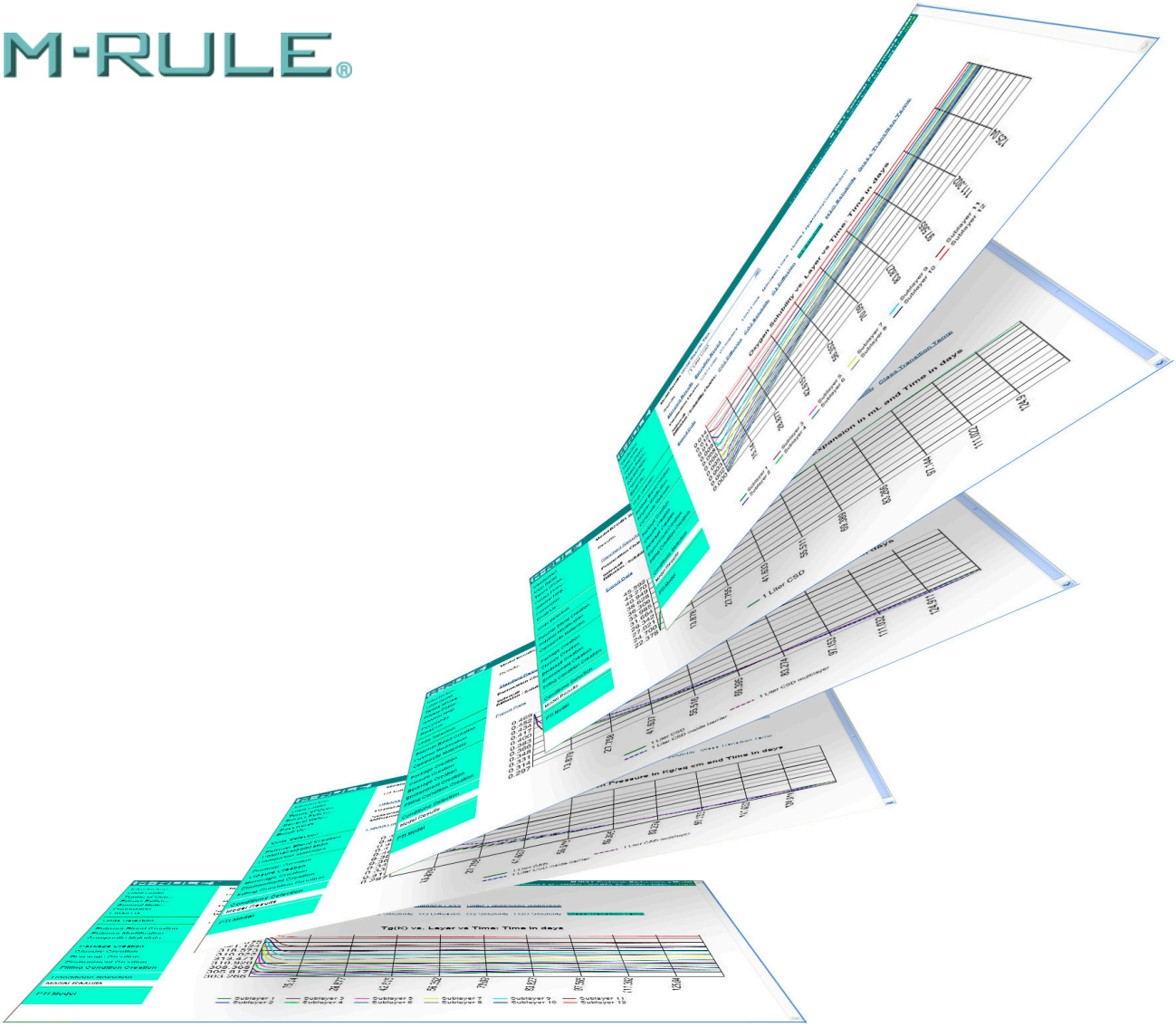
M-RULE®



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

A powerful permeation model for predicting the performance
of packaging under a broad range of environmental conditions.

V.02.15

Table of Contents

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.

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 equilibriums, 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 package finish; 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 using their computers, without first having to create physical containers. This not only saves them time and money, but also allows them to explore more packaging options.

How this model differs from other models

Most other shelf-life models used in the packaging industry are one of two varieties: they are either simple, one or two parameter empirical models with rather limited predictive capability, or they are based on detailed sectioning and analysis of pre-existing packages -- testing often more tedious and costly than performing the permeation test itself.

The empirical approach does not provide quantitative predictive capability over an extended range of package, beverage, or environmental conditions, while the testing approach inherently can only reveal the performance of a package already in production. Neither approach fulfills the need of the packaging industry for a quick, reliable, and quantitative predictive tool for package permeation performance that 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. The M-RULE® Container Performance Model fills that gap.

Typically, other 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. 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 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.

For these reasons, the M-RULE® Container Performance Model for Beverages 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 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 Explorer browser. Through this 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 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 three layers in the closure, as well as the environmental conditions and filling conditions to be simulated. The model then calculates from first principles:

1. The permeability of the specified material(s) and the package volume expansion and creep as a function of time, temperature, humidity, package materials, and container pressure;
2. The permeation of CO_2, O_2, N_2, and H_2O through that package for a program-defined time increment;
3. The change that permeation has on the beverage CO_2, O_2, N_2, and H_2O content;
4. The change (if selected) in the Vitamin C content of the beverage; and
5. The consumption of oxygen and oxygen scavenger (if selected) in either the bottle sidewall, closure, or both.

The model then iterates to the next time interval, and repeats all of the above calculations. After the model has run for the user-specified time, the model transfers the calculation results to the user's 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 download the results into Excel-readable .cvs files for further analysis.

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 Internet Explorer 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

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 that 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 and product performs 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" the model should report results in. 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 CO_2:

- The Coca-Cola FT-IR method measures the concentration of CO_2 gas inside an empty bottle, plus the amount of CO_2 dissolved in the bottle sidewall.

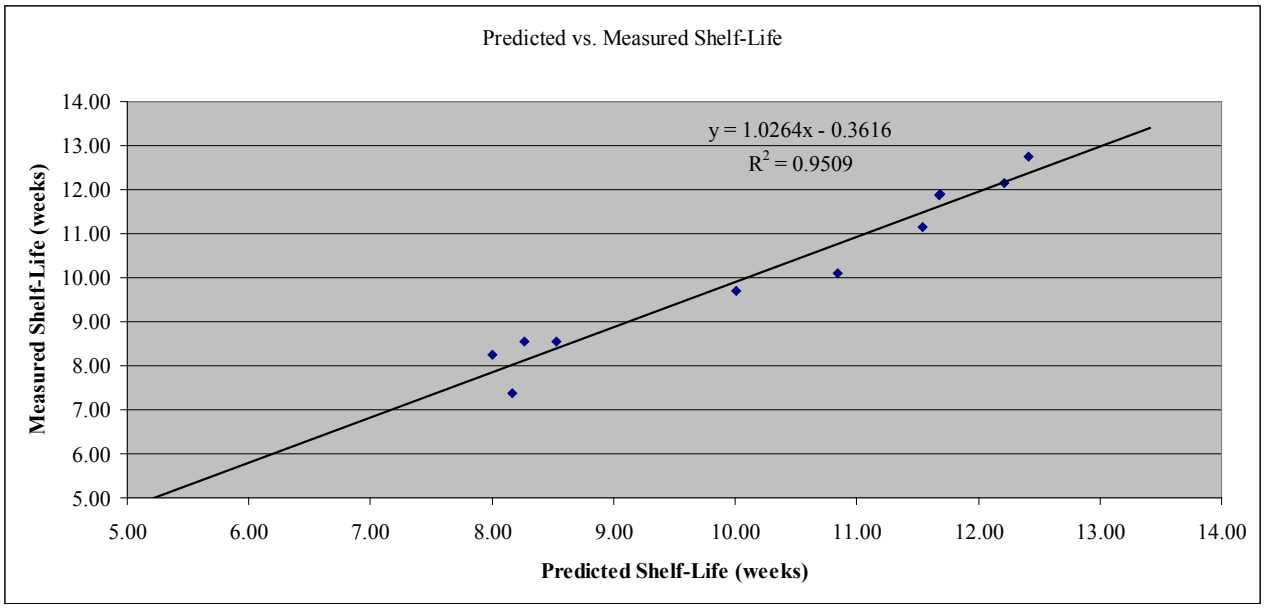
- The Zahm-Nagel test measures the pressure of gas in the headspace of a bottle, and from that is inferred the concentration of CO_2 in the beverage.
- Mocon Whole Package testing measures the rate of loss of CO_2 by measuring the rate that CO_2 reaches the exterior of the package, and from that is inferred an interior CO_2 concentration over time.
- The gravimetric method measures the total weight of CO_2 in the container and container sidewall, plus the weight of oxygen, nitrogen, and water. The gravimetric method inherently does not account for volume expansion and creep.

For CO_2, the decision was made to have the M-RULE® Container Performance Model for Beverages report the CO_2 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 contained 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.

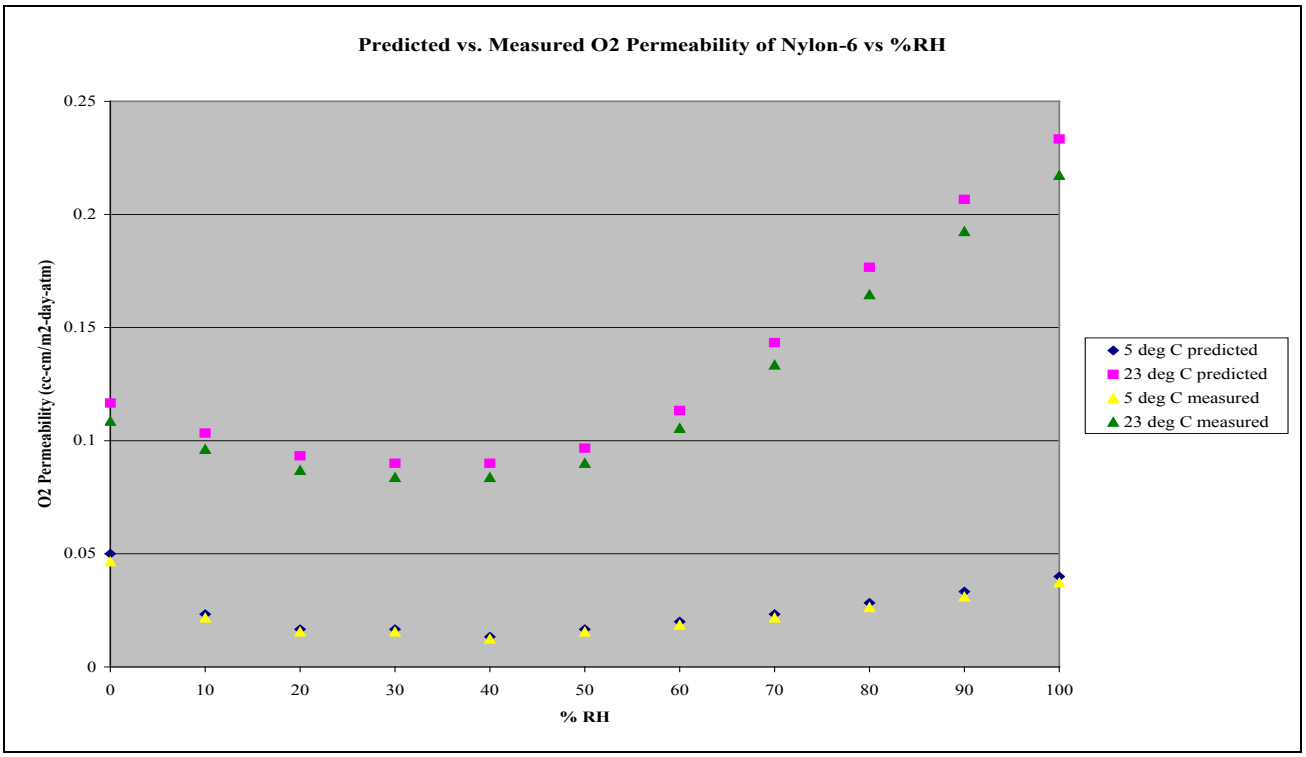
There are two important consequences of these choices. The first consequence is that the values the model reports may be different than what you have measured for your containers in the past. (Note: in the validation work, we emulated the different test methods to confirm the validity of the model.) The second consequence is you now have a "truer" 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 accuracy and robustness of this M-RULE® Container Performance Model has been established 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. For example, CO_2 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 CO_2 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.



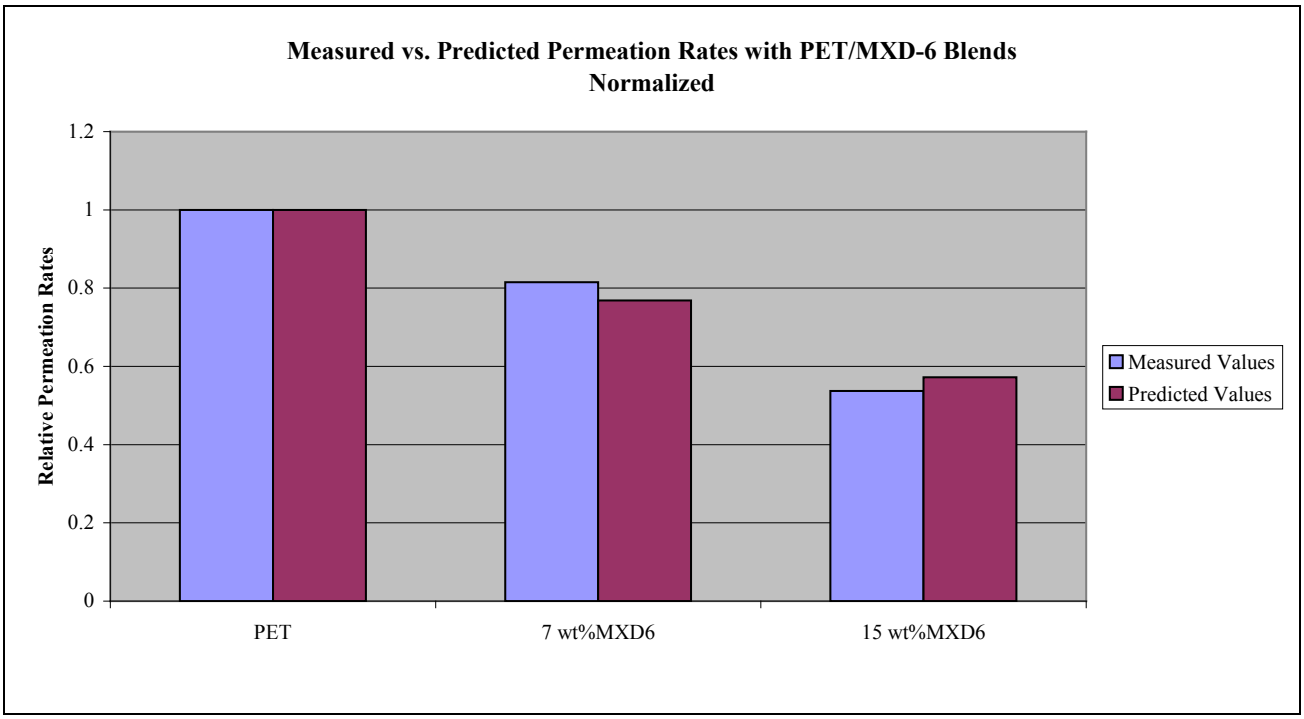
A more rigorous validation of the fundamental strength of the model can be found in the graph below, which shows the model's predicted oxygen permeability of nylon-6 as a function of both relative humidity and temperature compared to measured values reported by Gavara and Hernandez.[1]



[1] *Gavara, Rafael and Hernandez, Ruben J., "The Effect of Water on the Transport of Oxygen through Nylon-6 Films," in Journal of Polymer Science: Part B: Polymer Physics, Vol. 32, 1994, pp. 2375-2392.*

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

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 this graph, 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) 128-bit encryption -- the world's most powerful encryption technology. This applies for both domestic and export versions of Internet Explorer. SSL encrypts all information exchanged between our Web server and our clients using a unique session key. To securely transmit the session key to the client, our server encrypts it with the client's public key. Each session key is used only once during a single session (which may include one or more transactions) with a single customer.

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 located at the Peak-10 Data Center, one of the premier data centers in the southeast. Peak-10 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 rented and/or shared server space, M-RULE® resides entirely on our own state-of-the-art hardware. We use high-end industry standard Dell and Compaq 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)
- Internet Explorer 5.0 or higher (Internet Explorer is downloadable from a link on the site)
- Excel 97 or higher (for data downloading)
- Adobe Acrobat Reader (downloadable from the site)

Hardware Requirements

For the end user, the hardware requirements are also relatively straightforward. It is recommended that you have at least a 266 MHz Pentium II processor, with 64 MByte of RAM.

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

Bottlers & Other End-Users

For bottlers and other end-users, this M-RULE® Container Performance Model 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.

A second important benefit is that the model allows you to determine if your package is under- or over- engineered for a particular application -- and if it is, the model helps you determine what are the most cost-effective changes that would allow you to meet your specifications.

A third benefit is that, 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.

A fourth 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, this M-RULE® Container Performance Model 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.

A second benefit is that the model 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.

A third benefit is that the model gives you a powerful tool to use in achieving package approval by your end-user. Almost all other 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 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, 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, this M-RULE® Container Performance Model 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 also determine what research will not.

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

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 providers (SBA-CCI Inc., MXI Modeling, Inc., Polynovation, Inc., and Plastic Technologies, 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.

If you have questions regarding subscriptions and terms of use, please contact:

John Maddox
E-mail: j.maddox@sba-cci.com
Phone: +1 904 382 8735
Fax: +1 904 212 1362

Per-Use Basis

Plastic Technologies, Inc. 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:

CAE and Simulation Services
E-mail: VPSupport@plastictechnologies.com
Phone: +1-419-867-5424
Fax: +1-419-867-7700

Subscriber Support

Subscribers may contact SBA-CCI by clicking the *E-mail us* button within the model. Questions will be routed to the appropriate party.