

Remote Sensing from 700 mm: Challenges and Potential

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Abstract

Remote sensing from 700 km, the nominal height for broad coverage, earth observation satellites, has advanced over the decades such that now, with adequate atmospheric correction, the instrument acquired radiance can be converted to spectral reflectance with sufficient accuracy for many applications. Industrial applications require quantitative analyses of material properties and abundances that far exceed those so far obtainable from orbital sensors using the sun as a source, viewing through a changing atmosphere. Although the physics of reflectance spectroscopy is the same for measurements from orbit and over the conveyor belt at 700 mm from the sample material, the needs for illumination, sample presentation and signal-to-noise ratio drive different approaches for close-up remote sensing. This paper will attempt to illuminate the accuracy, illumination, calibration and stability requirements as well as solutions for systems used to make quantitative, real-time measurements of the properties of rocks on conveyors in industrial applications. Quality reflectance spectroscopy has the promise of making a step change in the efficiency of materials processing in factory settings.

Introduction

The last three decades have seen great strides in the use of imaging reflectance spectroscopy to unlock the secrets of the composition of surfaces all over our planetary system, including Earth. On Earth, we have the advantage of visiting the sites measured and checking our hypotheses. Even then, field spectrometers are needed to validate the measurements from orbit and help steer the sample collection efforts. The physics of the interaction of photons with surfaces is the same throughout the known universe. However, there are still many obstacles to acquiring all the information available in the scattered signal, not the least of which, for the Earth, is the intervening atmosphere with clouds, varying illumination angles, surface heterogeneity, particle size, shadowing, moisture and a variety of other aspects, including the effects of ants.

In this paper, I deal with problems that are simplified by the fact that many of the variables have been eliminated and imaging is not required. On the other hand, there are requirements for precise constituent analysis and a reckoning of the value added to an industrial process, and the intervening atmosphere is still a problem even at 700 mm above a moving sample. The following discussion revolves around what is required to apply reflectance spectroscopy techniques to the analysis of natural materials on conveyors that rarely stop.

Industrial Measurement Requirements

Reflectance spectroscopy is used in many industries, in particular, food, agriculture and pharmaceutical manufacturing. All industries have some form of quantitative laboratory analysis of their products for process control and to meet regulatory requirements. Reflectance spectroscopy can play an important role in bringing

laboratory-grade analysis to at-line and in-line measurement environments. These have the advantage of near-real-time analysis so that material properties can be held to tighter tolerances resulting in cost savings. Each application has its precision and accuracy requirements. For example, in the manufacture of cement, the combination of Ca, Si, Al and Fe oxides must fall within approximately $\pm 1\%$ of the Lime Saturation Factor (Taylor, 1997). The measurements of the composition of the quarry limestone are carried out every hour, usually with automated sample collection and analysis by X-ray fluorescence (XRF). In an average cement plant, approximately 3000 tons per hour travel on belts to stockpiles. If the quarry is homogeneous in composition, standard XRF techniques will suffice. However, if not, then other techniques such as prompt gamma neutron activation analysis (PGNAA) or NIR can provide higher time resolution.

In heap leach operations for copper ore processing, the gangue mineralogy, which usually makes up more than 99% of the ore mined, is very important to the efficient recovery of copper. Parameters such as heap permeability and mineral acid consumption can be calculated from quantitative mineralogy. Reflectance spectroscopy is being applied more and more to increase the number of samples analyzed in the laboratory. Ultimately, over-the-conveyor systems will be used at critical points in the workflow to provide detailed metallurgical parameters very rapidly (Goetz, et al., 2009).

Data Quality Requirements

Essentially all applications of reflectance spectroscopy in industrial environments must yield quantitative results. The analysis requires the development of predictive models using statistical techniques. Building an initial calibration model consists of five basic steps: (1) assembling a set of samples that is representative of the materials desired for analysis; (2) measuring the reflectance spectra of those samples; (3) analyzing the samples for the properties of interest using a reference method; (4) using statistical techniques to relate the collected spectra to the corresponding values of the measured properties; and (5) applying chemometric regression methods to calculate the calibration equation (Martens and Naes, 1991; Workman, 2008). The partial least squares (PLS) technique applied to first derivative spectra is the most commonly used for model development

Maintaining high precision and accuracy requires that spectrometers used to gather model spectra must be matched with those that make the ongoing measurements. This means virtually identical wavelength and resolution calibration and high signal-to-noise ratio (SNR). Ongoing radiometric calibration is required to account for drift in the instruments and the illumination system. A common reflectance standard is required to which all the model and sample spectra can be anchored. The stability must be maintained while the instruments operate 24 hours a day in dusty environments for months without servicing.

Measurement System Considerations

Signal-to-noise ratio

Figure 1 illustrates the need for very high SNR values to detect subtle absorption features.

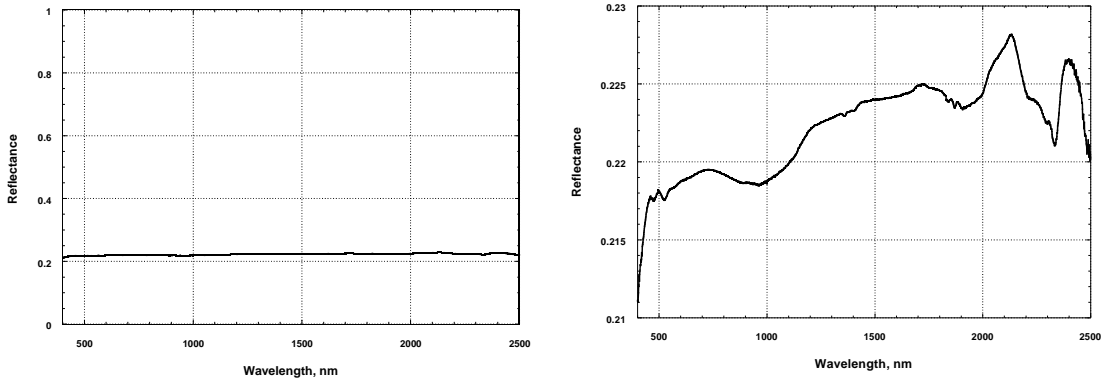


Figure 1. Spectral reflectance of < 200 μ m quarry limestone plotted at two different magnifications of the ordinate. With an intense light source it is possible to see features consistently with absorption depths of less than 0.1%.

Illumination

Since the depths of absorption features are related to concentrations, a very high SNR on the order of 10,000:1 is required to satisfy the requirements for high, concentration precision. The difference between passive Earth remote sensing and remote sensing in the industrial environment is the fact that in the latter it is possible to control the illumination source. Figure 2 illustrates the comparative measured radiances from the two sources.

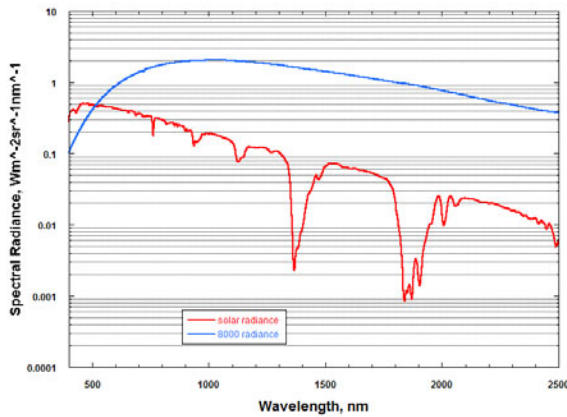


Figure 2. Solar radiance measured from a Spectralon® standard at approximately noon in May at 40°N. The quartz halogen 575W lamp in the ASD QS8000 elliptical illumination head produces a measured radiance from a crown-glass-covered Spectralon panel that is a factor of 30 greater at 2200 nm.

If the reference panel were not glass-covered against dust contamination, in this plot, the lamp source would be 40 times greater than the sun at 2200 nm. The oxygen, water vapor and CO₂ absorption features are clearly visible in the solar radiance

measurement. The QS8000 head is mounted approximately 1.5 m above the conveyor creating a 3 m path from the lamp to the spectrometer. The path length is sufficient to cause absorption in the 940, 1140, 1380 and 1900 nm bands caused by water vapor in the path. This can be normalized out by taking a measurement of the reference panel at the level of the samples on the conveyor. However, just as in the Earth-orbit to ground path, the water vapor concentration is changing constantly. Figure 3 demonstrates what can happen over time as the weather conditions change in plant facilities that are open to the elements.

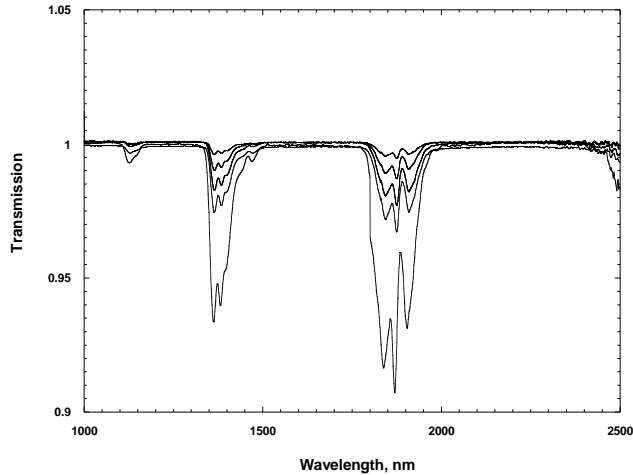


Figure 3. Spectra taken of the Spectralon reference standard, serving as a sample, as the relative humidity changed from 20%, at which the system was normalized, to 60%.

The spectral measurement system is much more sensitive to humidity changes than any other kind of sensor. Hence, ASD does not make use of the water vapor band spectral ranges in model development except when analyzing for moisture content in materials, in which case the liquid water signal normally overwhelms the water vapor signal.

Particle Size and Shadowing Effects

Another reality that must be accounted for is the variation of particle size in rock materials coming from crushers. In many operations, ore or quarry rock enters the conveyor stream at the <100mm size fraction but there are also large quantities of fine material. The fine material partially covers the freshly exposed rock surfaces and, of course, the depths of spectral absorption features are affected. The depths of the absorption features are the primary basis for concentration determination in the predictive models. Experience has shown that the averaging effect of acquiring spectra from a conveyor that is moving at 2 meters or more per second reduces the scatter associated with particle size differences.

An additional effect has to do with shadowing by large blocks that are illuminated from above. This effect has been reduced considerably in the ASD QS7000 and 8000 illumination heads by locating the receiving optics coaxially with the illumination source. This configuration is equivalent to observing the full moon at zero phase which

eliminates any topographic shadowing. The setup for this experiment is seen in fig. 4a. Here the QS8000 system is set to observe a tray of copper ore sample, fig.4b, that is rotated slowly. The resulting spectra are shown in fig. 5.

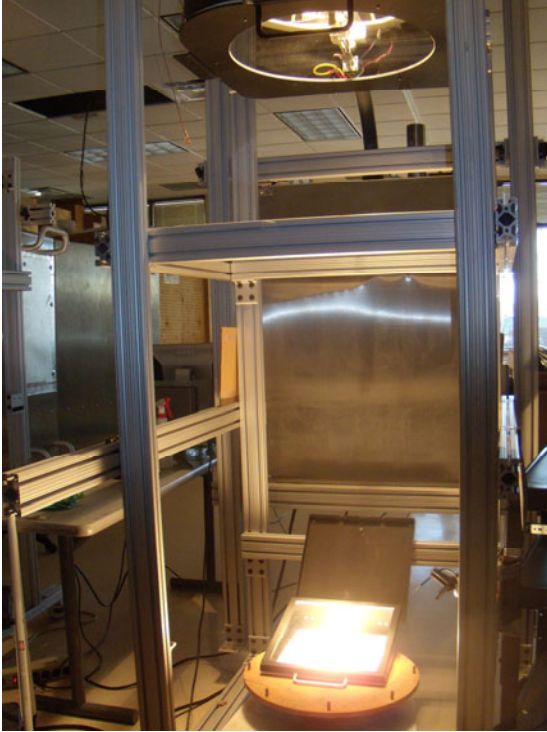


Figure 4b. Rotating pan of copper ore, particle size < 30 mm.

Figure 4a. The ASD QS8000 illumination shining on a glass-covered Spectralon panel. The input fiber for a second ASD FS3 spectrometer is mounted at 45° on the right. The illumination head contains a coaxially-mounted, off-axis parabolic mirror that directs the scattered light from the sample to the spectrometer in the instrument cabinet

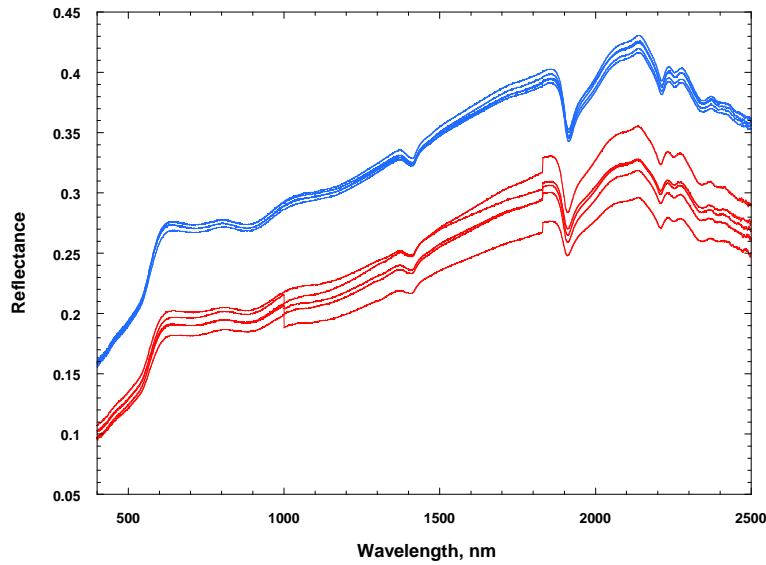


Figure 5. Reflectance spectra of the ore sample shown in fig. 4b. rotating at approximately 15 rpm. The blue spectra were acquired by the coaxial optics in the illumination head shown in figure 6. The red spectra were acquired with an identical spectrometer acquiring data at 45° to the illumination axis. Each spectrum represents a one-second average of ten scans.

In figure 5, the steps in the red spectra at 1000 and 1800 nm are caused by the shadowing and an uneven illumination of the optical fibers in the bundle. The standard deviation in the reflectance values at 2100 nm is 0.5% for the blue spectra and 2.1% for the red spectra, a factor 4 difference. A greater deviation of the reflectance values leads to a greater uncertainty in the quantitative model results.

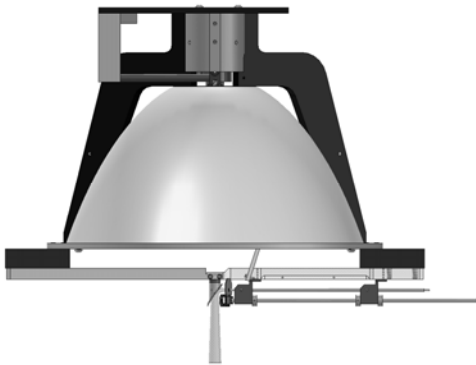


Figure 6. ASD QS 8000 illumination head consisting of an elliptical mirror and 575W quartz halogen lamp. The scattered signal from the sample surface is directed into the spectrometer fiber optic bundle by an off-axis parabolic mirror mounted coaxially with the illumination mirror. The sample surface is approximately 1.5m below the head. A mirror is moved into the beam in front of the fiber optic to direct it toward the internal reference.

Calibration and Stability Requirements

Sensors that provide data and information for a process control loop in a plant must be able to function reliably, 24 hours a day, for months between maintenance cycles. This constraint places stringent requirements on stability of the spectrometer and light source operating in often dusty environments. Since there are inevitable changes in the halogen lamp source as it ages and sensitivity changes in the spectrometer associated

with temperature, a technique for measuring and compensation of the changes is required. In addition, since the quantitative model was developed with samples thought to span the range of concentrations of constituents before system installation, there must be a method to track the quality of the model results and flag any anomalies. These anomalies could come from either instrument or illumination discrepancies or, most likely, from materials whose constituent concentrations fall outside those used in creating the model.

For measuring changes in the product of the lamp radiance and the spectrometer sensitivity, a Spectralon® white reference standard is mounted to the surface of the illuminator mirror. To access the radiance of the internal reference standard, a mirror is rotated in front of the fiber optic bundle. In a normal operation this internal calibration is recorded every 10 minutes. After installation and after each lamp change, an external reference is placed at the level of the conveyor samples and the “adjustment file” is calculated as the ratio of the radiances of the internal reference and the external reference.

$$\rho = \frac{L_s}{L_i} \frac{L_i}{L_e} \quad (1)$$

where ρ is the spectral reflectance, L_s is the spectral radiance from the measured sample, L_i is the spectral radiance from the internal reference and L_e is the spectral radiance from the external reference. The λ subscripts have been omitted for clarity. $\frac{L_i}{L_e}$ is the

“adjustment file” that is applied to all spectra measured. The result is that all reflectance measurements are bound to the external reference, which is considered invariant. This method allows the inter-comparison of models developed with different spectrometer systems and allows for replacement of spectrometers if necessary. Experience has shown that the measurements of L_i are generally stable to ± 0.1 % over a 24 hour period, which is sufficient for modeling purposes. As the lamp filament changes through boil-off and re-deposition of the tungsten in a halogen lamp, the distribution of illumination at the measurement plane can change and the adjustment file may have to be recalculated. This effect is most pronounced near the end of bulb life and may be detected in the quality of the model results.

The Mahalanobis (M) distance is a measure of the probability that, in this case, a spectrum is part of the model set. It is given in standard deviations and a value of greater than 3 is considered the maximum deviation allowed. A measurement with an M-distance greater than 3 is considered an outlier which can be caused by a sample that lies outside the range of constituent values used in the construction of the model or an instrument/lamp system malfunction. In practice the M-distance is called the measurement quality index (MQI). MQI values can be incorporated into alarm settings in process control software.

Typical Results

Copper ore

The heap-leach process is the most widely used technique to separate copper minerals from gangue. The gangue mineralogy plays an important role in the agglomeration step before the material is put onto the heap. Here factors such as

mineralogy and particle size play a role in acid consumption. On the leach heap, permeability and acid consumption play a major role in the economics of copper extraction. Again, mineralogy is important and in some locations smectites play a major role in the permeability of the pile.

Figure 7 shows spectra of a subset of samples acquired by the QS 8000 from the rotating pan shown in fig. 4b for modeling purposes.

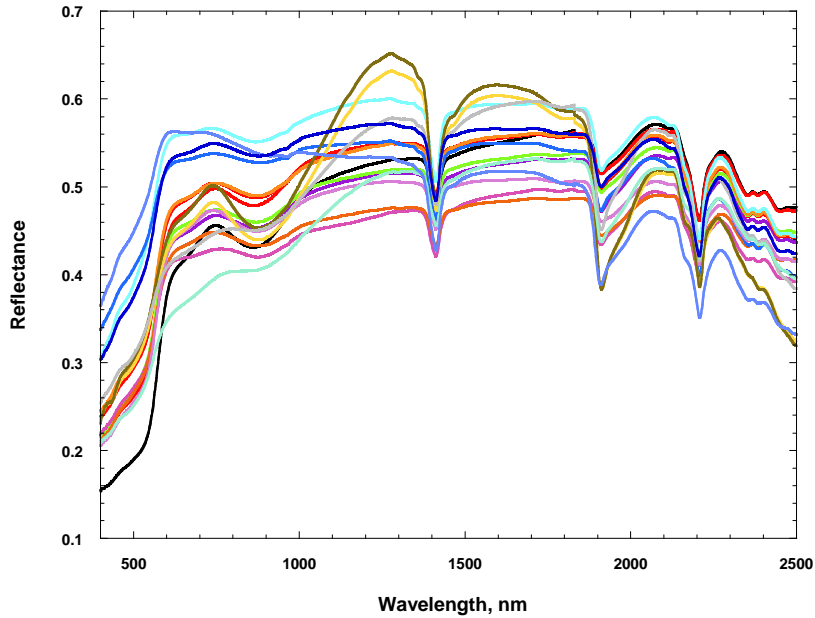


Figure 7. Reflectance spectra of 17 samples of copper ore from a set of 45 used to develop quantitative mineralogical models.

From the 45 sample spectral data, a quantitative model was developed for a variety of minerals. The reference data were constituent percentages measured by quantitative X-ray diffraction (XRD). Figure 8 shows the performance of a model for kaolinite.

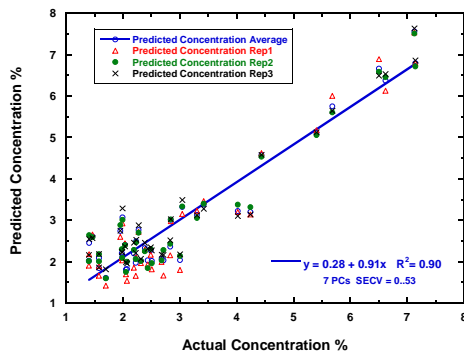


Figure 8. A predictive model for kaolinite. The data were acquired from the samples on the rotating pan shown in fig. 4b. Between each repetition the pan was stopped and the sample hand mixed. In general, the standard errors are approximately 10% of the concentration range or less. (Goetz et al., 2009)

At ASD, our experience has been that the errors are greater in the reference measurements than in the spectral measurements. This has been verified by using two different reference methods on the same sample set. In general, reference measurements using QEMSCAN produce better models with smaller standard errors of prediction (SEP) than with XRD (Dan Shiley, private communication).

Oil Shale

VNIR/SWIR reflectance spectroscopy has been used to study the state of kerogen in oil shale (Rowan et al., 1991; Rowan et al, 1995) Oil shale must be heated to drive out the organic constituents, and the concentrations of kerogen as well as moisture are important in the economics of the process and can be measured using modeling techniques. Figure 9 shows a sample of the oil shale spectra.

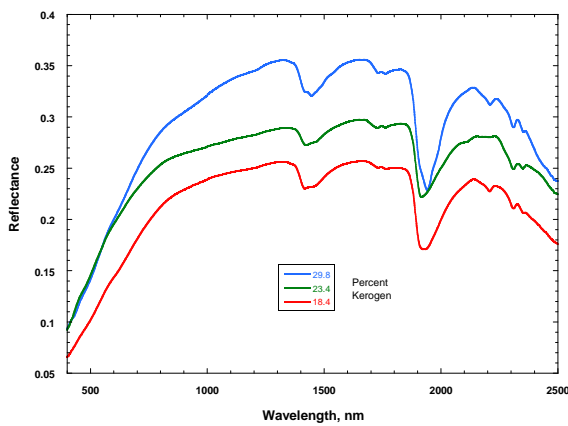


Figure 9. Three reflectance spectra of oil shale samples having different concentrations of kerogen.

Figure 10 a,b show the results of modeling to produce concentrations of kerogen and moisture.

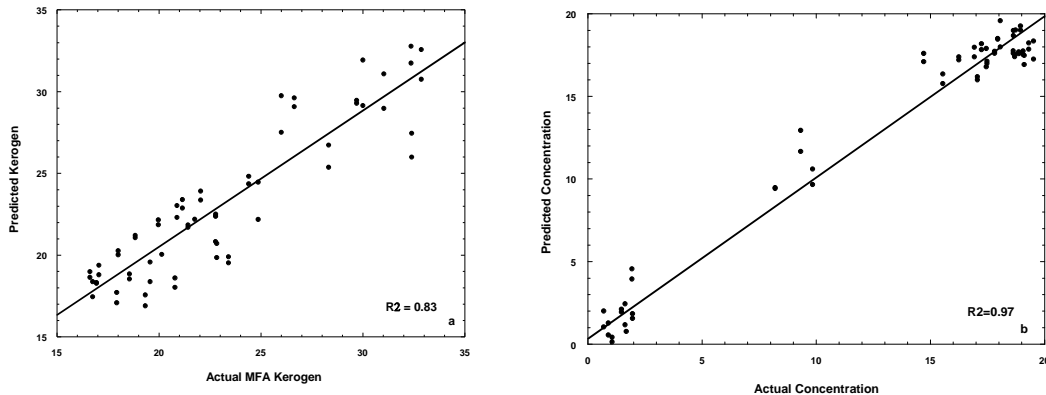


Figure 10. a) Model for the concentration of kerogen in oil shale samples provided by Shale Tech Inc of Rifle, Colorado. The reference method is Modified-Fischer analysis. b) The moisture content model is based on the oven dry weight method. (Courtesy Dan Shiley, ASD Inc.)

Pulp Manufacturing

During the conversion of wood chips to pulp that is later used to make paper, CaO or lime, is used and in the process converts to CaCO₃, or lime mud, which is then recycled to CaO in a rotary kiln at high temperature. The knowledge of the moisture content is important to the economics of fuel consumption in the kiln. Since there are other impurities in the CaCO₃ besides water, a complete spectrum must be used in the model to cover the variability in mud composition and produce accurate measurements of moisture content, or its complement, solids.

Figure 10 shows a portion of the running measurement of the solids content from a QS 7000 system acquiring data over a conveyor belt and applying the measured spectra to the prediction model over a 500 minute period. The solids measurements are determined from the application of spectra averaged over a one minute interval. The MQI, discussed above, yields a measure of the confidence in the reported model value. Values above 3 indicate that new samples should be retrieved from the conveyor and run through the primary reference method and then added to the sample data base to be used in updating the model.

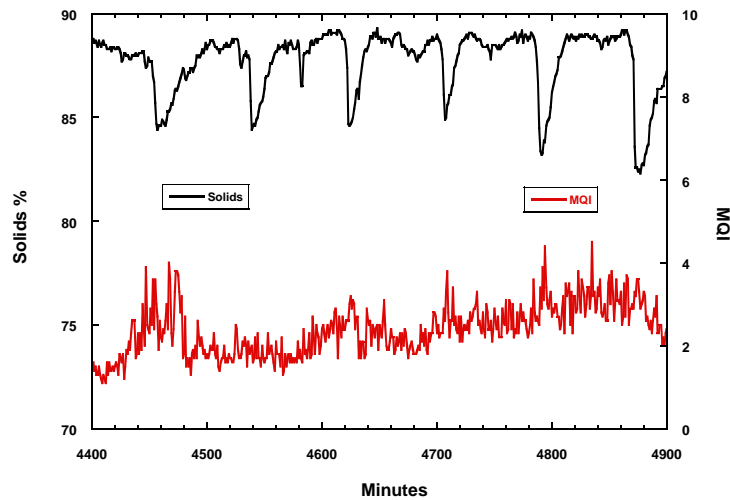


Figure 10. A continuous 500 minute trace of the results of the solids model for lime mud running under a QS 7000 instrument installed over a continuously operating conveyor belt feeding material into a rotary kiln.

Conclusions

Quantitative analysis of reflectance spectra is possible to a precision of value to industrial processes if analysis systems are able to obtain high signal-to-noise ratios, overcome variance caused by shadowing, maintain stability and have the ability to reference each spectrum to a fixed standard. The steps required have been outlined here and model results show that this non-contact, non-destructive technique can produce high-quality information for a variety of industrial processes.

References

- Goetz, A. F. H., Curtiss, B. and Shiley, D. A., 2009, Rapid gangue mineral concentration measurement over conveyors by NIR reflectance spectroscopy, *Minerals Engineering*, **22**, 490-499.
- Martens, H., and Næs, T., *Multivariate Calibration*, 1991, Wiley, New York.
- Petersen, D. L., Aber, J.D., Matson, P. A., Card, D. H., Swanberg, N., Wessman, C., Spanner, M., 1988, Remote sensing of forest canopy and leaf biochemical contents, *Remote Sensing of Environment*, **24**, 85-108.
- Rowan, L. C., Salisbury, J. W., Kingston, M. J., Vergo, N. and Bostick, N. H., 1991, *J. of Geoph. Res.*, **96**, 18,047-18,057.
- Rowan, L. C., Poole, F. G. and Pawlewicz, M. J., 1995, The use of visible and near-infrared reflectance spectra for estimating organic matter thermal maturity, *AAPG Bulletin*, **79**, 1464-1480.
- Taylor, H. F. W., 1997, *Cement Chemistry*, 2nd ed., Thomas Telford, London, 459p.
- Workman, J.J., Jr., NIR Spectroscopy Calibration Basics. *Handbook of Near-Infrared Analysis*, ed. D.A. Burns and E.W. Ciurczak, 2008, CRC Press, pp.123-149.