CITRINE INFORMATICS

Using AI to Cut Costs and Maintain Flammability Compliance in Polyurethane Foams

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THE MULTI-DIMENSIONAL POLYMERS CHALLENGE

Competing Performance Objectives
Balancing thermal conductivity, flammability and density.

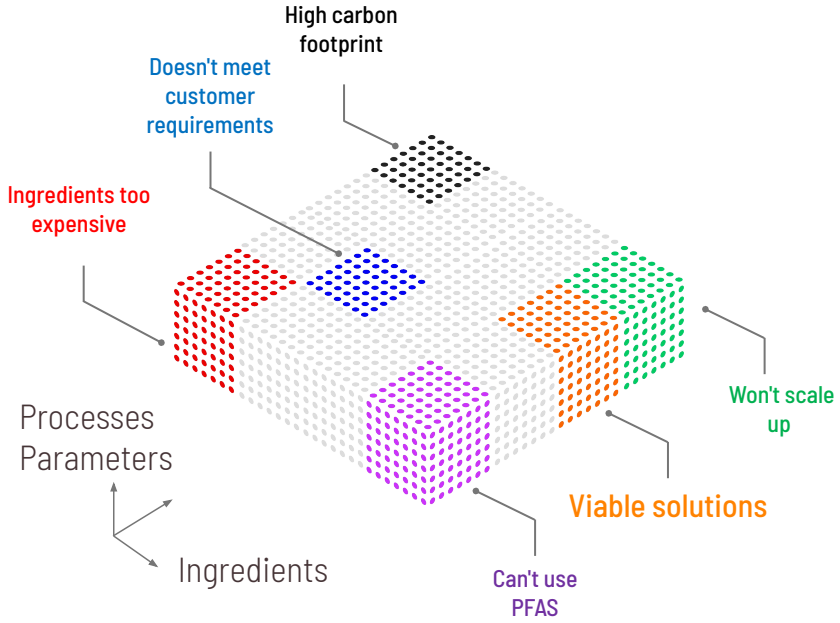
Evolving Regulatory Landscape
Adapting to restrictions on chemicals like PFAS and phthalates while meeting safety standards

Sustainability Mandates
Meeting targets for recycled content and growing demand for compostable alternatives

Supply Chain Volatility
Managing disruptions and mitigating rising raw material costs through innovation

TRADITIONAL WORKFLOWS

- You can’t test everything
- Teams that rely on intuition alone narrow the space too early
- Weak candidates survive too long, strong candidates arrive late



You can explore all options using AI

"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

SPEEDY STARTER FORMULATIONS AND MORE EFFICIENT TESTING

HUNTSMAN
BUILDING SOLUTIONS

- A multinational developer and manufacturer of polyurethanes that are regulated and need to pass stringent flammability tests before getting market approval.
- Their products cover a wide range of applications with different requirements and allowed ingredients.

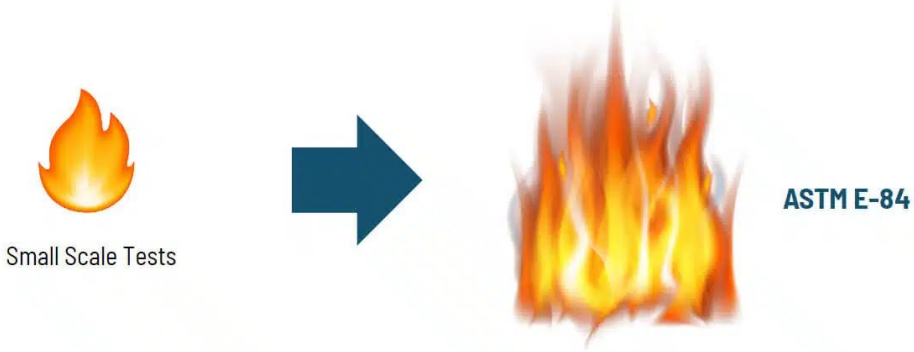
The Objectives

- Establish an **accelerated development** framework, speeding up the creation of starter formulations.
- Transform a starting formulation into a formulation capable of **passing ASTM E-84.**
- Reduce the number of l**arge scale fire tests** needed to create a compliant product.
- Deepen **materials understanding** of the complex chemistry involved.

SPEEDY STARTER FORMULATIONS AND MORE EFFICIENT TESTING

The Process

- An AI model to predict structural stability, insulation and flammability properties was developed.
- The formulation team has learned how to use the model to predict starter formulations for different applications by changing the allowed ingredients and target properties.
- A model was created to predict the results of the large-scale flammability tests, based on small scale tests.



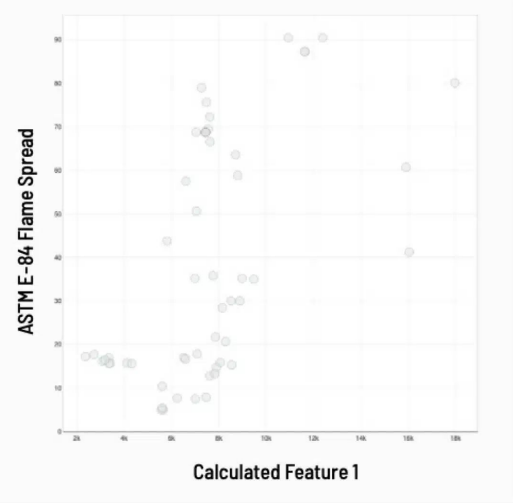
First Win

"In the old workflow, it took a chemist 6 months to come up with a starter formulation. With the platform, they can get a starter formulation on day 1."
R&D Technical Manager

SPEEDY STARTER FORMULATIONS AND MORE EFFICIENT TESTING

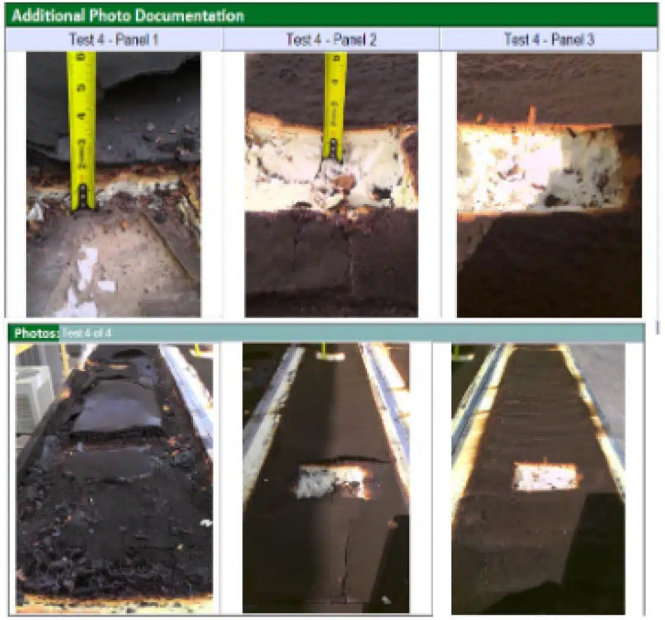
The Outcome

The connection between bench-top and large-scale tests is now better understood and **fewer large scale tests fail.**



Better understanding of what features can be used to predict flame spread.

Better Predictions of whether formulation will fail large scale fire test.



Condition	ASTM E-84 FSI	ASTM E-84 SDI
Prediction	15.56 +/- 5	457.53 +/- 40
Actual	15	450

BUILT FOR SCIENTISTS, NOT DATA SCIENTISTS

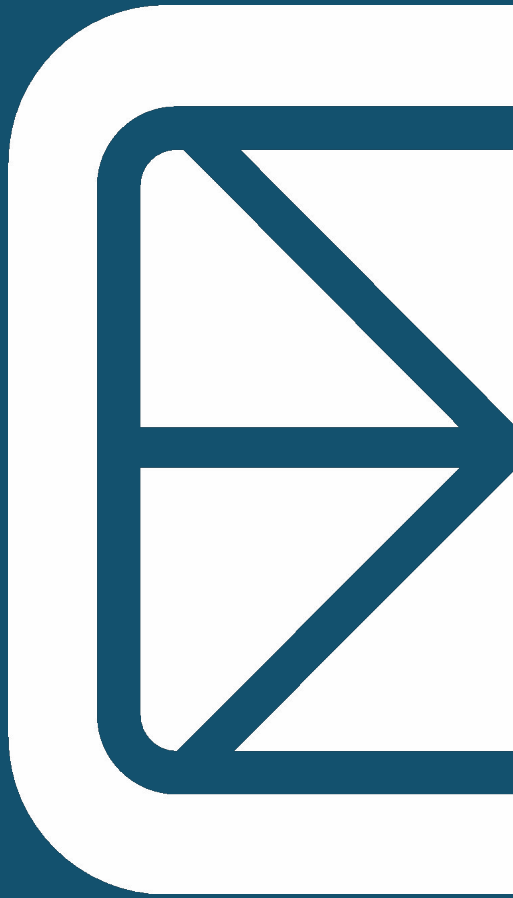
Ease of use matters because adoption matters

"The great thing about the platform is you don't have to be a data scientist to use it. The vast majority of the people using it are just my regular chemists and formulators."

David Cranfill, Technology & Innovation Director, Huntsman Polyurethane

Practical implication for R&D managers: your team can start with the data they already have, then build confidence through a focused technical win.

How does this work?



Iterative AI-driven Experimentation Workflow

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

Generate ranked list of potential experiments

- Predicts properties
- Estimates uncertainty of predictions

Safe bets

Exploratory Experiments

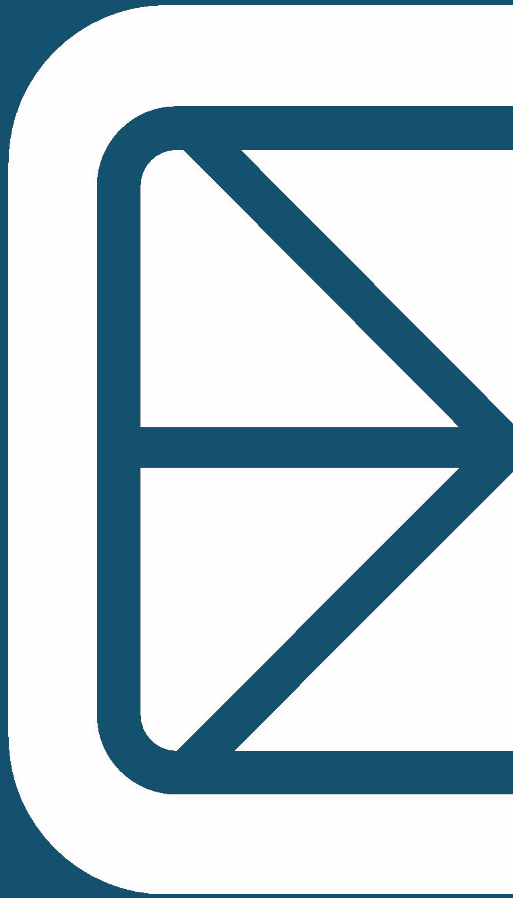
Extra information that reduces number of experiments needed.

Take strategic experiments to the lab

Learn from the results and make the AI smarter

DEMO

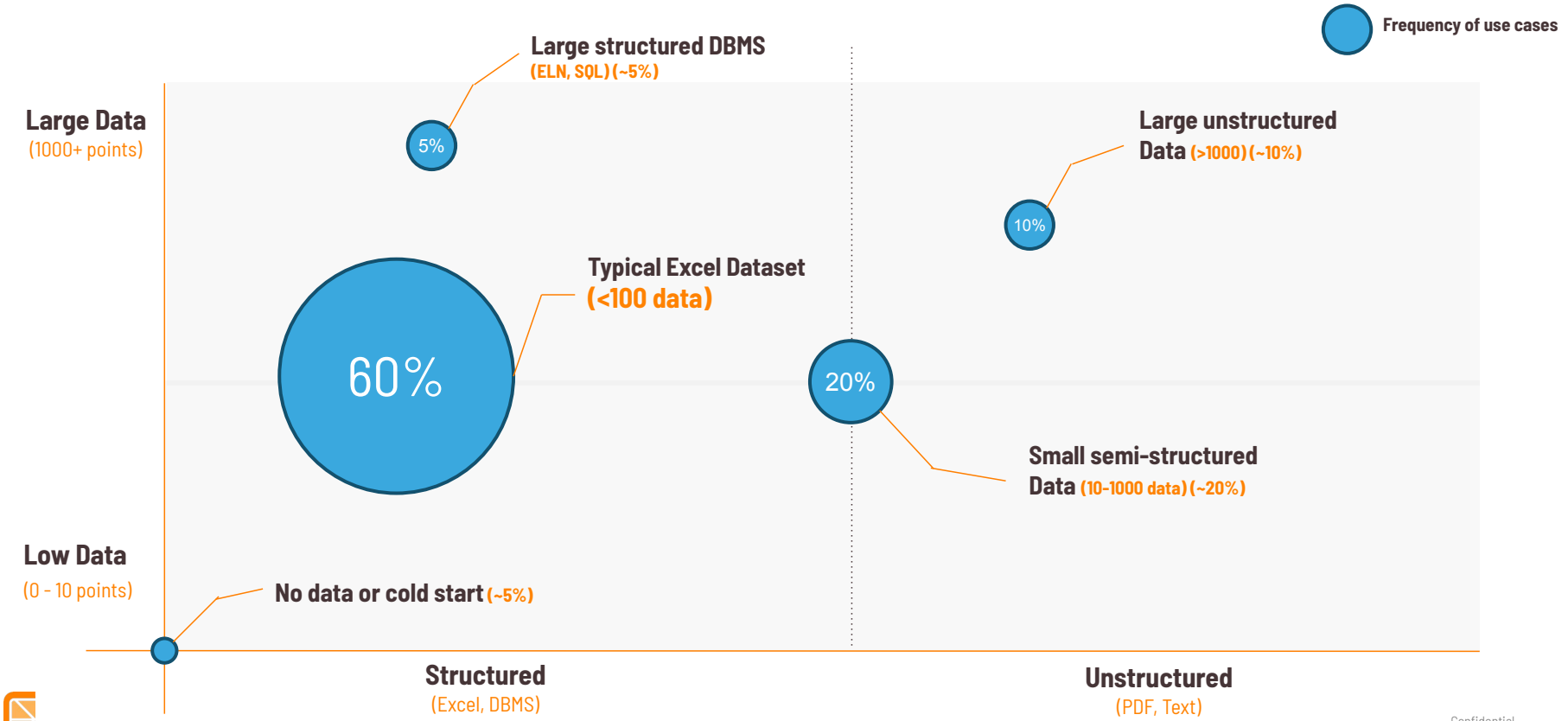
Our tips



EVERYTHING STARTS WITH DATA

But you don't need as much as you think

> *The thing that I liked about Citrine is you do not need a huge amount of data to get started.*
>
> David Cranfill, Technology & Innovation Director, Huntsman Polyurethanes



HOW TO GET AN EARLY WIN

Do not start with a massive data project

01

Pick one formulation problem

Choose one bottleneck with clear business value, such as fire-test reduction or ingredient-cost pressure.

02

Use the data you already have

Messy historical and bench data are enough to start ranking better experiments.

03

Constrain the search space

Set practical ingredient, process, and compliance boundaries before modeling.

04

Scale after a technical win

Build trust through one project, then expand to adjacent foam families or test workflows.

CITRINE CUSTOMERS DELIVER RESULTS AT SCALE

Currently on our platform each month

380
Projects worked

550
AI models deployed

70,000
Experiment suggested

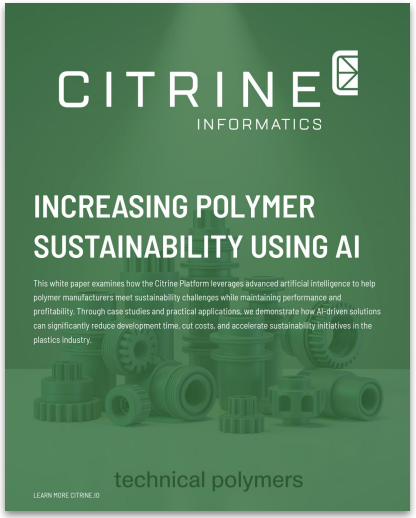
Start now

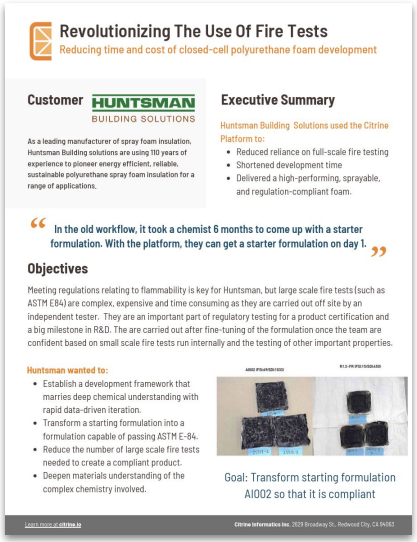
6.5 days
to first experiment suggestions

25 weeks
to first technical win

Median values

MORE RESOURCES ON AI AND PLASTICS





Contact us to get a copy of the paper info@citrine.io