Performance of European Artificial Neural Network (ANN) Calibrations for Moisture and Protein in Cereals Using the Danish Near-Infrared Transmission (NIT) Network

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ABSTRACT

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Three problems need to be addressed in networks of Infratec Grain Analysers: 1) the networks are not interconnected, 2) the partial least squares (PLS) calibrations used so far have to be individually adjusted for bias when transferred to the slave instruments, and 3) the calibrations are not entirely stable over time. Nonlinear artificial neural network (ANN) calibrations based on a large common European data set (≈4,000 samples in the training sets and ≈1,000 samples in the stop sets) were introduced to overcome these constraints. The performance of these ANN calibrations was compared with Danish PLS models for protein and moisture in cereals during the 1998 harvest in Denmark, and subsequently with PLS models based on the same European data set. ANN models were more accurate than PLS and, unlike PLS, were linear and transferable up to 25% moisture. It is suggested that the improved performance of the ANN models is attributable to the modeling technique rather than the size and nature of the European data set. In most cases, ANN models could be applied directly and without bias adjustment to slave instruments. The ANN models were also more stable, they required fewer bias adjustments or remodeling over time compared with Danish PLS models. ANN calibrations using shared data have been adopted for commercial use in several European countries and work is in progress to develop global ANN models for determination of protein in wheat and barley.

The Danish near-infrared transmission (NIT) network, based on Infratec 1221 and 1229 Grain Analysers from Foss Tecator AB (previously Perstorp Analytical Tecator AB), was established in 1991 and is now the predominant system for quality assessment of crops in Denmark. Until recently, the measurements were exclusively based on partial least squares (PLS) calibrations, using 100–150 Danish and Swedish samples. Büchmann and Runfors (1995) described the basic features of the Danish network, and a procedure for bias-adjusting the instruments for the determination of protein, moisture, starch, and Zeleny (sedimentation value) in grains, and oil and moisture in rapeseed. Since then, a calibration for gluten in wheat has been introduced.

Since 1991, similar PLS-based networks involving more than 3,000 Grain Analysers have been established throughout Europe, North America, Australia, and elsewhere in the world. Although these networks perform well, some general constraints have become apparent: 1) The networks are not interconnected, but are based on different PLS models and local reference laboratories, and are thus not ideal for international crop trading. 2) Plots of PLS predicted results against reference chemical values tend to be curvilinear, notably for moisture. 3) Practical experience has shown that, for optimal performance, slave instruments must be individually bias-adjusted when transferring the PLS calibrations from the submaster. This standardization procedure becomes even more complicated if moisture is to be measured, because a separate set of standardization samples is required for each instrument to avoid moisture changes during repeated usage. 4) The PLS calibrations are not completely stable over time (a typical example is given below in Table III). The modem system may be used for calibration updates, but as the Grain Network often is used for payment both for protein and moisture, any adjustment of the calibrations has huge economic consequences both for farmers and grain traders. From a practical point of view, it is therefore necessary to keep a balance between calibration stability and accuracy.

To overcome these constraints, the use of regression modelling using nonlinear artificial neural networks (ANN) was proposed. The use of neural networks for agricultural applications has been reported by several authors (Hervas et al 1994; Hana et al 1995, 1997; Lo 1995) but usually with relatively small numbers of samples. The idea that ANN combined with very large data sets displaying great diversity with respect to variety, and growing and harvest conditions would provide an advantage in prediction of protein and moisture in cereals was first suggested by Büchmann (1996). To further the idea, nine European NIT networks formed an informal group called The European Grain Network in early 1995. The common European ANN calibrations were used commercially for the first time in 1996 in the Swedish Agrolab NIT network (Agronet). In 1997, the ANN calibrations were also used in England, Scotland, and a newly established network in the Ukraine. Finally, more than half of the Danish NIT instruments were converted to ANN calibrations in 1997. (The remaining instruments were still based on Danish PLS models in 1998.) In this article, we report on our experiences from the 1998 harvest in Denmark. The reliability of the common European ANN calibrations in terms of accuracy, stability, and transferability were compared with the performance of the Danish PLS models. Subsequently, the performance of PLS models based on the common European data set was also assessed.

MATERIALS AND METHODS

Common European Data Set

Very large sets of European grain data collected during the 1991–1997 harvests, comprising NIT-scans and reference values for protein and moisture, were transferred to Foss Tecator by members of the European Grain Network for development of the European ANN models used during the 1998 harvest. Included were both winter and spring cultivars of soft wheat (but only few samples of durum wheat); winter barley (mostly feeding cultivars) and spring barley (mostly malting cultivars). For reference analyses for moisture, each network used the oven-drying method (ISO 712). One of the participating laboratories used a Kjeldahl method (ICC 105) for protein, while the rest used the Dumas technique. Annual ring tests, based on 10 fresh wheat samples originating from two to three European countries, were conducted between the participating laboratories. Bias adjustments between laboratories were not required for moisture, but minor adjustments (typically in the ±0.2% range) were applied to harmonize protein levels. The vast majority of scans came from 12 different Infratec Analysers, but scans from four additional instruments were also included. All models for both ANN and PLS were developed by Foss Tecator, Sweden.

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ANN Calibration Models

Sample observations (i.e. NIT-scans plus reference values) representing the harvests in Europe from 1991 to 1997 were used to develop ANN calibration models. All NIT scans were subjected to a proprietary mathematical preprocessing stage before artificial neural network calibrations were developed using the back propagation method. The protein model combined wheat and barley; the moisture model combined wheat, barley, oats, and triticale; a separate moisture model was developed for rye during the 1998 harvest. Details of the ANN calibration models used at the beginning of the 1998 harvest in Denmark are shown in Table I. These ANN models were used commercially on 80 instruments.

PLS Calibration Models

At the start of the 1998 harvest, the Danish PLS calibration models were based on 100–150 samples collected in Denmark, most of them in 1996 and 1997. A separate model was required for each species. These Danish PLS models were used commercially on 68 instruments. Subsequent to the 1998 harvest, the European PLS models were developed for comparative purposes; these models were not used commercially. The protein and moisture models were based on the data used in a training set for the corresponding ANN models (Table I, 4182 and 4261, for protein and moisture respectively).

Infratec Types

The European spectra used for calibration development were collected using Infratec types 1221, 1225, and 1229. All instruments measure whole-grain samples, using an 18-mm path length. Performance was evaluated with instruments from the Danish Network. Before the 1997 harvest, the Danish network consisted of 142 slave instruments and four backup instruments. Two instruments were sited at the reference laboratory. The submaster was used for calibration work, while the second instrument was used to monitor the submaster. Of 148 instruments, 12 slaves and one backup instrument were either Infratec type 1229 or the latest version of type 1221, both of which can support ANN and PLS calibrations simultaneously. The remaining 135 instruments were earlier Infratec type 1221 which could not support ANN calibrations. It was decided to upgrade 67 of these instruments (including the two submasters) to type 1229 specifications. It thus became possible to use ANN calibrations on a total of 80 instruments, while 68 field instruments remained unmodified.

TABLE I

Number of Data Records in Training and Stop Sets for the Artificial Neural Network Calibration Models Used at the Start of the Danish 1998 Harvest

	WBP14: Protein (DM) in Model Applicable to Wheat and Barley		WBMO8: Moisture in Model Applicable to Wheat, Barley, Oats, and Triticale		WBRM1: Moisture in Model Applicable to Rye	
	Training	Stop	Training	Stop	Training	Stop
Wheat	2,024	456	2,088	457	1,657	317
Barley	1,851	431	1,965	514	1,471	349
Durum wheat	307	89	79	26	…	…
Oats	…	…	129	44	…	….
Rye	…	…	…	…	71	15
Total	4,182[a]	976	4,261[a]	1,041	3,199	681

[a] These data sets were used for development of the European partial least squares (PLS) models for protein and moisture, respectively.

Evaluation of Accuracy and Stability

The evaluation was based exclusively on Danish samples from the 1998 harvest. Seven elevator sites throughout Denmark submitted a total of ≈100 samples of each commodity. Each sample weighed ≈5 kg and was of typical commercial quality. The samples were mechanically cleaned and transferred to the reference laboratory at The Plant Directorate, Ministry of Food, Agriculture, and Fishery, Lyngy, Denmark. The procedures used for sample inspection, NIT scanning, and reference analyses (protein by Kjeldahl, moisture by oven-drying) have all previously been described (Büchmann and Runfors 1995). At the start of the harvest, scans from a given set of samples were used to predict both a set of ANN and PLS values (Danish models only) for a given constituent, which were then compared with the same set of reference data. The statistics of the two calibration models could therefore be directly compared. Although later it proved necessary to update some of the models by adding 1998 samples, all statistics presented here refer to the models in use at the beginning of the harvest.

Preharvest Standardization Control

Ten large primary samples of barley and 10 of wheat from the 1997 harvest were subdivided to form 96 final sample sets using a procedure previously described (Büchmann and Runfors 1995). All samples except one contained <15% moisture. One set of final samples was scanned on each of the ANN instruments and four sets of final samples were scanned on the first submaster; all scans were saved electronically. All statistical computations were performed by comparing ANN prediction results from a particular instrument, commodity, and constituent with the average of the corresponding predictions on the submaster (hence, the quadruplicate determinations on the submaster). Reference analyses were not employed in this context.

Standardization Control with High-Moisture Samples

Normal standardization control is always performed with fresh samples at the onset of a harvest. In 1998, wet samples did occur, but only later during the season. Therefore, the high-moisture standardization evaluation was conducted separately from the ordinary

TABLE II

Accuracy: SubMaster Statistics for Danish 1998 Grain Samples Measured with the European Artificial Neural Network (ANN) Calibrations Compared with Danish and European Partial Least Squares (PLS) Models

				European ANN		Danish PLS		European PLS	
Grain	Constituent	*n*	Range	SEP[a]	RPD[b]	SEP	RPD	SEP	RPD
Winter and spring barley	Moisture	61	13.6–25.4	0.22	12.2	0.75	3.5	0.69	3.8
	Protein	61	7.7–13.9	0.31	5.1	0.36	4.4	0.39	4.1
Winter wheat	Moisture	83	12.7–28.1	0.26	11.0	1.10	2.6	1.13	2.5
	Protein	78	8.7–14.5	0.23	5.0	0.38	3.0	0.39	2.9
Triticale	Moisture	42	13.4–25.0	0.20	11.1	PLS models not available			
Rye	Moisture	73	11.8–30.4	0.47	6.9	PLS models not available			
Oats[c]	Moisture	38	14.3–32.5	0.41	8.1	PLS models not available			

[a] Standard error of prediction.

[b] Standard deviation in the population of prediction samples divided by the SEP for the same samples.

[c] One sample of oats >30% moisture was underestimated by >2%; if this sample is removed, the SEP becomes 0.25 and the RPD 9.1.

control. Five large primary samples of barley and five of wheat from the 1998 harvest were subdivided into individual sample sets as described above. The moisture content in the samples was 18.8–23.4%. One sample set was used for each of 16 randomly chosen ANN instruments, and four sets were measured on the submaster. The scans were not saved electronically. Again, comparisons were only made to the submaster results.

Statistics

The RPD is defined as the SD in the population of prediction samples divided by the standard error of prediction (SEP) for the same samples. The SD of differences (SDD) is the random error when transferring a calibration from the submaster to a population of slave instruments and is computed in the same way as SEP. All other statistics used to evaluate performance have previously been described (Büchmann and Runfors 1995).

RESULTS AND DISCUSSION

During growing and harvesting in Denmark in 1998, the climate was wet, cold, and overcast during most of the growing season. In many parts of the country excessive rain caused increased nitrogen uptake and, hence, severe lodging. Lodging further reduced the light energy available for photosynthesis, which aggravated poor kernel development. Finally, grain crops were attacked by *Fusarium* fungi during and after flowering in many parts of the country. The harvest was delayed and very wet, resulting in extremely high moisture levels in the crops and additional attacks from fungi.

For the main crops, barley and wheat, the values for the standard error of prediction (SEP) for moisture measured with ANN were low (Table II) resulting in RPD values >10. At very high moisture levels, the ANN predictions were still linearly correlated to the reference values but were slightly less accurate as compared with predictions in the normal range. In contrast, the Danish PLS models could not be used reliably at ≈18% moisture, where the predicted values were both erratic and far lower than the reference data. Figures 1 and 2 illustrate typical ANN and PLS predictions, in this case for moisture in barley. Attempts to improve the accuracy by adding high-moisture samples to the PLS models were not very successful (data not shown). It should be noted that because of these problems it was decided that PLS moisture values >19.5% from the instruments should not be printed nor displayed.

For the other grain crops, only ANN models were available commercially. The SEP value for triticale was as good as those for wheat and barley. For rye, the SEP was somewhat higher, as the ANN model overestimated moisture at >20%. A similar observation was made in Sweden, where the same model was used (T. Olsson, Agrolab Sweden, *personal communication*). After adding very moist rye samples to the ANN model, the SEP value was reduced to 0.29. A similar improvement was observed in Sweden. The SEP for oats was rather high because one sample at >30% moisture was underestimated by >2%. If this sample is omitted, the SEP is reduced to 0.25 and the RPD increases to 9.1.

For protein in barley, the SEP value for the combined crop ANN model was smaller than that of the Danish PLS model. One sample with a highly unusual scan fitted badly with both calibration models, and, hence, had a very poor repeatability. The average value for four determinations of the sample was used for both the PLS and the ANN predictions. The ANN predictions for protein in wheat were more accurate than the PLS results but the difference was less pronounced than with moisture. It should be noted that all the Danish samples were soft cultivars. The same ANN calibration gives comparable results for protein with soft wheat samples from other parts of Europe. However, protein in durum wheat can not yet be predicted with similar accuracy (H. Andrén, Foss-Tecator, *personal communication*). In general, the problems encountered during the 1998 season resulted in somewhat higher SEP values for both the ANN and the PLS models compared with the respective ANN and PLS results from 1997 as well as the PLS results from previous years (Büchmann and Runfors 1995). However, the extreme conditions in 1998 also highlighted the extent of improvement in accuracy with the ANN calibrations, particularly for moisture.

Subsequent to the 1998 harvest, new combined crop protein and moisture PLS models were developed on the same sample sets that were used to generate the ANN calibrations. The statistics for wheat and barley are shown in Table II, and the prediction plot for moisture in barley is shown in Figure 3. These European PLS results closely resemble those from the Danish PLS model, even though the European calibration set contained much more variation in terms of moisture range, sample origin, and instrument difference than the much smaller Danish calibration set. In a preliminary study based on a smaller European data set (≈2,000 samples), Büchmann (1996) also observed lower SEP values for the ANN models

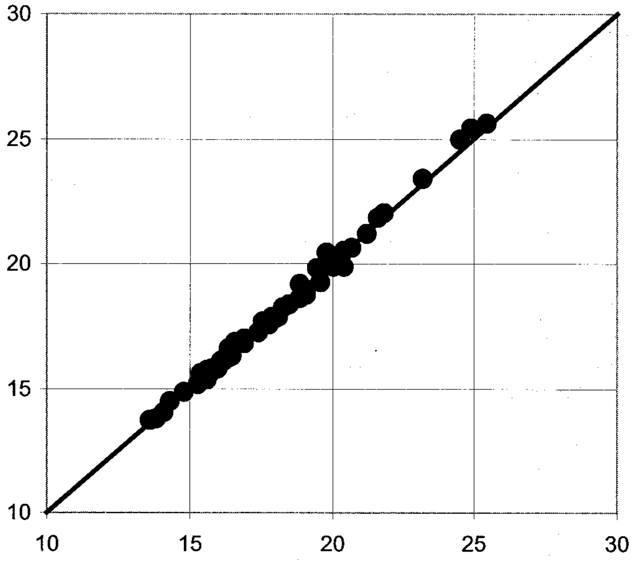

Fig. 1. Moisture values from the submaster predicted with the European Artificial Neural Network (ANN) model plotted against reference values by oven drying for spring barley samples from the 1998 harvest.

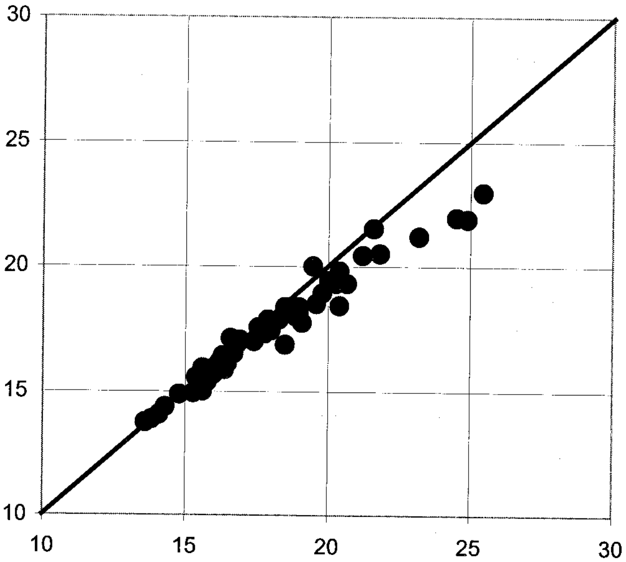

Fig. 2. Moisture values from the submaster predicted with the Danish Partial Least Squares (PLS) model plotted against reference values by oven drying for spring barley samples from the 1998 harvest.

compared with the corresponding PLS figures, even though the two models were based on the same calibration set. It is thus suggested that the improved performance of the ANN models is attributable to the modeling technique rather than the size and nature of the European data set.

The less a calibration model needs to be changed over time, whether through bias adjustment or remodelling, the more stable it is. The ANN calibrations for protein and moisture in barley were completely stable during the entire 1998 harvest (Table III). In comparison, new Danish PLS models had to be developed for both constituents in barley. In wheat, the ANN calibration for moisture was not changed in any way; two small bias adjustments were made to the ANN protein model. The PLS models for both moisture and protein had to be updated with 1998 samples during the harvest. For the minor cereals, only ANN models were available. For rye, a new model was developed to improve the accuracy at >20% moisture as mentioned above. For triticale and oats, only minor bias adjustments were necessary. The common European ANN calibrations were, in general, more stable than the Danish PLS models. The same observation was made in the Danish network in 1997. Calibration updates can be efficiently transferred to all slave instruments by means of the modem system. However, such updates are still a cause of great practical concern to the grain industry which tries to dry, store, and segregate crops to very close moisture and protein tolerances. The improved stability of the ANN models is, therefore, of great practical significance.

It is advisable to check the standardization and general performance of all the slave instruments just before a new harvest season. The preharvest standardization was done using stored and rather dry wheat and barley samples from the 1997 harvest. Statistics for the preharvest standardization control of all of the ANN instruments in the Danish network are shown in Table IV, using barley as an example. For moisture, the ANN calibration was applied directly to both the submaster and all the other ANN instruments without any additional individual bias or bias-slope-adjustment. The average of the bias values for the 79 instruments was 0.07 higher than the bias of the submaster. Thus, the submaster deviated slightly from the mean of the population of slave instruments in this respect. The SD of the 79 bias values was 0.06; this indicates that 95% of the instruments in the population should have bias values differing $<\pm 2 \times 0.06 = \pm 0.12$ from the level of the submaster. These tolerance limits were in good agreement with the actual bias values observed. The SD value of 0.06, describing the bias variation between uncorrected ANN instruments, is almost as good as the average SD value observed immediately after applying individual bias adjustments to a population of 128 PLS-based Infratec 1221 instruments (Büchmann and Runfors 1995). The random error (SDD) of transferring the ANN moisture model to the 79 instruments was 0.06, on average. The comparable average SDD value for the 128 PLS instruments evaluated in 1994 was more than twice as high as the ANN figure from 1998 (Büchmann and Runfors 1995). The average slope was 0.98, very close to the theoretical value of 1. For protein in barley, the calibration was applied directly to the submaster and to 76 of the 79 ANN instruments. A computer simulation using data from 1996 revealed that the remaining three instruments had incorrect biases for both wheat and barley protein compared with the submaster. The three instruments have since been thoroughly checked, but the reason for the bias problems is not understood. However, in the standardization control in 1997, the three instruments behaved as they did in 1996, so the 1996 biases could be used to correct the 1997 readings. The same 1996 values were also used as bias correction for the three instruments throughout the 1998 harvest and were consequently also applied before the present statistical calculations for protein.

The SD of the biases between the 79 ANN instruments was 0.09 for protein in barley. This figure is somewhat higher than the comparable figure observed with the 128 PLS instruments in 1994 immediately after an individual bias adjustment was applied. However, over the course of a year, the SD for the corrected PLS instruments degraded to a higher value than the one given here for the (almost) uncorrected ANN instruments (Büchmann and Runfors 1995).

The average SDD value for protein in barley was 0.17 with the ANN instruments, which is slightly lower than the value of 0.20 observed previously with PLS instruments (Büchmann and Runfors 1995). The average protein slope was 0.97 for the ANN instruments; once again close to 1. The statistical figures for wheat closely resemble those for barley. For protein, the three deviating instruments were once again corrected individually, using the bias values for wheat from 1996.

The conclusion taken from these experiments is that instruments using PLS models have to be individually adjusted, notably if moisture is to be measured. Rippke et al (1996) conducted a transferability study of protein and moisture in corn and soybeans using PLS-based Infratec equipment. Their values for bias variation and SDD closely resemble those published for the PLS-based Danish network for cereals (Büchmann and Runfors 1995). To correct for the instrument differences, Büchmann and Runfors (1995) recommended a simple bias adjustment of each instrument, while Rippke et al (1996) suggested an optional slope adjustment as well. In contrast, the common European ANN calibrations may, in nearly all cases, be transferred to the slave instruments without further modification. The improvements are more pronounced with moisture than with protein, which was the case with the accuracy. Probably, the improved transferability is related to the fact that scans from more than 20 instruments (typically local submasters throughout Europe) were used when developing the ANN models. In practical terms, the improved transferability greatly facilitates the management of a NIT network. Additionally, the random transfer error (SDD) is lower for the ANN calibrations than for the PLS models. It should be noted, however, that the SDD values observed are not of a random nature only. The most striking example is the plot of the individual SDD values for moisture in wheat against the corresponding slope values (Fig. 4). The SDD figures form a highly regular "V", with a minimum at slope values of ≈1. It is therefore possible to further reduce the transfer error by introducing an

TABLE III
Stability: Dates for Bias-Adjustments and Development of Updated Calibration Models for Cereals During the 1998 Harvest in Denmark

		Artificial Neural Network Models		Danish PLS Models[a]	
Grain	Constituent	Bias-Adjustment	Update	Bias-Adjustment	Update
Winter and spring barley	Moisture	no	no	+0.1(27/8/98)	20/8/98
	Protein	no	no	no	15/9/98
Winter wheat	Moisture	no	no	no	27/8/98
	Protein	–0.1(21/8/98) –0.1(8/9/98)	no	–0.1(28/8/98)	10/9/98
Triticale	Moisture	–0.1(19/8/98)	no	PLS model not available	
Rye	Moisture	–0.1(14/8/98)	19/8/98	PLS model not available	
Oats	Moisture	+0.1(7/9/98)	No	PLS model not available	

[a] European partial least squares (PLS) models were developed for comparative purposes only and were not in commercial use during the 1998 season.

individual slope correction for each instrument. However, to avoid systematic errors at the upper and lower ends of the ranges, slope corrections must be based on a large number of standardization samples displaying great variation with respect to both moisture and protein. While samples displaying a broad variation in protein are available throughout the year, grain samples with a natural, high moisture level simply cannot be procured before a new harvest when it is most advisable to perform the standardization control. The SDD values for instruments corrected for bias (but not for slope) do not, however, constitute a major practical problem, and a complicated correction procedure is therefore hardly justified. Returning to the three atypical instruments, it is not a permanent solution to apply an individual adjustment to a few analyzers (even if correct), as all the instruments have to be controlled regularly to identify problematic instruments. (The current instruments were only identified by means of standardization scans collected in 1996 for the sake of individual corrections of the PLS models.) Work is in progress to simplify the control procedure and rectify the problematic analyzers.

TABLE IV
Preharvest Standardization Control: 1997 Barley Sample Statistics for 79 Infratec 1221/1229 Instruments Compared with the SubMaster After Transfer of the European Artificial Neural Network Calibration BY218040

	Bias	SDD[a]	Slope
Barley moisture			
Average	0.07	0.06	0.98
SD[b]	0.06	0.02	0.03
Min.	–0.07	0.02	0.91
Max.	0.24	0.15	1.08
Barley protein[c]			
Average	–0.04	0.17	0.97
SD	0.09	0.04	0.04
Min.	–0.24	0.08	0.85
Max.	0.15	0.24	1.05

[a] Standard deviation of differences.
[b] Standard deviation.
[c] For three instruments, individual bias corrections for protein based on 1996 measurements were applied before the statistical evaluation.

TABLE V
Bias Statistics for 16 Infratec 1221/1229 Analyzers Compared with the Submaster, Using the Common European Artificial Neural Network Calibrations BY218040 and HV508040 for Barley and Wheat and Fresh, Wet Samples from the 1998 Harvest

	Barley	Wheat
Average moisture content in control samples	21.4	21.0
Average bias compared to submaster	0.17	0.00
Standard deviation of biases	0.15	0.16
Minimum bias	–0.06	–0.32
Maximum bias	0.40	0.20

The wet harvest offered a rare opportunity to evaluate the effectiveness of standardization at high moisture levels using fresh 1998 samples of wheat and barley. The statistics for this extra standardization control of 16 randomly selected ANN instruments in comparison with the submaster are shown in Table V. As the PLS read-out values were not reported for moisture readings of >19.5%, the high moisture standardization control could only be evaluated with ANN analyzers. There were only five samples of barley and wheat in the control sets, so the evaluation was limited to statistics for the biases only. The average bias of the slave instruments tested deviated slightly from zero for the barley samples but was exactly 0.0 for wheat (Table V). The SD for the biases was roughly twice as high as the comparable SD values for the dry preharvest samples (Table IV). Even then, one may conclude that the analyzers were well aligned with respect to bias at very high moisture levels. This observation agrees with the fact that the ANN calibrations were very accurate, also in the high moisture range. It also underlines the arguments advanced above for not attempting to reduce the calibration transfer error by introducing a slope correction to the individual slave instruments.

CONCLUSIONS

The common European ANN calibrations for moisture in wheat and barley had lower SEP values compared with the PLS models also used in Denmark. The PLS results for moisture levels >≈18% were inaccurate, while the ANN predictions were linear at >25% moisture in the various commodities tested. For protein in wheat and barley, the ANN models were also more accurate than the PLS calibrations but the difference was less pronounced than with moisture. It is suggested that the improved performance of the ANN models is attributable to the modelling technique rather than the size and nature of the European data set. The extreme harvest conditions in 1998 in Denmark highlighted the practical importance of the improved accuracy of the ANN calibrations. The ANN

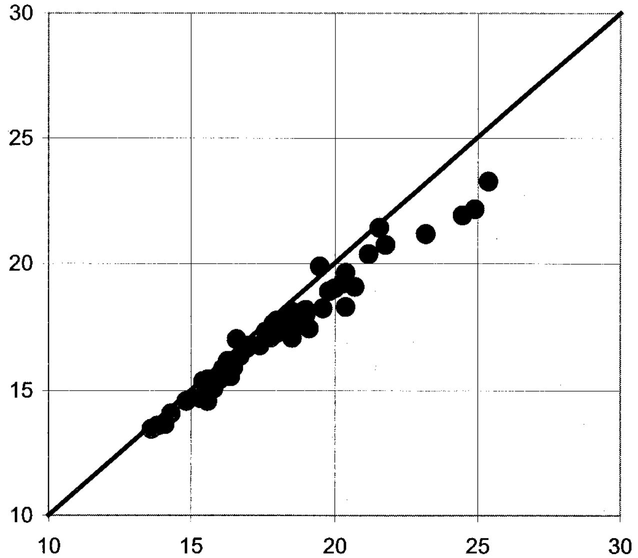

Fig. 3. Moisture values from the submaster predicted with the European Partial Least Squares (PLS) model plotted against reference values by oven drying for spring barley samples from the 1998 harvest.

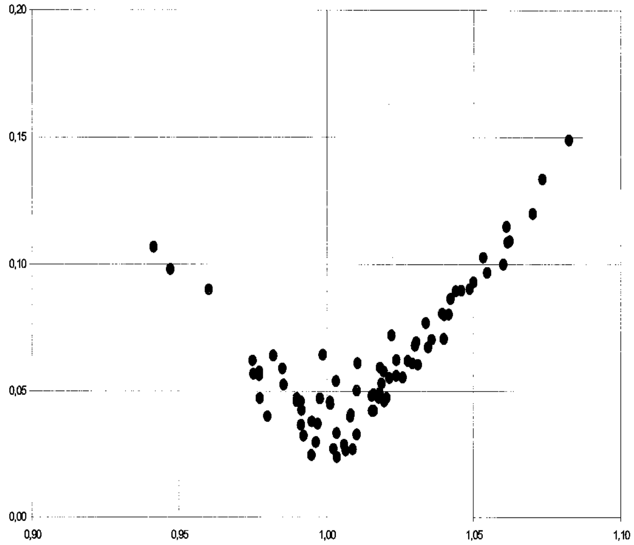

Fig. 4. Relationship between standard deviation of differences for moisture values in wheat and slope of corresponding regression lines when data from individual instruments are plotted against values from the submaster during preharvest standardization trials in Denmark in 1998.

calibrations were, in general, more stable than the Danish PLS models. The improved stability is of great practical importance to both the grain farmer and the grain industry. To ensure an acceptable transferability, NIT analyzers based on PLS models must always be individually adjusted for bias or bias-slope, notably if moisture is measured. The ANN moisture models may, in contrast, be applied directly to all the slave instruments without bias correction. For protein, however, three of the ANN instruments differed from the general pattern and had to be individually bias corrected. The random error (SDD) when transferring ANN calibrations to the slave instruments was lower than with the PLS models. Again, the improvement was most pronounced for moisture. It is possible to further reduce the transfer error by introducing a slope correction individually for each instrument. The SDD values for the uncorrected instruments do not, however, constitute a major problem and a complicated correction procedure is not justified. Good transferability greatly facilitates the management of a NIT network. The wet harvest offered an opportunity to evaluate the effectiveness of the instrument standardization with fresh high-moisture samples. The analyzers are well aligned with respect to bias also at very high moisture levels. This observation agrees with the fact that the ANN calibrations are very accurate throughout the moisture range. Only ANN results from Denmark have been discussed here. The same European ANN models were, however, also used commercially in a number of other European countries during the 1998 harvest. The common ANN calibrations are expected to be adopted in even more European Infratec networks in 1999 (H. Andrén, Foss-Tecator, *personal communication*). Work is in progress to develop ANN calibrations for protein in wheat and barley combining the European data with a great number of measurements from North America and Australia. If such an approach is feasible, the resulting ANN calibrations would constitute global models in the literal sense of the word.

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LITERATURE CITED

Büchmann, N. B. 1996. NIR networking–The ultimate control. Pages 479-483 in: Near Infrared Spectroscopy: The Future Waves. Proc. 7th Int. Conf. on Near Infrared Spectroscopy. A. M. C. Davies and P. Williams, eds. NIR Publications: Chichester, UK.

Büchmann, N. B., and Runfors, S. 1995. The standardisation of Infratec 1221 near infrared transmission instruments in the Danish network used for the determination of protein and moisture in grains. J. Near Infrared Spectrosc. 3:35-42.

Hana, M., McClure, W. F., Whitaker, T. B., White, M. W., and Bahler, D. R. 1995. Applying artificial neural networks: I. Estimating nicotine in tobacco from near infrared data. J. Near Infrared Spectrosc. 3:133-142.

Hana, M., McClure, W. F., Whitaker, T. B., White, M. W., and Bahler, D. R. 1997. Applying artificial neural networks. II. Using near infrared data to classify tobacco types and identify native grown tobacco. J. Near Infrared Spectrosc. 5:19-25.

Hervas, C., Garrido, A., Lucena, B., Garcia, N., and De Pedro, E. 1994. Near infrared spectroscopy for classification of Iberian pig carcasses using an artificial neural network. J. Near Infrared Spectrosc. 2:177-184

ICC. 1995. Standard Methods of the International Association of Cereal Science and Technology. Standard 105/2. Determination of crude protein in cereals and cereal products. ICC: Vienna.

ISO. 1985. Cereals and Cereal Products. Determination of moisture content (routine reference method). Standard 712, 2nd Ed. International Organization for Standardization: Geneva.

Lo, S.-C. 1995. Rapid classification and blends analysis of tobacco mixtures using near infrared and artificial neural networks. Pages 441-447 in: Near Infrared Spectroscopy: The Future Waves. Proc. 7th Int. Conf. on Near Infrared Spectroscopy. A. M. C. Davies and P. Williams, eds. NIR Publications: Chichester, UK.

Rippke, G. R., Hardy, C. L., Hurburgh, C. R., and Brumm, T. J. 1996. Calibration and field standardisation of Tecator Infratec analysers for corn and soybeans. Pages 122-131 in: Near Infrared Spectroscopy: The Future Waves. Proc. 7th Int. Conf. on Near Infrared Spectroscopy. A. M. C. Davies and P. Williams, eds. NIR Publications: Chichester, UK.

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