



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

This powerful permeation model predicts the performance of packaging for liquids under a broad range of environmental conditions.

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

The M-RULE® Container Performance Model for Beverages 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. This M-RULE Model® is the only predictive model for beverages that is commercially available across the plastics packaging industry. Since its introduction in 2002, it has been extensively validated by our users. To date, the M-Rule® Container Performance Model for Beverages has been used in over 125,000 package simulations.

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 containers. Those permeants are *carbon dioxide*, *oxygen*, *nitrogen* and *water*.

- *Carbon dioxide loss* is a pervasive issue in the carbonated soft drink (CSD) industry. It is the predominant controlling factor for shelf-life and beverage quality for CSDs in plastic containers.
- Next in importance to carbon dioxide loss is *oxygen ingress*. Oxygen can affect beverage quality in a number of ways. It can react with contained vitamins (especially vitamin C), and it can react with color and flavor components (especially in the presence of light).
- An increasing number of packages are pressurized with nitrogen in order to facilitate processing, or to exclude oxygen. While *nitrogen loss* is not a significant issue for some barrier packages, it can be substantial for thin-wall containers and/or highly permeable materials.
- *Water loss* or *ingress* can have a significant effect on product quality, especially for a product that needs to be held at a controlled humidity in order to maintain freshness.

How this model addresses permeation

The M-RULE® Container Performance Model for Beverages 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 interior concentration of carbon dioxide, oxygen, nitrogen and water, including:

- Volume expansion and creep as a function of time, temperature, material composition, modulus, 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
- Solubility of the permeant gases in the bottle sidewall and closure as a function of temperature, material composition, pressure and humidity.

Thus, the M-RULE® Model is inherently capable of accurately predicting package performance over a wide range of material, package, beverage 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 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 bottlers, 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 Beverages takes all of these issues into account with a robust comprehensive approach. The M-RULE® Model calculates the concentration, diffusivity, and the impact of temperature and stress on all of these permeants concurrently and with each time increment. Thus, it inherently calculates the impact of all these interactions on the permeation of each component.

In addition, for each time increment, the M-RULE® model can calculate the impact of contained Vitamin C and oxygen scavengers on the concentration of oxygen inside the package and in the package sidewall and closure.

Operation of the Model

The M-RULE® Container Performance Model for Beverages is a web-based tool that you access through your internet browser.

Through your browser interface, you create/select the material composition(s), the package design, the closure design, the beverage, the time/temperature environment, the filling conditions and the test options desired.

The model allows you to specify up to seven sidewall layers, each of which 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 your package.

You can also specify up to five layers in the closure, as well as the environmental conditions and filling conditions to be simulated for the package.

The model works by iterating through the following steps:

1. The model divides the container 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 and time increment 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 by the amount that has diffused into (or out of) the package, and calculates the change in pressure in the container, the resultant change in stress on the package sidewall, and the change in the package volume as a result of these stresses.
7. The model then calculates the change that permeation has had on the beverage CO₂, O₂, N₂ and H₂O content.
8. It then calculates the change (if selected) in the vitamin content of the beverage.
9. Next it calculates the consumption of oxygen and oxygen scavenger (if selected) in either the bottle sidewall, closure, or both.
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 calculation. 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 brimfull; any initial starting temperature; and any temperature 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 shows the M-RULE software interface for creating a filling condition. On the left is a green sidebar menu with options like Introduction, User Guide, Units Selection, and Filling Condition Creation (which is highlighted). The main area is titled 'Filling Condition Creation' and contains various input fields and buttons. At the top, there's a dropdown menu for 'Choose a Filling Condition' set to 'Example Conditions 3[sg]', with 'Add' and 'Delete Multiple' buttons. Below that is a text field for 'Filling Condition name' set to 'Example Conditions 3', with 'Save' and 'Delete' buttons. The main section contains several rows of input fields: 'Filling temperature' (71.6 deg F), 'Time at fill temperature' (2.000 Hours), 'Relative Humidity at filling' (50 %), 'Storage time between blowing and filling' (0.000 days), 'Storage temperature' (32 deg F), 'Relative Humidity during storage' (50 %), 'Induction time after blowing' (0.000 days), and 'Nitrogen fill pressure' (0.000 Kg/sq cm). There are also three sets of radio buttons for 'Beverage degassed of O2?', 'Headspace degassed of O2?', and 'Sidewall degassed of O2?', each with 'Yes' and 'No' options and a '% Degassed' field set to 100. At the bottom, there are 'Save As:' and 'Cancel' buttons.

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 inputs 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, often unappreciated influences/interactions between the co-permeants, the package, 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, we have deliberately allowed the user to input a wide range of filling and environmental conditions, so all the environments that your product might see 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 the entire package development process.

Data Outputs

In developing this M-RULE® Container Performance Model, considerable thought went into which “test method” should be used by the model for reporting results. This is a significant consideration, because there are a wide range of test methods available for each permeant, and each method performs (and measures) something different than every other method. Thus, for example, for CO₂:

- The Coca-Cola FT-IR method measures the concentration of CO₂ gas inside an empty bottle, plus the amount of CO₂ dissolved in the bottle sidewall.
- The Zahm-Nagel and CarboQC tests measure the pressure of gas in the headspace of a bottle, and from that is inferred the concentration of CO₂ in the beverage.
- Mocon Whole Package testing measures the rate of loss of CO₂ by measuring the rate that CO₂ reaches the exterior of the package, and from that is inferred an interior CO₂ concentration over time.
- The gravimetric method measures the total weight of CO₂ in the container and container sidewall, plus the weight of oxygen, nitrogen, and water. The gravimetric method inherently does not account for volume expansion, CO₂ sorption, and creep.

For CO₂, the decision was made to have the M-RULE® Container Performance Model for Beverages report the CO₂ concentration in the beverage itself, which is the value that all of the above methods attempt to measure, and which is the critical factor for product quality.

The same criterion is used for oxygen, since the internal oxygen concentration is what affects product quality.

For nitrogen, the decision was made to report results as absolute nitrogen pressure, since that is the criterion that is most often used for assessing loss of this permeant.

For water, results are reported as the gain (or loss) in units of mass from the package interior.

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 simulated the different test methods to confirm the validity of the model.)
- The second consequence is you now have a “truer” picture of your container’s performance with respect to the package contents and the impact of the package parameters on that performance.

(Note: If the “Chilled CO₂ Test” option is selected in the model, the CO₂ values reported will reflect the CO₂ content during testing, as opposed to CO₂ content during storage.)

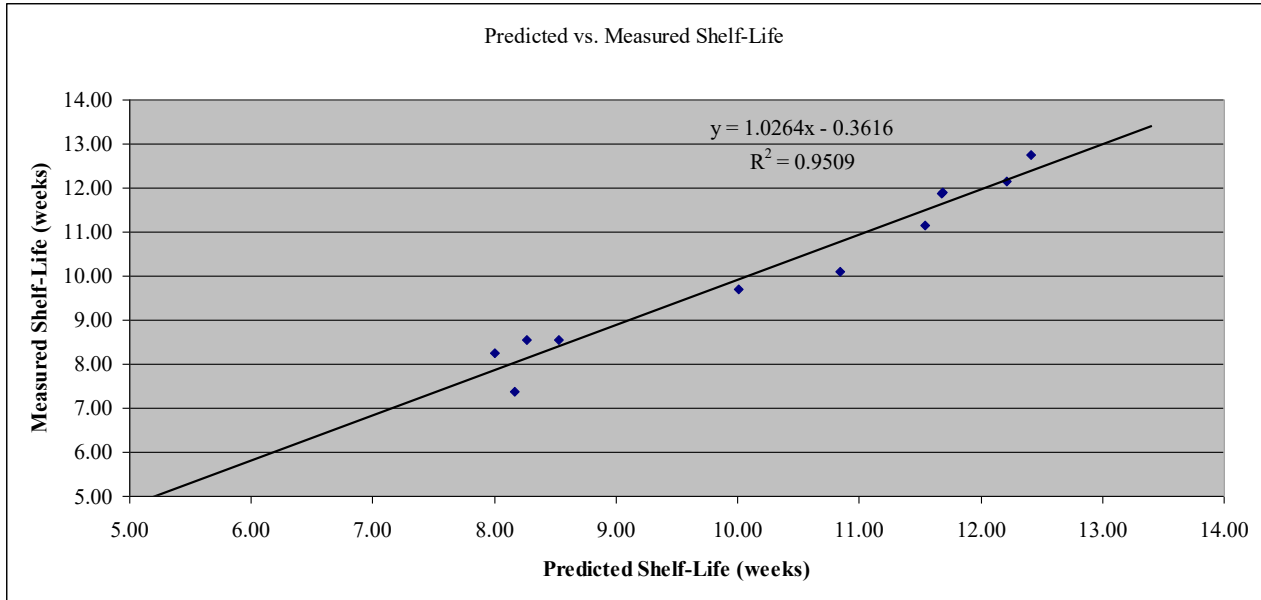
Validation of the Model

The M-RULE® Container Performance Model for Beverages was introduced to the packaging industry in 2002. The accuracy and robustness of the model 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. To date, the model has been run over 125,000 times.

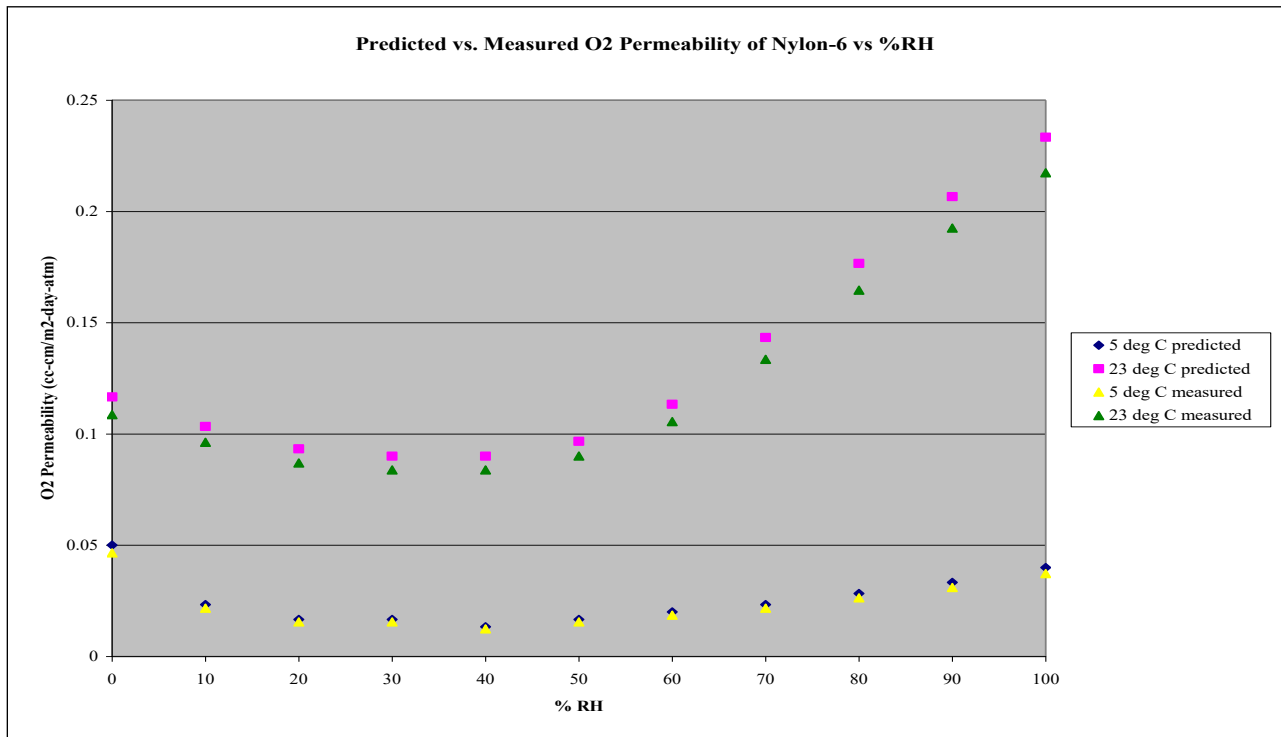
For example, CO₂ loss has been validated against polyester monolayer, barrier coated, and multilayer containers ranging in size from 250 ml to 2 liter (compared using both the FT-IR and Zahm-Nagel as the test methods). A small sample of that validation work is presented in the graph below, where the measured CO₂ shelf-life of a range of PET monolayer packages are plotted against the predicted values for those same packages.

Note: in the graph below, the measured and predicted shelf-life are plotted as x,y co-ordinates. Plotted this way, a perfect correlation would result in a least squares fit with a slope of 1.00, an intercept of 0.00, and a correlation coefficient of 1.00.

Given the intra-lab errors associated with the measured shelf-life values (often +/- 0.5 weeks, or more), we can conclude that the model results are well within the error limits of the experimental method.



A more rigorous validation of the fundamental strength of the model can be found in the graph below, which shows the model's predicted oxygen permeability of nylon-6 as a function of both relative humidity and temperature compared to measured values reported by Gavara and Hernandez.¹



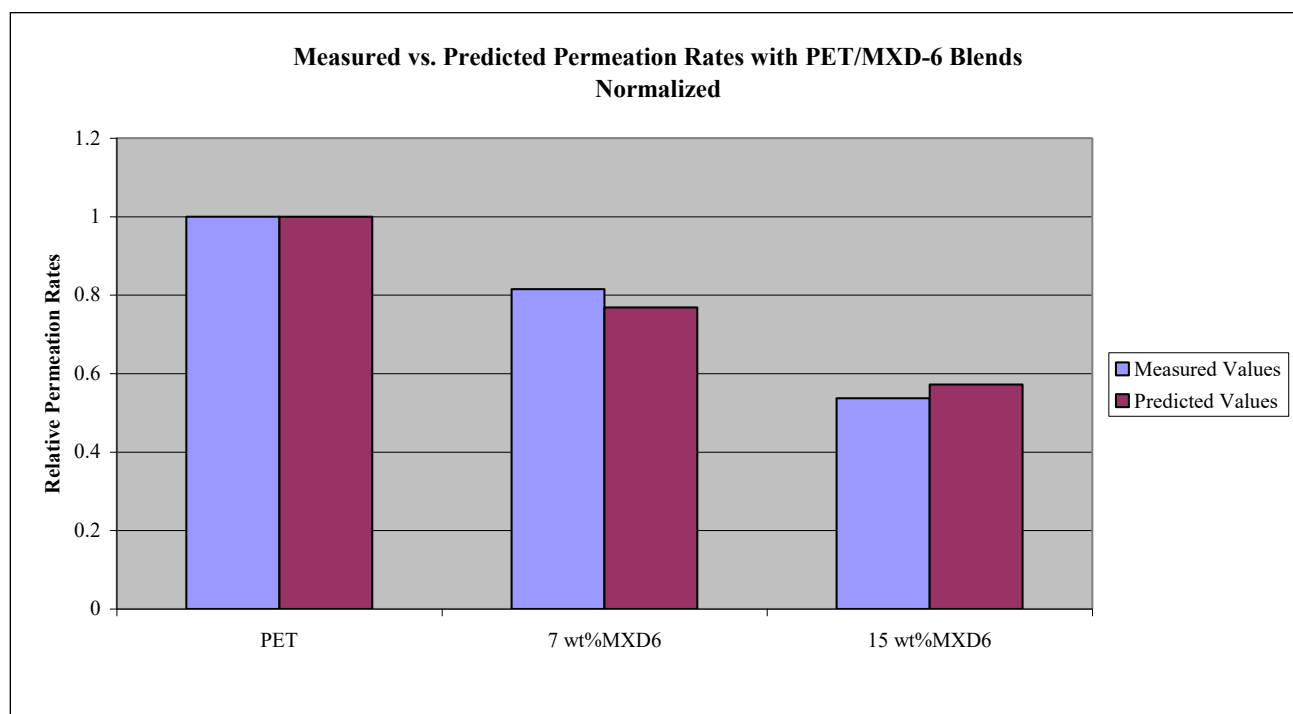
¹ Gavara, R, Hernandez, RJ. 1994. The effect of water on the transport of oxygen through nylon-6 films. J Polym Sci: Part B: Polym Phys. 32: 2375-2392.

A testament to the predictive power of the M-RULE® model is its ability to predict, from first principles, the complex non-linear impact of humidity on permeability in this system.

Another test of the validity of the model is in the mixing rules used to generate polymer blends. The graph below shows the permeation rate for PET/MXD-6 blends with different weight percent MXD-6.

In the graph below, the measured values are taken from Mitsubishi Gas Chemical Technical Report TR No. 91001-E, Tables 10 and 11. The predicted values are from the model for a package with the same wall thickness.

To facilitate comparison, both sets of values are normalized, with the respective permeation rates for PET being set to 1.0.



The model has also been validated for Vitamin C degradation and water loss. Additional validation work has shown the accuracy of the M-RULE® Model in predicting the performance of oxygen scavengers in both monolayer and multilayer constructions.

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.

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 Beverages

Bottlers, Brand Owners & Other End-Users

For bottlers, brand owners, and other end-users, the M-RULE® Container Performance Model for Beverages is a valuable tool for determining 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 Beverages is a valuable addition to your regular routine 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 end-user. 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, 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 this M-RULE® Container Performance Model. With it, you can quickly create new, cost-effective, innovative packaging with assurance 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 Beverages 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 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, you can 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 Beverages handle?

Oxygen (O₂), Nitrogen (N₂), Carbon Dioxide (CO₂), Water Vapor (H₂O), and optionally Hydrogen (H₂).

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, through 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 during stretch-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. Through 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 (as achieved in stretch-blow molding). If you are modeling an extrusion blow-molded container, you will have to modify the material to give it an appropriate orientation and crystallinity.

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, Vitamin C loss (and other oxidizable ingredients) 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 R^2 value > 0.95 . (See graphs in the earlier section entitled “Validation of the Model.”)

How precise is the model?

As is generally known, experimental accuracies/errors associated with a single traditional test of these components (CO_2 , O_2 and Vitamin C) are not insignificant. In contrast, the M-RULE® Container Performance Model for Beverages 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 these traditional test methods. And because the model calculates the actual concentrations present in the container (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, beverages, 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?

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 parameters 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? What happens to my data? Can anyone see my data?

Every time you create a blend, package, closure, beverage, scenario, 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 until you delete it.

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 the Executive Report link on the Model Results page, you will open a report that contains all of your Conditions Selection information as well as the Standard Results information. You can right-click on the report to print the Executive Report or to save a copy of the report to a file on your computer. You can also copy the report into a Word document by using Word's "select, copy, and paste" functions.

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 bottle blowing 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 notes 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 or e-mail. This high level of support is included in the subscription.

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

This model 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 M-RULE® Container Performance Model for Beverages 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 Beverages. *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

Access Options

Access to the M-RULE® Container Performance Model for Beverages is available through paid subscription or through a “per-use” basis.

Subscription Basis

When you subscribe to this model, 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 Beverages. If you have questions regarding subscriptions and terms of use, please contact:

John Maddox

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Phone: +1 904 382 8735

Fax: +1 904 379-1755

www.sba-cci.com

Per-Use Basis

[Plastic Technologies, Inc.](http://PlasticTechnologies,Inc) (PTI) is authorized to run the M-RULE® Container Performance Model for Beverages as a service for others on a per-use basis. If you have questions about this option, please contact:

Email: info@pti-usa.com

Phone: +1-419-867-5424

Fax: +1-419-867-7700

Subscriber Support

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.