TRANSFORMING CUSTOMER RESPONSIVENESS

WITH AI-DRIVEN TECHNICAL SERVICES

In today's rapidly evolving chemicals industry, the ability to respond quickly and accurately to customer demands separates market leaders from followers. As brands increasingly demand sustainable, bio-based alternatives without compromising performance, technical service teams face mounting pressure to **deliver innovative solutions faster** than ever before. Traditional formulation development processes—characterized by time-consuming iterative testing, lengthy stability studies, and trial-and-error experimentation—can no longer keep pace with market demands.

This white paper explores how artificial intelligence is fundamentally transforming the formulation development landscape, enabling chemicals suppliers to achieve unprecedented levels of customer responsiveness while simultaneously reducing development costs and accelerating time-to-market. Through platform-based AI modeling, companies can now create **reusable predictive assets that empower technical service teams** to rapidly evaluate formulation alternatives, predict performance outcomes, and confidently recommend optimized solutions to customers in days rather than months.

APPLICATION MODELS: CREATING REUSABLE AI ASSETS FOR CUSTOMER SUCCESS

The paradigm shift enabled by AI-driven formulation platforms centers on a fundamental concept: transforming experimental data and domain expertise into reusable predictive models that can be rapidly deployed across multiple customer scenarios. Unlike traditional one-off development projects where knowledge remains siloed in lab notebooks and individual scientists' experience, application models become organizational assets that compound in value with each use and can be leveraged across the team.

CREATING AN APPLICATION MODEL

01

BUILD THE FOUNDATION

Historical experimental data, ingredient properties, and process parameters are structured and stored in a centralized platform.

02

TRAIN PREDICTIVE MODELS

Machine learning algorithms identify patterns and relationships between formulation inputs and performance outcomes.

03

DEFINE SEARCH SPACES

Constraints around allowable ingredients, concentrations, and processing parameters ensure recommendations are commercially viable.

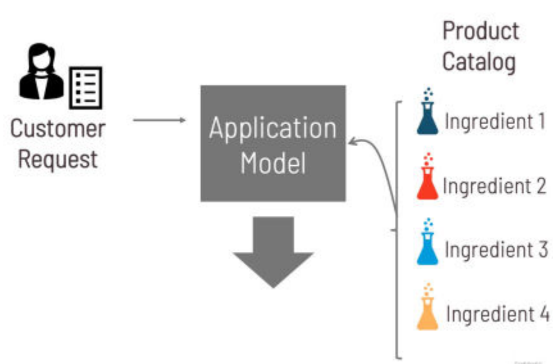
04

DEPLOY FOR CUSTOMER RESPONSE

Technical service teams leverage application models to rapidly evaluate alternative ingredients and generate data-backed recommendations.

DEPLOYING AN APPLICATION MODEL

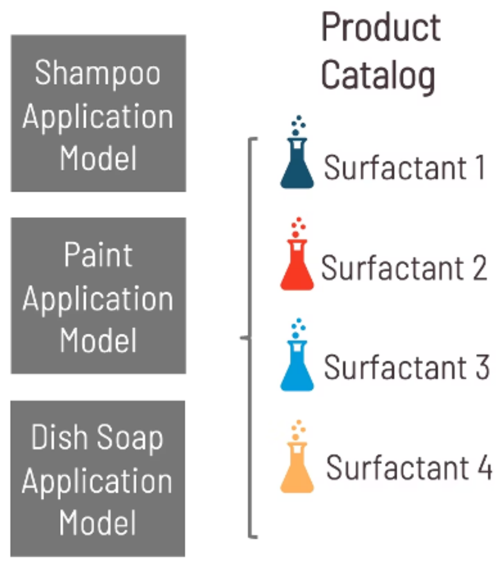
This approach transforms the economics of customer technical service. Models created for one customer project become immediately applicable to future requests. When another customer approaches with similar but distinct requirements, technical teams can simply adjust the targets and constraints within the existing model framework, **generating new recommendations in hours** rather than starting from scratch. This reusability creates a multiplicative effect on ROI, as each model becomes more valuable with each subsequent application.



RESPONSE

- Which product will perform best
- What quantity
- How much does it cost
- What performance can it achieve

> *"**I'd love to have 10 of these projects going.** I want more application data to drive deeper conversations around subjects our customers care about."* - Stepan Business Manager



Multiple application models can be connected to the product catalog

THE CUSTOMER CHALLENGE: BALANCING SUSTAINABILITY WITH PERFORMANCE

REAL-WORLD SCENARIO

Consider a typical request faced by surfactant suppliers today: a major shampoo brand needs to reformulate a popular product with plant-based surfactants to meet growing consumer demand for natural ingredients. However, the reformulation must maintain critical performance parameters that consumers expect.

Non-negotiable requirements include:

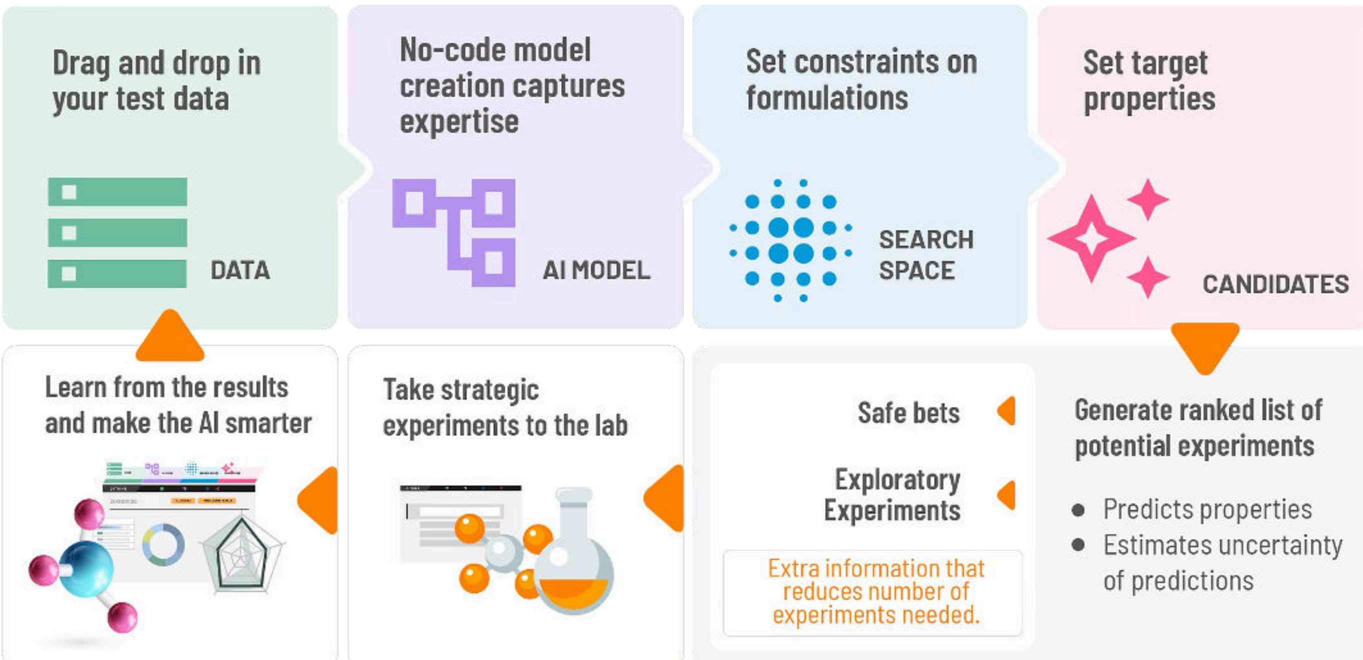
- Maintaining viscosity within established specifications
- Preserving the product's rheology profile
- Ensuring long-term formulation stability
- Matching or exceeding current performance benchmarks

The challenge for the surfactant supplier becomes clear: which plant-based surfactant will perform optimally in this specific formulation matrix, and at what concentration should it be used? Traditional approaches would require extensive experimental design, multiple testing cycles, and weeks or months to reach confident recommendations.

The Stakes: Delayed responses to reformulation requests can result in lost business opportunities, while rushed recommendations without adequate testing risk product failures and damaged customer relationships.

STEP 1 - CREATE THE APPLICATION MODEL

Using your historical data and understanding of your customer's formulation and requirements, create a model to predict the properties specified in the customer request - in this case, viscosity, rheology type, stability and cleaning power. Run experiments to improve the accuracy of the model and validate its predictions.



DATA INTEGRATION

Upload historical experimental data including ingredient compositions, processing parameters, and measured properties. Ensure ingredients in your product catalog are well characterized.

MOLECULAR CHARACTERIZATION

Chemical structures converted to SMILES strings enable computation of 127+ molecular descriptors.

MODEL TRAINING

AI algorithms identify patterns linking ingredient properties and molecular features to performance outcomes.

MODEL REFINEMENT

If a customer request is pushing the boundaries of what is currently possible, a couple of small batches of experiments might be needed.

STEP 2 - FROM DATA TO INSIGHTS

COMPREHENSIVE PROPERTY TRACKING

For each ingredient in the model dataset, the platform captures:

- **Molecular structure** encoded as SMILES strings for computational analysis
- **Physical properties** including molecular weight, density, and solubility parameters
- **Chemical characteristics** such as functional groups and reactive sites
- **Performance attributes** relevant to specific application areas

Simultaneously, measured properties of final formulations are systematically recorded, creating a rich dataset that links molecular inputs to performance outputs. This bidirectional data capture—from molecular features through formulation composition to final properties—enables the AI to identify subtle structure-property relationships that might escape human observation.

GENERAL PROPERTIES

MEASUREMENT TEMPLATE

Properties

PROPERTY	RUN	UNITS	SPEC	UNITS
Viscosity Category	HIGH			
Rheology_Type	OTHER			
Viscosity at Zero Shear Rate	4528	MPa·s		
Log10 - Viscosity at Zero Shear Rate	3.7			

SHAMPOO FINAL PROPERTIES STORED

By representing molecular structures as SMILES (Simplified Molecular Input Line Entry System) strings, the platform automatically computes over 127 molecular descriptors that capture key structural features, functional group characteristics, and physicochemical properties.

INGREDIENT PROPERTIES STORED

GENERAL PROPERTIES

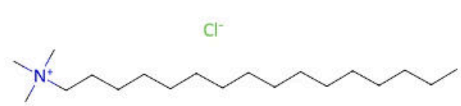
MEASUREMENT TEMPLATE

Properties

PROPERTY	RUN	UNITS	SPEC	UNITS
Hydrophilic - COOH	0			
Hydrophilic - N+	1.0			
active_matter in percent	25			
Hydrophilic - Cl-	1.0			
Hydrophilic - Na+	0			
Hydrophilic - SO3^-	0			
Price in Dollars per lb	20			
Hydrophilic - Ether - O	0			
water_content in percent	75			
Hydrophilic - OH	0			
Alkyl Chain Length	16			
Griffin Method HLB Values	8.8			
Hydrophilic - NH	0			
Lipophilic - Alkyl CH2/CH3	16			
Hydrophilic - K+	0			

STRUCTURAL FORMULAS

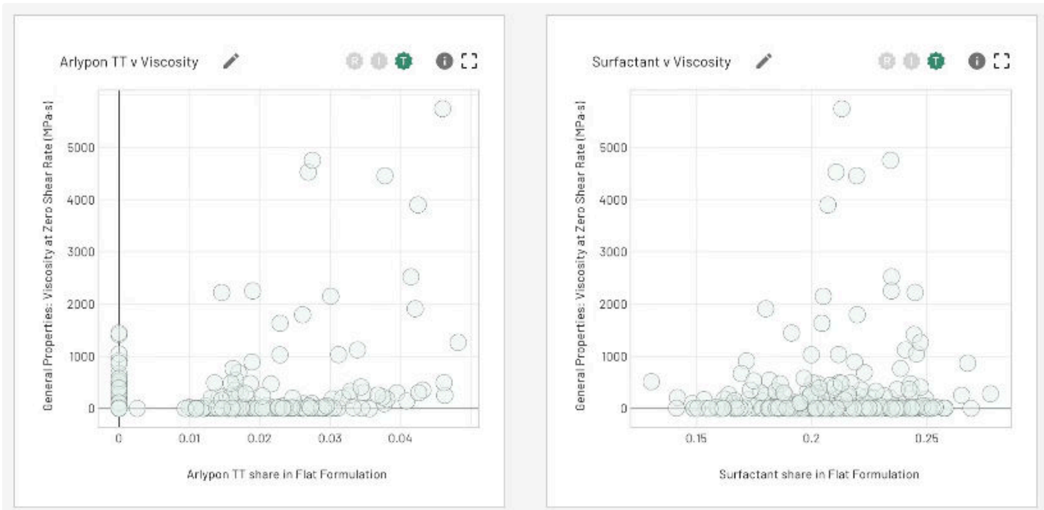
CCCCCCCCCCCCCCCC[N+](C)(C)C.[Cl-]



The predictive capability of AI-driven formulation platforms stems from their ability to connect molecular structure with macroscopic performance—a relationship that has traditionally resided in the tacit knowledge of experienced formulators.

DATA VISUALIZATION AND PATTERN RECOGNITION

One of the most immediate benefits of platform-based formulation development is the ability to visualize complex relationships within experimental data. Traditional spreadsheet-based approaches struggle to reveal multi-dimensional patterns, while AI platforms automatically generate insightful visualizations that accelerate understanding and hypothesis generation.



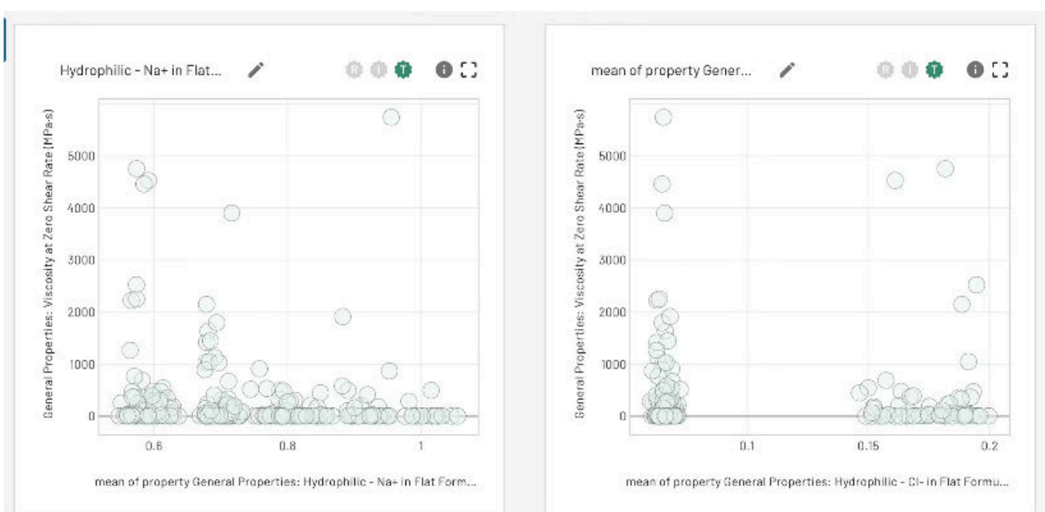
Consider the relationship between surfactant concentration and viscosity in the shampoo formulation example. Platform visualization immediately reveals a non-linear relationship: viscosity rises steadily as surfactant share increases to approximately 22%, then unexpectedly decreases at higher concentrations. This insight—which might require extensive manual plotting and analysis to uncover—becomes immediately apparent through automated data exploration.

TREND IDENTIFICATION

Automatically detect non-linear relationships and optimal operating windows across multiple variables simultaneously.

CORRELATION ANALYSIS

Reveal unexpected connections between molecular features, process parameters, and performance outcomes.



These visualizations serve multiple purposes: they accelerate initial understanding of formulation behavior, support quality control by identifying anomalous results, facilitate communication between R&D teams and business stakeholders, and ultimately build confidence in the AI models by demonstrating their foundation in real experimental data.

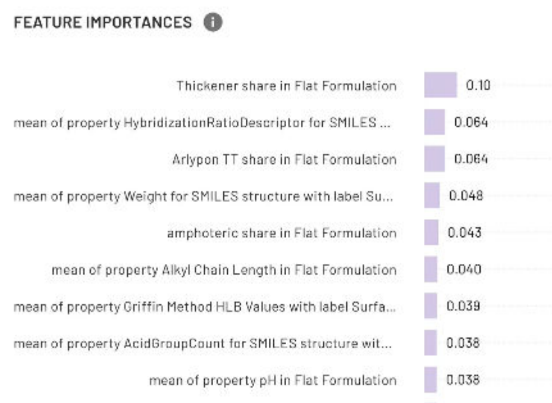
STEP 3 - CHECK THE MODEL AND LEARN FROM IT

FEATURE IMPORTANCE ANALYSIS

A critical concern when adopting AI for technical decision-making is the perceived "black box" nature of machine learning algorithms. Advanced platforms address this concern head-on through comprehensive interpretability features, particularly **feature importance analysis** that reveals which factors most strongly influence predicted outcomes.

When predicting formulation stability, for example, the platform ranks the relative importance of various inputs—ingredient molecular descriptors, concentration ranges, process parameters, and interaction effects. This transparency serves multiple essential functions for R&D leadership:

- **Validation:** Expert formulators can verify that the AI is weighting factors consistently with established chemical principles
- **Discovery:** Occasionally, the analysis reveals unexpected factors that influence performance, leading to new insights
- **Confidence:** Understanding model reasoning builds trust
- **Improvement:** Feature importance guides targeted data collection to strengthen model predictions



> "We understand our own laboratory more than before. It's fun to work in this way."
>
> *— Oliver, Technical Application Lead, Dorfner*

TRANSPARENCY AND TRUST: AI AS A FLASHLIGHT, NOT A BLACK BOX

The metaphor of a "flashlight in a dark room" perfectly captures the value proposition: AI doesn't replace human expertise—it amplifies it by illuminating patterns and relationships that would otherwise remain hidden in complex, multi-dimensional data spaces. This augmentation of human capability, rather than replacement, represents the true promise of AI in formulation development.

STEP - 4 STRATEGIC SEARCH SPACES

Search spaces—structured sets of constraints that bound the universe of possible formulations to those that are technically feasible, commercially viable, and regulatory compliant.

INGREDIENT CONSTRAINTS

Specify allowable ingredients, including required substitutions (plant-based surfactants) and exclusions (parabens, sulfates). Multiple search spaces can accommodate regional regulatory variations.

CONCENTRATION BOUNDS

Set minimum and maximum concentrations for individual ingredients and ingredient classes to ensure formulation.

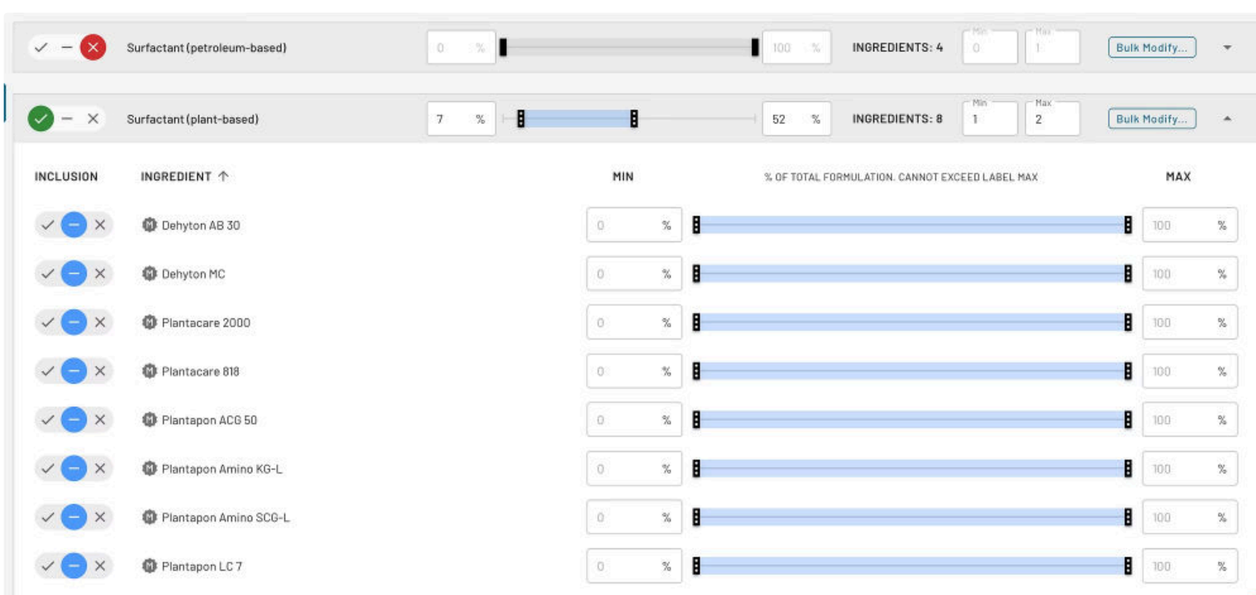
PROCESS PARAMETERS

Define acceptable ranges for mixing conditions, temperature profiles, pH adjustment protocols, and other manufacturing variables.

PRACTICAL EXAMPLE: SHAMPOO REFORMULATION

For the plant-based shampoo project, the search space includes:

- All plant-based surfactant alternatives in the supplier's portfolio
- Maximum of 10 total ingredients (formulation simplicity)
- Exclusion of parabens and sulfates (clean label requirements)

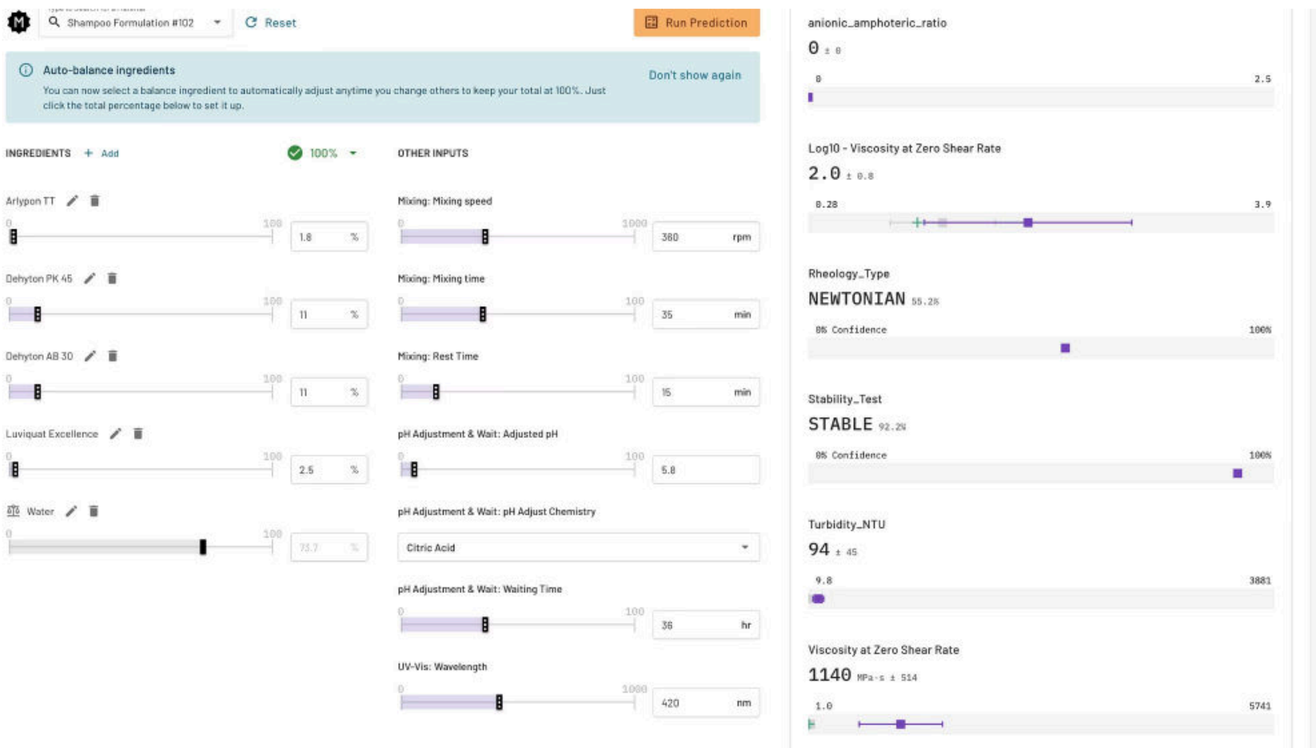


STEP 5 - SET TARGETS AND RUN MODEL

Upon receiving a customer request, the technical services team can leverage the Citrine Platform to:

A: MODEL EXPLORE - QUICK PROPERTY PREDICTIONS

Utilize ***Model Explore*** to predict the properties of new formulations. For instance, with plant-based surfactants substituted for previous petroleum-based ones, the model can be run to assess if the proposed formulation is expected to remain stable and exhibit appropriate viscosity.



B: AI-GUIDED EXPERIMENTATION FOR NEW FRONTIERS

Should a request push the boundaries of current capabilities, leading to high uncertainty in model predictions within that specific region of the search space (due to limited prior experimental data), the platform can address this. In such cases, the customer's desired properties are set as targets, and the AI model is run over the appropriate search space to generate suggested experiments. These experiments are designed either to meet the targets, show promise for future development, or strengthen the predictive power of the model in the area requested by the customer. Once these experiments are conducted, and the model is retrained and improved, it can then provide precise recommendations on optimal surfactant performance, recommended quantities, and the achievable technical performance for the given surfactant.

PROVEN RESULTS: INDUSTRY CASE STUDY DEMONSTRATES TRANSFORMATIVE IMPACT

The theoretical advantages of AI-driven formulation development translate into concrete business outcomes across the chemicals and consumer products industries. A representative case study illustrates the versatility of the platform approach.

STEPAN COMPANY: SCALING AI ACROSS MULTIPLE PROJECTS

Stepan® is a global specialty and intermediate chemical supplier of chemical ingredients and formulations. They initially piloted AI-driven formulation development for a liquid dishwash project. The business manager's enthusiastic response—"I'd love to have 10 of these projects going"—reflects the platform's ability to drive deeper technical conversations with customers while simultaneously improving internal efficiency. The reusable model framework enables Stepan to rapidly respond to diverse customer reformulation requests, transforming technical service from a cost center into a competitive differentiator.

LIQUID DISHWASH FORMULATIONS

Models, datasets, and search spaces become reusable assets for similar projects

CROP PROTECTION FORMULATIONS

Predict surfactant stability and appearance for customer applications

SPRAY FOAM FORMULATIONS

Improved polyol formulations for spray foam insulation

> *"**I'd love to have 10 of these projects going.** I want more application data to drive deeper conversations around subjects our customers care about."* - Stepan Business Manager for the Liquid Dishwash Project

THE PATH FORWARD: ACCELERATING YOUR MATERIALS INNOVATION JOURNEY

STRATEGIC IMPERATIVES FOR R&D LEADERSHIP

For R&D directors and technical service leaders evaluating this opportunity, several strategic considerations merit attention:

1. **Platform thinking:** Approach AI adoption as building reusable assets, not executing one-off projects
2. **Data readiness:** Begin organizing historical experimental data to maximize near-term ROI
3. **Cultural preparation:** Foster organizational openness to AI-augmented workflows and decision-making
4. **Pilot selection:** Identify high-value customer relationships where enhanced responsiveness creates competitive advantage
5. **Expertise partnership:** Leverage vendors with proven implementation experience to accelerate adoption

RESPOND QUICKER

Transform technical service from reactive problem-solving to proactive solution delivery, winning business through superior responsiveness.

ADOPT EASILY

Platform architecture integrates with existing laboratory workflows and data systems, minimizing disruption during implementation.

TRUST EXPERIENCE

Partner with teams possessing a decade of proven success rolling out AI across chemicals and materials organizations.

READY TO ACCELERATE YOUR MATERIALS INNOVATION?

Discover how Citrine Informatics can transform your application engineering processes, and drive measurable commercial success.

Contact us to explore how AI can revolutionize your technical service capabilities: info@citrine.io