A successful story of an Internet-enabled NIR system

Ching-Hui Tseng, Nan Wang, Kangming Ma

Cognis Corporation, AgoSolutions/QTA, 4900 Este Avenue, Cincinnati, OH 45232, USA

Introduction

Near Infrared (NIR) technology has been used in agriculture for a long time but the advantages of NIR still have not been fully utilized.[1] An NIR system can be designed to be a single trait analyzer, such as a moisture analyzer, an oil analyzer or a protein analyzer. This kind of NIR system has the advantages of a rugged design with easy operation at a lower price to be used at the grain handling or processing locations by minimally-trained operators. However, the application of each analyzer is limited. The user also has to purchase and maintain several different analyzers if more than one grain or one trait have to be analyzed.

An NIR system can also be a high performance spectrometer covering a wide spectral range, having good wavelength accuracy, and high spectral resolution for more complicated applications. However, it is usually more expensive, less rugged and needs specialists to build and maintain application methods. In order to overcome the problems of the simple-NIR and full-functioned NIR while maintaining the advantages of both systems, an Internet-enabled NIR system was developed.

Internet-enabled NIR system

This Internet-enabled NIR system, named QTA™(Quality Trait Analysis), is composed of a central processor, many rugged, easy-to-operate, full-functioned client NIR systems, the Internet and any computers connected to the Internet (shown as Figure 1).

All the calibration models are stored in the central processor. The user of the client NIR system only has to use the web browser to go to the QTA™ website (www.QTA.com), choose the material (such as canola seeds, wheat, soybean, sunflower, corn etc.) and the traits (such as oleic acid, linolenic acid, moisture, protein, oil etc.) to be analyzed. Then follow the instruction to measure the NIR spectrum of the sample. The obtained spectrum and the user input will be sent to the central processor via an Internet connection. The central processor uses the specified calibration models according to

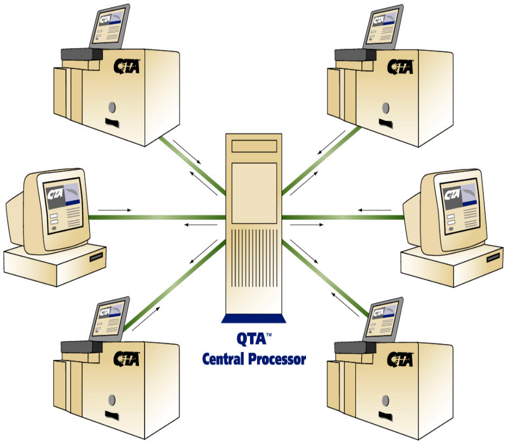

Figure 1. Internet-enabled NIR system

the user input for the prediction of the incoming NIR spectrum. The predicted results are then returned to the client NIR system for display and stored in the central database for future access.

Figure 2 shows the rugged full-functioned client NIR system. It is based on Bruker Matrix FT-NIR system with an integrating sphere and PbS detector. The sampling system is a rotating cup with a glass bottom with the diameter of about 100mm. The NIR beam illuminates an area approximately 20 mm in diameter at one time. When starting a measurement, the cup starts to rotate and a tumbling device also moves the sample material from the bottom layer to the upper layers. Therefore, this system can be used to analyze inhomogeneous solid materials including powder, small grain, large grain, pellets etc. The Bruker Matrix system is designed to work in a production environment. It is waterproof, dust-proof and very rugged. An industrial rugged notebook computer with touch screen function is also integrated with the NIR system.

Figure 2. A rugged FT-NIR system for multiple trait analysis

Why FT-NIR?

Fourier transform (FT) NIR system has the advantages of covering full NIR spectral range (from 12500 cm^{-1} to 4000 cm^{-1} or 800 nm to 2500 nm), good wavelength accuracy (within 0.05 cm^{-1}) and flexible spectral resolution (2 cm^{-1} to 256 cm^{-1}). With the capability of full NIR spectral range, any spectral change in the first overtone, the combinational, the second overtone, the third overtone or the fourth overtone spectral regions due to compositional change can then be used to calculate the compositional property. Therefore, it can be used to develop more NIR applications in comparison to the NIR systems using only a small spectral region. The flexibility of the spectral resolution also allows the method developer to optimize the measurement parameters according to the application requirements. Normally, with the same sample scanning time, a NIR spectrum with a lower spectral resolution exhibits a better signal-to-noise ratio and a NIR spectrum with a higher spectral resolution is typically noisier. Therefore, if an application needs to distinguish minor concentration differences, a low-resolution measurement with good signal-to-noise ratio should be applied. On the other hand, if an application needs to distinguish detailed spectral features, a high-resolution measurement and a longer scanning time should be applied. In addition, with the flexibility of the spectral resolution, FT-NIR can be adjusted to simulate the spectrum of any type of NIR system, including a different brand of FT-NIR, dispersive NIR, AOTF NIR, diode array NIR etc. It is then possible to transfer calibration models from any type of NIR system to the Internet-enabled NIR system.[2] In some cases, if a fast measurement is required, a low-resolution measurement with a short scanning time will be applied. Since the wavelength drift has been known to be an important factor affecting the NIR prediction accuracy, the wavelength accuracy of FT-NIR also makes the Internet-enabled NIR system easier to share calibration models between different client NIR units.

Why the Internet?

Internet technology is the most popular technology in this century and most of the educated people in the world know how to use a web browser to access the Internet. From the above description, we know that there are many advantages of using an FT-NIR system. However, it is not easy for a non-professional user to fully utilize these advantages. In order to have the NIR technique to be widely accepted, the use of the system must be as easy as possible. The addition of Internet capability makes the FT-NIR system easy to use for anyone. The QTA™ users do not have to know how to choose NIR measurement parameters, how to develop calibration models, or even how to maintain calibration models; these are all taken care of by NIR experts at the QTA™ central location.

Via Internet, it is possible to remotely monitor the instrument performance, and in many cases, identify and solve problems remotely. Since all the models are stored at the central processor, they can be remotely developed or modified by NIR experts at the central location and used by all the client NIR systems simultaneously. Therefore, even without on-site NIR experts, the NIR applications for a client NIR system can still be easily expanded.

Data storage and management are other advantages of the Internet-enabled NIR system. Since all the spectra and predicted results are stored in a database that resides at the central location, either the current analyzed data or the historic data can be made available to your central office, laboratory personnel, or business personnel anywhere in the world for their use in managing the business.

Centralized model building

QTA™ builds shared models for the entire networked NIR units not calibration models for individual NIR analysers. It is very important that these models predict consistent results of the same sample from different client NIR analyzers. QTA™ uses special calibration techniques to compensate for instrument variances of the FT-NIR systems, so the calibration model can be shared by different NIR units including the units already in service. For example, a normal PLS calibration model of oleic acid content in canola seeds was built using 150 NIR spectra obtained from a FT-NIR system (M102). The calibration result shows the R^2 (determination coefficient) of 94.26% and RMSECV (root mean squared error of cross validation) of 0.55% with the linolenic acid content ranged from 60.62% to 76.19%. Two samples with the oleic content of 70.45% and 76.09% were measured in duplicate by 14 other FT-NIR systems. The prediction errors are shown in Table 1 and illustrated in Figure 3. There are many predictions with the errors much more than twice of the standard error (95 % confidence interval) of the calibration. This calibration model cannot be shared by the Internet-enabled NIR systems. With a QTA™ treated calibration model, the prediction errors are shown in Table 2 and illustrated in Figure 4. It is obvious that the QTA treated model is consistent and can be shared by different FT-NIR systems.

QTA models not only compensate for hardware variances, but also for variances from sample and environmental changes. Therefore, the same sample measured by the instrument at different locations, different days or after hardware changes (such as light source and laser replacement etc.) still produce consistent results.

Table 1. Prediction errors of oleic acid content of two samples measured by 15 FT-NIR systems using a normal PLS model

Instrument	Prediction errors			
	Sample 1(70.45% oleic)		Sample 2 (76.09% oleic)	
	Measure 1	Measure 2	Measure 1	Measure 2
M101	-0.466	-0.786	-0.94	-0.861
M102	0.219	-0.203	0.166	-0.109
M104	2.872	2.557	1.986	2.059
M105	0.3	-1.251	-0.135	-0.578
M108	4.17	3.301	2.907	2.228
M109	2.889	2.668	2.065	1.898
M113	4.985	4.078	3.824	3.634
M115	3.289	2.27	2.072	2.134
M118	2.261	1.667	1.318	0.957
M119	3.699	2.785	2.496	2.078
M120	2.061	1.283	0.563	0.518
M122	1.351	0.316	0.154	0.232
M124	3.052	2.34	1.92	1.687
M125	3.674	2.232	2.59	2.293
M129	2.48	1.822	1.375	1.285

Table 2. Prediction errors of oleic acid contents of two samples measured by 15 FT-NIR systems using QTA calibration model

Instrument	Prediction errors			
	Sample 1(70.45% oleic)		Sample 2 (76.09% oleic)	
	Measure 1	Measure 2	Measure 1	Measure 2
M101	0.319	-0.349	-0.011	-0.118
M102	-0.145	-0.136	0.087	-0.115
M104	0.267	-0.176	0.225	0.126
M105	0.608	-0.285	0.114	0.354
M108	0.567	-0.074	0.008	0.603
M109	-0.159	-0.484	-0.119	0.026
M113	0.461	0.625	0.205	0.107
M115	0.199	-0.089	-0.017	0.05
M118	0.59	-0.06	-0.094	0.103
M119	0.306	-0.344	0.582	-0.072
M120	-0.371	-0.447	-0.208	-0.398
M122	-0.076	-0.037	-0.416	-0.298
M124	0.234	-0.223	0.338	-0.408
M125	0.602	-0.184	0.53	0.206
M129	-0.049	-0.526	-0.026	0.125

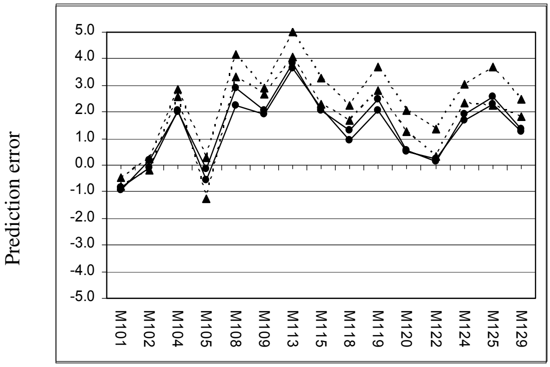

Figure 3. Prediction errors in Table 1

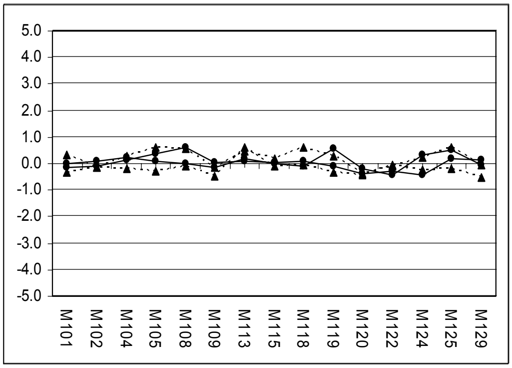

Figure 4. Prediction errors in Table 2

Conclusion

QTA™ makes it possible to have full-functioned FT-NIR systems operated by non-experts. Temperature-compensated models of QTA™ also allow users to operate NIR analyzers without the need of climate controlled conditions. The model sharing capability will enable individual QTA™ analyzers to perform unlimited application analyses. The plug-and-play models are made available over the Internet for immediate use from any QTA™ client analyzer. The low labor costs also greatly reduce the impacts of expensive equipment.

QTA™ started the evaluation application in 2000 and the commercial application in 2001. Currently, there are 20 QTA™ NIR systems installed in Canada for field service. More QTA units and more application models will be added for service this year. The successful story of QTA™ indicates the use of Internet-enabled NIR will become an important trend for NIR applications in the near future.

References

1. I. Ben-Gera, and K. H. Norris, *Isr. J. Agric. Res*. **18,** 125 (1968).
2. D. E. Root, W. Muller, K. Vonbargen and T. G. Kelley, *N.I.R. News*, **14(2),** 8 (2003)