THE METAL PACKAGER

Building a compass for AI innovation in metal packaging coatings

February 27, 2024

(https://metalpackager.com/2024/02/building-a-compass-for-ai-innovation-in-metal-packaging-coatings/)

Cameron Brown, application research scientist, and Kuo-Hsiang Raye Chang, advanced application development scientist at Eastman's (https://www.eastman.com/en) coatings division, discuss how the company is benefiting from artificial intelligence (AI) and machine learning (ML) to develop a new class of exceptionally durable polyester resins for can coatings.

Identifying magnetic north in the can coatings industry

Metal packaging coatings are highly formulated products, used in a complex landscape that allows for various formulation combinations, combined with different types of metal substrate and curing conditions. Additionally, a variety of application testing methods are being used to mimic the experience of the coating

during can fabrication, filling, shipping and storage. Navigating this landscape and identifying the most promising formulations can be a daunting task. Sound navigation requires a reliable compass.

Compasses are rather simple devices consisting of a magnetized needle that can pivot to align itself with magnetic north. But what is magnetic north in the can coatings industry? That answer depends on where you are in the value chain. For chemical material suppliers, it can be that elusive material ingredient that brings unique adhesive or flexibility properties. For formulators, it can be a more sustainable coating that is formulated without bisphenol A (BPA) but has equivalent performance to coatings that do contain BPA. For can makers, it can be a novel can design that enables a reduction in the amount of metal used while still maintaining the structural integrity of the can.

Once you have identified your magnetic north, you can begin constructing your compass. You will need two major components to your compass: a magnetic needle that guides you towards your magnetic north, and a baseplate in which to mount that needle.

The baseplate is the foundation of your compass. It is used to build out and support the rest of your compass. Think about what sets your organisation apart. What are your core competencies? These will be key components of your baseplate. At Eastman, our baseplate consists of our long history of innovation in ester and polyester chemistry and our unique manufacturing capabilities in these areas.

The tools to design products faster

The needle in a compass is made of magnetized metal. The needle of innovation is made of a team of people working together towards a common goal. What that goal is will determine what kind of "magnetism" you will need this team to have. In general, it will consist of product and application development, manufacturing and technical service scientists and engineers working alongside dedicated marketing, sales and financial folks. Eastman invests heavily in its human magnetism, providing state-of-the-art instrumentation and access to literature and raw materials, as well as encouraging collaboration and exchange of ideas with academic and industrial partners.

Having a compass is just a stepping stone to an innovative solution. How you use and maintain that compass is also critical. We believe a strong commitment to understanding structure-process-property relationships of our target applications is vital to the long-term success of our organisation. Building these relationships

gives our scientists the tools to design new products quicker and to rapidly respond to issues facing our customers. We call this the application research mindset and have a specific team dedicated to these fundamental efforts.

Eastman's resin systems for high-performance can coatings

Utilising our compass and mindset has allowed us to create a new class of exceptionally durable polyester resins from a unique monomer called 2,2,4,4-Tetramethyl-1,3-cyclobutanediol, or TMCD. These are commonly known as Eastman Tetrashield protective resin systems for metal packaging coatings. Tetrashield resins deliver a unique balance between chemical resistance, hydrolytic stability, solubility and flexibility.

Of course, writing about how to enhance innovation in the metal packaging industry would not be complete without mentioning recent advances in AI and ML. It is well-known that to reap the true benefits of AI you need to have a well-thought-out strategy if you want to implement AI/ML in your innovation workstream.

The backbone of the Tetrashield AI infrastructure revolves around a ML model that predicts structure-process-properties relationships of unformulated polyester resin properties. This general polyester resin model acts as the foundation for individually connected application-based formulation models for specific coatings applications such as three-piece cans, full aperture and easy-open ends for food. These models help ensure formulators get the best performance from Tetrashield resins by suggesting starting point formulations faster. To date, we have seen on average a 20% reduction in the amount of experimental lab work needed to complete a project using these models. The percentage reduction in experimental resources and the percentage of time devoted to data capture/retrieval are derived from internal Eastman AI/ML projects.

Taking advantage of AI/ML models

While our internal models are created and maintained by Eastman's R&D and computer scientists, we also actively collaborate with external partners to maintain our competitive advantage. For example, in collaboration with the University of Tennessee at Knoxville we have developed a multitask ML architecture that relies on polymeric features and graph neural networks to predict polyester properties (https://www.nature.com/articles/s41524-023-01034-3). Additionally, we also work with Citrine Informatics to utilise their world-class ML models for materials science innovation. By leveraging the expertise and knowledge gained through these partnerships, Eastman is continuously improving

our ML models to better analyse and understand the resin and formulation landscape. This enables the identification of innovative solutions in a more efficient and timely manner.

We have found that the biggest bottleneck in taking advantage of AI/ML is not in building these models, but rather in locating, reformatting and validating data itself. One of the key challenges faced by research laboratories in every discipline is the collection, storage and retrieval of data. With the introduction of new test methods, materials and processes, managing and organising data has become increasingly complex. Moreover, ensuring the level of detail required for comprehensive analysis adds to the challenge. It is further compounded by the need to retrieve and access old data from files.

Altogether, these challenges constitute on average about 80% of the time and resources needed to successfully build a new AI/ML model at Eastman, regardless of whether we build that model internally or make use of an external platform. To address these challenges, automated systems are being developed to capture resin and formulation characterisation data into a standardised relational database, streamlining data management processes. Building such a database allows us to take advantage of AI/ML models and build data visualisation tools to aid in seeing what has been done and where any gaps may still be.

In conclusion, innovation is an evolving process that takes a lot of time and effort. Hiring a team of scientists is only a part of the story. If you want to do it effectively, your AI strategy must be well aligned with your overall growth strategy, and you must give your team the tools necessary to guide you through uncharted territory. Doing so can help your bottom line and help change the world in a material way.
