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A WHITE PAPER FROM FOSS:

ROBUSTNESS OF GLOBAL PREDICTION MODELS FOR FT-IR DAIRY EQUIPMENT

ANALYTICS BEYOND MEASURE

By: Per Waaben Hansen
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Data & Algorithms, Research & Development, FOSS Analytical A/S
fossanalytics.com

Introduction

Prediction model maintenance and monitoring is an important quality assurance task when working with indirect methods such as FT-IR milk analyzers. It can be very costly due to the need for wet chemistry results. Furthermore, adjustments based on wet chemistry data are prone to errors due to the error from the chemical method.

With the most modern FT-IR equipment and prediction models the work can be significantly reduced by utilizing the inherent robustness of the current models.

Objective

A study of the stability of commercial ready to use prediction models was performed, focusing on two important aspects: 1) The robustness of the results towards different milk types (skim, raw, and homogenized milk), and 2) the seasonal variation of the results. The results were benchmarked against simple prediction models developed on a small data set.

Methods

Two MilkoScan FT1 instruments were used for the study.
Standard reference milk samples (skim, raw, and homogenized milk) were measured biweekly on two different MilkoScan FT1 instruments for more than one year. Fat was analyzed using the Röse-Gottlieb method (IDF1/ISO1211).

Two versions of the prediction models for fat in milk were used for the study:

- Old model: A traditional filter model based on only four spectral regions (fat, protein, lactose, and baseline) – i.e. the basic milk fat model from MilkoScan FT120
- Current model: A spectral model based on milk data collected from MilkoScan FT1 worldwide, covering all seasons and milk types, version 2.4.0 for MilkoScan FT1

Overall accuracy

First of all, the overall accuracy of the two instruments using the two different fat prediction models was tested. A general slope/intercept was applied to match the wet chemistry data with the predictions, whereas no correction for seasonal variations was applied. The performance results are shown in Table 1.

Table 1: Calculated performance for the two MilkoScan FT1 instruments using two different prediction model versions for fat. Each milk type is slope/intercept adjusted individually, except for "All milk" where one common slope/intercept correction is applied to all sample types.

		Number of samples		Accuracy		Repeatability	
Model	**Sample type**	**Instr. 1**	**Instr. 2**	**Instr. 1**	**Instr. 2**	**Instr. 1**	**Instr. 2**
Old	Homogenized milk	62	63	0.025	0.027	0.006	0.006
	Raw milk	164	159	0.043	0.035	0.009	0.007
	Skim milk	62	61	0.018	0.019	0.005	0.004
	All milk	**288**	**283**	**0.046**	**0.040**	**0.008**	**0.006**
Current	Homogenized milk	62	63	0.022	0.019	0.008	0.008
	Raw milk	164	159	0.030	0.023	0.012	0.009
	Skim milk	62	61	0.015	0.015	0.005	0.003
	All milk	**288**	**283**	**0.027**	**0.021**	**0.010**	**0.008**

The following can be deducted from Table 1:

- The performance in terms of accuracy is generally better for the current compared to the old prediction model for fat.
- This is particularly noticeable for the combined "All milk" group for the old prediction model where the accuracy for the combined group ("All milk") is inferior to any of the individual groups ("Homogenized", "Raw", "Skim"). This indicates that there are sample type specific slope/intercepts and that they cannot be combined.
- On the other hand, this is not the case for the current prediction model where the "All milk" accuracy falls between the results for the individual milk types.

This shows that the current model is able to handle different milk types and hence the slope/intercept correction scheme can be simplified to only one correction per parameter (fat, protein, lactose, etc.), irrespective of milk type. This means that fewer samples are required to validate and maintain the slope/intercept adjustment, saving cost.

Seasonal variation

The same data set was used for studying the seasonal stability of the old and current fat prediction models. The weekly biases are shown in Figure 1A (old model) and 1B (current model).

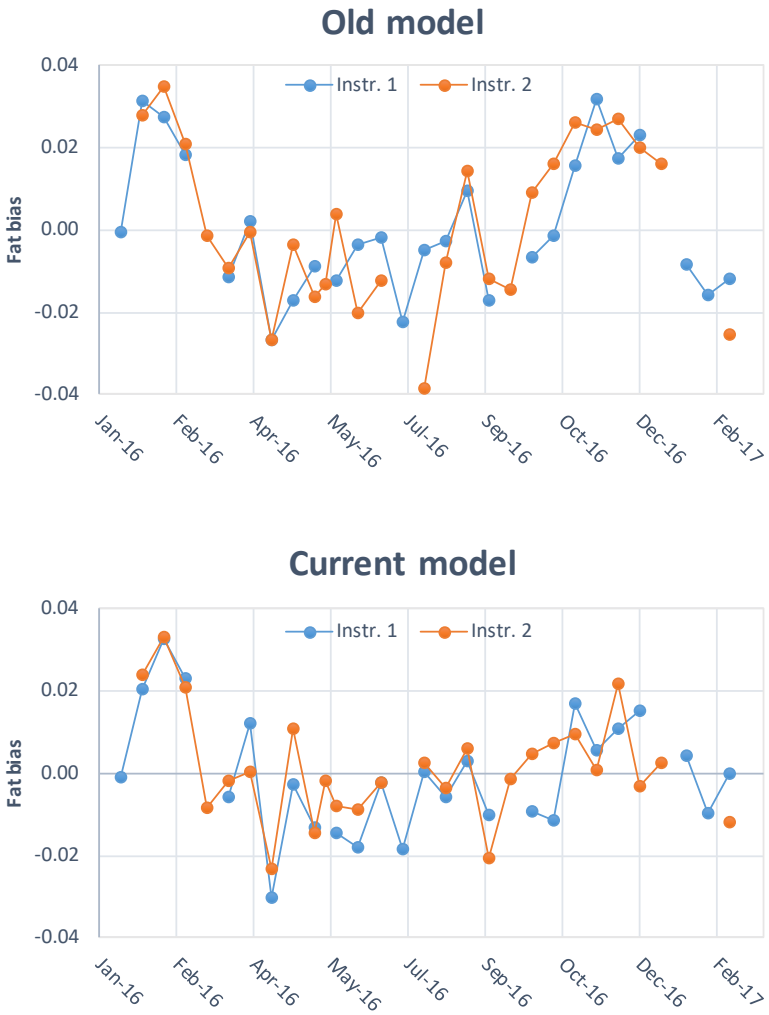

Figure 1: Weekly biases for the old (A) and current (B) models.

The seasonal variation for fat for the two instruments is significantly lower for the current model compared to the old model. This means that fewer slope/intercept adjustments are required to maintain the performance when using the current model, further reducing the need for costly wet chemistry results.

Conclusion

With FT-IR spectroscopy it is possible to establish global calibration models that are robust towards sample type and seasonal variations, reducing the need for costly wet chemistry data for continuously adjusting the results.

Fat in milk is used as the example in this white paper, but the conclusions are applicable to all major components predicted with global models in milk.

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FOSS
Foss Allé 1
DK-3400 Hilleroed
Denmark

Tel.: +45 7010 3370
Fax: +45 7010 3371

info@foss.dk
www.fossanalytics.com