Obtaining value from a feed/forage lab engagement

Florida Ruminant Nutrition Symposium
February 27, 2024

Ralph Ward
Cumberland Valley Analytical Services

Role of the feed lab

• Execute defined peer reviewed assays
  • AOAC, AOCS, AACC, ASTM, NFTA
  • Journal published assays
  • Lab results should be able to be associated with specific assays
  • Assay definitions should be published and easily located

• Ensure quality control in execution of assays
  • What are the quality control systems in the laboratory?
  • Is there a quality control officer?
  • How are samples controlled?
  • How are samples ground / processed?
Role of the feed lab

- Execute quality control (proficiency) programs
  - NFTA
  - AAFCO
  - AOCS
  - AACC
  - BIPEA
- Execute under ISO 17025 or other quality assurance program (?)..
- Manage internal data in a well-developed LIMS (laboratory information management system).
- Execute and report results in an agreed upon time-frame.
- Communicate and manage client data effectively.
- Effective communications between lab and the client.

Potential roles of the feed lab

- Assist in interpretation of data
- Nutritional support
- Research support
- Method development research
- Provision of data libraries
- Sample collection and transit (“drop box” system)
- Farm sampling services
- Improved time in transit execution
U.S. forage lab industry engagement

- Unique to global ruminant industry
- Many small labs in the 1980's that engaged the new technology of NIR
- Initially, questionable NIR results but set the stage for rapid low-cost analysis
- Services available as the role of forage quality became recognized and ration modeling started in earnest.
- Low cost, rapidly available lab services underwrote the development of the ruminant nutritional services industry in the U.S.
- Lack of external lab quality regulation allowed for labs to keep costs low.
- Routine testing has implemented the concept of process control and mitigation of variation in feed sources.
- Significant value contribution.

U.S. feed lab evolution

- Formerly many small chemistry labs served the U.S. feed industry.
- Small lab ownership was not carried forward, labs closed or were bought out in successive lab aggregations.
- Technology has allowed large feed manufacturers to internalize QC.
- In the U.S. only a few large providers of feed analysis services.
- Forage lab analysis for ruminant purposes now resides with 4 primary labs in the U.S.
Quality control systems vs sample cost

- Extensive quality control system engagement by labs is a requirement in many industries.
  - Example: EPA certifications for environmental work.
- In EU in many cases feed lab service provision requires ISO or similar certification.
- These quality control systems drive up costs but don’t always bring functional value, especially in forage testing where needs are different.
- Forage and feed lab quality control systems will evolve over time.

As a lab client, becoming familiar with forage and feed lab processes will allow for improved value in the absence of these programs and will assist in keeping costs low and routine analysis affordable.

Chemistry versus NIR utilization

- In the U.S., >90% of routine analysis for forage and ingredient quality is by NIR.
NIR History

- Described in literature as early as 1939
- Dr. Karl Norris and coworkers first applied the concept to agricultural products in 1968 with instrumentation at a USDA research lab.
- Dr. John Shenk, a plant scientist at Penn State pushed Dr. Norris to consider the use of NIR for evaluating forage quality (published communication) and in 1976 it was demonstrated that absorption at specific wavelengths was correlated with chemical analysis of forages.

In 1978 a portable unit was designed for use in a van on farm and at hay auctions. This developed into a university extension program using mobile NIR vans in PA, MN, WI, and IL.

- By the early 1980’s, several companies were manufacturing commercial units.
- At Penn State, John Shenk and his associate Mark Westerhouse became the world’s leading authority on the development and use of NIR for agricultural applications.
What makes a good NIR equation?

• Just because a lab generates a nutrient value on an NIR report does not mean that the number has value!
  • “Good” calibration statistics do not guarantee a good equation.
  • Large numbers of samples do not guarantee a good equation.
  • Having samples “over many seasons” does not necessarily make for a good equation.
  • Having good calibration statistics is not a guarantee of a good prediction.
  • Is the reported nutrient a NIR prediction, a calculation, or a value based on an NIR calibration.

So, what makes for a good NIR equation?

What makes a good NIR equation?

• Applying NIR to an organic constituent that has C-H, O-H, N-H, or S-H bonding
• A broad range of like characteristic spectra
  • From a defined feed type such as “hay” or “corn stover”
• A set of spectra that uniformly covers the spectral range of a defined feed material
  • This can be the hard part, obtaining a representative set of materials
• Accurate chemistry information for the nutrient being calibrated!
  • Chemistry analysis is difficult to do on a large set of samples and costly
• Equation statistics that provide a high R2 and low Standard Error of the Calibration (SEC)
• Validation of the equation against a broad range of routine samples
• Validation of the of the calibration samples against the general population
• Does the predicted nutrient have prediction value?
1163 samples labeled DDGS

100 samples labeled DDGS, linear selection
Large set of calibration spectra versus a selected set

7900 corn silage spectra for selection process
Selected corn silage spectra
Amino acid calibration, uNDF calibration

Starch Evaluation by NIR
CVAS Calibration Statistics

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<td>Corn Grain</td>
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Comparison of Starch by Chemistry and NIR

![Graph showing comparison of starch by chemistry and NIR with correlation coefficient r^2 = 0.94 and RMSE = 1.21.]

New Report Reference Information

- **Nutrient Z Score**
  - How far is the value from the mean
- **Nutrient Global “H”**
  - How far is the spectra from neighbors in the population
- **Nutrient RPD value**
  - What is the prediction value for the nutrient

This information will assist the user in knowing if the reported information has decision value.
What is a “Z score?”

- A Z score is the number of standard deviations that a value is above or below the mean value.
- The Z score is a single value that provides understanding of how far a nutrient value falls from the mean. It is a more descriptive way of understanding how a value relates to a population.
What is the sample definition for a population for comparing a sample?

- We often compare samples to “range values”, perhaps a mean and plus/minus 1 SD.
- To obtain value from comparisons define objectives and use the appropriate summarized population!
  - Corn distillers
  - Low fat distillers
  - High protein distillers
  - Wheat distillers
- Large population averages do no change significantly over time
  - U.S. corn silage analysis averages do not vary much from year to year.

What is a Global H value?

- Statistical Term
- The “H” refers to the “Hat” or “^”
- The value is the squared distance between a sample spectrum and the average spectrum sample in a population
- A low H, or distance, means that the sample belongs to the population (<3)
- A very high H means that the sample probably does not belong to the population (>7?) while an intermediate value (3 to 5) means that the calibration may benefit by adding the sample to the calibration set.
- The Neighborhood H value is the distance of the between a spectra and its nearest neighbor spectra and should be <.6.
GH evaluation across 15,000 samples, 3 corn silage calibrations

Three calibrations were evaluated by applying them each to a set of 15,000 sample spectra. The GH values generated for each sample were summarized by calibration.

- Random spectra selection for general nutrients (developed from 1154 samples)
  - GH Average = 1.16, SD = .50
- Linear spectra selection for amino acids (255 samples)
  - GH Average = .82, SD = .48
- Linear spectra selection for uNDF calibrations (305 samples)
  - GH Average = .58, SD = .32
What is RPD?

• RPD is the “ratio of performance to deviation”.
• A mathematical definition would be $\text{RPD} = (1-R^2)^{-0.5}$.
• Practical definition is the “Standard Error / Nutrient Standard Deviation”
# CVAS NIR Calibration Statistics for uNDF in Corn Silage

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The NIR Team
Representing over 50 years of experience!
NIR Technology Application

Handheld NIR Opportunities

• Several models of handheld NIR available in the market.
  • NeoSpectra
  • Trinamix

• Easily portable, few moving parts, advanced spectrophotometric capabilities.

• Good operating apps to work from phone for scanning and basic data management.

• Calibration statistics on dried ground material can be quite good.

• Affordable pricing.
Handheld NIR Limitations

• Sample presentation to the NIR unit is a challenge for obtaining precise and repeatable results.
• Sample homogeneity is a key requirement for precision NIR analysis.
• As-received samples that are coarse and/or have high moisture may not provide reliable results.
• Predictions on ingredients can be acceptable if the material is ground.
• Matching of instruments can create problems in deployment of calibrations.

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Dried ground corn silage model performance

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CP model

Cross-Validation

R² = 0.87 RMSE = 0.56 Bias = -0.00 RPD = 2.74
Handheld NIR Opportunities

• Match the technology to the optimal use.
• Speed of access to information is only of value as that information allows for time-sensitive decisions to be made.
• Does the technology bring value or require time, capital, administrative, and technical resources?

Use case: Receiving soybeans at the mill

• High oleic soybean genetics are coming into the marketplace.
• Mills receiving these soybeans need to know in real time if the beans being delivered are high oleic.
• The NeoSpectra NIR unit will allow the mill to effectively determine whether soybeans are high oleic or traditional genetics.
NIR Predicted Oleic Acid vs Chemistry, High Oleic versus Traditional Genetics

(\% of DM)

Future Opportunities

• VNIR Hyperspectral imaging

A technology that uses sensors to collect a broad range of spectral data in the NIR and visible regions on a pixel basis evaluating a material multidimensionally using advanced computing to derive relationships.

Used in a variety of quality evaluations such as food quality control

There is significant research to apply this in various quality control realms.
Galaxy is an on-site food test for lab technicians and plant operators. It integrates end-to-end testing, processing, and visualization capabilities into a single test.
Future Opportunities

- Reducing analytical error through replication:

\[ SE = \frac{\sigma}{\sqrt{n}} \]

- Improved quality of calibrations.
- Expanded calibrations or new calibrations built around specific materials or forage species.
- Expert systems to develop information from sample comparison to the population or recognizing change over time.
- Increased understanding of what data is important in recognizing quality and variation over time.
Obtaining value from a feed/forage lab engagement

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