Computer Aided Formulation

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EXECUTIVE OVERVIEW

This document describes OPM Product Development’s Computer Aided Formulation solution. Whether it’s the Research and Development (R&D) lab or the Production environment, simulations can be run to play out “what if” scenarios, saving the time and cost of using actual materials and equipment. Alternate items and lots can be plugged in to achieve the best blend. Product targets can be specified for ingredient optimization. In-process production can be fine-tuned for available inventory or changes in the manufacturing conditions. Security and business rules are enforced to provide a controlled yet flexible working environment so many users can benefit from these tools, and productivity can be maximized.

INTRODUCTION

Managing materials efficiently is critical to process manufacturers in order to minimize costs, maximize inventory and resource utilization, and meet product and/or customer specifications. Optimizing formulas is a necessary tool in any process industry. Further to that point, in industries such as Chemicals, Food and Beverage, Pharmaceutical and Biotech, optimizing batches based on the chemical properties and costs of raw materials is an integral part of their business practices.

Using computer-aided formulation can provide the following benefits:

1. The ability to get products to market more quickly
2. The ability to scope out ideas without need for expensive and time-consuming experimentation and testing
3. Greater “workbench” capabilities, providing researchers with more options to pursue ideas
4. The ability to re-direct research efforts early on if results prove to be unprofitable
5. Simplify installations and integrations by eliminating other applications currently being used for advanced formulation.
WHAT IS COMPUTER AIDED FORMULATION?

Computer Aided Formulation is a process where R & D scientists such as formulation chemists or food technologists rely on a computer to handle the mathematical models involved in determining the best formulation to meet product specifications rather than using a more traditional method like the Pearson’s Square. Oracle Process Manufacturing offers two methods of helping to design a formula – a predictive or ‘what if’ analysis called the Simulator, and a target based tool called the Optimizer.

The Simulator allows users to see the impact on a product when new ingredients are substituted, quantities are changed, different lots and sublots of materials are selected, or a characteristic of one of the materials is modified. Any changes made to the formulation are recalculated to display the new product totals.

The Optimizer takes the reverse approach; the user specifies product targets that must be met, selects the materials that can be adjusted, and has the optimizer automatically recalculate and adjust the formulation to meet the new targets.

FORMULATING IN AN R & D LABORATORY

Requirements for a new product are normally given to a formulator in R & D, and may originate from Sales and Marketing, customers, or regulatory agencies. New materials may be required, in which case these must be analyzed to determine their chemical, physical or nutritional properties. Experimental items can be established for these “unapproved” items; they can be entered quickly and used in experimental formulas. These items do not require any details to be entered other than their technical properties, and do not have to undergo the normal New Item Introduction process. This also means that they cannot be seen by or used in the production process.

The formulator must then design a new formula – many times an existing formulation is used as a starting point and then modified to meet the new specifications. The Simulator and Optimizer can be used to design this new formula, using criteria such as cost, potency, color or other parameters. All of the ingredients and their properties are loaded into these tools by selecting the name and version of the formula.

Once the output quantity and product targets are specified, the relevant materials are recalculated to meet the product specifications. Once an optimum formulation is decided upon, the formula can be saved and sent for approval.

After test batches are performed, the results are submitted for review. If the formula produces yields as expected, it can then be sent for approval for production use. At this point, the formula is validated to see that no experimental items exist, which means that the ingredients must be fully defined and approved.
MANAGING VARIABILITY IN PRODUCTION BATCHES

Similar to formula simulation and optimization, an in-process batch can be loaded into the Simulator to refine or change the final output. A batch may need “tweaking” once the properties of the raw materials are determined. In industries that process agricultural raw materials, the quantity of certain ingredients may vary depending on the quality of the other raw materials.

A work-in-process batch can be loaded into the Simulator, along with the actual or available inventory and its properties. The user can view the technical properties for each ingredient, or ingredient lot, and its effect on the product properties. By designating various quantities for the available lots, the production engineer can determine the best inventory to be used for the batch. Additionally, they can add ingredients and view the effect of the new material on the final product. The Optimizer can be used to modify the quantities using any of the technical parameters for the product.

Once the input and output quantities are finalized, the batch can be uploaded into production, along with any allocated inventory lots.

INDUSTRY SOLUTIONS

Food and Beverage/Consumer Packaged Goods

Any company working with farm-based raw materials must deal with variability from lot to lot. Properties such as percent butterfat need to be balanced out with other ingredients in order to yield a certain quantity with the appropriate fat content. The Food and Beverage industries are especially sensitive to the characteristics of their materials in order to ensure a consistent product with an anticipated shelf life. Food and Drug Administration regulations also have a major impact on this, such as standards of identities for jams and jellies that designate the proportions necessary to label a product as such.

Chemicals

Chemical companies normally need to optimize formulas. Since specific grades of raw materials are ordered from an approved list of vendors, the lots they receive are relatively stable. Therefore, the batch does not usually require optimization at the lot level, but the formula must use the correct combination of ingredients. Laboratory batches are used while the formula is still in the experimental phase, so the Optimizer could be used to correct those preliminary production runs.

Life Sciences

Pharmaceutical and biotechnology companies need to yield products with consistent technical characteristics. It's very important that each lot of raw material lot is tested for potency and other factors, and that each finished product meets exacting specifications. The Food and Drug Administration (FDA) has an influence over these industries, along with the high cost associated with the
materials and research required to bring a drug to market. Initial profitability is an important element and requires formula and batch optimization. The ability to optimize batches using lot specific data in a simulated environment provides time and cost savings. Often, products from different batches harvested during their lifecycle must be blended together to achieve the desired properties. Computer aided formulation makes predicting these blended outcomes possible.

**USING COMPUTER-AIDED FORMULATION**

Computer-aided Formulation is a feature of the Oracle Process Manufacturing (OPM) New Product Development application. It relies primarily on setup in the New Product Development application. The required setup consists of:

1. Designating a Laboratory organization
2. Defining global or organization-specific technical parameters
3. Determining the display of technical parameters
4. Entering technical data for items or lots/sublots

Once the technical information has been entered, simulations can be run on formulas or batches and the results can be optimized and saved for future use.

**Designating a Laboratory Organization**

The laboratory organization is the organization under which the simulation will be run. In Process Manufacturing, it is established as an OPM Organization, and given a designation of “Laboratory”.

The laboratory organization must be assigned to the user, via the profile option **GMD: Default Laboratory Organization**. Additionally, the user must have this organization assigned to them under User Organizations.
Figure 2: User Organizations provide access to the organization in OPM

Users can run simulations on formulas from any OPM Organization. The Laboratory Organization is used to retrieve technical data for the item and lots.

### Defining Global and Organization Technical Parameters

Technical parameters are the characteristics of an item that you want to measure or calculate. They can be measurements such as “percent butterfat” or “pH”, or they can be expressions that are calculated based on other technical parameters. Technical parameters can be linked to Quality Tests from the OPM Quality application. Technical parameters can be specific to a laboratory organization, or global and used by all organizations. You can decide on the technical parameters that are used by all organizations in your company and those that are limited to one organization.

### Types of Technical Parameters

There are several types of technical parameters, in addition to one required technical parameter. The technical parameter called Density must be set up for every item in a formula. This technical parameter is used for other calculations, such as weight and volume totals and percents. Density is automatically created for every lab organization, but the value for Density must be entered for each item as Item Technical Data (see following section on entering item data).

The other supported technical parameter types include:
1. Weight Percent – This is typically entered as a percent for each ingredient and then a total weighted percent is computed for the product.

2. Volume Percent – This is a percent entered for each ingredient and a total weighted volume is computed for the product. Similar to weight percent, although computed on volume. When a conversion from weight to volume is needed, then the Density technical data is used.

3. Specific gravity – This is the relative density for the ingredient (usually at a certain temperature) and is used to compute the specific gravity for the product.

4. Cost – A cost per unit figure is entered for each ingredient or byproduct and used to compute the total unit cost for the product.

5. Equivalent Weight – Equivalent weight for the product can be calculated by setting up this technical parameter for an “atomic weight” and entering technical data for each item’s valence.

6. Quantity per weight – Quantity per weight is the quantity of the material required for the formula/batch divided by the weight in another unit of measure.

7. Expression or Product Expression – This is a technical parameter that is calculated, using supported mathematical functions or other technical parameters. Supported mathematical functions include Addition, Subtraction, Multiplication, Division, Power, Square Root, Common Logarithm, Natural Logarithm, Summation of Ingredients (ISUM) and Summation of Byproducts (BSUM). The variables that can be used in expressions include other technical parameters, along with the fixed variables QTY$ and VOL$.

Figure 3: Technical parameters are established on this form
Examples of Technical Parameters

Here are examples of technical parameters, which you will see used in Simulation examples later on.

<table>
<thead>
<tr>
<th>Parameter Type</th>
<th>Description</th>
<th>Example</th>
</tr>
</thead>
<tbody>
<tr>
<td>Character</td>
<td>Any characters which represent technical information</td>
<td></td>
</tr>
<tr>
<td>Numeric</td>
<td>Number or value</td>
<td></td>
</tr>
<tr>
<td>Validation List</td>
<td>List of valid values that can be assigned</td>
<td>Color: list of values may be RED, BLUE, GREEN</td>
</tr>
<tr>
<td>Boolean</td>
<td>0 or 1 to represent False or True, respectively</td>
<td>Yes or No condition which may be evaluated by an expression</td>
</tr>
<tr>
<td>Expression</td>
<td>Algorithm entered using supported or defined variables</td>
<td>PARAM1+PARAM2</td>
</tr>
<tr>
<td>Weight Percent</td>
<td>This gives you the percent of the total weight for a specific parameter and is often used to measure total percents solid.</td>
<td>Fat Percent Solids Non-Fat Percent BRIX</td>
</tr>
<tr>
<td>Volume Percent</td>
<td>This gives you the percent of the total volume for a specific parameter. It is similar to weight percent, except that it applies to the volume UOM.</td>
<td>Potency Moisture</td>
</tr>
<tr>
<td>Specific Gravity</td>
<td>This is a relative density. It is usually calculated for a specific temperature.</td>
<td></td>
</tr>
<tr>
<td>Cost</td>
<td>The unit cost of the item</td>
<td>Standard or forecasted cost of an item</td>
</tr>
<tr>
<td>Equivalent Weight</td>
<td>This is the atomic weight of an element divided by the valence it assumes in a chemical compound</td>
<td></td>
</tr>
<tr>
<td>Quantity Per Unit</td>
<td>This parameter is calculated based on the primary inventory unit of measure (versus a Mass unit, which may differ)</td>
<td></td>
</tr>
<tr>
<td>Product Expression</td>
<td>Algorithm entered using supported or defined variables</td>
<td>SQRT(PARAM1)</td>
</tr>
</tbody>
</table>

These are the supported mathematical expressions that can be used for a Product Expression or Expression technical parameter type. Expressions give you flexibility in computing any technical parameter. The expression cannot contain any spaces.
<table>
<thead>
<tr>
<th>Symbol</th>
<th>Meaning</th>
<th>Example</th>
</tr>
</thead>
<tbody>
<tr>
<td>+</td>
<td>Addition</td>
<td>PARAM1+PARAM2</td>
</tr>
<tr>
<td>-</td>
<td>Subtraction</td>
<td>PARAM1-PARAM2</td>
</tr>
<tr>
<td>*</td>
<td>Multiplication</td>
<td>PARAM1*PARAM2</td>
</tr>
<tr>
<td>/</td>
<td>Division</td>
<td>PARAM1/PARAM2</td>
</tr>
</tbody>
</table>
| POWER  | Take value to the power indicated | POWER(PARAM1,2) – This will multiply PARAM1 by itself  
POWER(PARAM1,3) – This will multiply PARAM1 together 3 times (equivalent to PARAM1*PARAM1*PARAM1) |
| SQRT   | Square Root              | SQRT(PARAM1)                         |
| LOG    | Common Logarithm         | LOG(PARAM1)                          |
| LN     | Natural Logarithm        | LN(PARAM1)                           |
| ()     | Parentheses              | (PARAM1+PARAM2)/(PARAM3-PARAM4)      |
| QTY$   | Variable that represents the quantity of an ingredient or byproduct | QTY$*2                              |
| VOL$   | Variable that represents the volume of an ingredient or byproduct | VOL$*2                              |
| ISUM   | Sums the parameter or value for all ingredients | ISUM(PARAM1)                         
ISUM(QTY$) – this will give you a summation of the ingredient quantities |
| BSUM   | Sums the parameter or value for all byproducts | BSUM(PARAM1)                         
BSUM(QTY$)  
BSUM(VOL$) |

**Linking Technical Parameters to Quality Results**

When you implement OPM Quality, you can link technical parameters directly to Quality Tests. This is done on the Technical Parameters form. The quality test can be from any organization. When a technical parameter is linked to a quality test, then the value for that parameter is taken from either the most recent test result (via a quality sample) or from the quality specification.
For certain quality tests, you can change the technical parameter type. Quality tests with data types of numeric range or numeric range with display text can be changed at the technical parameter level to a data type of weight percent, volume percent, equivalent weight or quantity per unit. The data type field is editable for these quality test types only. One reason to change the data type when linking to a quality test is for the use of the optimizer. The technical parameter types of weight percent, volume percent, equivalent weight and quantity per unit are the only four types that can be used with the optimizer. Other quality test types remain the same data type when linked to a technical parameter, for example, a list of test values cannot be changed to another type of technical parameter.

**Displaying Technical Parameters**

Technical parameters are assigned to items using Technical Parameter Sequences. The sequences allow you to configure which parameters are displayed for an item. They also allow you to enter technical data for an item. If a parameter is not applicable to an ingredient or product, then you delete the sort number. You can also change the sort number to modify the order in which a parameter is displayed in the Simulator. A row for Density automatically displays with a sort sequence of 1. You can select both global and organization parameters to be displayed.

Technical parameter sequences can be established at 3 levels:

1. By item (product and ingredient)
2. By item category
3. By organization

The parameters are retrieved first for an organization and item, then by organization and item category and finally by organization. The item category used for technical parameters is set via a profile option GMD: Technical Parameter Category Set. You can set this category to any item category to which your items are assigned.
Entering Item Technical Data

Technical data can be entered for an item after the parameter sequences are established. You must enter a value for Density for all items. Other parameters may or may not require data; if the value is not entered here, it can be entered on the Simulator and later updated to the item technical data. Item technical data can be entered for an item, lot/sublot, formula or batch.

If there is quality data at the lab level, then the most recent quality test results will default to the item technical data. When values are obtained from quality results, then a Quality Control checkbox is marked next to the parameter and the value cannot be changed. When the technical data pertains to a batch, then the quality data is pulled from data owned by the plant. For items or batches where there are no results, the quality specification target values are used instead.

![Technical data can be entered for an item, lot, formula or batch](image)

Loading a Formula into the Simulator

Once a formula and the appropriate technical data have been set up, you can load the Simulator and try “what-if” scenarios on the formula. The technical information displays from either item technical data or quality results, depending on your setup, and values can be modified or entered directly on the Simulator. Formulas are retrieved into the Simulator using the “Find” (flashlight) icon and displayed along with technical data.
Figure 6: The Simulator with a Formula and Technical data loaded

At the formula level, the quality data owned by the lab is first retrieved, and then quality data for the formula is queried. The Quality Source option on the Actions menu takes you to a view of the quality record that is the source of the simulator values. A right mouse click also indicates the quality record on the status line. The Simulator considers all sample dispositions, with the most recent results displayed. When no quality results exist, the quality specification target values are used. The specification must have an approved specification validity rule to be taken into account by the Simulator. Quality data owned by other plants or labs for an item can also be used for a simulation. The user must invoke the LOV in the Plant column for the item or lot in order to display quality results from other organizations.

Optimizing a Formula

The Optimizer is launched from a button on the Simulator. If an item has parameter values, it is displayed on the Contributing Tab. Items with no values are displayed on the Non-Contributing Tab. The only parameters used by the Optimizer are those with a technical data type of weight percent, volume percent, equivalent weight and quantity per unit. The “Calculate” checkbox for an ingredient is marked when that ingredient is designated as a buffer on the formula. The user can also manually set it in the Optimizer for other ingredients; marking the checkbox does not change the formula, but allows you to perform additional optimizations.

In the following example, there are 3 ingredients, but the technical data applies to only two of the ingredients.
A formula or batch is loaded into the simulation tool with the following values:

<table>
<thead>
<tr>
<th>Ingredient</th>
<th>Lot</th>
<th>LBS</th>
<th>FAT</th>
<th>SNF</th>
</tr>
</thead>
<tbody>
<tr>
<td>RCM</td>
<td>10</td>
<td>94</td>
<td>4%</td>
<td>8%</td>
</tr>
<tr>
<td>Cream</td>
<td>32</td>
<td>3.5</td>
<td>20%</td>
<td>25%</td>
</tr>
<tr>
<td>SMP</td>
<td>44</td>
<td>2.5</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Std. Milk</td>
<td>501</td>
<td>100</td>
<td>4.46%</td>
<td>8.4%</td>
</tr>
</tbody>
</table>

Two technical parameters have been established, FAT, which represents the percentage of butterfat in the milk, and SNF, which is the percentage of non-fat solids. Both technical parameters are classified as “Weight Percent”.

The FAT content in Cream is changed from 20% to 25% and it is selected for recalculation, meaning that its quantity will be adjusted to meet the total FAT content for the product. This will also require an adjustment in the quantity of Skim Milk Powder (SMP) to compensate for the total output quantity in pounds (LB). The SMP quantity has an ingredient tolerance level of +/- 1.00 KGM, so the quantity for this ingredient cannot be more than 3.25.

The FAT content of Cream was increased by 25% (from 20% to 25%). In order to maintain a total FAT content of 4.46% and 100 LB, the quantity of Cream has been decreased to 2.80 LB, and the quantity of Skim Milk Powder (SMP) was increased.

In another example, the formula is for Ice Cream Mix. The ingredients consist of cream, milk, sweetener, stabilizers and emulsifiers. The formulation needs to conform to a certain fat percentage, as well as a percentage for non-fat solids. When there are several ingredients that contribute to both of those measures, then the optimizer is an ideal tool to help compute the required quantities. For the ingredients where there is only one source, the quantity can be computed using the
Simulator or other tools. For our Ice Cream Mix formula, the initial quantities are established as:

<table>
<thead>
<tr>
<th>Ingredient</th>
<th>LBS</th>
<th>FAT</th>
<th>SNF</th>
</tr>
</thead>
<tbody>
<tr>
<td>Stabilizer/Emulsifier</td>
<td>0.65</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>RCM (skim)</td>
<td>40</td>
<td>0%</td>
<td>9%</td>
</tr>
<tr>
<td>Cream</td>
<td>32.5</td>
<td>40%</td>
<td>5.4%</td>
</tr>
<tr>
<td>SMP</td>
<td>11.85</td>
<td>0%</td>
<td>97%</td>
</tr>
<tr>
<td>Sucrose</td>
<td>15</td>
<td>0%</td>
<td>0%</td>
</tr>
<tr>
<td>Ice Cream Mix</td>
<td>100</td>
<td>13%</td>
<td>16.85%</td>
</tr>
</tbody>
</table>

The skim milk and skim milk powder are two sources of the non-fat solids; those are the ingredients we want to modify to achieve our target of 11% solids, while keeping the fat percentage for the ice cream mix at 13%.

Bringing this into the Simulator, we can see the current percentages. We have a fat percentage of 13%, but the non-fat solids are higher than our target.

Using the Optimizer, we set the target for SNF (Solids Non-Fat) to 11%, and check the Calculate box for the Skim Milk (Milk) and SMP (Skim Milk Powder) to recalculate those quantities.
The adjusted quantities are 46.65 LBS for RCM and 5.2 LBS for SMP. The equations behind this are as follows:

If $X = \text{SMP}$ and $Y = \text{RCM (Milk)}$, the equations that need to be solved are:

(a) $X + Y = 100 - 32.5 - 15 - 0.65$

(b) $0.97X + 0.09Y = 0.11(100) - ((0.54)(32.5))$

Equation (a) becomes $X + Y = 51.85$ and equation (b) becomes $0.97X + 0.09Y = 9.245$.

By solving these two equations, using substitution of one of the variables (for example, the variable $Y$ in equation (b) can be substituted with information from the first equation), we can state $Y = 51.85 - X$, so that equation (b) becomes:

$0.97X + 0.09(51.85 - X) = 9.245$

Then $X = 5.20$ LBS.

And $Y = 46.65$ LBS.

**CONCLUSION**

Computer aided formulation provides a way to develop and optimize formulas as well as production batches. With integration to Oracle Process Manufacturing Process Execution and Quality applications, you can leverage existing data to develop your formulations, optimize inventory utilization and produce consistent, high-quality product. New functionality will be introduced in succeeding releases to complement these features and provide more robust formulation tools.