CITRINE INFORMATICS

THE FUTURE OF CONSUMER PACKAGING:

DRIVING SUSTAINABILITY WITH MACHINE LEARNING TECHNOLOGIES

This white paper explores how artificial intelligence and machine learning technologies are revolutionizing the consumer packaging industry, enabling companies to meet sustainability goals while maintaining performance and cost efficiency. As regulatory pressures increase and consumer preferences shift toward eco-friendly solutions, AI-powered approaches offer unprecedented capabilities to optimize multi-dimensional packaging challenges with fewer experiments, faster development cycles, and more innovative outcomes.

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THE MULTI-DIMENSIONAL PACKAGING CHALLENGE

Today's packaging manufacturers face an increasingly complex set of challenges, balancing competing objectives like performance, sustainability, cost, and regulatory compliance. Traditional development approaches often force compromises, intensified by supply chain disruptions, fluctuating raw material costs, and stringent regulations. Growing sustainability mandates from consumers and corporate initiatives further pressure the industry to reduce environmental footprints while maintaining product integrity.

> "In learning this field, we're always told that while our goals are **faster, better, cheaper,** we'll only ever be able to get two of the three. With ML, there is now potential to get all three."
>
> – Senior R&D Scientist

COMPETING PERFORMANCE OBJECTIVES

Optimize for strength, barrier properties, weight, and cost while maintaining product integrity. These often conflict, making traditional optimization difficult.

EVOLVING REGULATORY LANDSCAPE

Tightening global chemical restrictions, like PFAS bans, demand reformulation without performance loss – a significant R&D challenge.

SUSTAINABILITY MANDATES

Corporate goals, consumer demand, and regulations drive calls for more recycled content, reduced material usage, and compostable alternatives, without compromising packaging function.

SUPPLY CHAIN VOLATILITY

Disruptions and price fluctuations require adaptable formulations and quick identification of alternative materials to ensure production continuity and cost efficiency.

These challenges cannot be effectively addressed through traditional trial-and-error or Design of Experiments (DOE) alone. The vast complexity of potential formulations makes comprehensive exploration impossible without advanced computational methods.

ACCELERATING INNOVATION WITH AI-DRIVEN APPROACHES

Traditional product development involves sequential experimentation, where each new variable significantly increases the number of time-consuming tests required. Machine learning-driven approaches accelerate this process by virtually exploring vast design spaces, allowing AI algorithms to assess millions of promising formulations that meet complex criteria simultaneously.

By predicting properties and estimating success likelihood, this computational approach allows researchers to strategically prioritize lab testing, delivering concrete business advantages.

50-80%

FEWER EXPERIMENTS

Customers achieve target properties with dramatically fewer physical experiments compared to traditional Design of Experiments or trial-and-error approaches.

2 YEARS

DEVELOPMENT TIME SAVED

AI-driven approaches can shave years off development timelines for complex reformulation projects.

MILLIONS

FORMULATIONS SCREENED

AI can evaluate millions of potential formulations virtually before suggesting optimal candidates for physical testing.

These capabilities are not theoretical. Leading companies in consumer packaging have implemented AI-driven development and achieved remarkable results, especially for challenges like PFAS elimination while maintaining performance.

A SELECTION OF OUR CUSTOMERS DEVELOPING MATERIALS OR ADHESIVES FOR PACKAGING

TerraSafe Materials LYB LyondellBasell Braskem ARKEMA

CASE STUDY: REMOVING PFAS IN ADHESIVES

THE CHALLENGE

A global materials conglomerate faced a critical business challenge: reformulating their entire pressure sensitive adhesive product line to eliminate PFAS (per- and polyfluoroalkyl substances) while maintaining mechanical performance. Traditional approaches would have required years of incremental testing across thousands of potential formulations, threatening their competitive position and regulatory compliance timeline.

THE PROCESS

MONTH 1

Trained internal team on AI platform, rapidly achieving autonomy and establishing model parameters.

MONTH 3

Screened millions of potential formulations computationally, narrowing to 30 viable candidates for physical testing.

MONTH 4

Identified breakthrough candidate formulation meeting all performance criteria without PFAS compounds.

MONTH 6

Team expanded capabilities with 25 user models, quadrupling projects and platform utilization.

THE OUTCOME

Successfully reformulated their product line to exclude PFAS, saving **2 years** of R&D work on a 5-year project timeline while maintaining all performance characteristics.

CASE STUDY: REMOVING PFAS IN ADHESIVES

KEY IMPLEMENTATION INSIGHTS

The success of this project hinged on several critical factors that can be applied across various packaging innovation challenges:

DATA INTEGRATION

The team leveraged existing experimental data, combining historical results with domain expertise to create robust initial models.

CLEAR CONSTRAINTS

Precise definition of performance requirements and material constraints enabled focused exploration of viable alternatives.

ITERATIVE APPROACH

Rather than seeking a perfect solution immediately, the team used an iterative process where each round of testing improved model accuracy.

CONVERGENT INTELLIGENCE

Integration of materials science expertise with data science capabilities accelerated the identification of non-obvious formulation opportunities.

This case demonstrates how AI-driven approaches can transform seemingly intractable formulation challenges into manageable projects with predictable timelines and outcomes. The same methodology can be applied to numerous packaging innovation challenges, from biodegradable barrier films to lightweighting initiatives.

MULTI-LAYER PACKAGING OPTIMIZATION: A PRIME AI APPLICATION

Multi-layer packaging is a prime application for AI-driven development. These complex structures combine various materials to achieve specific barrier, mechanical, and aesthetic properties. AI approaches excel at systematically navigating the inherent trade-offs often found in traditional development, allowing for optimal solutions across competing objectives like recyclability and cost.

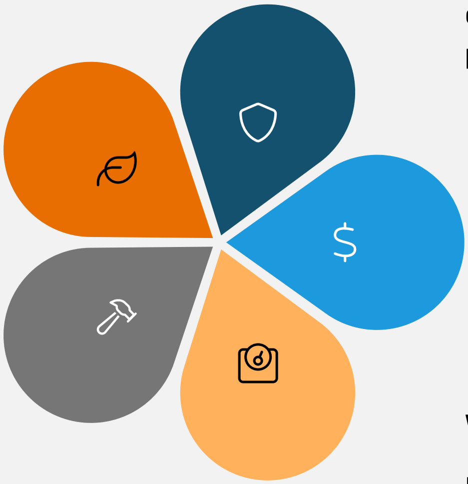
BALANCING COMPETING OBJECTIVES

BARRIER PROPERTIES

Ensuring effective protection against moisture, oxygen, light, and contaminants throughout the product lifecycle

BIODEGRADABILITY

Meeting consumer and regulatory demands for environmentally friendly end-of-life options while maintaining product protection



PRODUCTION COST

Optimizing material selection and processing parameters to maintain commercial viability and competitive pricing

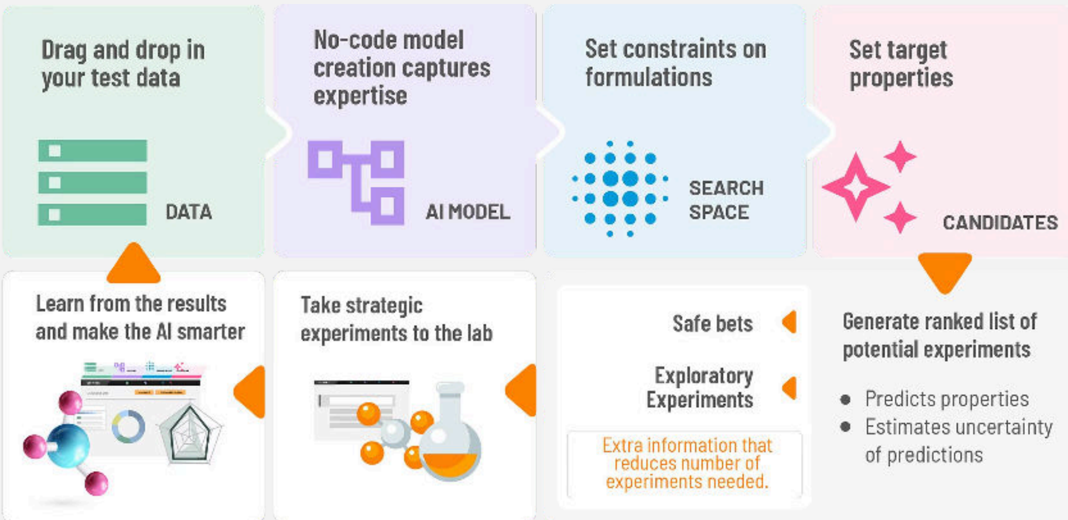
MECHANICAL STRENGTH

Ensuring durability throughout the supply chain, preventing product damage, and maintaining consumer experience

WEIGHT REDUCTION

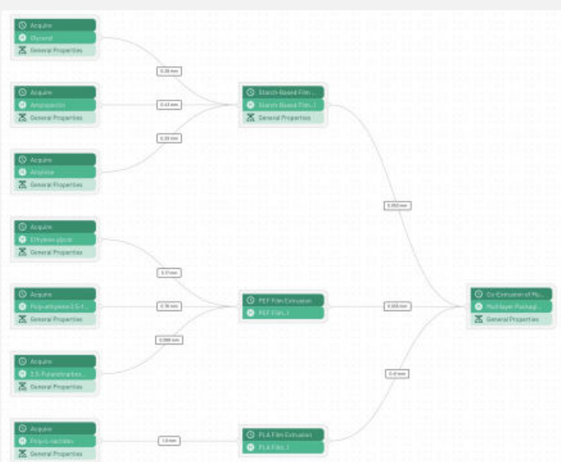
Minimizing material usage to reduce transportation costs and environmental impact without compromising structural integrity

IMPLEMENTATION APPROACH



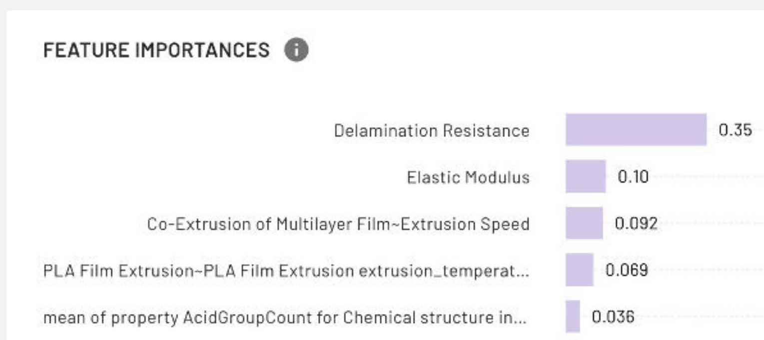
The chemically-aware, no-code Citrine Platform allows packaging engineers to evaluate thousands of potential material combinations, layer configurations, and processing parameters using fewer experiments. The result is faster development cycles, more innovative solutions, and packaging that more effectively balances multiple competing objectives.

DATA STORED IN INTERACTIVE PROCESS DIAGRAM

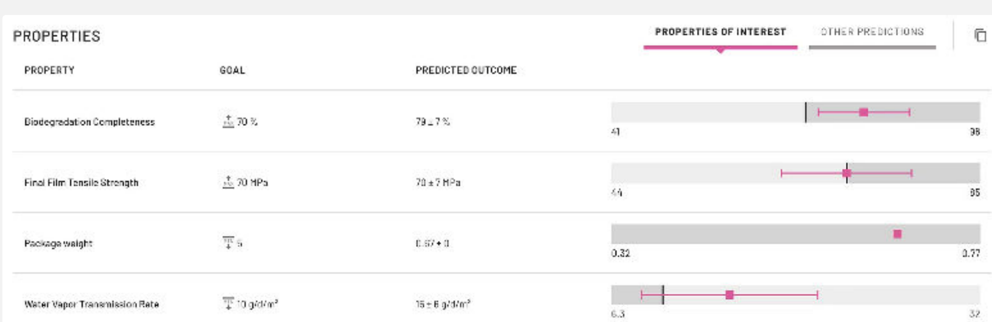


AI MODEL PROVIDES INSIGHT

Factors important for each prediction are shown. In this case Biodegradation completeness is strongly related to delamination resistance.



FOR EACH PROPOSED CANDIDATE MATERIAL PROPERTY PREDICTIONS COME WITH ERROR BARS



PROPERTY	GOAL	PREDICTED OUTCOME	
Biodegradation Completeness	70 %	79 ± 7 %	41 – 98
Final Film Tensile Strength	70 MPa	70 ± 7 MPa	44 – 85
Package weight	5	0.67 ± 0	0.32 – 0.77
Water Vapor Transmission Rate	10 g/d/m²	15 ± 6 g/d/m²	6.3 – 32

STRATEGIC RECOMMENDATIONS FOR AI ADOPTION

AI-driven development offers a significant competitive edge for packaging and consumer goods companies. Successful adoption requires a strategic approach aligned with organizational size and objectives.

SMALL COMPANIES

- Use AI to reduce research costs and compete effectively.
- Leverage AI to focus on niche applications.

MEDIUM-SIZED COMPANIES

- Leverage agile decision-making to rapidly test and scale AI.
- Identify high-ROI initial projects.
- Define clear success metrics.

LARGE COMPANIES

- Utilize extensive historical data.
- Apply transfer learning across products and teams.
- Establish centers of excellence.

KEY SUCCESS FACTORS

1 CLEAR BUSINESS OBJECTIVES

Focus AI initiatives on specific, measurable challenges with high business impact (e.g., PFAS replacement, weight reduction).

2 INTEGRATE DOMAIN EXPERTISE

Involve materials scientists and engineers in model development and validation for industry-specific knowledge.

3 ITERATIVE PROCESSES

Continuously improve models and experimental results by testing little and often.

4 MEASURE AND COMMUNICATE VALUE

Track metrics like development time reduction and successful innovations to quantify ROI and build support.

CONCLUSION

The future of consumer packaging hinges on balancing performance, sustainability, and cost. AI offers powerful tools to navigate this, enabling faster innovation and efficient resource use. Organizations embracing AI today will gain significant competitive advantages as market pressures evolve.

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