COMMENTARY

AI-Powered Formulation Development: The Future is Here

Takeaways

AI-powered formulation enables science-based innovation to rapidly meet new market demands.

Centralized digital lab environments drive speed, agility, and collaboration in R&D.

Generative formulation and Virtual Twins improve sustainability, reduce costs, drive efficiency and speed, and enhance compliance.

Dassault Systèmes' Perfect Formulation solution, delivered by the **3D**EXPERIENCE platform, delivers comprehensive end-to-end transformation of the formulation lifecycle.

Introduction

Today's R&D organizations operate in a highly complex and rapidly evolving environment. Companies in the food, beverage, cosmetics, and other formulation-driven industries are under intense pressure to innovate faster, more sustainably, and with fewer resources. They must respond to increasingly sophisticated market demands while navigating a dense and evolving web of global regulatory requirements. Success depends on their ability to formulate and reformulate products that meet nutritional, sensory, cost, and sustainability goals—often simultaneously.[1]

CIMdata sees several global megatrends that are reshaping the current industrial landscape. Climate change and environmental degradation are forcing companies to design for sustainability from the outset. Health concerns and the rising cost of healthcare are pushing innovation toward preventative wellness. A projected global population of nearly 10 billion by 2050 will demand safe, affordable, and sustainable products at scale. At the same time, economic uncertainty, political instability, and post-pandemic volatility continue to add additional layers of complexity.

Consumer tastes and preferences are more dynamic than ever. Shoppers demand healthier ingredients, clearer labeling, ethical sourcing, and full transparency. Brands must respond quickly, accurately, and credibly, and do so while regulatory pressures continue to increase. New and evolving mandates require real-time compliance, data traceability, and increasingly detailed disclosures. These forces, combined with a shortage of digital skills and siloed data systems, leave many R&D teams struggling to keep pace.

Finally, the amount of product reformulation has dramatically increased the R&D workload. The race for innovative new products continues, while the resources needed to refresh and reformulate existing

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products across the core portfolio have skyrocketed. Ingredient shortages, cost pressures, shifting regulations, and evolving consumer preferences make reformulation a continuous necessity. This environment places R&D at the strategic center of next-generation product development and demands a fundamental rethinking of how innovation is conceived, designed, and delivered.

The Case for Digital Science-Based Innovation

The path forward lies in embracing digital, science-based innovation. Traditional R&D methods—manual, isolated, and iterative—cannot meet the demands of today's markets. Companies must transition from reactive approaches to proactive, predictive, and data-driven innovation processes. Artificial intelligence (AI) and machine learning (ML) are beginning to play a pivotal role in this transformation.

AI-powered formulation offers a smarter, faster way to design and optimize products for market readiness. It enables teams to explore a broader range of formulation alternatives, model consumer preferences, and predict how a product will perform under real-world conditions. With these capabilities, R&D can drastically reduce the need for physical experimentation, shorten development cycles, and improve first-time-right success rates.

Figure 1—AI-Powered Formulation and Simulation Accelerates Innovation
(Courtesy of Dassault Systèmes)

Generative formulation represents a breakthrough. By leveraging large volumes of historical and real-time experiment data, teams can create intelligent models that recommend optimal formulations to meet multiple target parameters. These parameters can include texture, stability, viscosity, cost, consumer liking, nutritional profiles, process, environmental impact, and others found to be critical to a company's ever-evolving fit-for-market characteristics. This approach enables knowledge capitalization and accelerates product development by leveraging powerful, data-driven models.

Virtual Twin technology not only mirrors physical objects but enables the simulation of their behavior and evolution during the life of the product. This power allows in-silico testing of formulations, packaging, and even consumer preferences. Teams can simulate different scenarios, anticipate issues early, and refine

designs without the time and cost of physical trials. With Virtual Twins, sustainability, regulatory compliance, and consumer likability can be validated virtually, long before a product reaches the physical world.

A unified digital platform can be an accelerator of such an environment. It breaks down silos across R&D, manufacturing, marketing, and compliance by enabling shared access to data and knowledge. It can speed up data collection and cleaning in order to feed AI models. Continuous learning loops then feed real-world outcomes back into the models, enhancing accuracy and insight over time. In turn, digital workflows structure and standardize processes, increasing visibility, control, and reproducibility.

Ultimately, CIMdata posits that digital science-based innovation enables organizations to accelerate time-to-market, reduce costs, increase collaboration, and deliver better, more sustainable products that will win with consumers. Compliance becomes embedded in the process, not an afterthought. The result is a leaner, smarter, and more resilient approach to product development.

Dassault Systèmes: Perfect Formulation, Enabled by the 3DEXPERIENCE Platform

Perfect Formulation is a Dassault Systèmes industry solution experience (ISE). It has been specially designed to address the modern-day challenges and needs of formulation-driven R&D organizations. Perfect Formulation provides a comprehensive, connected environment that integrates all aspects of formulation development—from ideation, development, and lab testing to regulatory compliance, packaging design, artwork creation, downstream manufacturing, and product launch in one cohesive environment.

Perfect Formulation harnesses the power of AI and predictive modeling to accelerate formulation optimization. It enables generative formulation by leveraging multi-sourced datasets to recommend formulations that meet business, technical, and consumer needs. From viscosity and texture to stability and consumer liking, all multiparameter attributes can be optimized through intelligent models. This smart capability can be used on its own or combined with broader functionality.

Beyond AI-powered formulation development, the solution enables design-for-cost strategies, helping organizations reduce sourcing costs. It integrates regulatory tools like FoodChainID to embed compliance directly into workflows, enabling real-time validation and reducing the risk of costly delays. By managing lab operations through structured workflows, Perfect Formulation can facilitate everything from sample tracking and method execution to data capture and analysis.

Perfect Formulation ensures cross-team collaboration and secures data continuity from the lab bench to downstream specification management. Structured version control and traceability support robust quality assurance and simplified audits.

As part of the **3D**EXPERIENCE platform, Perfect Formulation benefits from integration with other Dassault Systèmes capabilities. For example, this includes powerful material and ingredient science, enabling scientists to conduct multi-scale and multi-physics modeling and simulation. The Dassault Systèmes' platform enables seamless end-to-end data flows from ideation to manufacturing to commercialization.

This unified platform supports cross-functional collaboration, drives faster decision-making, and enhances the scalability of R&D operations. From artwork creation to structured specifications, from lab testing to market launch, all stages of development are aligned on a single source of truth. The solution enables openness to connect to third-party tools, expanding the solution's reach and adaptability.

Perfect Formulation, available from the **3D**EXPERIENCE platform, offers a transformative opportunity: a digital backbone for science-based innovation that is agile, intelligent, and future-ready.

Conclusion

In today's competitive and rapidly shifting market landscape, the ability to innovate quickly, sustainably, and scientifically defines success. AI-powered formulation is no longer a future vision—it is a present competitive advantage. CIMdata is impressed with Dassault Systèmes' AI-powered formulation capability and believes organizations must rethink their R&D strategies to embrace digital transformation and data-driven development.

The integration of generative AI, Virtual Twins, and centralized lab data platforms empowers R&D teams to move faster, make smarter decisions, and deliver better products. Sustainability and compliance can be embedded by design, not retrofitted under pressure. Consumer satisfaction, cost control, and speed to market can be achieved in parallel.

Dassault Systèmes' Perfect Formulation solution provides an end-to-end digital environment for transforming formulation development. It enables companies to create innovative products that meet the demands of a complex world while reducing costs, enhancing collaboration, and increasing agility.

CIMdata strongly encourages companies in formulation-driven industries—such as food, beverage, and cosmetics—to evaluate Dassault Systèmes' Perfect Formulation solution. For R&D teams tasked with achieving more with less, and for executives seeking to future-proof their innovation pipelines, CIMdata believes Perfect Formulation provides the tools, insights, and agility necessary to succeed in the race for science-based innovation.

About CIMdata

CIMdata, a global strategic management consulting firm, provides services designed to maximize an enterprise's ability to design, deliver, and support innovative products and services. For more than forty years, CIMdata has provided industrial organizations, providers of digital technologies and services, and investment firms with world-class insight, expertise, and best-practice methods on a broad set of product lifecycle management (PLM) topics and the digital transformation they enable. CIMdata also offers research, subscription services, publications, and education through certificate programs and international conferences. To learn more, visit www.CIMdata.com or email info@CIMdata.com.