STEPAN'S JOURNEY WITH CITRINE INFORMATICS

– ACCELERATING CUSTOMER WINS THROUGH PLATFORM MODELING

Stepan S.

EXECUTIVE SUMMARY

- ▮ TECHNICAL TARGETS SURPASSED IN THREE ROUNDS OF EXPERIMENTS

- ▮ PLATFORM MODELS ENABLE IMPROVED CUSTOMER RESPONSIVENESS AND WIN CONTRACTS

- ▮ SURFACTANT INTERACTION INSIGHTS ARE INVIGORATING THE TEAM

CUSTOMER

Stepan® is a global specialty and intermediate chemical supplier of chemical ingredients and formulations. It produces surfactants, polymers, and specialty products used in industries such as cleaning, personal care, agriculture, and rigid foam insulation.
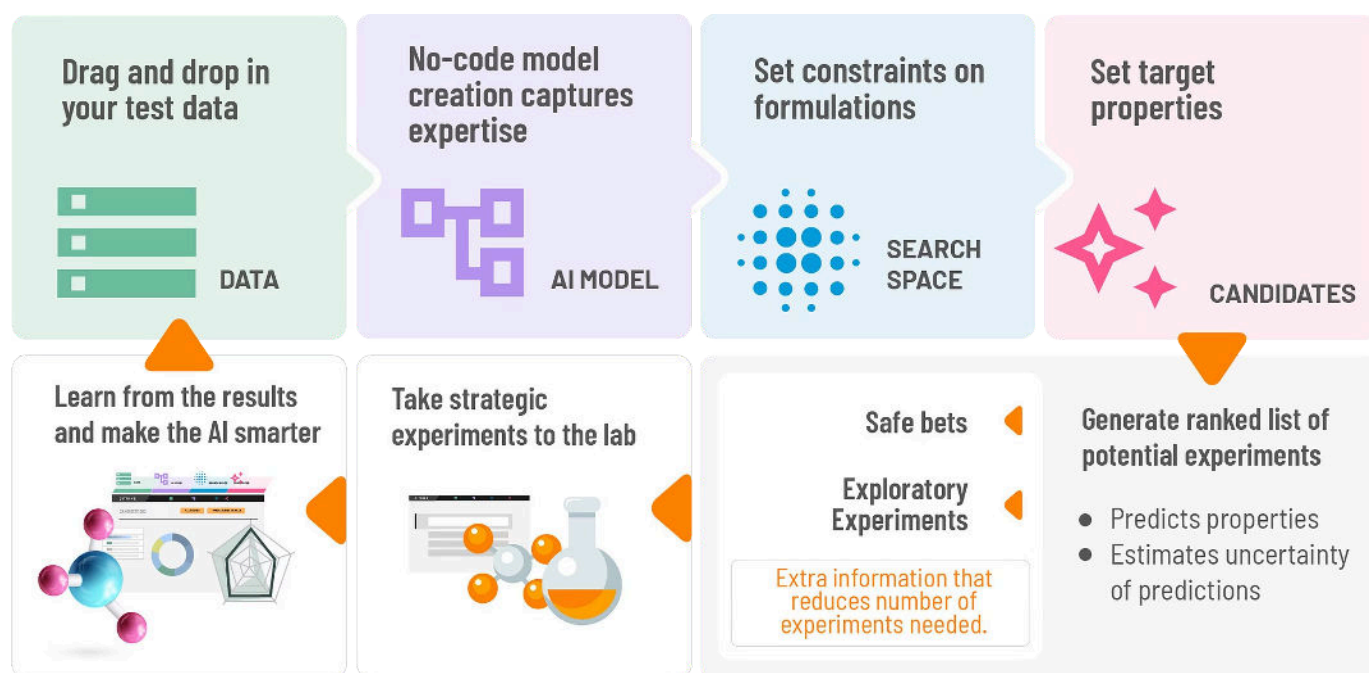
PROJECT 1 OBJECTIVE

A Stepan customer requested a new liquid dishwash formulation with the same cleaning performance but at a lower price point.

PROCESS

The Stepan team worked on this project autonomously, easily picking up and running with the Citrine Platform after their initial training. They used the recommended iterative, AI-driven experimentation process, building an AI model to predict cleaning performance and cost. The model suggested candidate formulations with the highest likelihood of success to test. The Stepan team chose a selection of these candidates to produce and test, inputting the test results back into the Citrine Platform and then retraining the AI models to increase its accuracy and get updated suggestions.

Drag and drop in your test data — DATA

No-code model creation captures expertise — AI MODEL

Set constraints on formulations — SEARCH SPACE

Set target properties — CANDIDATES

Learn from the results and make the AI smarter

Take strategic experiments to the lab

Safe bets
Exploratory Experiments
Extra information that reduces number of experiments needed.

Generate ranked list of potential experiments
- Predicts properties
- Estimates uncertainty of predictions

UNEXPECTED FORMULATIONS

The first suggestions by the Citrine Platform were not the usual suspects. One member of the Stepan team with 30 years of experience remarked that they would not have tried that formulation combination. However, in just three rounds of iteration, the suggested formulations were outperforming cleaning performance targets.

RESULTS AND WIDER BENEFITS

RESULTS

Stepan provided two formulations to the customer based on the Citrine model: a formulation that met the cost target, as well as a slightly higher cost formulation that met all performance targets. Stepan's customer was impressed with the performance formulation and was happy with the trade-off between technical performance and cost. Based on this work, the customer has expressed interest in bringing future formulation projects to Stepan.

WIDER BENEFITS

Beyond accelerating development and enabling the team to surpass technical targets, the Stepan team values the ability to see how chemical features and raw materials are influencing the predictions of technical properties. They were able to gain insight from data analysis in the platform and identify the importance of interactions between surfactants and other ingredients. This improved the mental models of the systems they are working on.

SCALABILITY AND KNOWLEDGE RETENTION

The models created for the liquid dishwash project can now be used on other similar projects with slightly different target properties. The dataset, models and search spaces (set of constraints on allowed ingredients and process parameters) have become reusable assets. The deep knowledge the veteran formulator used to augment the AI model is now codified and can be used by less experienced employees.

APPLICATION ENGINEERING

Stepan is currently working on several "platform models" across multiple application areas in multiple markets, including crop protection in Agriculture and polyol formulations for Spray Foam insulation. A platform model is one where application engineers working with customers can use it to quickly find the best formulation by using the same model and tweaking the targets and constraints according to customer requests. Using Citrine is enabling Stepan teams to improve customer responsiveness, leading to new business opportunities.

LIQUID DISHWASH FORMULATIONS	CROP PROTECTION FORMULATIONS	SPRAY FOAM FORMULATIONS
Models, datasets, and search spaces become reusable assets for similar projects	Predict surfactant stability and appearance for customer applications	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

AMBITIONS

Citrine identified the development of clear KPIs as one of the critical factors that influences the success of our customers. As part of the kick-off at Stepan, they developed a set of year one KPIs, including the ambition to get 20 projects to the candidate generation stage on platform and to achieve five technical wins. The Stepan Team has already achieved their five technical wins, including the liquid dish formulation. Citrine's customer success team is delighted to partner with a customer having such vision and drive.

20

PROJECT TARGET

Separate projects on platform before year end

5

TECHNICAL WINS ACHIEVED

> "We are delighted to partner with a customer that has such vision and drive." Citrine Informatics Customer Success Manager.

READY TO ACCELERATE YOUR MATERIALS INNOVATION?

Discover how Citrine Informatics can accelerate your R&D, optimize your formulations, and drive commercial success, just like Stepan. Our platform transforms materials development with AI-driven insights, turning ambitious goals into tangible results.

Contact Us   **Request a Demo**