Beyond the Spreadsheet

Exploring an ideal computer tool for nutritional supplements and food products

By **James T. DeGroff**
FORMULATOR Software, LLC

THE NUTRIENT SUPPLEMENT FOOD technologist and formulation chemist require an electronic laboratory notebook created specifically to meet nutritional application requirements. Formulation software must provide the tools to create and organize nutritional materials data throughout the lifecycle of the product. In addition, it should provide data management tools to more efficiently develop formulations to meet nutritional product label claims, hit cost targets, and provide nutritional supplement labels as developed by the end user, while tracking and meeting regulatory and QC test requirements. The formulation system should also provide a collaborative development environment that is secure, audited and economical to configure, implement and expand. The system's architecture should support technical field service configurations, multi-laboratory data exchange, toll manufacturer data exchange, and multi-lingual regulatory output.

James T. DeGroff is managing partner of FORMULATOR Software LLC. He has managed the development of formulation software for more than 30 years for nutritional products, foods and beverages, cosmetics, specialty chemicals and other formulation industries. He can be reached at jdegroff@formulatorus.com.

BEYOND THE SPREADSHEET

The Issue

Many nutritional product development laboratories develop and manage their new and revised product formulations either manually or, at best, with custom spreadsheets for formula development, meeting nutritional product label requirements, product costing, small production operations, and even tracking inventory. The use of spreadsheets provides valuable calculation tools to the individual end user. While they fill short-term needs, in the long run spreadsheets present numerous issues.

- Security is poor to nonexistent
- Auditing is extremely difficult
- Changes are not logged
- Crash recovery is only as good as the most recent back-up
- Searching for specific formulas or raw materials meeting given requirements is difficult
- Analysis is fixed; changes require re-programming the spreadsheet(s)
- No intermediate formula analysis is available without extensive programming
- Cost updates are problematic and are often difficult to apply at an intermediate level

The Solution

The solution to this issue is acquiring formulation software for the basic laboratory system for nutritional supplements, which has all the functions required in a laboratory development or piloting environment. This should include features such as the following:

- Security is set at user, group and module levels; formulas can be divided into groups, and users can be restricted to "no access" or "read-only access" to these groups
- Auditing is automatic, and revisions are user/date/time stamped
- Electronic Lab-Book FDA CFR 11 compliant data logging
- SQL Server/MySQL versions provides up-to-the-minute crash recovery
- Raw materials and formulations can be searched by a multitude of conditions, with spot "where used" and full search-and-replace capabilities
- Automated nutritional formulation tools are flexible and defined by the end user by objective, including overage by nutrient
- Nutritional supplement labels can be outputted in a variety of formats directly from newly developed formulas
- Multi-level intermediate analysis is standard
- Cost updates can be integrated off the shelf from ERP or accounting data and then propagated to any number of levels in the database

In addition to solving the most pressing spreadsheet issues, formulation software should also provide:

- Certificates of Analysis (CofAs)
- Specifications for contract manufacturer suppliers
- Electronic signature capture
- Formula dilution/calculation adjustment and targeting
- Test, QC, pilot, production batch and related QC and adjustment histories
- Project and time management, tying together all sampling, development and testing
- Properties, data elements and calculations are configurable by the end user

R&D Data

The first step in creating an electronic lab-notebook is to decide which database manager to use. In the past, spreadsheets were extended and often tied to databases such as dBase or FoxPro. These older databases had their own security and scalability issues. Modern relational database management systems are designed to work efficiently on most Microsoft Windows and Open Source servers (i.e. Linux), and are constantly evolving. Ideally, formulation software should work with most leading edge databases — a common data interface should support Microsoft Access, MSSQL Server, Sun Microsystems' MySQL, and Oracle, independent of the specific database management system. Further, the information and user functions on screen should be the same regardless of the database chosen.

The extensible software design approach provides a series of tools and utilities that allow the user to create his own criteria for nutritional data and mathematical functions in the software. Rather than hard-coding the functions, a formulation program should allow the user to create his own units of measure (weight and volume), physical properties, equations, QC functions, tests and testing criteria, hazardous materials criteria by CAS and EINECS number, repeated phrases, repeated manufacturing instructions, cost criteria, auto numbering schema, inventory status and conversions. It should also allow the user to add additional raw materials, formula, nutritional criteria, dosage sizing and hazardous materials fields.

Ultimately, formulation software should rely on user-created raw materials with the appropriate nutritional calculation by dosage or serving size. Formulas can then be used as raw materials within other formulas. When using formulation software such as FORMULATOR, nutrient label product requirements with overage are entered by nutrient. This particular type of software allows the user to select nutrient raw material candidates. Then it automatically formulates the product and provides dosage criteria and cost analysis of the new formula. With user approval the program can then output a supplemental label, along with the dosage as a tablet/capsule or quantity

to be packaged directly from the formulation. QC test requirements are linked to each formula singularly or as a series of tests. Regulatory criteria can be identified first by raw material, then by formula.

Once a formula is ready, a test batch can be created with the amounts for each material, instructions and the QC tests to be run and recorded by formula by test batch. Users can add notes in most of the critical areas of the program. Notes should provide basic formatting and font selection. Cut and paste from other documents should also be supported.

A logical layout and progression is important to using and understanding complex software. Even more helpful are linkages between modules and set-up and configuration, with the availability of extensive context-sensitive help-windows. In a good program, links between functions and set-up screens make it easy to add and modify fields and functions. The program will also allow the user to view and work with multiple compares, of various formulas, of the nutritional and cost equation results for a series of formulas, and to look back on every change in a formula since it was first developed.

Security of Program and Data

Spreadsheets have little security. A database management system (such as Microsoft SQL Server or Sun Microsystems MySQL), on the other hand, provides not just security, but also scalability, back-up and recovery, and auditing. Security on each table can be set by user or group. This can range from "full access" to "read only" to "no access."

Beyond basic database security, a good lab e-notebook program also provides application level security; regardless of the database security levels, it should provide each user or group of users a set of security privileges for each module in the system, ranging from "Administrator" to "Supervisor" to "Add/Update/Delete" to "Read Only" to "No access," for example.

Each user or user group can also be prevented from viewing any cost data within the system. For many companies cost of materials and formulas is privileged information. Your application security should ensure that specified users have absolutely no access to any cost information.

Security can also be set up by type of formula. This is desirable for companies with separate research groups and plant support chemists. It allows research to use a common materials database, yet keep future development limited to those authorized to be working on them. A good program will also support electronic signature capture for accounts requiring sign-off at critical points in the formulation, QC, or batching process.

E-notebook software like FORMULATOR runs on a modern database platform and will outperform spreadsheets in reliability of use, speed of nutritional balancing and formulation, collaborative development, security of technology, and transfer to production. Cost analysis using database information assures that quotations cover not only the current raw material and container cost, but labor and overhead as well. The information gathered in a well managed database will also assure valid input for regulatory worker safety MSDS and hazardous label creation. ■