Near infrared networking—the ultimate control

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Near infrared reflectance and transmittance networks in agriculture

In a near infrared (NIR) reflectance or transmittance network, the calibrations are developed on a "sub-master" instrument by comparing NIR reflectance/transmittance readings for typical samples with the corresponding reference values. The calibrations can then be transferred to a population of "slave" instruments. Usually, the calibrations are transferred from a central computer to the slaves by means of ordinary telephone modem connections, allowing an almost simultaneous update of all slave instruments.

There are several advantages of running NIR reflectance/transmittance networks:

- Many slave instruments can be easily supervised and updated.
- The calibration cost per instrument can be reduced.
- Local operator influence on the results can be virtually eliminated.
- A high degree of analytical reliability can be ensured where it counts, i.e. in the industrial environment rather than in the laboratory.
- The instrument-to-instrument variation can be reduced to a level below the comparable laboratory-to-laboratory variation.

Examples of NIR transmittance networks

The first large-scale NIR transmittance network was introduced in Denmark in 1991 based on Infratec 1221 instruments from Tecator AB. Since then, similar Infratec networks have been established in many parts of the world. Some examples are:

- *Denmark:* The national network with 130 users. Wheat, barley, rapeseed and rye.
- *Austria:* The national network (Raiffeisen) with 60 users. Wheat and barley.
- *Germany:* The North German network (Raiffeisen Nord) with 10 users. Wheat and barley.
- *Austria/Germany*: The regional malt network (Doemens) with 21 users. Wheat, barley and malt.
- *France:* The regional network (GIE) with 55 users. Wheat and barley.
- *France:* The regional network (Ceralliance) with 30 users. Wheat and barley.
- *Great Britain:* The network in England and Scotland with 22 users. Wheat and barley.
- *Belgium:*The network of Station de Haute Belgique with 3 users. Wheat and barley.
- *Sweden:* The Agrolab network to be established with 6 users. Wheat and barley.
- *USA*: The Iowa State network (Dupont) with 25 users. Corn.
- *USA:* The Anheuser Busch network with 35 users. Barley, malt and rice.
- *USA/Canada:* The Continental network with 400 users. Barley and wheat.
- *Canada:* The Canadian Grain Commission network with 54 users. Barley and wheat.

- *Australia:* The Barley Board network with 10 users. Barley.
- *Australia:* The Western Australia network (CBH) with 200 users. Barley and wheat.

In most of the networks the number of instruments keeps increasing; the figures quoted above are from July 1995.

Recently, several networks based on Grainspec instruments from Foss Electric have been established including three in Canada, one in Australia, one in France and one in the USA.[1]

Standardization of slave instruments in a NIR reflectance/transmittance network

In theory, a sub-master calibration can be transferred to all field instruments in a network without modification. In practice, however, calibration transfer introduces two sources of analytical variation:

- A *random transfer variation* superimposed on the random calibration error. The random transfer variation is expressed using the term standard deviation of differences (*SDD*) but is calculated just as the standard error of prediction (*SEP*) that describes the calibration error.
- A *systematic transfer variation* that equals the bias difference between the sub-master and the individual slave instruments.

To optimize the performance of a population of instruments, the sub-master calibration therefore has to be adjusted to each slave instrument individually, i.e. the instruments have to be standardized. For NIR reflectance instruments a set of mathematical standardization algorithms has been described.[2] For the Infratec NIR transmittance instruments, it often suffices with a simple bias-adjustment, specific to the slave-instrument and calibration in question. A complete standardization procedure based on fresh samples of grains and rapeseed has been developed for the Danish NIR transmittance-network. The procedure has been described in detail elsewhere.[3] Some findings shall be briefly referred to below.

The random transfer variation (*SDD*) between the field instruments and the sub-master (*cf.* Table 1) is usually small compared with the accuracy of the calibration itself (*SEP*; typical prediction values from 1994 are quoted). Thus, random transfer variation between the field

Table 1. Standardization of NIR transmittance instruments in Denmark in 1994. The calibration accuracy of the sub-master compared with the random transfer variation between sub-master and field-instruments.

Constituent	Sub-master, *SEP*	Average of 128 NIR transmittances, *SDD*
Barley protein	0.23	0.20
Wheat protein	0.25	0.13
Barley moisture	0.19	0.14
Wheat moisture	0.26	0.09
Wheat starch	0.59	0.21
Wheat zeleny	3.6	1.4
Rapeseed oil	0.65	0.48

instruments and the sub-master is usually not a major practical problem with an Infratec NIR transmittance network.

The systematic transfer variation is reduced by applying instrument-specific bias values using a set of fresh standardization samples on all the instruments right at the onset of a new harvest. The effect of the standardization was studied on 22 randomly selected slave instruments in the Danish network. In Figure 1 the results for barley protein are shown as an example, evaluated with an independent set of twelve subdivided barley samples. Note that the results from all the 22 instruments are plotted on top of each other. The "Bias SD" in the legend box shows the standard deviation among the 22 bias values obtained for the slave instruments. After the standardization procedure the instrument-to-instrument variation was thus much smaller than the comparable variation between reference laboratories.

A proposal for a large-scale, common European NIR transmittance network

The networks established up to now ensure comparable measurements within each network but not between the various networks, as each network is calibrated and monitored using its own reference laboratory. Furthermore, the calibrations are developed using conventional linear mathematics (PLS), limiting the variability that may be handled. The networks are thus not harmonized and therefore not ideal for international grain trade.

Turning briefly to another area of agriculture, compound animal feeds have conventionally been considered difficult to measure using near infrared in transmission mode. Highly useful results may, however, be obtained using artificial neural network calibrations (NN) instead of conventional mathematics such as partial least squares (PLS). Infratec 1255 NIR transmittance analysers from Tecator using neural network calibrations have thus been successfully used for at-line control of compound feeds in fifteen Danish feed mills since 1993.[4]

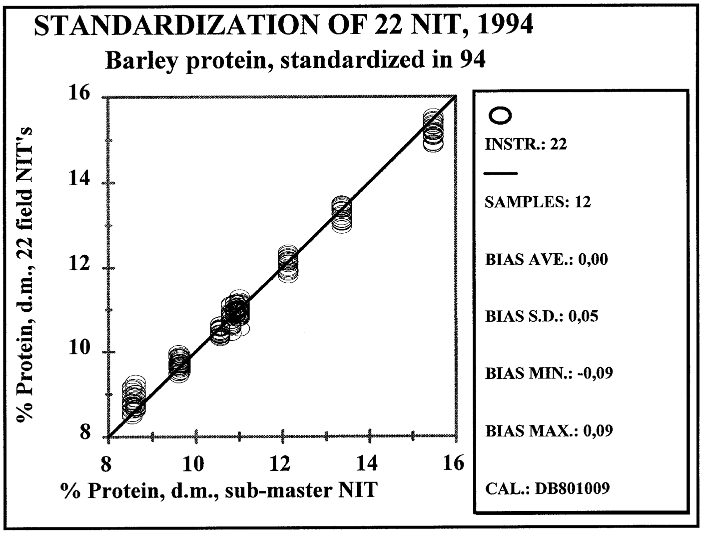

Figure 1. Standardization of NIR transmittance instruments in Denmark in 1994. The variation between 22 randomly selected field instruments measured on twelve sub-divided barley samples just after standardisation for the 1994 harvest.

Table 2. Accuracy of calibration models based on neural networks (NN) and partial least squares (PLS) respectively, predicted with grain samples from Northern and Central Europe from 1991 to 1994.

	N in test set	Range in test set	*SEP* for NN	*SEP* for PLS
Wheat protein	238	8.2–22.7	0.31	0.39
Barley protein	360	7.8–17.5	0.35	0.41
Wheat moisture	198	10.2–25.7	0.28	0.49
Barley moisture	320	8.4–22.1	0.28	0.47

The results with compound feeds show that NN calibrations can handle very large data sets, that the calibrations are highly linear and that the calibrations are transferable. Based on these experiences, the present author and Tecator has proposed trying the NN calibration technique on a very large set of European NIR transmittance-data displaying great variation in terms of harvest-year, climate, varieties etc. The goal is to install NN-calibrations on the existing Infratec instruments in Europe, allowing a common, seamless grain-quality system to be established. As an added advantage, one could hope for more reliable and more robust and therefore cheaper calibrations.

To further the idea of a common European NIR transmittance network, an informal project group named “The European Grain Network” was established during the spring of 1995 encompassing the above-mentioned European networks.

Feasibility of using artificial neural networks

The present members of the group agreed to share data on common parameters such as protein and moisture. Thus data from 1991 to 1994 were collected from the participating networks, allowing Tecator to assess the feasibility of using neural network calibrations. The data sets comprised approximately two thousand NIR transmittance scans each for barley and wheat. The corresponding chemistry values for protein and moisture derived from the individual reference laboratories; to reduce the influence of laboratory-to-laboratory variations, the chemistry values were corrected for laboratory bias differences before use. For each commodity the data set was split in a training set (for the actual calibration), a stop set (to evaluate the progress of the training) and a prediction set (to allow an evaluation of the calibration with an independent sample set). These samples sets were then used to compare neural network calibrations with classical PLS calibrations. The results are quoted in Table 2.[5]

The results in Table 2 show that the NN calibration technique may be used for grain samples from a very large region. Also, the prediction results are better compared with similar PLS results obtained with the same data set split in the same way.

The evaluation of the European NN calibration for barley and wheat will be continued during the 1995 harvest.

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