
Merging of spectral datasets from different MIR instruments used in the routine analysis of milk

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This work is performed in the framework of the OPTIMIR project. It aims to develop innovative farm management web applications based on the use of infrared spectroscopy analysis of milk to enable a sustainable and profitable management of the milk production. Mid Infrared (MIR) spectroscopy has been the method of choice worldwide for quality control during routine milk testing. It allows a fast, non destructive and screening quantification of milk chemical properties, as the content of fat, protein and lactose. In this project, the MIR spectrum will be used with a different purpose and will be considered as a reflexion of cows' state in order to obtain indicators concerning fertility, health and feeding among others. This innovative approach of using MIR needs the support of important spectral databases associated to reference values for each of the properties to be studied. For this reason, a large number of commercially available MIR spectrometers from different manufacturers installed in different laboratories from four different countries were used. Because of differences of the instrumental responses between different MIR spectrometers, spectra obtained on one instrument cannot readily be compared to a library acquired on a different instrument. Moreover, the use of calibration models developed on an instrument with MIR spectra obtained on another instrument will usually lead to an increased uncertainty of the prediction model. Then, spectral corrections adapted to each instrument (standardization) are needed. In this work, the piecewise direct standardization (PDS) has been used in order to reduce the inherent instrument to instrument variability. The obtained results have shown a very good correlation between all the spectra and repeatable results across instruments, which is an indication that a common database could be constructed and would permit to develop MIR breeding tools which should be easily implemented in practice in many different countries

Abstract



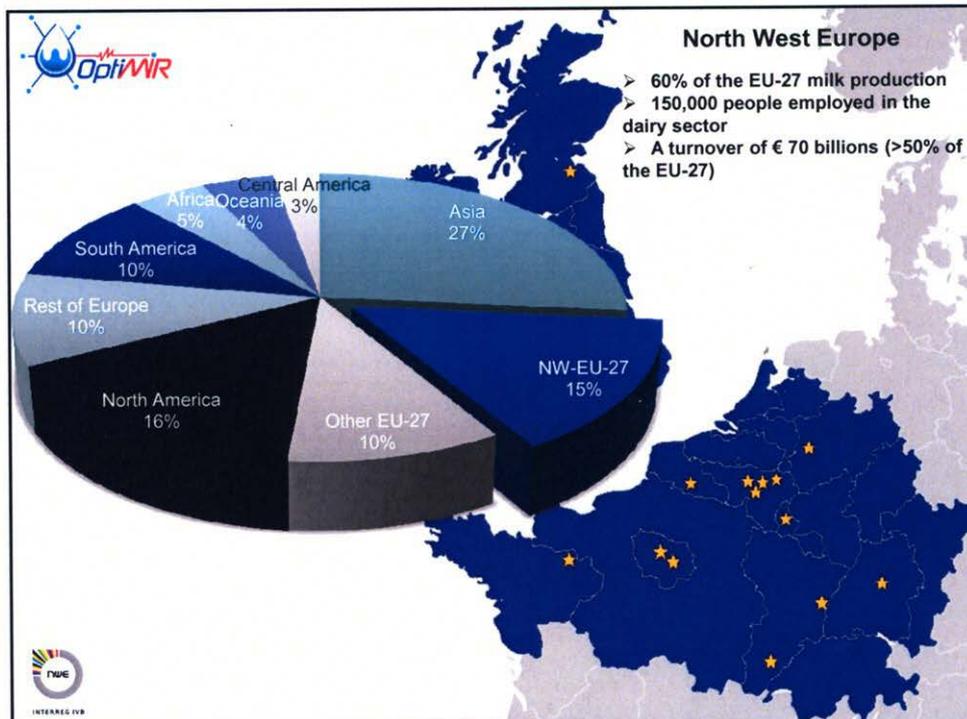

**MERGING OF SPECTRAL DATASETS FROM DIFFERENT MIR
INSTRUMENTS USED IN THE ROUTINE ANALYSIS OF MILK**



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Cork – 28 May 2012






The Project

17 partners and 1 sub-contracting partner / 6 countries

Milk recording organizations	Country	Research Units	Country
AWE asbl	BE	Institut de l'Elevage	FR
Chambre régionale Agriculture Alsace	FR	Gembloux Agro-Bio Tech (ULg)	BE
ADECL62 (Pas-de-Calais)	FR	CRA-W (DVPA)	BE
CLASEL (Sarthe & Mayenne)	FR	TEAGASC	IR
SCL25 (Doubs et territoire de Belfort)	FR	Scottish Agricultural College	UK
France Conseil Elevage	FR	University of Hohenheim	DE
LKV Baden-Württemberg	DE		
LKV Nordrhein-Westfalen	DE		
National Milk Recording	UK		
 Irish Cattle Breeding Federation	IR		
 CONVIS	LU		

Laboratory	Country
Comité du Lait asbl	BE





AIMS

To improve the profitability and sustainability of the dairy sector by providing milk producers with innovative **standardized management tools based on association between MIR milk records and cows' status.**

To reduce the costs of production through **improved daily herd management.**

To bring opportunities to access competitive markets by measuring quality traits linked to **higher added value** (e.g. low-cost measure of food label claims).

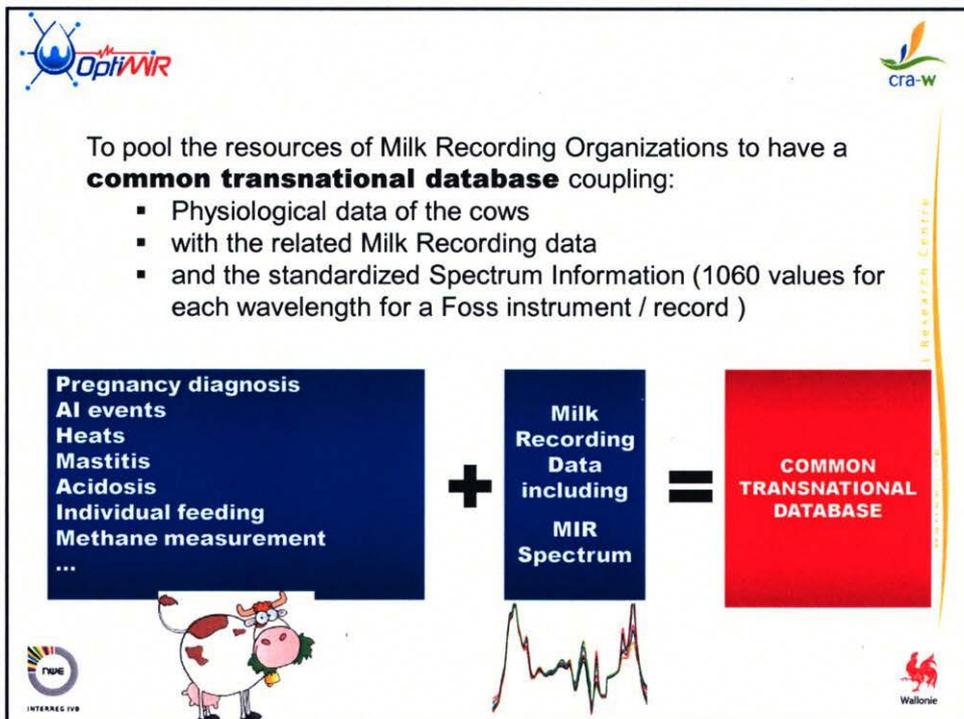
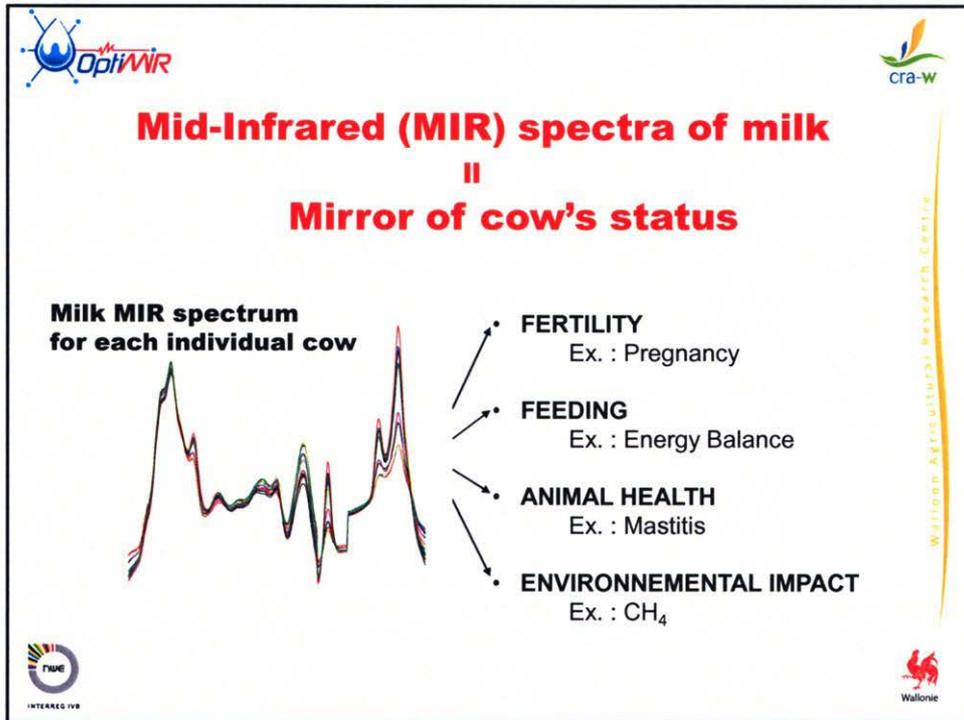
To decrease the impact on the environment (quantification of methane and nitrogen production).

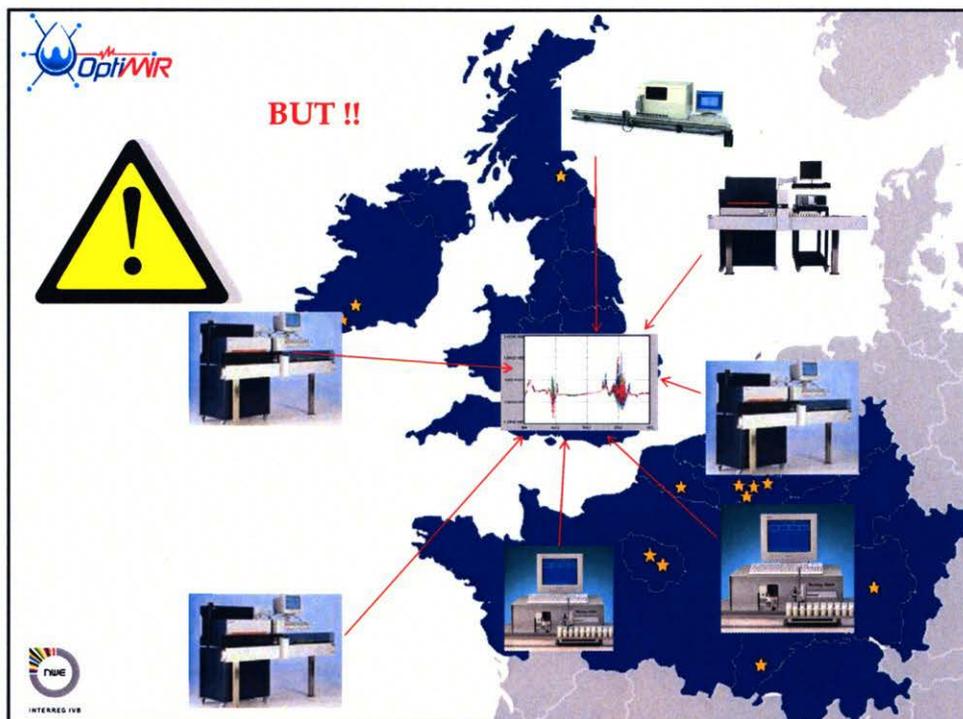
costs of feeding with **energetic balance indicator**

veterinary costs with **early diagnosis of mastitis**

costs of semen straws with **insemination predictor**



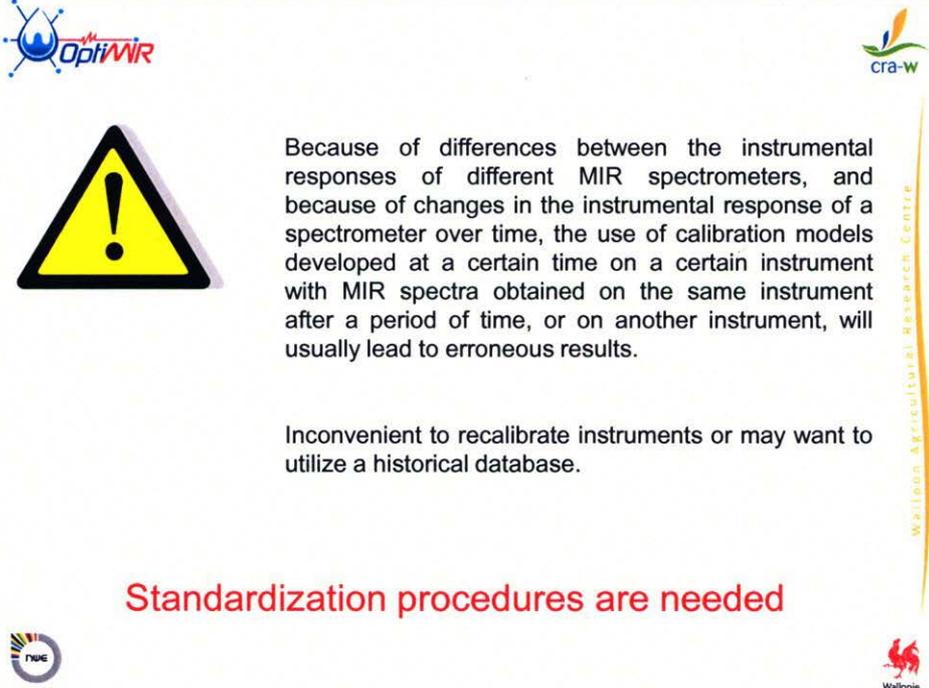




Because of differences between the instrumental responses of different MIR spectrometers, and because of changes in the instrumental response of a spectrometer over time, the use of calibration models developed at a certain time on a certain instrument with MIR spectra obtained on the same instrument after a period of time, or on another instrument, will usually lead to erroneous results.

Inconvenient to recalibrate instruments or may want to utilize a historical database.

Standardization procedures are needed



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A decision needs to be made which instrument will be declared as **MASTER** instrument, the remaining instruments will be used as **SLAVE** instruments.

An own unique **standardization model for every master-slave** combination needs to be designed, describing the shift between the particular slave instrument and the master instrument

In order to be able to perform data standardization between the master and a slave instrument, an equal amount of measurements have to be done with both instruments.

New measurements will be later standardized using the standardization models built.



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STANDARDIZATION APPROACHES

Find a transformation that maps the response of the slave instrument onto the master instrument

- Direct and piece-wise direct standardization
- ...

Process the data from both instruments in a way that makes the differences disappear

- baselining and derivatizing
- multiplicative scatter correction, FIR filtering
- orthogonal signal correction
- prediction augmented classical least squares
- generalized least squares
- explicit deresolution
- ...



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PIECE-WISE DIRECT STANDARDIZATION (PDS)

Proposed by Wang et al.

This method transfers the MIR spectra from the instrument on which they were collected ('slave') to the instrument on which the calibration model was developed ('master').

PDS is based on the fact that the spectral information contained in a certain wavelength on the master instrument is highly correlated to the spectra of neighbor wavelengths on the slave instrument.





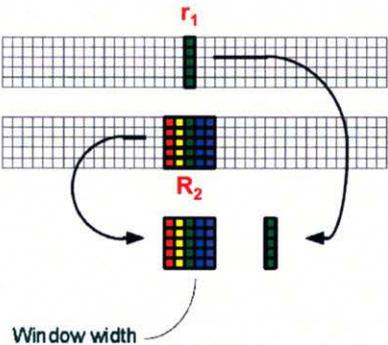


PIECE-WISE DIRECT STANDARDIZATION (PDS)

The PDS method is based on the fact that the spectral variation of spectroscopic data is limited to small regions. In PDS, the response r_1 of the standardization samples measured at wavelength j on the 'master' instrument is related to the wavelengths located in a small window (R_2) around j (neighbouring) measured on the 'slave' instrument:

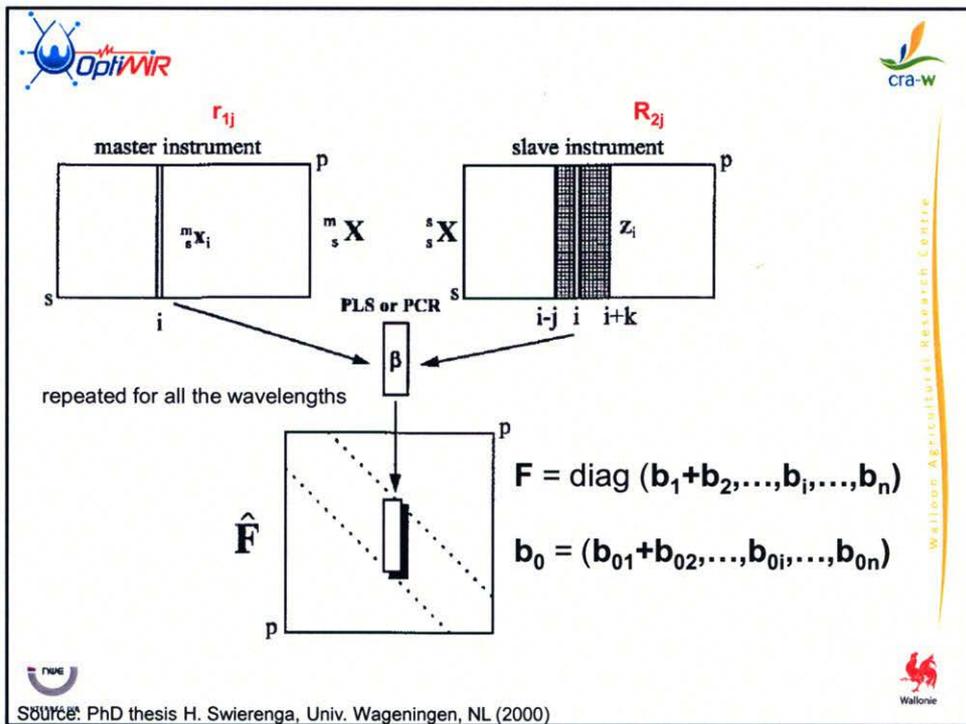
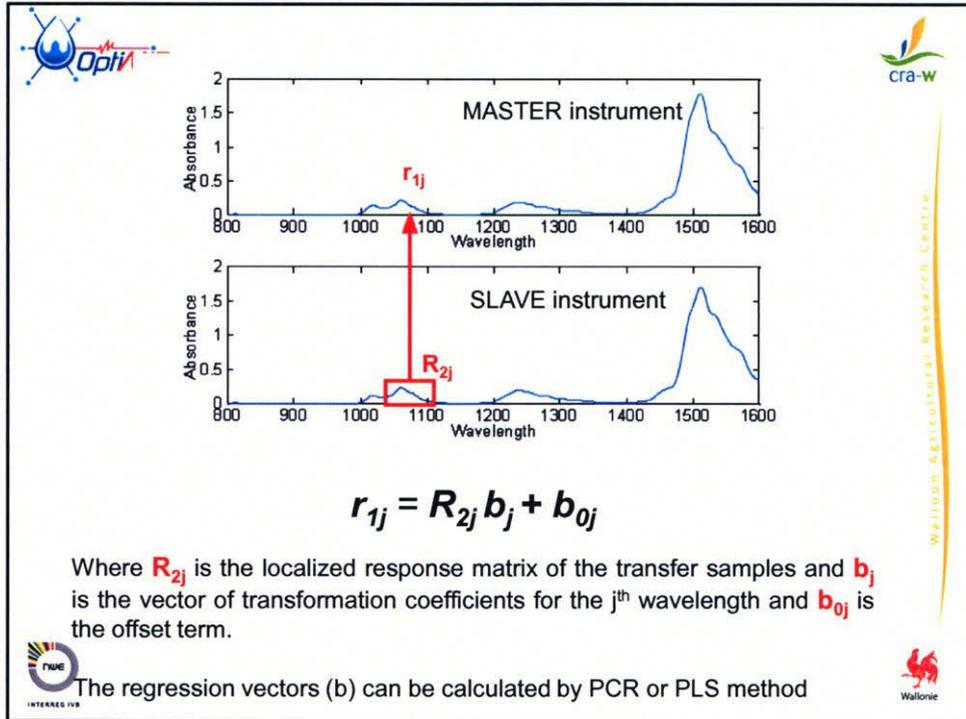
Master

Slave






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The F matrix and the b_0 vector are used to correct new spectra measured in the slave instrument, $r_{2,unk}$

$$(R_{2,unk})_{std} = r_{2,unk} F + b_0$$



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SOME RESULTS

OptiMIR Standardization of February – March 2012

- 25 laboratories
- 50 instruments
- 600 samples

Master FOSS (Battice Foss05009)



Protocol of the standardization procedure

Mars 2012 - 2013

Préparé: Dominique, Gilbert, Jean-François, Wang, Nam Nguyen

Contact address :

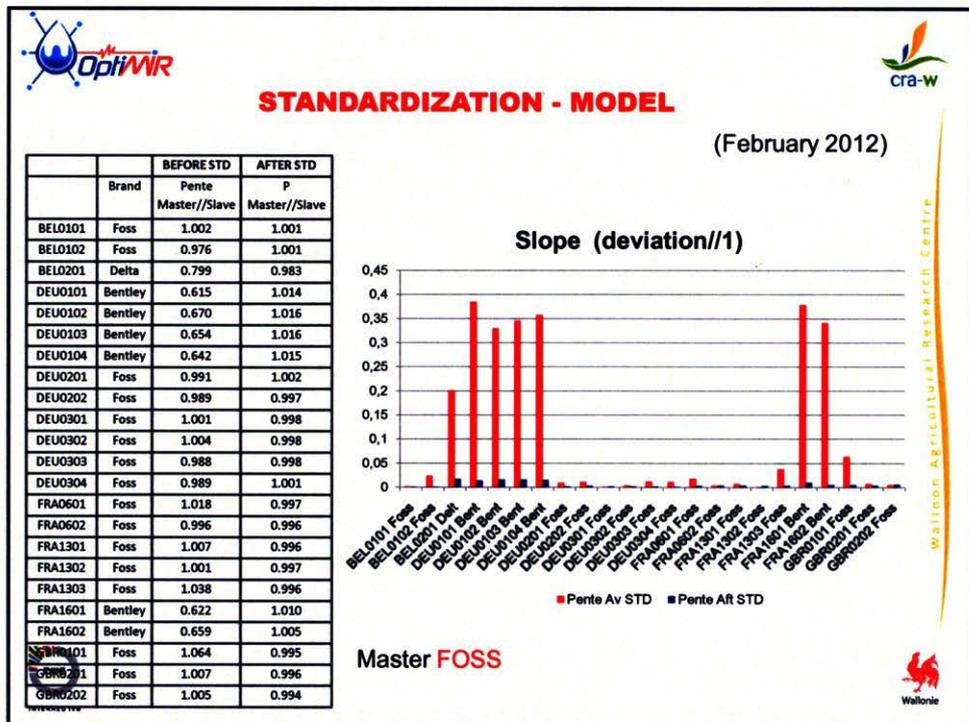
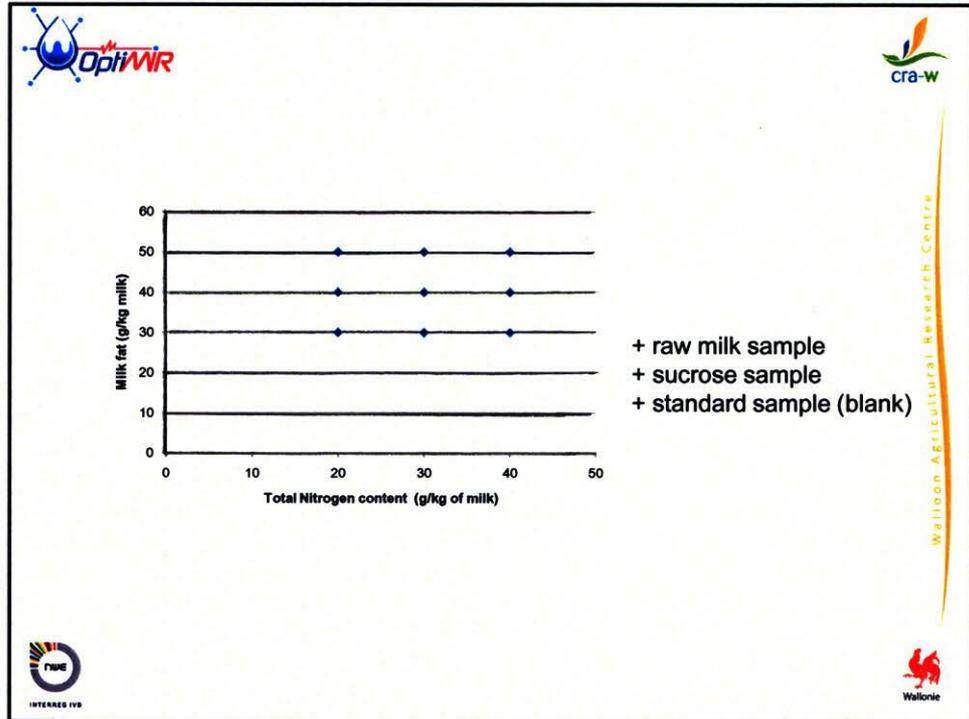
For any problems, please contact Gilbert Ortel or Frédéric Dubarney
Gilbert.Ortel@cra.wallonie.be or Frederic.Dubarney@cra.wallonie.be

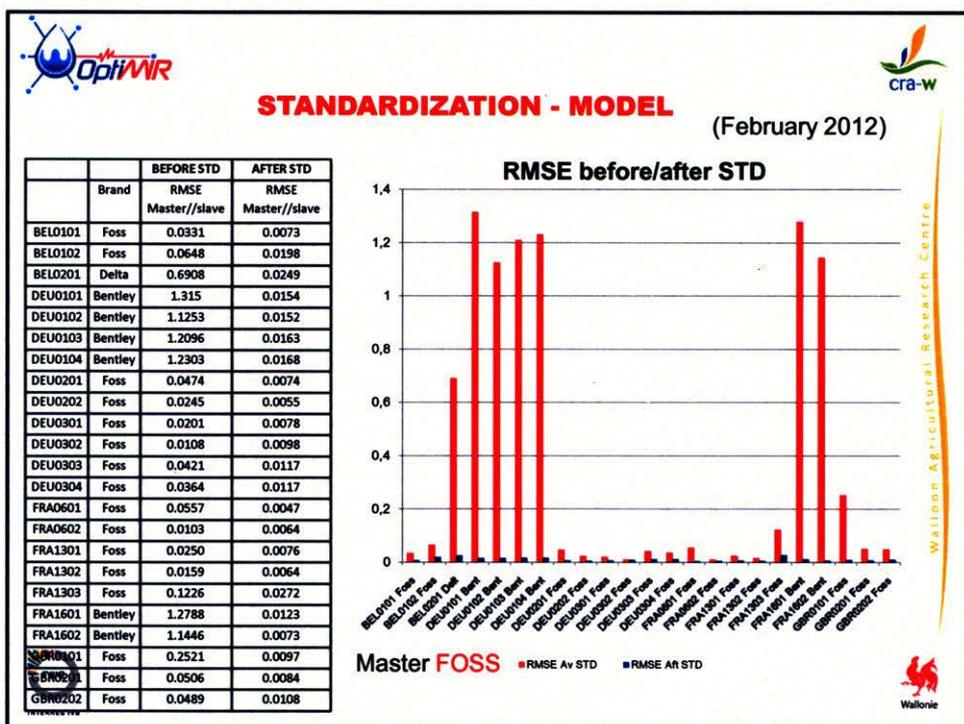
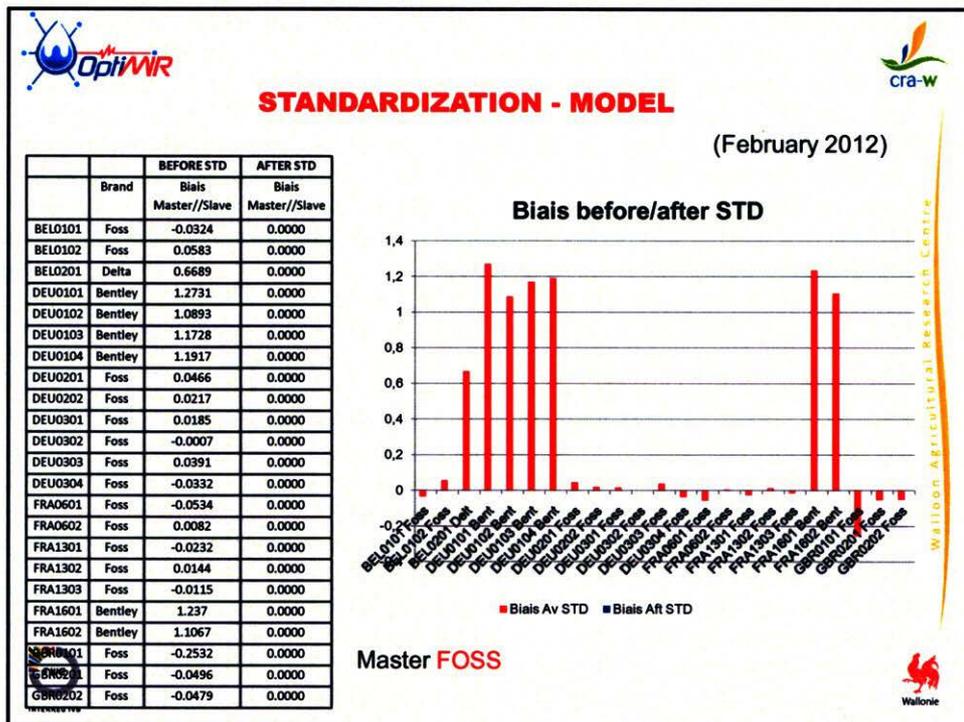
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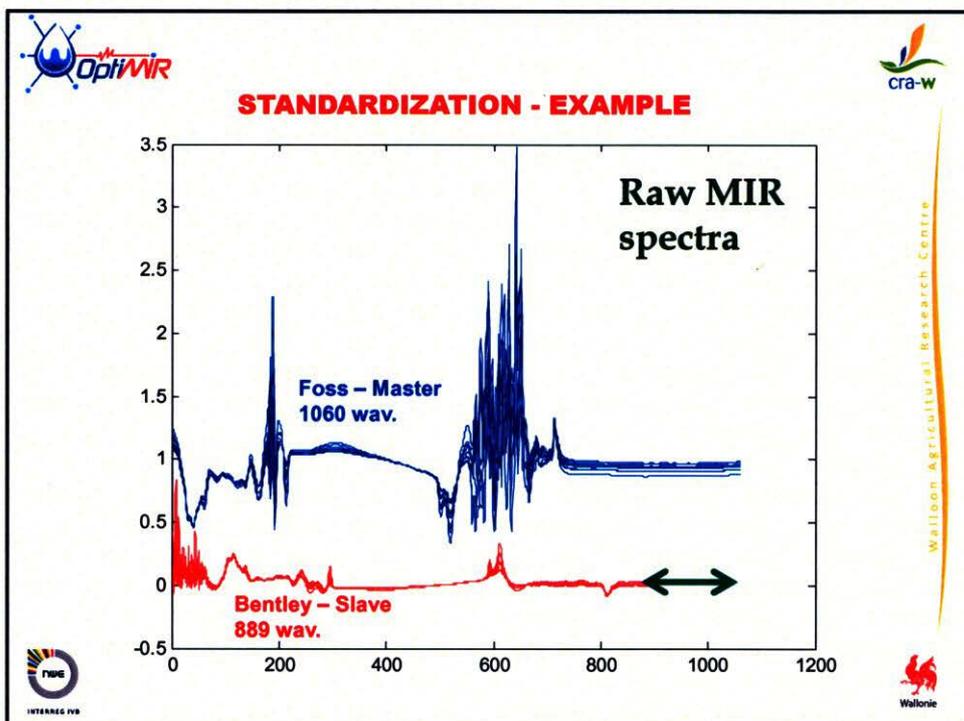
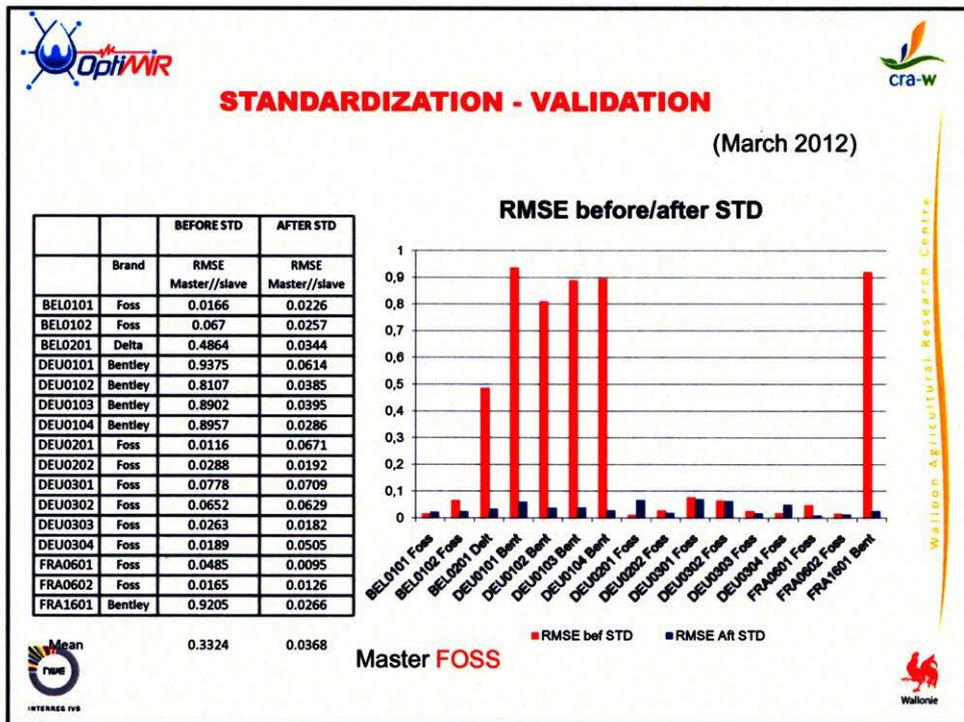


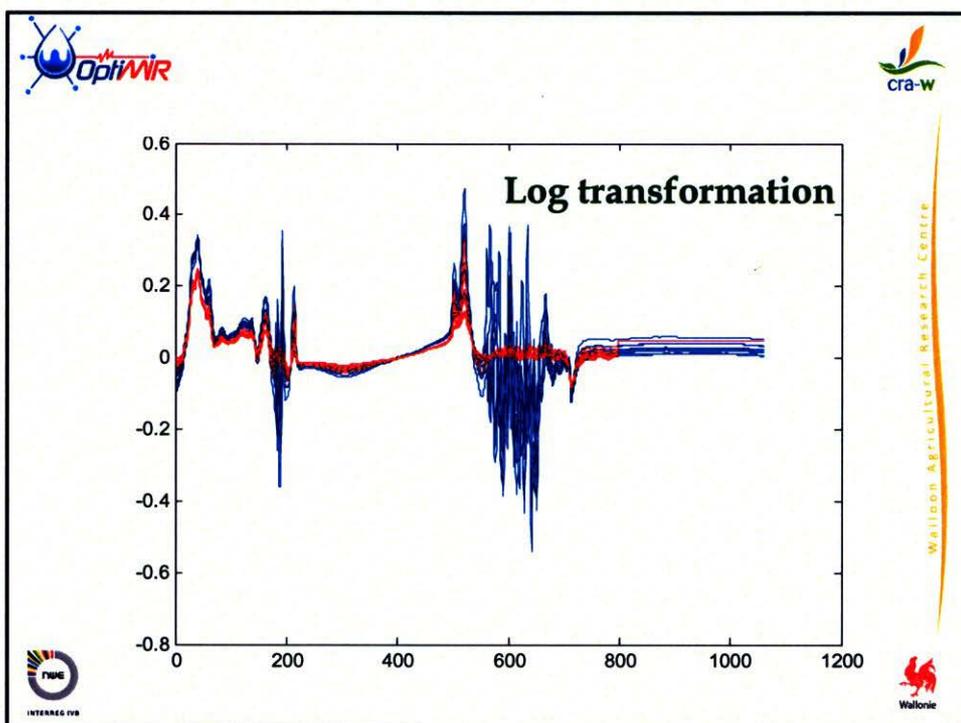
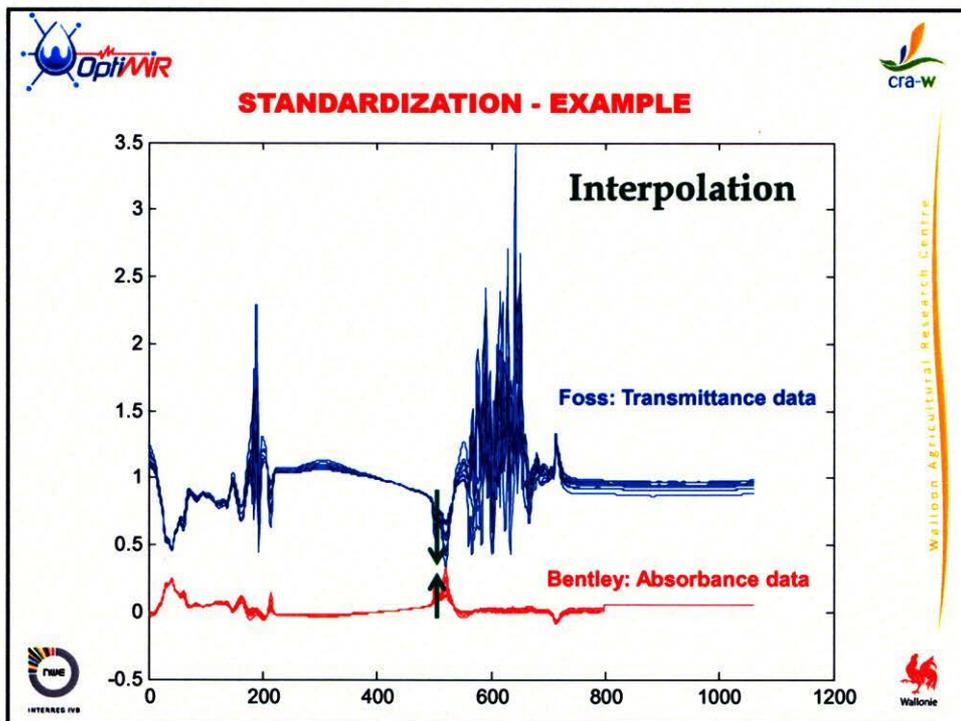

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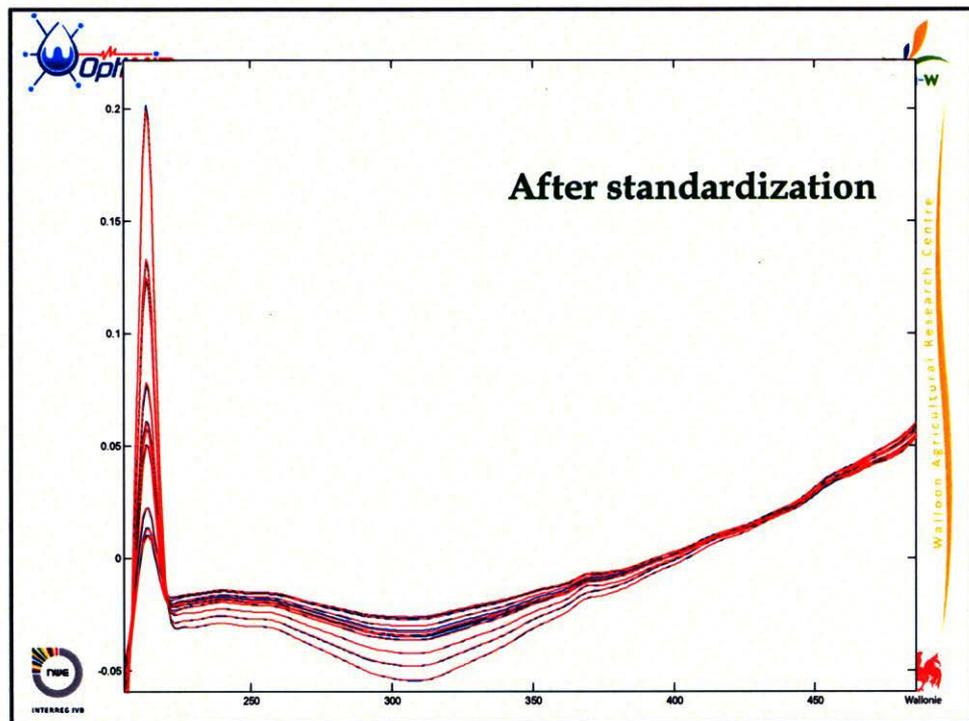
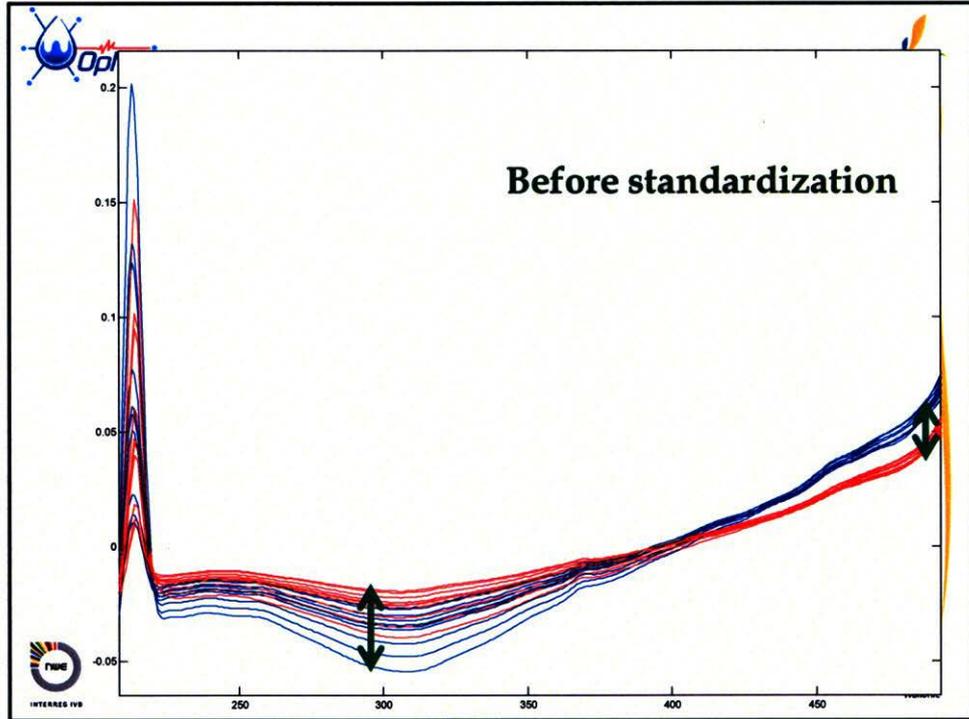


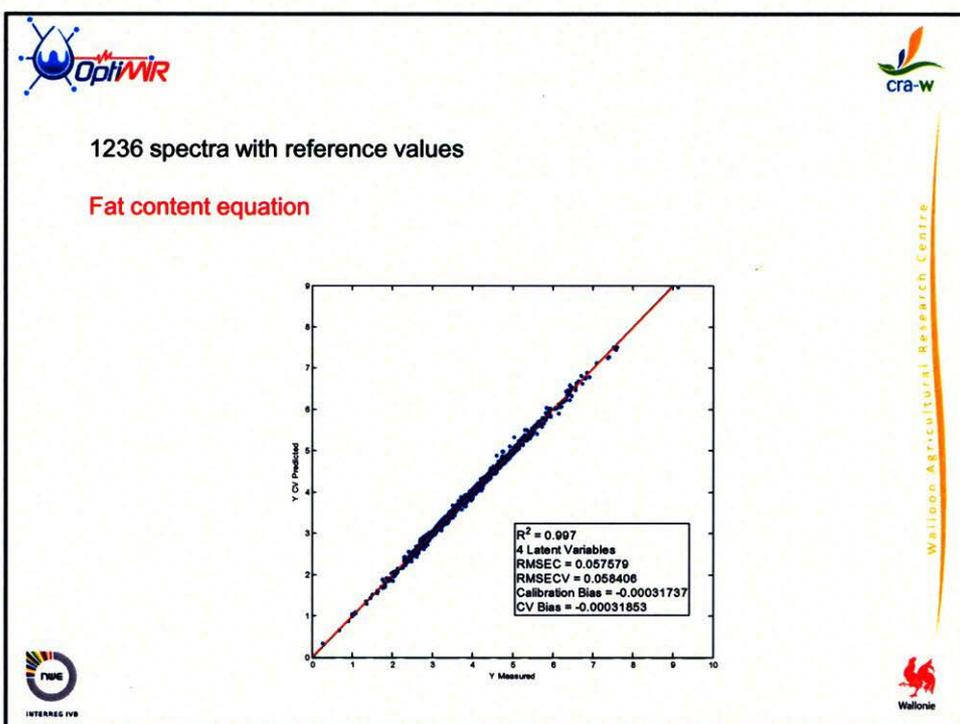
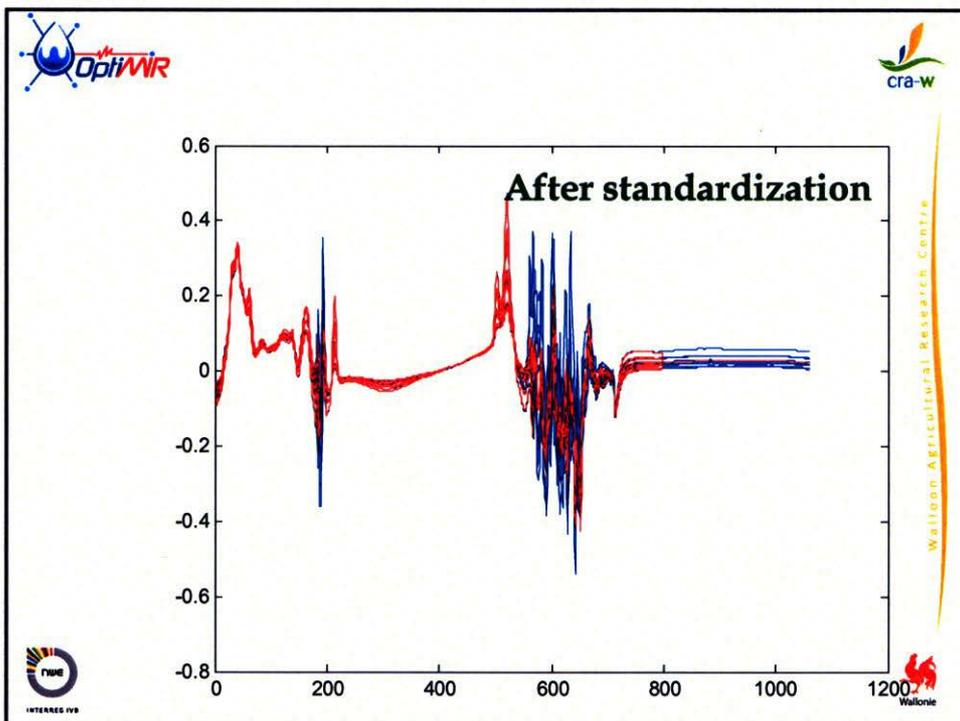


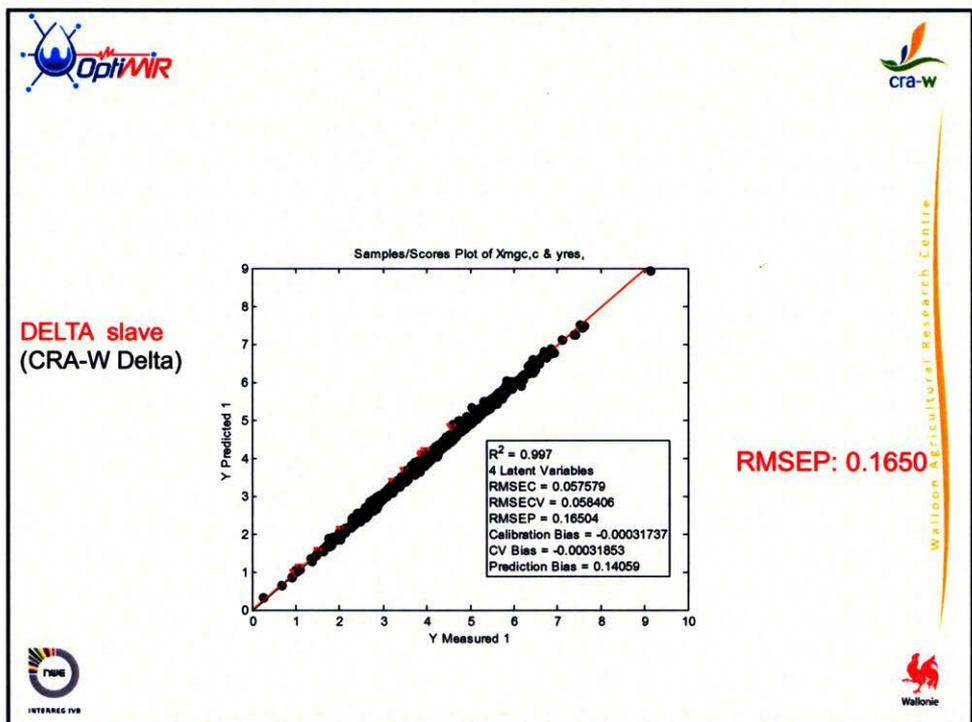
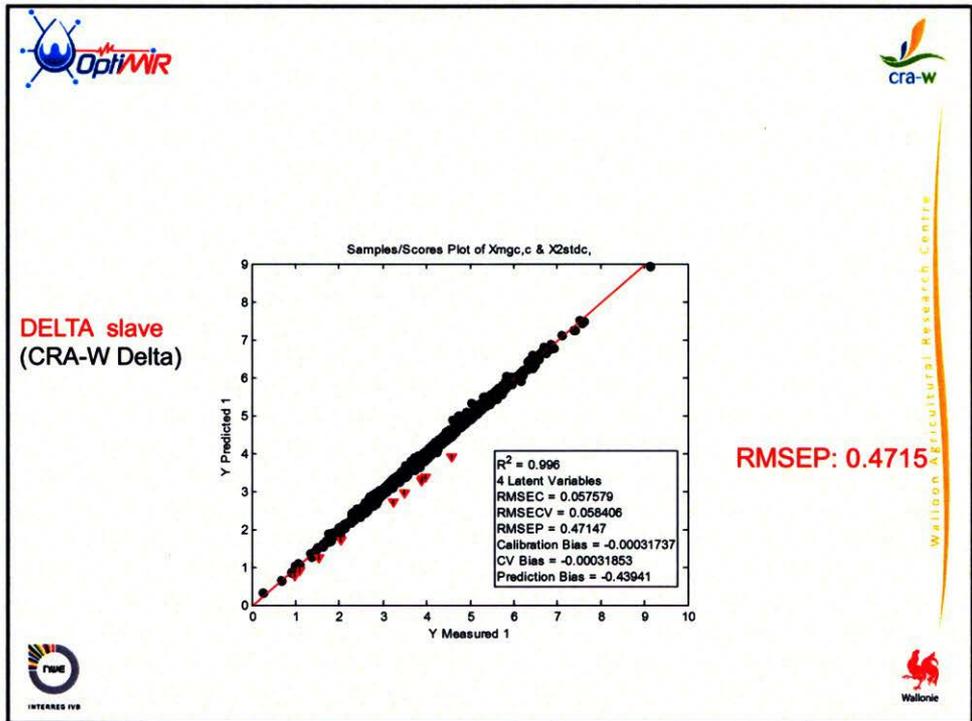




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CONCLUSIONS

The standardization correction using PDS seems to work correctly **during time for the different slave instruments** available, including different brands.

The use of this standardization method is a crucial step for the OptiMIR project because it will allow the use of **only one single equation by property** for all the different instruments.

Useful to pool the resources of milk recording organizations and research centres and MIR milk spectra to be used as **indicator of the cows' status**.

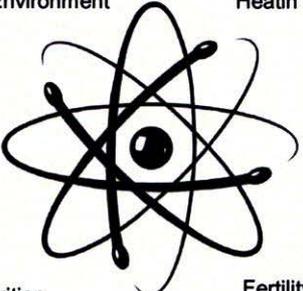



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