WHITE PAPER

Accelerate Innovation in Specialty Chemical Formulation and Development with Informatics-Derived Knowledge

Introduction

The global specialty chemicals industry, forecast to reach approximately 2.5 billion dollars by 2020,[1] is essential to innovation in industries ranging from cosmetics and construction to food and textiles. Manufacturers looking to maintain a pipeline of new and improved products that are safe and cost effective rely on specialty chemicals to improve the performance or function of their goods. It's a never-ending endeavor, with the goal of gaining market share by being fast – if not first – to market with a better solution.

According to IHS Markit, for specialty chemical companies to remain competitive, they must focus on innovation and sustainability. Rapid consumption of natural resources drives the need for sustainability, and innovation "is seen as the engine that determines progress in the sustainability area.[2]"

As value-added ingredients that give both consumer packaged goods (CPG) and industrial products their competitive edge, specialty chemicals are called on to deliver better safety profiles, regulatory compliance, and cost-to-performance ratios. To achieve the desired product-performance requirements, suppliers of specialty chemicals must have an intimate knowledge of the performance aspects that are responsible for the finished products' ultimate performance.

That knowledge comes from understanding the structure-property-performance relationship. This requires not only better experimental design and workflows, but also close collaboration among synthetic chemists and application chemists/formulators, as well as the marketers, business development personnel, and company leadership involved in new product development. Communication and information sharing must be optimized for efficient, fast development of safe and innovative consumer and industrial products.

Informatics Tools Optimize Productivity

Informatics solutions such as electronic laboratory notebooks (ELN) and data analytics platforms are the tools needed to acquire such knowledge, generate efficiencies, maintain compliance, and foster collaborations that drive productivity.

ELNs, combined with data analytics, contribute to the optimization of innovation in several ways:

- Increase the speed of innovation
- Increase the likelihood of success
- Assure the quality of the final product
- Minimize development and commercialization costs

The benefit of informatics tools is that the data streams (from molecules to formulations to properties to instrumental performance to subjective performance) can be easily compiled, grouped, sorted, and subsequently analyzed as part of the experimental process. Informatics allow a research team to get the most out of the experimental work and obtain structure-activity relationships (SAR) or structure-property-formulation-performance relationships. The informatics solutions, however, must be leveraged within an innovative experimental process.

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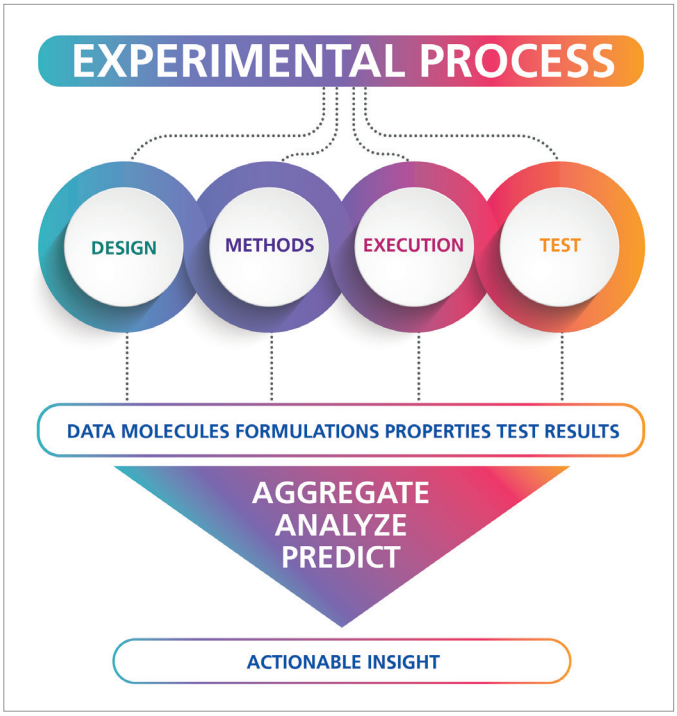

Figure 1. Materials Design Process: experimental workflow and resulting data driving decisions.

The Innovation Process

While some innovation stem from serendipitous discovery, much comes from tried-and-true processes and planning. Planning starts with business leaders working with marketing and business development teams to use customer insights to guide decisions around product development. Perhaps the competitive edge stems from a unique performance attribute, similar performance at a better price, or performance that offers a regulatory benefit. While regulatory restrictions are often initially seen as an obstacle, companies that are first to launch products that address regulatory concerns can be rewarded with increased market share.

Once product demands are identified, staff scientists, managers, and senior managers begin their planning to determine how discovery and development should be pursued. These decisions are based on:

- IP and existing competitor product landscape
- Chance for success or level of difficulty
- Expected timeframe for development work
- Regulatory and safety assessment
- Financial ROI

After this exploration and the green light is given to the project, a more detailed innovation planning process starts. This innovation process pathway begins at the experimental design stage, where new chemicals, novel polymers, and/or novel formulations are created. Next, these new chemicals, polymers, and formulations must be characterized such that their structure and composition is verified. After that, their performance is assessed, either by instrumental methods or subjective test methods. Similar synthesis procedures, analytical measurements, and performance tests can be quickly and efficiently planned using customized experiment templates in ELNs, such as PerkinElmer's E-Notebook and Signals Notebook™ solutions.

E-Notebook and Signals Notebook optimize innovation via:

- Better planning of research directions through ready access to additional information such as IP and chemical databases.
- Enhanced experimental planning by using design of experiment (DOE) and resources such as chemical property prediction and toxicity prediction.
- Access for all domains i.e. (chemistry, formulations, analytical sciences) to enable simultaneous work within an experiment.
- Better collaboration between decision makers, chemists and formulators, process and production engineers, and product testing experts as experiments and results are now accessible to all parties. Everyone can see the reasoning and decision making that goes into:
  - Work plan, experimental steps, and results.
  - Thought process and scientific/logical reasoning behind the plan and the science.
- Improved knowledge management, as record keeping of the results and methods allow for faster access to information, better and faster training of new new team members as well as more rigorous compliance management.

Types of Specialty Chemicals

Specialty chemicals can be polymeric or nonpolymeric additives used in chemical products; consumer products, such as hair and skin care, or fabric and home care goods; and industrial products from packaging materials to adhesives, inks, paints, nonwovens, and specialty coatings, or paper making and building materials.

Polymers may function as rheology modifiers or thickeners, emulsion stabilizers, binders for fibers such as paper or glass, suspending agents for particle dispersions, or surface modifiers for hair or skin conditioners and dual-use products (shampoo and conditioner in one).

Specialty polymers also include silicones that can be used to improve the strength or feel of materials, coatings for backings such as self-adhesive stamps or labels, defoamers for detergents and other products where surfactants are used and create foam. Fiber-binding polymers are used in hair sprays and paper making to create a strong hold or paper that doesn't easily tear.

Nonpolymeric specialty chemicals include surfactants, fragrance ingredients, and food additives. This includes surfactants used for emulsification and emulsion stability, foaming, cleaning or dirt removal, texture control in food and cosmetics, and film-formation in coatings.

- Enhanced communication among the research team and analytical testing groups. Test requests can be made by the research team and transferred to the analytical testing group who can post the results back directly to the sample resulting in enhanced productivity.
- Allow for knowledge development as analytical and performance data can be combined with structure information and formulation contents. Such connected data streams allow for continuous development and the optimization of structure/formulation-property-performance relationships.

What's more, E-Notebook and Signals Notebook are searchable such that information can be easily found by all team members. That data can then be analyzed using PerkinElmer's TIBCO Spotfire® data analytics and visualization platform. Interfaced to E-Notebook or Signals Notebook, it provides interactive access to the data as well as improved insight, particularly when compared to static reporting. This allows researchers to develop predictive structure-activity or structure-property-performance relationships that can generate new insights for home/fabric care, personal care, and other specialty chemical applications.

Data Analytics in Targeted Innovation

Structure/formulation-property-performance relationships are key to understanding the consumer or industrial product's performance, as well as predicting useful new chemical structures and product formulations that should be explored. The structure component of this relationship consists of novel chemical or polymer structures and/or formulations.

For instance, in the specialty chemical industry, polymer compositions and molecular weight variations are explored in order to obtain the right properties needed to achieve:

(i) Mechanical strength

(ii) Solubility in particular solvents

(iii) The right mechanical properties at elevated temperatures (glass transition related)

(iv) The right mechanical properties under various humidity conditions

(v) The desired electrical conductivity

(vi) The targeted rheology of the polymer in solution, or

(vii) A polymer with the right biodegradability profile

In the planning stages, the variables to be explored are identified, such as monomer types, monomer ratios, polymer molecular weight, extent of branching, and, potentially the degree of chemical-crosslinking. Experiment planning can be executed using software or manually by the subject matter experts. As a result, the large variety of polymer structures that can be made must be prioritized. This can be done by identifying the chemicals that are predicted to have unwanted physical properties. This filtering process can be executed using scientific software, such as TIBCO Spotfire® data visualization and analytics solution, to quickly analyze test predicted/estimated physical properties as solubility parameters, glass transition (Tg) predictors, and mechanical property predictors. This automated filtering process improves the experimental designs since it removes candidates that are very likely not going to have the desired physical properties. In addition, combining TIBCO Spotfire® with modeling applications can provide additional insight on prioritized candidates.

Another example would be the search for a surfactant that has the right combination of:

(i) Foaming behavior in the intended application

(ii) Ability to wet the surface for optimum coating efficiency

(iii) Emulsification power to create stable emulsions or to remove the right stain from a dirty fabric

(iv) The right biodegradability profile, or

(v) The right toxicity profile

Again, an experimental design is created, either by software or manually by experts, and the outcome filtered using informatics calculations to predict, properties like: logP (octanol-water partition coefficient), HLB (hydrophile-lipophile balance), foaming, type-of-emulsion predictors, endocrine disruption capability, biodegradability, activated sludge affinity, and toxicity.

Utilizing data analytics systems like TIBCO Spotfire® in the design phases optimize the discovery process, thus decreasing the innovation time as the chance for success of finding the right chemical is increased. As a result, time-to-market also decreases.

An additional benefit of the use of data analytics at the experimental design stage is that when the properties and performance tests are eventually obtained, informatics tools can be employed to correlate the chemical structures with the physical properties, their behavior in the formulations, and the ultimate performance. As such, optimized, tailored, and proprietary predictive models can be constructed for structure-property-performance or, in final products, structure/formulation-property-performance relationships to be exposed. Such relationships can be utilized for predictive purposes to:

(i) Speed up the innovative discovery process

(ii) Set performance-based specs for the new technology that allows for quality control targets for production

(iii) Troubleshoot performance issues, and

(iv) List the specifications that are essential to capturing underlying principles for inventions in future patents

Yet another area where data analytics can play an important role is the use of an ingredient database (commercial, public, or proprietary to the company) to gain information. This ranges from specific benefits of ingredients, such as the odor of fragrance ingredients; regulatory restrictions, such as for surfactants or biocides; or cost information. Such databases can be used to filter the molecule options to explore, or to weed out materials that should not be used in formulations.

Data Analytics in Formulation Management

In the specialty chemical or chemical industry in general, formulation development is as critical as the ingredients, with new chemical structures evaluated for their benefit in various consumer products. In addition to tracking the many variations' formulations, each formulation must be cleared for safety and labeling requirements and regional registration. Informatics tools employing databases of ingredients, excipients, commercially-available raw materials, and standard formulations will enable the formulators to quickly access information and make the best decisions, therefore increasing efficiency and saving evaluation time.

Signals Notebook and E-Notebook allow for the management of the entire formulation process, including experimental planning and management of materials, recipes, inventory, and formulation testing.

Leverage Informatics for Productivity

The productivity of specialty chemical innovation can be streamlined when powerful informatics solutions are introduced. Efficient planning in the early stages can be achieved with a combination of ELN and advanced data analytics, such as PerkinElmer's E-Notebook, Signals Notebook, and TIBCO Spotfire® integrated platforms, to perform experimental design , property prediction based filtering prediction, and analysis of high throughput methods. This is true especially when further filtering of the experimental options is necessary because of regulatory or cost limitations. Furthermore, an informatics-based understanding of the experimental results allow for better and continuous learning of the structure/formulation-property-performance relationships. These relationships, in turn, allow for improved performance-based specification settings of the product, as well as for the manufacturing process. As such, informatics-derived knowledge can lead to reduced and safety out-of-spec batches due to optimal quality control, reduced material waste, reduced production costs, and reduced consumer complaints.

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Global Chemical Company: Virtual Testing Optimizes High-Performance Formulations

When a global chemical company that develops innovative high-performance materials for polyurethane-based polymers needed help designing formulations to meet specific performance criteria, they turned to PerkinElmer for informatics solutions.

The company wanted to test as many variations of formulations as possible and, based on the results, decide which candidates to progress for further performance and cost evaluation.

The solution was a combination of ELN and data analytics. Using PerkinElmer's Signals Notebook, the company could create and plan experiments, create formulations, and send them for laboratory testing. Results of the tests were analyzed in TIBCO Spotfire® to identify candidate formulations with the desired performance criteria.

Further virtual exploration of formulation conditions was carried out using the PerkinElmer platform in combination with predictive analysis and expert modeling applications. This process allowed for significantly more virtual experiments to be carried out than would have been physically feasible in the lab. The virtual experiments enabled top candidate formulations to be selected for synthesis in the lab, with additional testing carried out to select the final candidate formulation. The company could also perform more analyses of performance/cost-cost/performance criteria for further optimization.

Combining Signals Notebook and TIBCO Spotfire® enabled this chemical company to virtually test formulations, significantly increasing the number of experiments – and therefore data for analysis – over actual experiments. It was able to optimize the cost of formulations with high performance, and to quickly and easily identify patterns, trends, and outliers in the large volume of test data to derive meaningful insights and identify a final candidate formulation.

Industrial Polymers: Global Data Accessibility and Knowledge Sharing Top Benefits of Informatics

With R&D and manufacturing labs spread across 20 countries, a global industrial company deployed PerkinElmer informatics to give its scientists and lab technicians full access to its treasure trove of experimental and quality data, as well as analytical capabilities to generate insights and share knowledge – furthering the company's innovation.

The company creates polymer, rubber, and organic-based products for the aerospace, automotive, and other industries. Scientists are working in both fundamental research and commercial industrialization for a variety of techniques and materials, from polymer and organics synthesis and rubber compounding to metal and textile reinforcements and tissues.

Understanding that expertise and knowledge is its strength, this company implemented PerkinElmer's E-Notebook laboratory notebook and TIBCO Spotfire® data analytics platform to create an optimal global data-gathering and knowledge-sharing environment. The informatics platform, a cornerstone of accessibility, sharing, and promotion of collected knowledge, serves the company in several key ways:

- Enhances collaboration and knowledge sharing across all global sites and functional areas
- Improves lab efficiency, particularly with more standardized workflows
- Preserves the flexibility required in R&D labs
- Harmonizes and improves the structuring of experimental results – which are then better exploited for data analytics
- Increases the speed and improves thoroughness of data analysis

E-Notebook, a core element for enterprise-wide knowledge management, delivers workflow-supporting functionality and enables this organization to store its data electronically so it can be immediately referred to and searched in the future. The solution also provides audit trail and sign-off/review functionality for IP and GMP compliance. Design of experiments can be reused, and all test results and notes are accessible. TIBCO Spotfire®, meanwhile, enables users to design their visualization dashboards to analyze datasets themselves, without seeking out IT to run reports. The platform enables fast and thorough data analysis compared to static reporting, leading to better and faster decisions, and analyses that can be broadly shared across the organization.

For more information visit www.perkinelmer.com/informatics.

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