

Overview to the M-RULE® Container Performance Model for *Foods*

This powerful permeation model predicts the performance of food packaging, medical and pharmaceutical packaging and sensitive electronics packaging under a broad range of environmental conditions.

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Introduction to the M-RULE® Container Performance Model for Foods

The M-RULE® Container Performance Model for Foods is a user-friendly, powerful and accurate permeation computational tool. With it, you can rapidly and quantitatively predict the performance of a wide range of packages and materials under a broad range of environmental conditions. Introduced in 2008, this M-RULE® Model is the only predictive model of its kind commercially available across the plastics packaging industry.

The M-RULE® Container Performance Model for Foods allows you to predict the impact of packaging on up to three different products simultaneously and to model up to two different packages inside an exterior package.

The model can calculate container performance not only for simple to complex food packaging, but also for packaging for pharmaceuticals, medical fluids, medical implant and diagnostic devices, sensitive electronics equipment, and any other packaging where sensitivity to moisture or other permeants is a critical issue.

Predicting Permeation and Container Performance with this Model

Why an understanding of permeation is important

All plastics permeate. This simple fact controls the quality of almost all products packaged in plastic containers and drives the specifications for most food, beverage and pharmaceutical products. Aside from flavor components, there are four major permeants that drive the performance specifications for plastic packages. Those permeants are *oxygen*, *water*, *nitrogen* and *carbon dioxide*.

- *Oxygen Ingress* is a pervasive issue in the food packaging industry. Oxygen can react with contained vitamins (especially vitamin C), and it can react with color and flavor components (especially in the presence of light). It is the predominant controlling factor for shelf-life and product quality for food in plastic packages.
- Next in importance to oxygen ingress is *moisture gain or loss*. Moisture can affect product quality in a number of ways. Every product has a preferred moisture content range, with levels above or below the target range impacting sensory performance and consumer acceptance.

Inherent to the M-RULE® Model is a first-principles prediction of moisture sorption for any specified product as a function of relative humidity and temperature.

- An increasing number of packages are purged with nitrogen in order to facilitate processing or to exclude oxygen. While *nitrogen loss* is not a significant issue with some barrier packages, it can be substantial for thin-wall packages and/or highly permeable materials.
- *Carbon Dioxide loss* or *ingress* can have a significant effect on product quality, especially for products that need to be held at a controlled level of CO₂ in order to maintain freshness.

How this model addresses permeation

The M-RULE® Container Performance Model for Foods operates by integrating the fundamentals of permeant diffusion and solubility through polymeric materials, permeant vapor-liquid equilibria, and time-dependent stress-relaxation behaviors with critically evaluated physical data for the component materials. It is therefore much more comprehensive than the empirical curve-fitting on which many other models are based. (See section below entitled “How this model differs from other models.”)

The M-RULE® Model quantitatively incorporates all the significant parameters affecting the concentration of oxygen, water, nitrogen and carbon dioxide in products, including:

- Volume expansion, contraction, and creep as a function of time, temperature, material composition, modulus, internal and external pressure, and humidity
- Permeation of carbon dioxide, oxygen, nitrogen and water as a function of time, temperature, material composition, pressure, stress and humidity (especially important for moisture-sensitive barrier materials like EVOH)
- Permeation through the package closure and package finish
- Solubility of the permeant gases in the product(s), package sidewall(s) and closure as a function of temperature, material composition, pressure, and humidity
- Product moisture content as a function of temperature and relative humidity

Thus, this M-RULE® Model is inherently capable of accurately predicting package performance over a wide range of material, package, product and environmental parameters—from first principles. *This makes it possible for users to examine an unlimited number of package options without first having to create physical containers.* This not only saves time and money, but also allows users to explore far more packaging options.

How this model differs from other models

The M-RULE® Model calculations are based on the application of physical laws and fundamental science via numerical integration. Other models are primarily data-driven empirical models that are restricted to a limited range of test data. Because of our fundamental approach, the M-RULE® Model can simulate scenarios and provide predictions well beyond the range of test data available to empirical models.

The M-RULE® Model fulfills the need of the packaging industry for a quick, reliable, and quantitative predictive tool for package permeation performance. Furthermore, the M-RULE® Model's approach provides brand owners, converters, package designers, and resin producers the capability of understanding how to rapidly and reliably optimize their package, their product, their production, and their distribution and storage conditions.

Typically, empirical models evaluate one parameter at a time (such as oxygen ingress), and treat it as independent from all the other parameters, such as carbon dioxide, water and nitrogen permeation. However, that approach requires an overly simplistic assumption: that diffusion and solubility of each of these permeants is independent of all the other permeants. In reality, this is not the case for the following reasons:

- The presence of moisture can decrease (or increase) the permeability of oxygen and carbon dioxide.
- The presence of carbon dioxide changes the solubility of both water and oxygen in the polymer matrix, and simultaneously affects the diffusivity and solubility of these permeants.
- Because of the limited solubility of oxygen in water, the presence of liquid water inside a container can strongly influence the apparent rate that oxygen will migrate into the container.
- Additionally, stress (from pressurization, for example) impacts the permeability of all these components. These effects can be quite significant. For example, a PET container pressurized with carbon dioxide can exhibit an oxygen ingress rate two to three times greater than the same container when unpressurized.

The M-RULE® Container Performance Model for Foods is designed to predict the interactions between products and packages. The user can specify up to three separate packages (one exterior and zero, one, or two interior packages), each containing a different product with different initial starting conditions.

A powerful feature of this model is its ability to accurately predict temperature-dependent moisture sorption as a function of relative humidity and food composition (using only carbohydrate, protein, and fat content of each product as inputs), eliminating the need for empirical moisture sorption vs. relative humidity measurements at different temperatures.

Along with moisture sorption, the model predicts the glass-transition temperature of the food product, which provides the user with an independent, non-empirical prediction of upper and/or lower moisture targets.

Because of these features, the M-RULE® Container Performance Model for Foods is able to calculate the concentration, diffusivity, and the impact of temperature and stress on all of these permeants concurrently and with each time increment, along with the concentration of each in

both the product(s) and in the headspace(s). Thus, it inherently calculates the impact of these interactions on the permeation of each component and the impact on each product.

In addition, for each time increment, the model can calculate the impact of contained vitamins and oxygen scavengers on the concentration of oxygen inside the package and in the package sidewall and closure.

Finally, the user can specify a respiration rate for each product and the consequential changes in moisture, oxygen, and carbon dioxide content—a feature useful for fresh vegetable packaging.

Operation of the Model

The M-RULE® Container Performance Model for Foods is a web-based tool that you access through your internet browser. As mentioned previously, the model allows you to predict the impact of packaging on up to three different products simultaneously and to model up to two different packages inside an exterior package.

Through your browser interface, you create/select the material composition(s), the package design(s), the closure design and the product(s). You also select the time, temperature, relative humidity and external pressure of the environment (up to 13 sequential intervals), as well as the filling conditions and the test options desired.

The model allows you to specify up to seven sidewall layers for each package. Each material can be either a material selected from the built-in database or a user-created blend of up to five materials (four polymers and one composite material).

In addition, you can select one interior and up to two exterior barrier coatings for each package. The exterior package can have a closure. You can specify up to three layers in the closure.

When you click Run Model, the following operations occur:

1. The model divides the package(s) and the closure into a pre-defined number of sublayers for each layer of material specified by the user.
2. Then, the model calculates an initial concentration of each of the permeants based on the calculated solubility of the permeants in each of the materials at the initial temperature and humidity defined by the user.
3. It next calculates the impact of each of these permeants on the free volume and the glass transition temperature of each of the layers.
4. The model next calculates the amount of stress and stress relaxation that occurs in a specific time increment and the influence of each permeant on the rate of that relaxation in each sublayer.

5. The model then calculates the diffusion factors for each of the permeants, and determines the diffusion that occurs in that time increment, and from that calculates the resulting concentration of each of the permeants in each of the sublayers.
6. The model next adjusts the concentration of each component in the interior of the package(s) by the amount that has diffused into (or out of) the package(s) and the amount dissolved in the product(s) and the Tg of the product(s), then calculates the change in pressure in the package, the resultant change in stress on the package sidewall, and the change in the package volume(s) as a result of these stresses.
7. The model then calculates the change that permeation has had on the product CO₂, O₂, N₂ and H₂O content.
8. It then calculates the change (if selected) in the vitamin content of the product.
9. If oxygen scavenging, vitamin degradation, or respiration is selected, the model then calculates the amount of oxygen reacting with any oxygen scavenger, vitamin, or food.
10. The model then iterates steps 3-9 until the designated run time is complete.

After the model has run for the user-specified time, the model transfers the calculation results to your individual database. You are then presented with the summary results of the calculations. You may then choose to view the results in graphical form and compare them to previous calculations.

You can also export the results into Excel-readable files for further analysis.

The Executive Report link opens a file that contains all your Conditions Selection information as well as Standard Results information.

Because the model uses numerical integration for its calculations, it is inherently more robust and flexible than models that rely on analytic solutions to the underlying differential equations. Thus, you can specify any starting boundary condition, such as sidewall degassed of oxygen, or not; whether the package is filled to any arbitrary level, up to the maximum package volume; any initial starting temperature; and any environmental profile over time.

The Inputs and Outputs Used in the Model

The model's interface provides a user-friendly, interactive environment for data creation, storage and selection. The model is designed to prompt you for all the relevant information needed to make an accurate prediction of a package's permeation performance, and to provide you the results in units you select.

Data Inputs

The M-RULE® Model input pages, like the example pictured below, have drop-down menus, side menus, and extensive data input fields so you can create data or modify existing data. Every input page also has a link to helpful “tips” that can guide you through the page. The model also accommodates different units of measurement, which are set by each user.

The screenshot displays the M-RULE Container Performance Model interface. The top navigation bar includes the M-RULE logo and a user login status: "You are logged in as Container Consulting, Inc. 1 temp17, temp17 Logout". A sidebar on the left lists various menu items, with "Filling Condition Creation" highlighted. The main content area is titled "Filling Condition Creation" and includes a link to "Filling Condition Creation Tips...". The interface features several input fields and controls for defining a filling condition:

- Choose a Filling Condition:** A dropdown menu set to "Test Filling" with "Add" and "Delete Multiple" buttons.
- Filling Condition name:** A text input field containing "Test Filling" with "Save" and "Delete" buttons.
- Filling temperature:** A numeric input field set to "22" with the unit "deg C".
- Time at fill temperature:** A numeric input field set to "1.000" with the unit "Hours".
- Relative Humidity at filling:** A numeric input field set to "50" with the unit "%".
- Storage time between blowing and filling:** A numeric input field set to "0.000" with the unit "days".
- Storage temperature:** A numeric input field set to "0" with the unit "deg C".
- Relative Humidity during storage:** A numeric input field set to "50" with the unit "%".
- Induction time after blowing:** A numeric input field set to "0.000" with the unit "days".
- Total internal pressure(absolute):** A numeric input field set to "1.033" with the unit "Kg/sq cm".
- Total external pressure(absolute):** A numeric input field set to "1.033" with the unit "Kg/sq cm".
- Product degassed of O2?:** Radio buttons for "Yes" and "No" (selected), with a "% Degassed" input field set to "0".
- Headspace Gas Composition:** Input fields for "2" (% O2), "0.03" (% CO2), and "50" (% RH).
- Sidewall degassed of O2?:** Radio buttons for "Yes" and "No" (selected).
- Package fill volume:** Radio buttons for "Nominal" (selected), "Brimfull", and "Empty".
- Save As:** A text input field and a "Cancel" button.

You may be surprised at first by what the model does (and does not) ask for as inputs. Many of the inputs you might expect are not required, because the model has built into it the mathematical relationships to derive them from the information you are asked to provide. (Those inputs, in turn, have been carefully chosen to be ones where the information should be readily available.)

Similarly, you may be surprised at the impact that your choice of initial conditions or package environment has on the shelf-life, even when the calculation is performed on the same package. This is often the result of sometimes subtle and often unappreciated influences/interactions between the co-permeants, the package(s), and the environment. Examining these influences in an interactive fashion can provide you with valuable insights into how your package may actually perform in the real world, and what specifications should be set for package approval.

An important consideration for any product is the environment to which the package (and product) will be exposed. Unfortunately, real-time simulation of all these different environments is virtually impossible in a laboratory environment. A practical consequence of this limitation is that package authorization specifications are generally tied to a single set of environmental conditions.

In developing this M-RULE® Container Performance Model for Foods, we have deliberately allowed the user to input a wide range of filling and environmental conditions, so all the environments that your product might encounter can be simulated. With this capability, you now have the opportunity to not only understand how your package performs and how the product behaves under these different conditions, but to also rethink and revamp your entire package development process.

Data Outputs

In developing the M-RULE® Container Performance Model for Foods, considerable thought went into how the model should report results. This is a significant consideration, because a number of different test methods have been developed for physically testing food packaging, and each of those methods measures something different than every other method.

In the M-RULE® Container Performance Model for Foods, the decision was made to report both the CO₂ concentration in the food and %CO₂ in the headspace. Because of the difficulty in actually measuring gas concentrations in food products, in the model it has been assumed that the solubility of CO₂ in food will mirror the CO₂ solubility in water.

The same assumption is used for oxygen. The concentration of dissolved oxygen and carbon dioxide can be expressed in a number of different units.

For nitrogen, the decision was made to only report %N₂ in the headspace.

For water, results for the product are reported as percent water content relative to the dry (water-free) product, since this is the most consistent and prevalent description for moisture content.

Also reported is %Relative Humidity (RH) in the headspace. For convenience in conversion of each headspace gas percentage to absolute concentrations in the headspace, the absolute total pressure inside the package is also reported.

There are two important consequences of the above choices:

- The first consequence is that the values the model reports may be different than what you have measured for your containers in the past. (Note: in the validation work, we emulated the different test methods to confirm the validity of the model.)
- The second consequence is you now have a “truer” and more accurate picture of your container’s performance with respect to the package contents and the impact of the package parameters on that performance.

Validation of the Model

The M-RULE® Container Performance Model for Foods is based on the same materials, science, algorithms and code developed for the M-RULE® Container Performance Model for Beverages, which has been the industry-standard tool for permeation prediction in the beverage industry since its introduction in 2002.

Consequently, the Model for Foods benefits from the in-depth validation and feature enhancements of the Model for Beverages. (For more information, please refer to the *Overview to the M-RULE® Container Performance Model for Beverages*, which is available via a link on the M-RULE® login page.)

The M-RULE® Container Performance Model for Foods was introduced to the packaging industry in 2008. The accuracy and robustness of the Model for Foods have been established over the years since then by extensive comparison with data generated with real-life packages. This validation has been conducted not only by Container Science, Inc., but also by external clients.

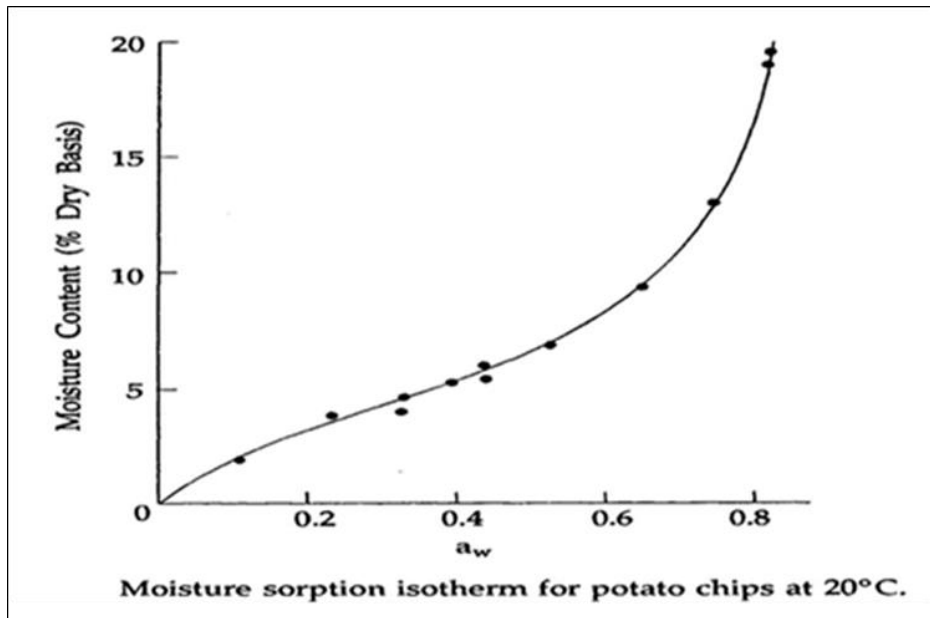
The M-RULE® Container Performance Model for Foods has been validated for vitamin loss through oxidation. Additional validation work has shown the model's accuracy in predicting the performance of oxygen scavengers in both monolayer and multilayer constructions.

As discussed previously, a first-principles prediction of moisture sorption isotherms is an important element of the M-RULE® Container Performance Model for Foods.

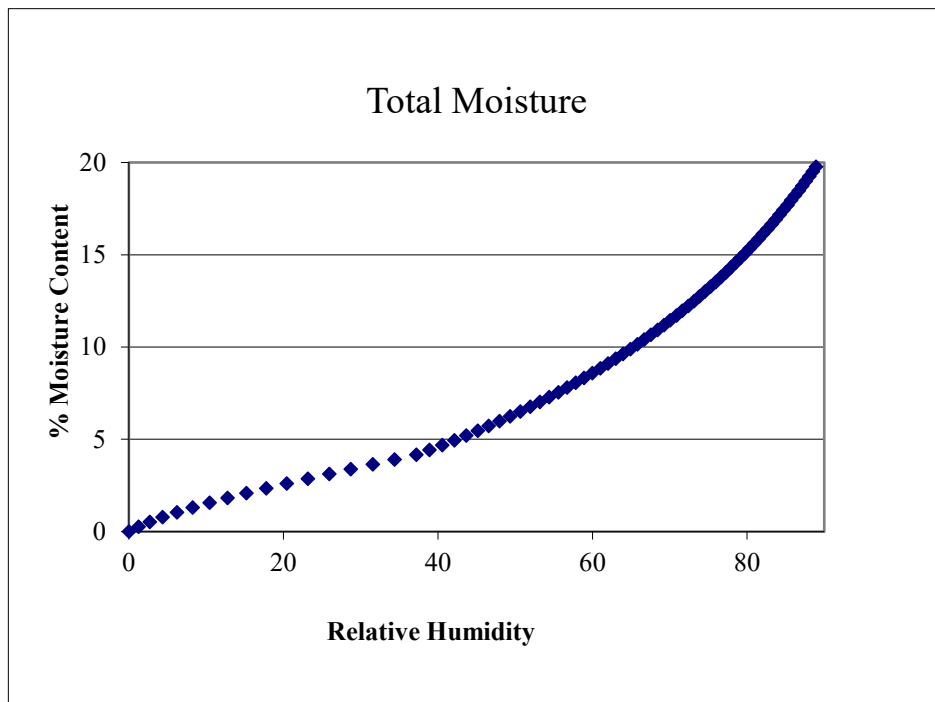
The graphs on the next page compare the measured moisture sorption isotherm for a food (potato chips) with the model's algorithm's prediction of the same (note: $a_w \times 100$ = relative humidity).

The only inputs required for the algorithm are the fat, protein, and carbohydrate content of the food – values which are readily available for most packaged foods.

Measured moisture isotherm¹:



M-RULE[®] Model prediction of moisture isotherm:



¹ Robertson, GL. 1993. Food packaging: principles and practice. New York (NY): Marcel Dekker, Inc. p.575. Print.

Security Features

Encryption

All pages of the M-RULE® application are secured via Secure Socket Layer (SSL) SHA-256—the world's most powerful encryption technology. The signature hash algorithm generates a digital fingerprint—also known as a "hash", "digest", or "checksum"—of information transferred during an SSL session. This fingerprint verifies that the information was not tampered with or corrupted between the server and client. These layers of privacy protection ensure that the user's information cannot be viewed even if intercepted by unauthorized parties.

Application

Each user of the system has a unique username and password. Like all other data transmissions between our clients and our server, the login screen is encrypted, which prevents any attempt to intercept username and password transmissions.

Network

M-RULE® is hosted at Flexential, one of the premier data centers in the business. Flexential provides a secure location that is protected against all types of breaches including fire, flood, and other natural disasters, failures of the main internet trunk lines, long-term power outages, sundry nefarious human actions and outright theft.

Hardware

Unlike many websites that are hosted on shared server space, M-RULE® resides entirely on our own private resources. We use high-end industry standard Dell and HP computational servers, multiple-location backups including offline data backup, and robust firewall hardware which prevents unauthorized access and automatically alerts our IT team about impending viruses or intrusions.

System Requirements

Software Requirements

For the end user, the software requirements are as follows:

- Microsoft Windows 98 or higher (or Mac equivalent)
- A modern browser
- Excel 97 or higher (for data downloading)
- Adobe Acrobat Reader (downloadable from the site)

Suggestions for Use of the M-RULE® Container Performance Model for Foods

Brand Owners & Other End-Users

For brand owners and other end-users, the M-RULE® Container Performance Model for Foods is a valuable tool to allow you to determine how any specified package is actually performing in the real world, or would perform under any defined set of filling/storage/distribution conditions. Thus, by using this model, you can determine how to optimize those parameters for your current packages, improve the quality of your product offerings, and extend the shelf-life of those products in the most cost-effective way.

The model also allows you to determine if your package is under- or over- engineered for a particular application or market. If it is, the model helps you determine the most cost-effective changes that would allow you to meet your specifications.

Because you can now evaluate many packaging options rapidly and at no incremental cost, you can explore far more choices than before, and introduce optimal solutions into the marketplace faster and more efficiently.

Another benefit is that the model allows you to determine, from first principles, what will *not* work – and hence, what packaging options to not carry forward to expensive prototyping.

Converters

For converters, the M-RULE® Container Performance Model for Foods is a valuable addition to your regular retinue of testing capability. With this model, you can examine the impact of resin selection(s) and material distribution(s) on the expected shelf-life of any specified container. This, in turn, allows you to understand what material and process parameters to optimize, and which ones are unimportant to package performance.

The model also allows you to optimize the package design and weight for each intended application and environment, and thus minimize the cost (and maximize the profit) for each of your package offerings.

With the M-RULE® model, you have a powerful permeation prediction tool to use in achieving package approval by your customer. Almost all physical testing required for package approval can be completed in a few hours or days. Permeation testing, on the other hand, often requires months. And, historically, failing (or passing) a permeation test did not provide information as to why the package failed or passed, or what changes needed to be made to meet the target specifications. With this M-RULE® Container Performance Model for Foods, you will be able to determine exactly what factors are affecting the package performance, and thus you will be able to quickly evaluate which changes will result in a cost-effective, acceptable package.

Package Designers and Developers

It is still common for a package development process to have multiple iterations, with each iteration involving tool cutting, resin processing, and permeation performance testing. Invariably, it is the permeation performance testing which is the largest hurdle, both in terms of testing time and potential for failure. A traditional approach for addressing this issue has been to create and test multiple package options in parallel. While this approach can reduce the development time, it can increase the cost of package development, and it still only allows evaluation of a limited number of options. Thus, the cost of package development (in terms of both money and time) can be a major limiting factor for new package development, and it is a major roadblock to the introduction of new packaging options.

By using the model in parallel with the design/development effort, package designers and developers can benefit from the M-RULE® Container Performance Model for Foods. With it, you can quickly create new, cost-effective, innovative packaging with confidence that it will meet the shelf-life requirements of the end-user. Additionally, because of the number of options available in material choices (blends, multilayers, barrier coatings, composites, and scavengers), filling conditions, environmental conditions, etc., you can explore a much wider range of packaging options than ever before and create packages that are tailored to meet the local needs of each market.

Resin Producers

For resin producers, the M-RULE® Container Performance Model for Foods offers the potential to expand your R&D capability. New resins can be evaluated quickly for shelf-life performance, new avenues for improving package performance can be identified, and competitive products can be quickly evaluated.

More importantly, this M-RULE® Container Performance Model for Foods allows you to evaluate new R&D opportunities quickly and reliably. You will be able to establish not only which research could lead to innovative, cost-effective new products, but equally important also determine what research will not.

For resin producers, the diffusion/solubility, polymer blend, polymer modification, and composite materials options are strongly recommended.

Frequently Asked Questions

What gases does the M-RULE® Container Performance Model for Foods handle?

Oxygen (O₂), Nitrogen (N₂), Carbon Dioxide (CO₂), Water vapor (H₂O).

Does the model include the effect of relative humidity on the moisture content of a food?

Of course. From the input parameters of serving size, grams of fat, grams of protein, and grams of carbohydrates, the model calculates the initial moisture content of the food and the relative humidity (water activity x 100) in the headspace above the food. For each time interval thereafter, the model calculates the change in the relative humidity, the corresponding change in moisture content, and the Tg (glass transition temperature) of the food. (Tg is a measure that correlates with crispness.)

How does the model handle crystallinity?

Built into the model's database is the as-molded crystallinity expected for each of the materials, as well as the crystallinity that would result from orientation of that material under the process conditions normally used in either extrusion or injection blow-molding.

These crystallinities are used by the model to correct the diffusion and solubility terms appropriately using well-established mathematical relationships (for example, Cussler's equation).

In addition, if you have purchased the Polymer Modification option, you will be able to change both the crystallinity and % orientation of the polymers and blends in the database.

How does the model handle orientation?

On orientation of plastic materials, some exhibit improved barrier because of alignment of the polymer chains. The impact of orientation is dependent on specifics of the molecular structure. The model contains appropriate factors for these different structural units. It calculates the impact of the orientation on diffusion terms using proprietary mathematical relationships.

A simplification in this model is the assumption that the maximum degree of orientation is achieved on injection blow-molding. This is a reasonable simplification, since optimal mechanical properties are also obtained at this point. In contrast, for extrusion blow-molded articles, little effective orientation is achieved. If you have purchased the Polymer Modification option, you will be able to vary the orientation of the polymers (and blends) in the database. In the Materials Database, the default assumption is 100% orientation. If you are modeling an extrusion blow-molded container, you will have to modify the material to give it an appropriate orientation and crystallinity. You can make these modifications using the Polymer Modification option.

How well does the model correlate with real world results, and what kind of validation has been conducted?

The model correlates within experimental accuracy for CO₂ loss, O₂ ingress and vitamin loss for all the experimental data against which we have validated. These validation studies have been conducted across a wide range of package sizes, construction, and test conditions (including temperature). The model's predicted shelf-life for these factors has been within the experimental accuracy of these real-world data in all cases tested to date; and, on average, the predicted shelf-life is at the mid-point of the measured values. Thus, a plot of predicted shelf-life vs. measured shelf-life gives a straight line that has a slope of 1.026, an intercept of 0.36 weeks, and an R² value > 0.95. Separately, the moisture sorption predictions of the model have been validated against published experimental data for a variety of food products.

How precise is the model?

As is generally known, experimental accuracies/errors associated with a single physical test method of these components (CO₂, O₂, water and vitamins) are not insignificant. In contrast, the M-RULE® Container Performance Model for Foods will always give you the same result for the same set-up conditions. By eliminating the measurement error variability from the overall package performance, the model inherently provides you with a more precise value for shelf life for any given package than if you were to use one of the traditional test methods. And because the model calculates the actual concentrations present in the package (rather than inferring the concentrations from indirect measurements), the results are inherently more accurate than those obtained from traditional experimentation. Furthermore, this provides a more accurate representation of what consumers will actually experience.

Some data is already loaded into the Model for packages, closures, products, environmental conditions and filling conditions. How am I supposed to use this information?

That information has been put into the model to provide users with examples of inputs. We cannot begin to incorporate all the actual conditions your packages might encounter, or the dimensional parameters for your packages. Those are inputs that you (or your company administrator) will need to provide.

What materials are available in the model?

The model includes a wide variety of polymers, ranging from polyesters (PET, PEN, PBT, PLA, PGA, etc.) to polyolefins (HDPE, LLDPE, PVA, EVOH, PCTFE, COC, etc.), to polyamides (Nylon 6, Nylon 66, MXD6, etc.), to polyacetal and polycarbonate. Any of these polymers may be blended with any other polymer or a composite material (such as nanoclay). Moreover, any material or blend may be further modified by changing its orientation, crystallinity, oxygen scavenging capacity or crosslink density.

What if I have a completely new material that I want to have available across my company, but not be System Global? How can I enter that information into the Materials database?

Other than via the Polymer Modification module, new data in the Materials database can only be entered by the M-RULE® IT team, and only after it has been critically evaluated for accuracy.

If you would like to have a new material entered, contact Container Science, Inc. at mrule@containerscience.com. Container Science, Inc. will provide to you the material parameters required and evaluate those values for accuracy. After that process has been completed, the new material can be entered into either the System Global or your Company Global Materials database, depending on your preference.

How do I know what materials to use for my package?

If you don't already have this information, ask your supplier or customer to provide you with specifications.

How does blend creation work?

Blend creation works by taking each of the selected resins and composite materials and combining the properties according to established mixing rules. These mixing rules have been validated for a wide range of materials, and have been found to be accurate and robust.

How can I save data? How can I share data? What happens to my data? Can anyone see my data?

Every time you create a blend, package, closure, product, environment, or filling condition, you will have the opportunity to save that information to your own personal database. Likewise, every calculation that you perform will be saved for later reference.

If desired, you can have records you have created in your personal database saved to your company's global database, so that anyone across your company can access them. That conversion is performed by the administrator assigned to maintaining your company's database (Company Global). Note: Conditions Selection and Model Results are not savable to a company global or system global database. To share that data, use the guest password feature of the model.

As long as your data is confined to your personal database, only you can access it. However, you can give temporary access to your data to other individuals by giving them guest privileges via password access.

In no cases can your or your company's data be accessed without specific, temporary permission being given by an authorized, designated administrator. Your data (and your company's data) is stored in its own specific memory location on a secure server that can only be password-accessed through the M-RULE® login page.

Can I get reports off of the model that summarize the inputs and results?

Of course. By clicking on the Executive Report link on the Model Results page, you will open a report that contains a complete summary of all your input conditions and summary results. You can then right-click on the report to print and/or save the Executive Report.

Can I export the data so I can do additional off-line data manipulation?

Yes. All calculation results that you have access to can be exported from the Model Results page into Excel-readable files, so that you can do further data analysis.

Why are some of the fields "grayed" out on some of the pages?

When you subscribe to the model, you purchase access to different capabilities specified in your subscription contract. If your subscription plan does not include certain capabilities, you can see the options related to those capabilities, but you cannot enter or choose data related to those parameters. Nor can you see results relating to those parameters. For example, if you have not subscribed to the H₂O permeation option, you will not be able to see the water loss from your package, even though the model has performed that calculation.

What kind of error checking is included in the model?

There are three levels of error checking in the model:

- 1) Simple error checking, to ensure that the inputted information is of the right format (numbers where numbers are required, for example), and material percentages total 100%.
- 2) Validity checking, to ensure that the specified package and environmental conditions are reasonable. For example, the model checks to make sure the closure matches the finish dimensions, and the package weight is consistent with the sidewall thickness specified.
- 3) Omission testing, to ensure that all the required parameters are entered. For example, if you ask the model to do oxygen scavenging on a package, it checks to make sure you have specified an oxygen scavenging material, and have inputted a time and temperature between package formation and filling.

How can I get training on the use of the model?

When you first subscribe to the M-RULE® Model, training is provided by Container Science, Inc. as part of the subscription fee. In addition, extensive help tips are included via links on each page within the model. Subscribers can also contact Container Science, Inc. directly by telephone or e-mail for additional support.

How can I get technical support while using the model?

Subscriber support is always available via the *Email Us* button within the model. Questions will be routed to the appropriate party. Requests for technical assistance will be directed to Container Science, Inc. Subscribers can also contact Container Science, Inc. directly by telephone. This high level of support is included in the subscription.

Disclaimers (cautions, restrictions, constraints) regarding Misuse of the Model

The M-RULE® Container Performance Model for Foods is not intended to be used to advertise or recommend one producer's materials over another. It is intended to be an objective assessment of the permeation of selected gases through these materials. Thus, all material properties included in the model have been critically and independently evaluated for accuracy. While specific resins may be identified by their trade names, this should not be considered an endorsement of any particular company's products.

Because there are so many variations that users of the model can perform to optimize their package options, and because there are so many external factors that can influence the final selection, we have chosen to not include any type of optimization routines in the M-RULE® Container Performance Model for Foods. *For the same reasons, Container Science, Inc. and its M-RULE® sales and marketing provider, SBAcci, Inc., cannot be held liable for any decisions made by the user regarding package selection based on results obtained from the model.*

The users of the model are reminded that permeation performance is only one of a number of material properties important to the final package. Other parameters that need to be considered in selecting the optimal material(s) for a package include clarity, color, processability, cost, availability, consumer preference, regulatory restrictions, etc.

Terms and Conditions of Use

The first time you log in to the model, you will be presented with the Terms and Conditions of Use. These must be accepted before you can proceed with access to the model. For subsequent reference, the Terms and Conditions of Use are always accessible via a link from the menu bar on each page of the model.

These Terms and Conditions apply to all users of the model (defined as any company subscribing to the model, and anyone within a subscription company who uses the model) and all components of the model. The Terms and Conditions also apply to users who have been granted temporary access to the model for evaluation purposes.

Subscription Information

When you subscribe to the M-RULE® Container Performance Model for Foods, you purchase unlimited access to the capabilities identified in your subscription contract for the specified contract period. There are a number of different subscription levels available, so that you can tailor the service to meet your specific needs.

SBAcci, Inc., based in Jacksonville, Florida, is the exclusive sales and marketing provider of Container Science's M-RULE® Container Performance Model for Foods. If you have questions regarding subscriptions and terms of use, please contact:

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