M-RULE®

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

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

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Table of Contents

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. This 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.

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 beverage 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 this 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 CO_2 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 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 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
- 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 using their computers without first having to create physical containers. This not only saves both time and money, but also allows them to explore far 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, product, 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 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. This M-RULE® Container Performance Model for Foods 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, this 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 example, 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.

In addition, the model 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.

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, 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 that model.

Operation of the Model

The M-RULE® Container Performance Model for Foods 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(s); the closure design; the product(s); the time, temperature, relative humidity, and external pressure of the environment (up to 13 sequential intervals); 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. The model then calculates from first principles:

For the outer package:

1. The permeability of the specified material(s) and the package volume expansion, contraction, and creep as a function of time, temperature, humidity, package materials, and external and internal 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 product and headspace CO_2, O_2, N_2, and H_2O content
4. The change (if selected) in the vitamin content(s) of the product
5. The change in CO_2, O_2, and H_2O content from respiration
6. The consumption of oxygen and oxygen scavenger (if selected) in either the package sidewall(s), closure, or both
7. The change in CO_2, O_2, and H_2O content of the food

For the first inner package (if present):

1. The permeability of the specified material(s) and the package volume expansion, contraction, and creep as a function of time, temperature, humidity, package materials, and external and internal pressure (in this case the external pressure is the internal pressure of the outer package)
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 product and headspace CO_2, O_2, N_2, and H_2O content
4. The change (if selected) in the vitamin content(s) of the product
5. The change in CO_2, O_2, and H_2O content from respiration
6. The consumption of oxygen and oxygen scavenger (if selected) in package sidewall(s)
7. The change in CO_2, O_2, and H_2O content of the food

For the second inner package (if present):

1. The permeability of the specified material(s) and the package volume expansion, contraction, and creep as a function of time, temperature, humidity, package materials, and external and internal pressure (in this case the external pressure is the internal pressure of the outer package)
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 product and headspace CO_2, O_2, N_2, and H_2O content
4. The change (if selected) in the vitamin content(s) of the product
5. The change in CO_2, O_2, and H_2O content from respiration
6. The consumption of oxygen and oxygen scavenger (if selected) in the package sidewall(s)
7. The change in CO_2, O_2, and H_2O content of the food

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 calculations. 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 the maximum package volume; any initial starting temperature; and any environmental 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 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 the M-RULE® Container Performance Model for Foods, 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 encounter 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 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.

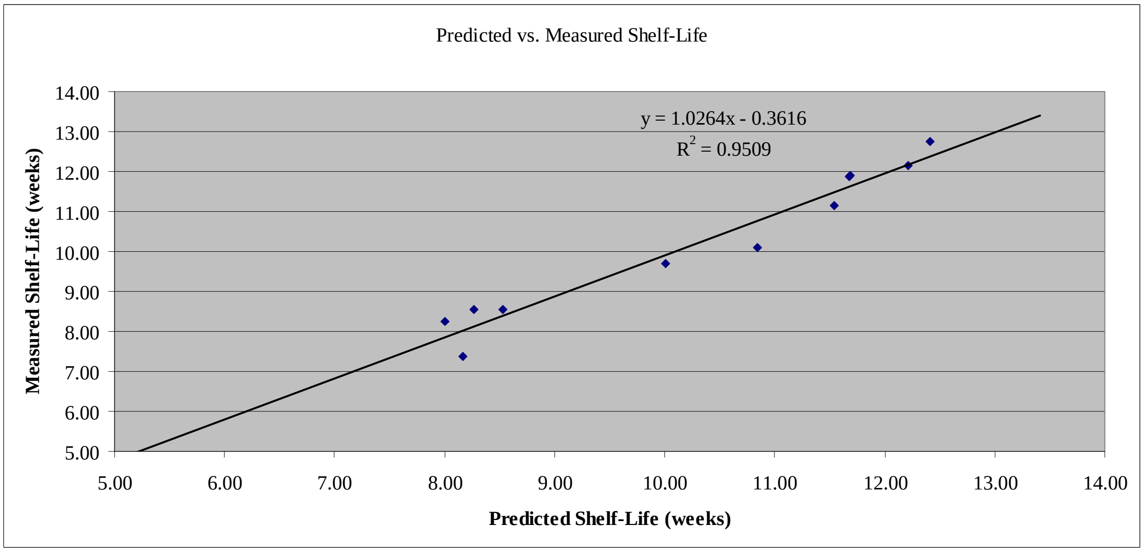
In the M-RULE® Container Performance Model for Foods, the decision was made to report both the CO_2 concentration in the food and %CO_2 in the headspace. Because of the difficulty in actually measuring gas concentrations in food products, in the model it has been assumed that the solubility of CO_2 in food will mirror the CO_2 solubility in water. The same assumption is used for oxygen. As in the model for beverages, 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 %N_2 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.

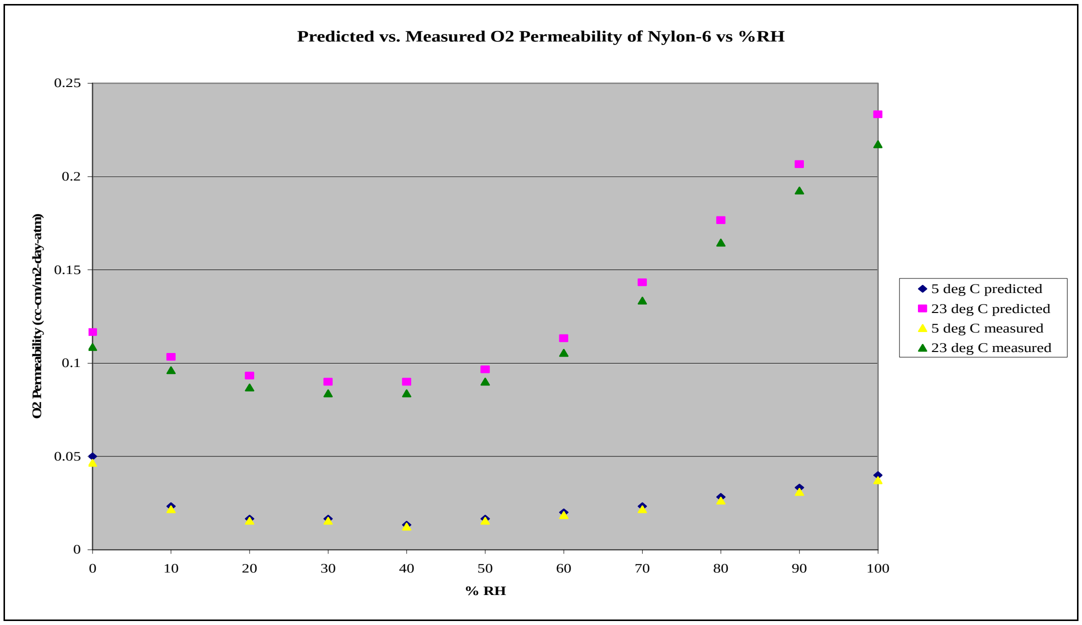
There are two important consequences of these choices. The first consequence is that the values the model reports may be different than what you have measured for your containers in the past. (Note: in the validation work, we emulated the different test methods to confirm the validity of the model.) The second consequence is you now have a "truer" 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 M-RULE® Models

The accuracy and robustness of the M-RULE® Container Performance Models have 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. 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.



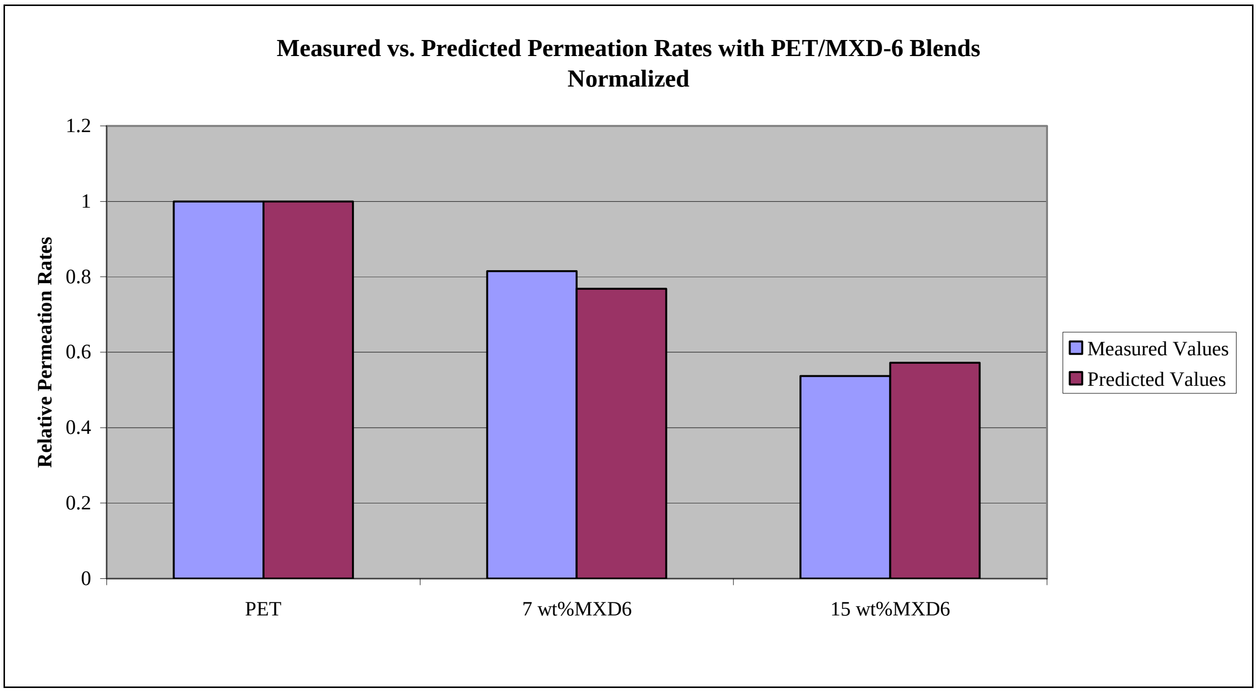
A more rigorous validation of the fundamental strength of the M-RULE® models can be found in the graph below, which shows the models' predicted oxygen permeability of nylon-6 as a function of both relative humidity and temperature compared to measured values reported by Gavara and Hernandez.[1]



[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.*

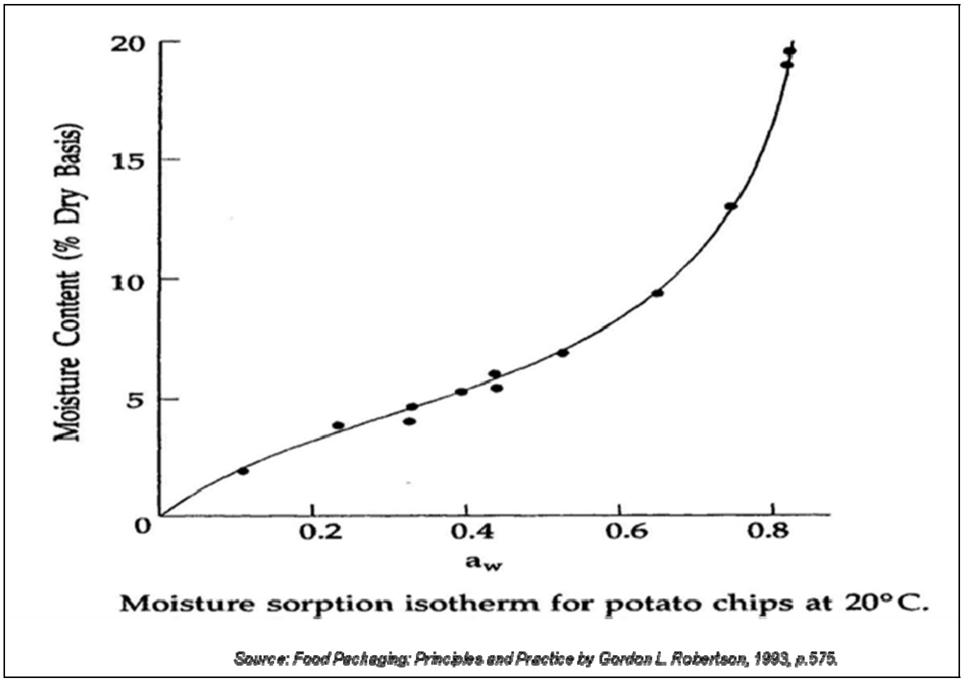
The M-RULE® models' ability to predict, from first principles, the complex non-linear impact of humidity on permeability in this system is a testament to the predictive power of the models.

Another test of the validity of the models 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 normalized to 1.0.

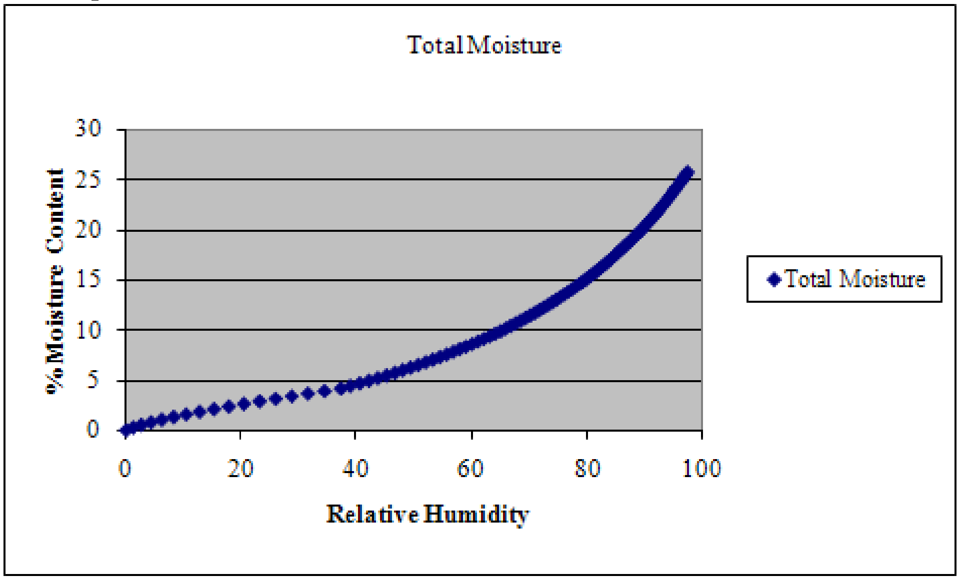


As discussed above, a first-principles prediction of moisture sorption isotherms is an important element of the M-RULE® Container Performance Model for Foods. The graphs on the next page compare the measured moisture sorption isotherm for a food (potato chips) with the model's algorithm's prediction of the same (note: a_w x 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 isotherm[2]:



M-RULE® Model prediction of moisture isotherm:



The M-RULE® Container Performance Models have also been validated for vitamin loss through oxidation. The Model for Foods allows up to two vitamins per package, each with different initial concentrations and different rates of reaction with oxygen. Additional validation work has shown the accuracy of M-RULE® models in predicting the performance of oxygen scavengers in both monolayer and multilayer constructions.

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[2] *Robertson, Gordon L., Food Packaging: Principles and Practice, Marcel Dekker, Inc., New York, 1993, p. 575.*

Security Features

Encryption

All pages of the M-RULE® applications 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 calculations) 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

Servers for the M-RULE® Container Performance Model for Foods are 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, the M-RULE® Container Performance Model for Foods 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 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.

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, 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.

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 customer. 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 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.

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 Foods 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 providers (SBA-CCI Inc., MXI Modeling, 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

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.

SBA-CCI, 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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