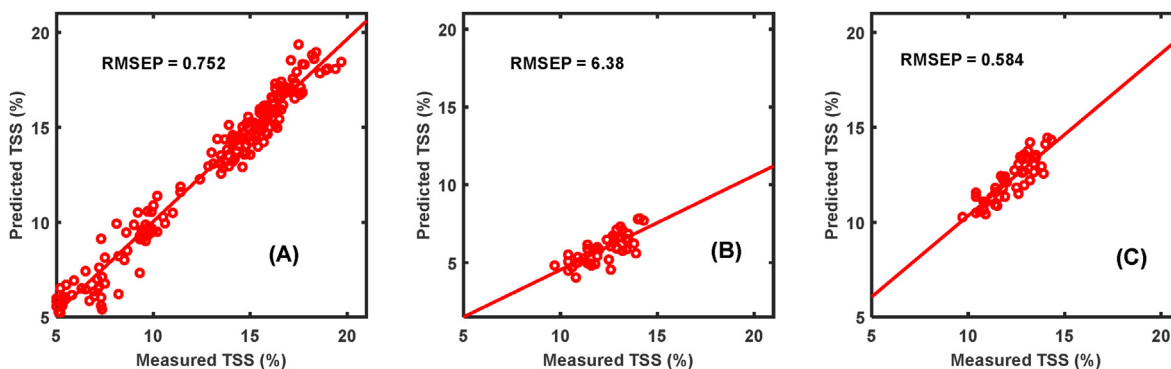
Fig. 6. A summary of model update for predicting total soluble solids in kiwi fruit. (A) Primary model tested on test set of primary batch, (B) primary model tested on local batch, and (C) primary model update and tested on local batch.
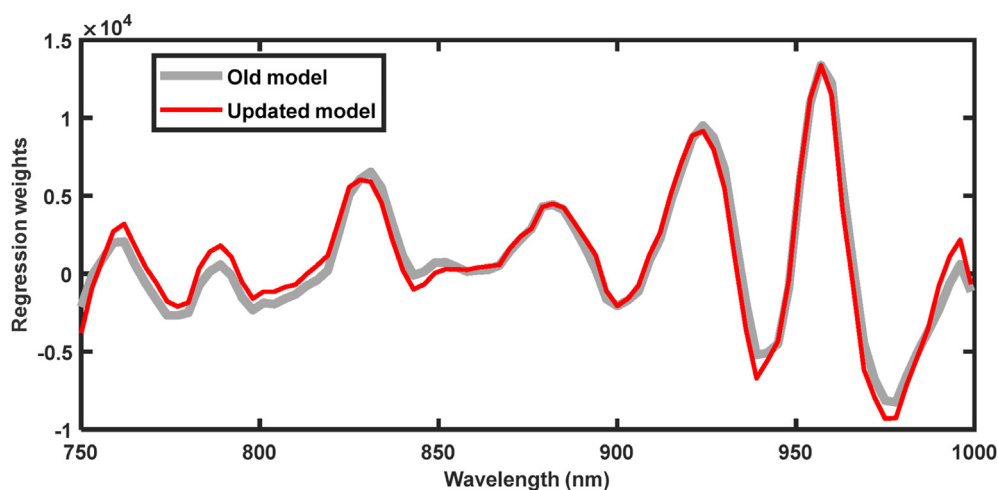

Fig. 7. The effect of model update on the regression coefficients of total soluble solids prediction in kiwi fruit.

expected to be a mix of biological variation and instrument differences.

3.3. Updating the transferred calibration model for new batches

In this study, for batch 1 of the pear fruit, two spectrometers were used to acquire the NIR spectra. To show the case of model updating of the transferred model, at first, the MC NIR model made on the LabSpec spectrometer was transferred to the Felix spectrometer using the fully supervised PFCE framework [16]. There was no interpolation needed before the CT because the spectra from the LabSpec spectrometer have spectral sampling at 1 nm, while the Felix spectrometer has a spectral sampling of 3 nm. The Labspec spectra were directly resampled to match the spectral sampling of Felix by selecting 1 out of 3 subsequent continuous spectral response variables. The transferred model reached a RMSEP 0.651% (Fig. 8A) on the test set of batch 1, greater than the RMSEP of the original Felix model (0.507%). The transferred model was directly used on batch 2, 3 and 4, and the RMSEP was increased in all batches compared to the performance of the original model. Such an increase in RMSEP indicates that the transferred model requires an update prior to being used in the new fruit batches. Hence, the transferred model was updated independently (second-row Fig. 8) and sequentially (third-row Fig. 8) with the PFCE approach. After the independent update for each batch, the RMSEP for batch 2, 3 and 4 were reduced from 1.713%, 3.177% and 2.077%−

0.512%, 0.408% and 0.485%, respectively. Similarly, for the sequential update, the RMSEP for batch 2, 3 and 4 were also reduced. However, the main benefit of the sequential update approach was related to a further reduction of RMSEP for batch 3 (0.408−0.402%) and 4 (0.485−0.466%). The reduction in RMSEP with the sequential approach shows that the updated transferred model was able to learn from the earlier batches. The evolution of regression co-efficients for the transferred model updated independently and sequentially were shown in Fig. 9A and B, respectively. The main difference in the regression coefficients of the transferred model and the regression coefficients of the subsequently updated models was the decrease in the regression weights at several regions over the spectral range. The differences in the regression coefficients were unique to the batches, however, it was difficult to extract chemically relevant information to conclude about the cause of variability in any new batch.

3.4. Posterior analysis to find the optimal number of sample size for model update with PFCE

To this end, the ability of the PFCE approach to perform parameter-free NIR model update for predicting key quality traits in pear and kiwi fruit was showed. However, in earlier sections, the total number of samples needed to perform the model update was set to 40% of the total samples selected by the KS algorithm. The selection of 40% of samples for the Kiwi case resulted in the
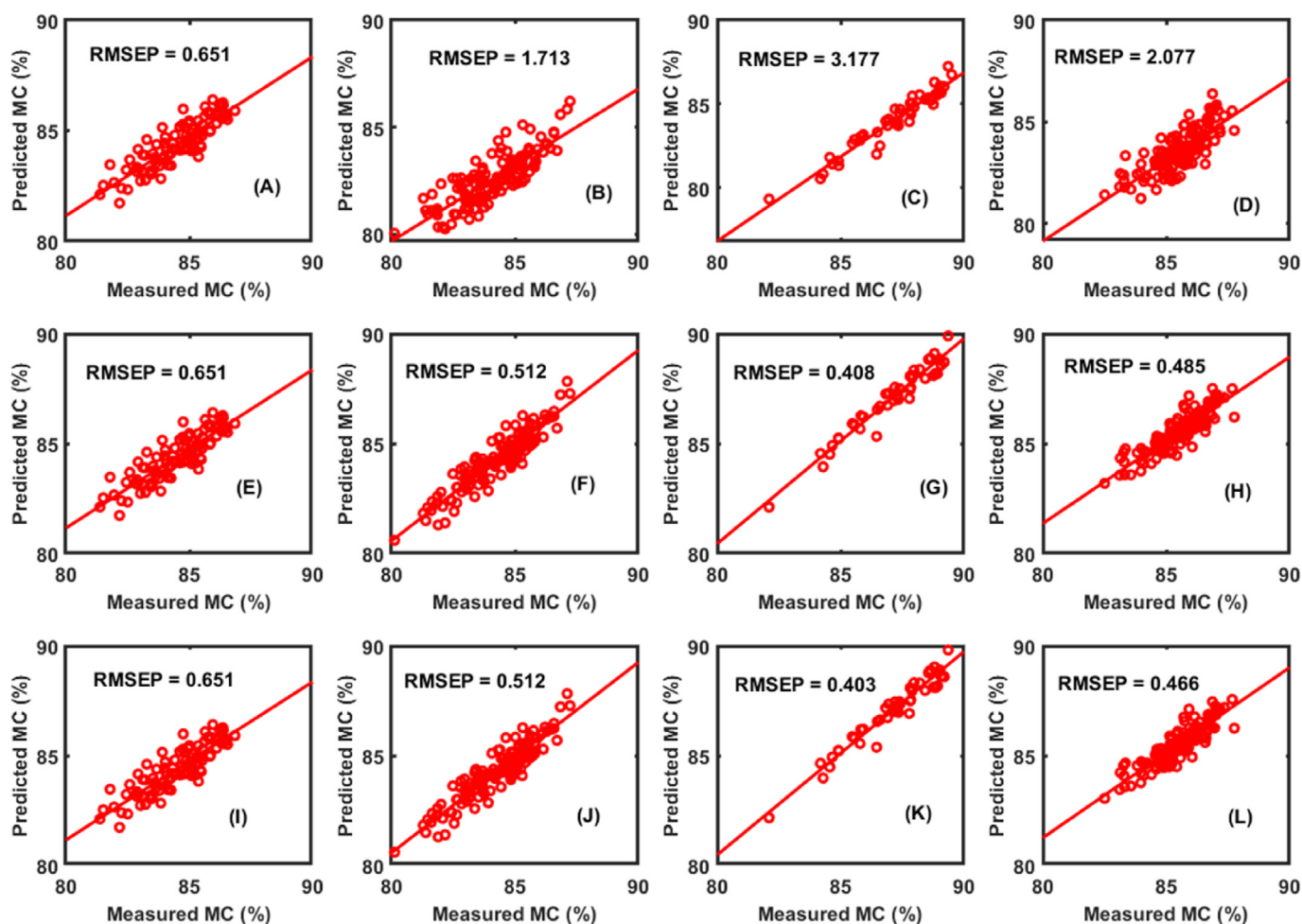
Fig. 8. A summary of performance of transferred model before and after model update for predicting moisture content (MC %) in pear fruit. Transferred model tested on (A) batch 1, (B) batch 2, (C) batch 3, and (D) batch 4. Transferred model updated independently for each batch and tested on (E) batch 1, (F) batch 2, (G) batch 3, and (H) batch 4. Transferred model updated sequentially and tested on (I) batch 1, (J) batch 2, (K) batch 3, and (L) batch 4.

selection of only 30 samples, while for the case of pear, the total number of samples selected were up to 92. One could expect that to use the PFCE approach in practice, the non-expert users would like to measure as low samples as possible to avoid unnecessary reference analysis of the samples and save time. Hence, to explore the effect of sample size on the performance of PFCE model update, a posterior analysis was performed. In the posterior analysis, the PFCE model update was performed with an increasing number of samples and later the performance of the model was tested on the left-out test set. The analysis was performed for both the pear as well as kiwi data set and the results were shown in Fig. 10. For pear (Fig. 10A), it can be noted that a small number of samples (~9) were sufficient to attain RMSEP lower than 0.56%. With increased sample size ~20 samples, the RMSEP further decreased. With a sample size of ~70, the updated model performed better than the primary model by reaching a RMSEP lower than 0.507% i.e., the RMSEP of the primary model. Hence, for practical use, either the model can be updated with a few samples i.e., ~9 or with a greater samples size of ~70 samples. The compromise will be in terms of analysing a small number of samples. In the case of kiwi (Fig. 10B), 9 samples were sufficient to achieve an error lower than 0.65%, which was already lower than the RMSEP of the original model i.e., 0.752%. The results suggest that a small number of samples were sufficient to update the NIR calibration related to fruit quality prediction.

4. Discussion

NIR models of fresh fruit lack robustness when used on a new batch or scenario having variability that was unmodeled [10,15]. This study also found that the PLS model made on one batch lacked robustness to precisely predict MC and TSS in the next new batches of pear fruit. Since all the fruit were of the same cultivar and measured with the same instrument using the standard protocol, the main reason for the model failure could be the biological variability in the pear fruit. There could also be some underlying minor causes of new variability such as the likelihood of instrument changes over 14-months (e.g., ageing light source, different measurement temperatures, etc.) and differences in sample manipulations regardless of having used the same protocol (different handling, or equipment differences in the drying oven, etc.). However, the models were successfully updated with the new semi-supervised approach and regained the predictive performance. Similarly, the online available model related to kiwi fruit failed when tested on a locally measured batch of fruit. Such a failure was expected as the measurements for the online model were performed by the instrument manufacturer using a similar (same type), but not the same (identical) instrument. In addition, the model was developed on a different fruit batch. Hence, the kiwi model update was a classic case of CT without standard, where the model of the primary instrument needs to adapt to the
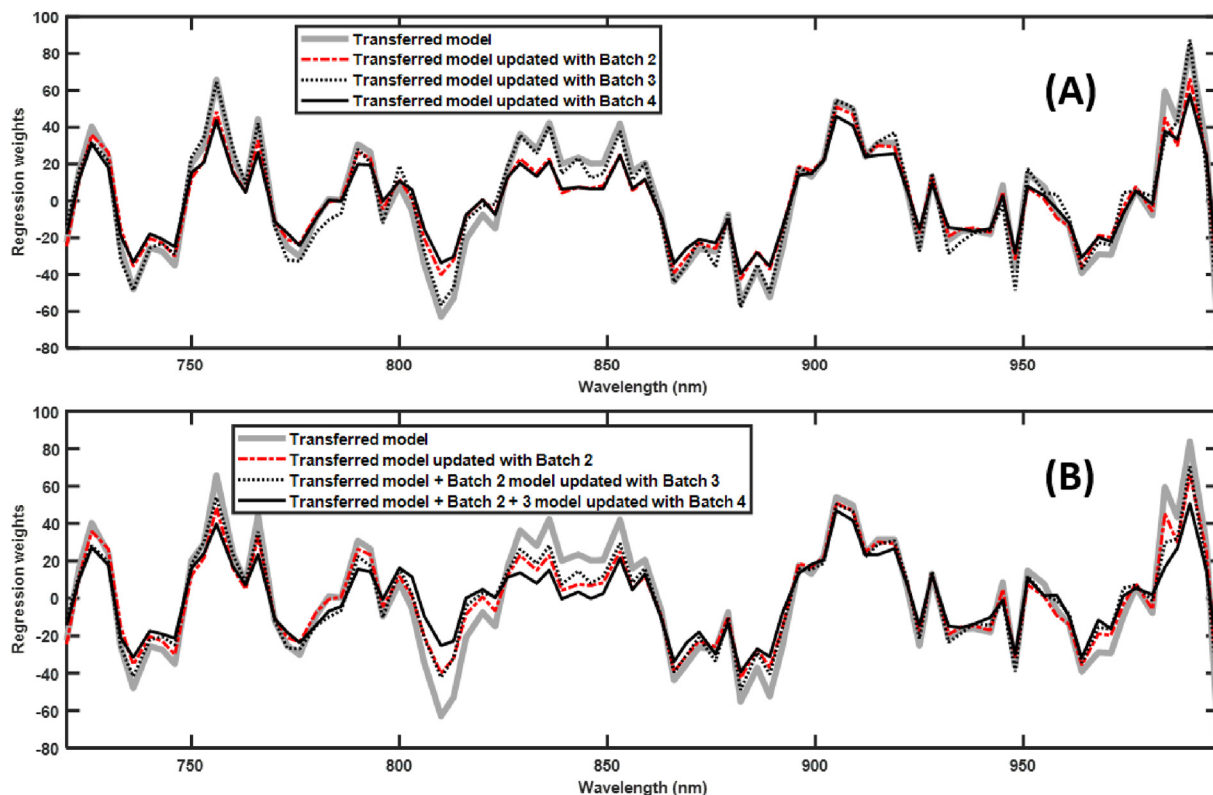
Fig. 9. The effect of model update on the regression coefficients of transferred moisture content prediction model for pear fruit. (A) Primary model updated independently for each batch, and (B) primary model was updated sequentially for each batch.
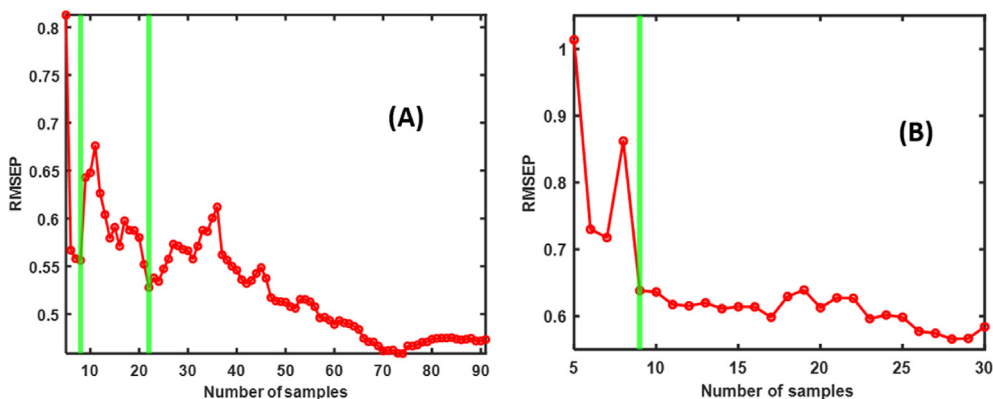

Fig. 10. Evolution of root mean square error of prediction (RMSEP) as the function of samples size. Updating the moisture content (MC %) prediction model made on batch 1 data of pear with data from batch 2 (A). Updating the Kiwi total soluble solids (TSS %) prediction model based on the data acquired in local laboratory experiment (B).

instrumental difference of the second instrument, but no standard samples can be measured on both the instruments as the primary instrument was not available. The semi-supervised approach presented in this study was successful in updating the online model to attain the CT without the need for any standard measurements on the primary instrument.

CT in the domain of NIR spectroscopy of fresh fruit is widely reported [20,21], however, there is still no work showed the robustness of the transferred model and its long-term usage such as on multiple fruit batches. This study for the first time presented such a demonstration where the model made on a batch was tested on 3 next independent batches measured along 14 months. Further, like the PLS model, the transferred model also lacked robustness

when tested on new batches. Hence, the transferred model was corrected with the same semi-supervised approach and regained the predictive performance when tested on multiple fruit batches.

In this study, the semi-supervised PFCE to update the primary model was used in two approaches. In the first approach, the model was independently updated for each next batch, while, in the second approach, the models were sequentially updated for the next batches. It was expected that the models being updated sequentially will be able to learn from all the earlier batches and may lead to improved prediction of MC and TSS, compared to the independently updated model. The results showed that the sequentially updated model (for both PLS as well as the transferred model) performed better than the independently updated model as

the RMSEP were lower for the sequentially updated models (Figs. 2, 4 and 8). The benefit of the sequentially updated model was however limited to batch 3 and 4 as batch 2 only had batch 1 prior to it to learn. In a practical scenario, sequential learning should be the preferred approach as the user can receive help from learning from all earlier batches, thus, along the time improving the robustness of NIR models.

Updating the NIR model is a key concern in the domain of fresh fruit analysis [12,13]. Several methods are available but require optimization of a range of parameters which makes them difficult to implement for a routine model update and analysis task [12,13]. Even a simple recalibration of PLS requires optimization of the LVs from scratch with cross-validation. In this study, for the first time, semi-supervised learning based on PFCE was showed to update the NIR models without any need for parameter tuning or optimization. The main benefit of the parameter-free approach is that it can be widely used and easily adapted to update PLS models and to even reach standard free calibration tasks.

5. Conclusions

The study concludes that the semi-supervised PFCE method was found to be an easy and fast approach to update the NIR calibration models for fresh fruit quality. In both the demonstrated fruit cases, the semi-supervised PFCE models regained the model performance and reduce the RMSEP. Semi-supervised PFCE can also be used to update the models transferred to a different instrument. The best way to use the semi-supervised PFCE for the NIR model update was found to be sequential as the models can continuously learn and improve from multiple batches along the time course. The semi-supervised PFCE approach can also be used to transfer the calibration models, especially when the primary instrument is not available for standard measurements. The semi-supervised PFCE can become a potential tool to support portable spectroscopy as the users can easily share their models without the need for complete recalibration of instruments.

Declaration of competing interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

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