

# MATERIALS WEEK EUROPE



## The next speaker is...



**Matthias Hermann**  
Solutions Engineer  
Citrine Informatics



*Smarter Formulations: Using AI to Cut Costs  
and Maintain Flammability Compliance in  
Polyurethane Foams*

Scan below for  
Conference Agenda



# Smarter Formulations:

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

# THE MULTI-DIMENSIONAL POLYMERS CHALLENGE



## Competing Performance Objectives

Balancing thermal conductivity, flammability and density.

## Evolving Regulatory Landscape

Adapting to restrictions on chemicals like PFAS.

## Sustainability Mandates

Meeting targets for recycled content.

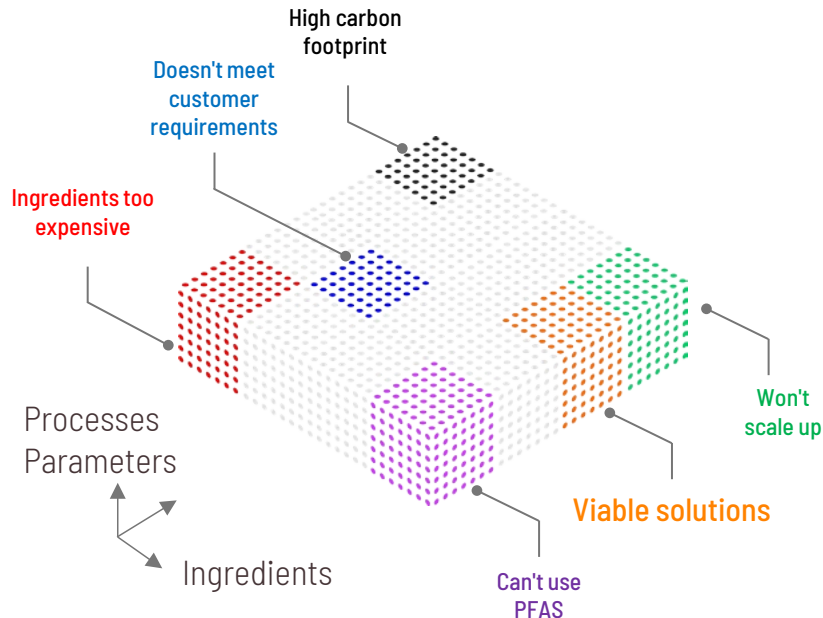
## Supply Chain Volatility

Managing disruptions and mitigating rising material costs.

# WITH AI YOU CAN

Explore all options - faster

## You can't test everything



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

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# SPEEDY STARTER FORMULATIONS AND MORE EFFICIENT TESTING

- 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.

## Objectives

- Establish an **accelerated development** framework.
- Transform a starting formulation into a formulation capable of **passing ASTM E84**.
- Reduce the number of **large 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.



Small Scale Tests



ASTM E-84

## 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."*

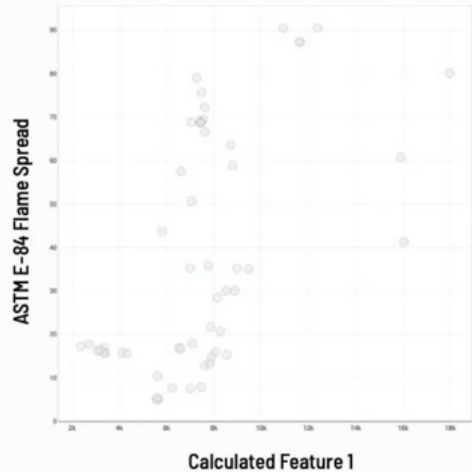
R&D Technical Manager



# SPEEDY STARTER FORMULATIONS AND MORE EFFICIENT TESTING

## The Outcome

The connection between benchtop and large scale tests is now better understood **fewer large scale tests fail.**



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

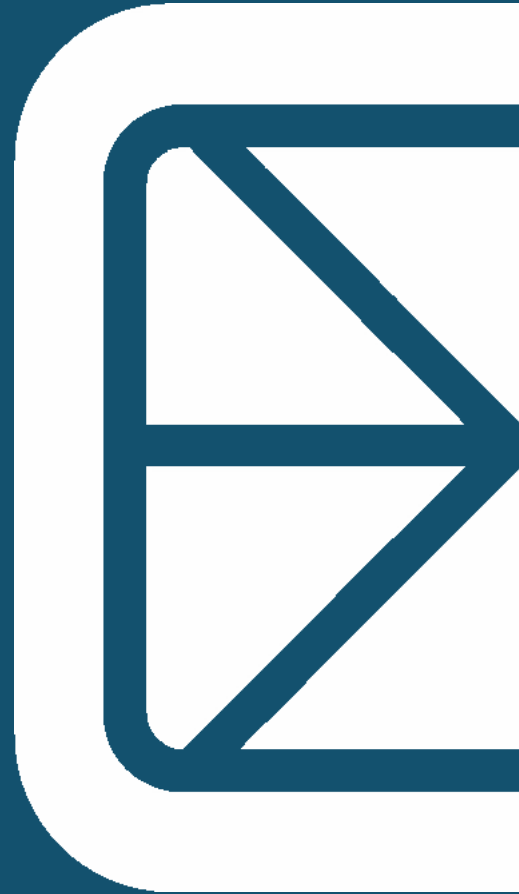
**Better Predictions** of whether formulation will fail large scale fire test.

Additional Photo Documentation

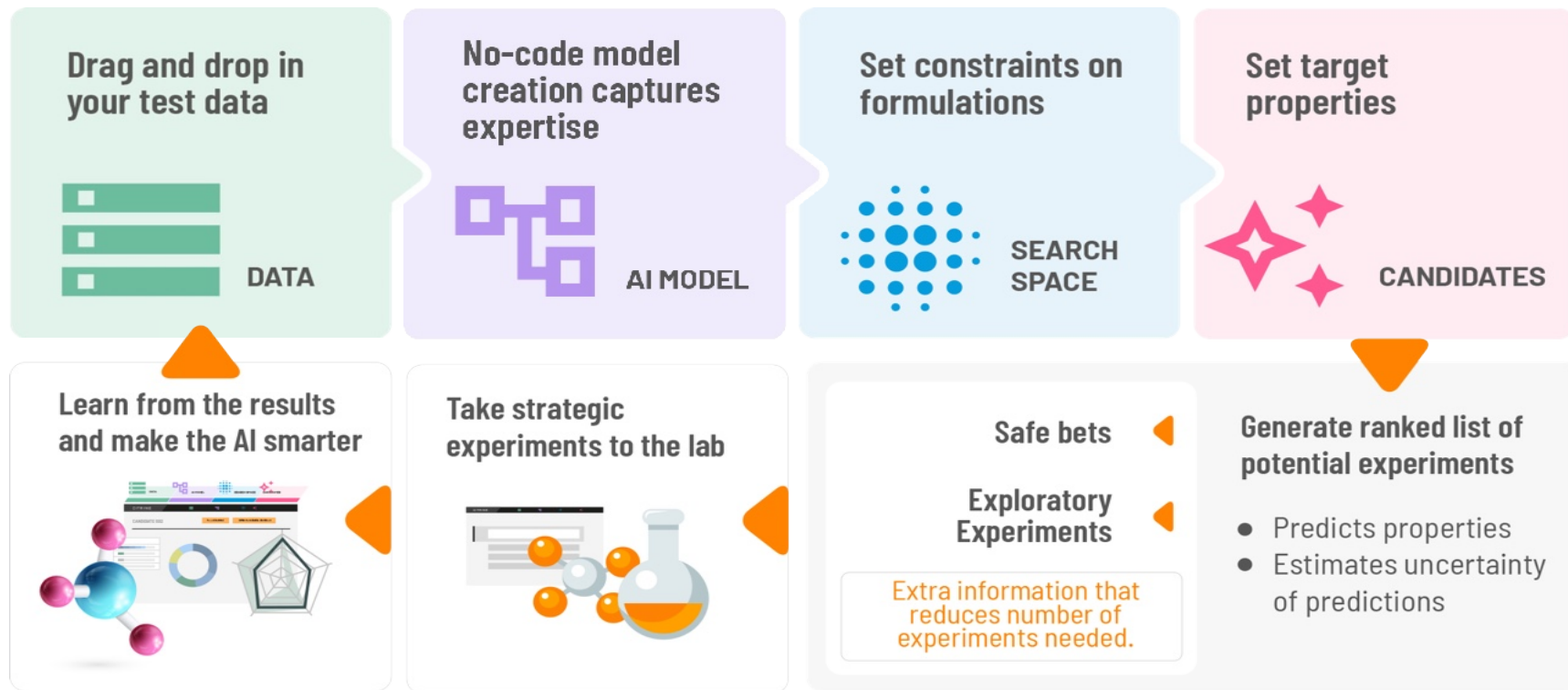
Test 4 - Panel 1	Test 4 - Panel 2	Test 4 - Panel 3
Photos: Item 4 of 4		

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

How does this work?



# Simple Iterative AI-driven Experimentation Workflow



SHOWING 39 OF 58 MATERIALS

Raw Ingredient (19)

Terminal (39)

- Exp\_1
- Exp\_10
- Exp\_11
- Exp\_12
- Exp\_13
- Exp\_14
- Exp\_15
- Exp\_16
- Exp\_17
- Exp\_18
- Exp\_19
- Exp\_2
- Exp\_20
- Exp\_21
- Exp\_22
- Exp\_23
- Exp\_24
- Exp\_25
- Exp\_26

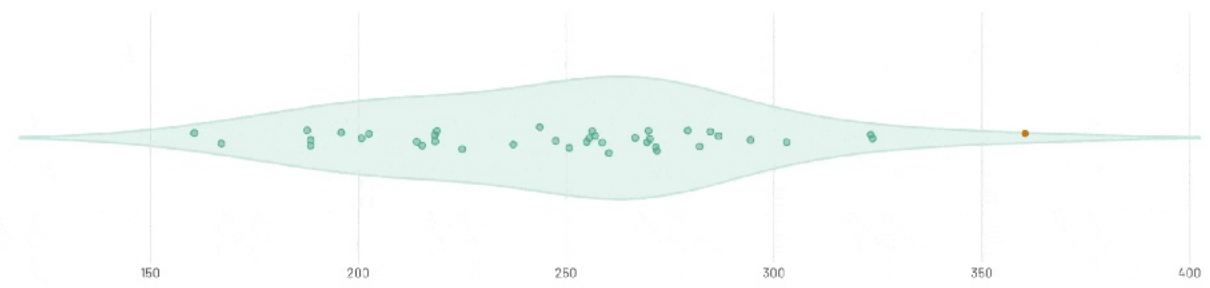
Distribution

⚠ 1 data attribute has values that are more or less than 1.5 times the Interquartile Range  
The presence of outliers may indicate an error in your data or atypical values that are not relevant for modeling. Inspect the data to assess whether outlier values need to be corrected or removed from the dataset.

SHOWING 1 OF 17 DATA ATTRIBUTES

Filter  
Attributes with outliers

⚠ Cell Size (µm)



BUILD

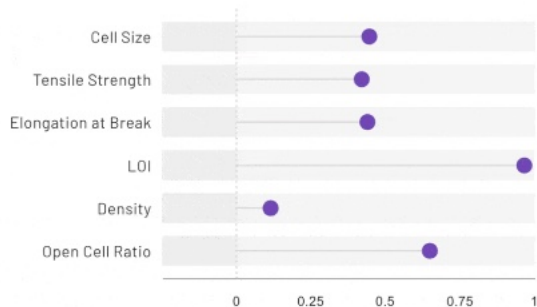
✓ TRAIN &amp; VALIDATE

**EVALUATE**

EXPLORE

Overall Model Performance ▾

## MODEL PERFORMANCE

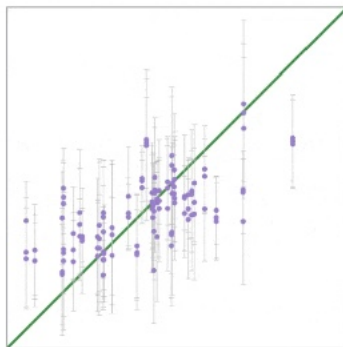
PREDICTIVE R<sup>2</sup> ⓘ

## EVALUATION SETTINGS ⓘ

NUMBER OF FOLDS	NUMBER OF TRIALS	IGNORE WHEN GROUPING
5	3	None

## PREDICTED VS ACTUAL

## Cell Size



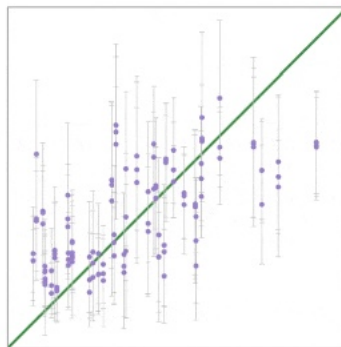
RMS ERROR ⓘ 32.0 ± 6.97

NDM ERROR ⓘ 0.729 ± 0.159

PREDICTIVE R<sup>2</sup> ⓘ 0.447

LOI

## Tensile Strength



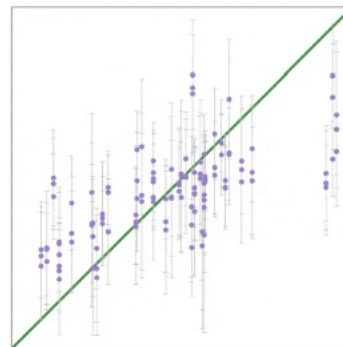
RMS ERROR ⓘ 3.40 ± 0.901

NDM ERROR ⓘ 0.739 ± 0.196

PREDICTIVE R<sup>2</sup> ⓘ 0.421

Density

## Elongation at Break

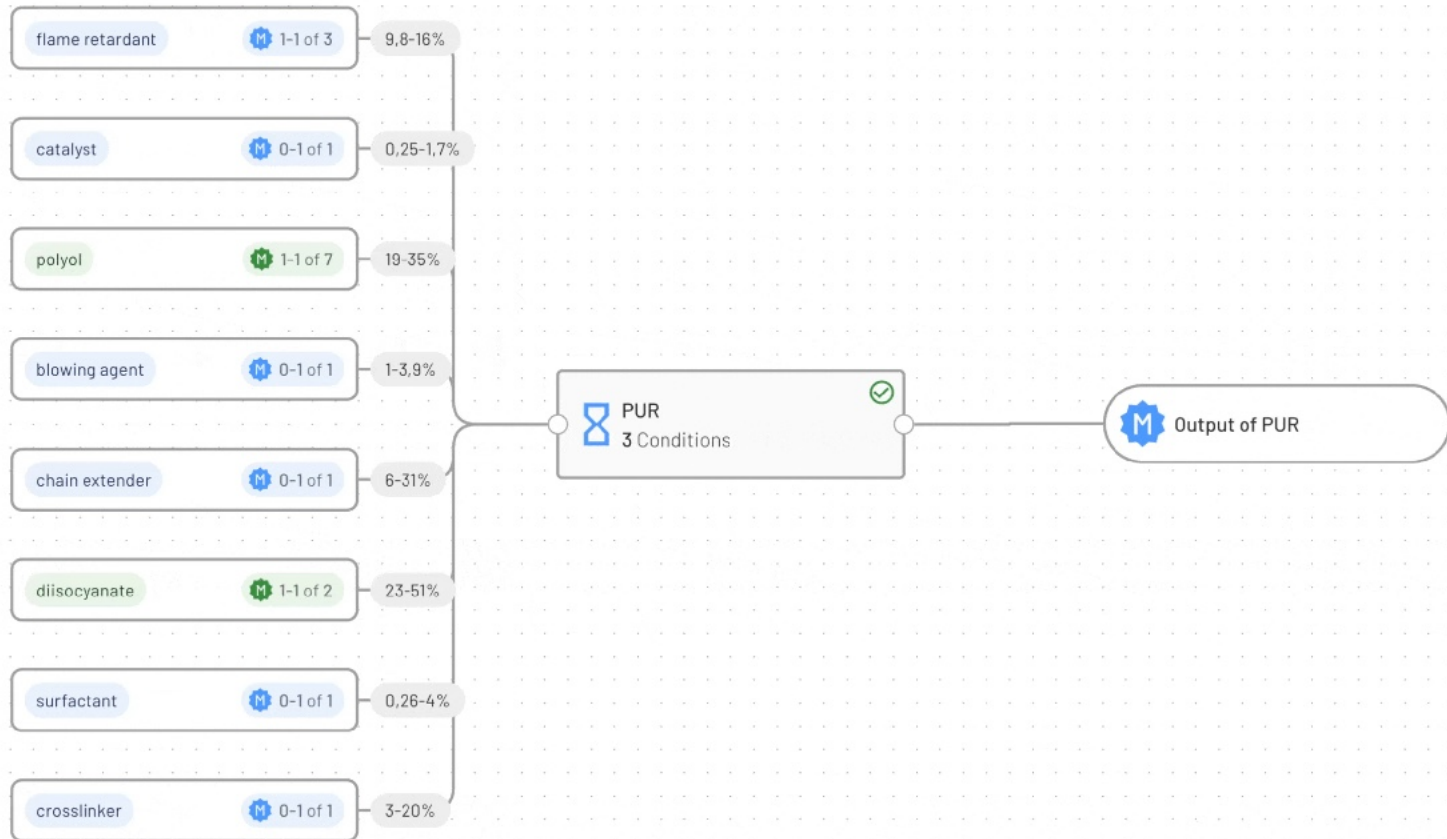


RMS ERROR ⓘ 56.8 ± 14.7

NDM ERROR ⓘ 0.728 ± 0.188

PREDICTIVE R<sup>2</sup> ⓘ 0.441

Open Cell Ratio



## OBJECTIVES & CONSTRAINTS

### OBJECTIVES:

- LOI > 24
- mean of property Cost in Flat Formulation < 2.71/kg
- Elongation at Break < 250%
- Density < 0.1g/cm<sup>3</sup>
- Open Cell Ratio > 0.6

### CONSTRAINTS:

No constraints selected

### SCORE TYPE:

Likelihood of Improvement

### CORRELATED SCORING:

- Cell Size
- Open Cell Ratio

100 of 100 Candidates

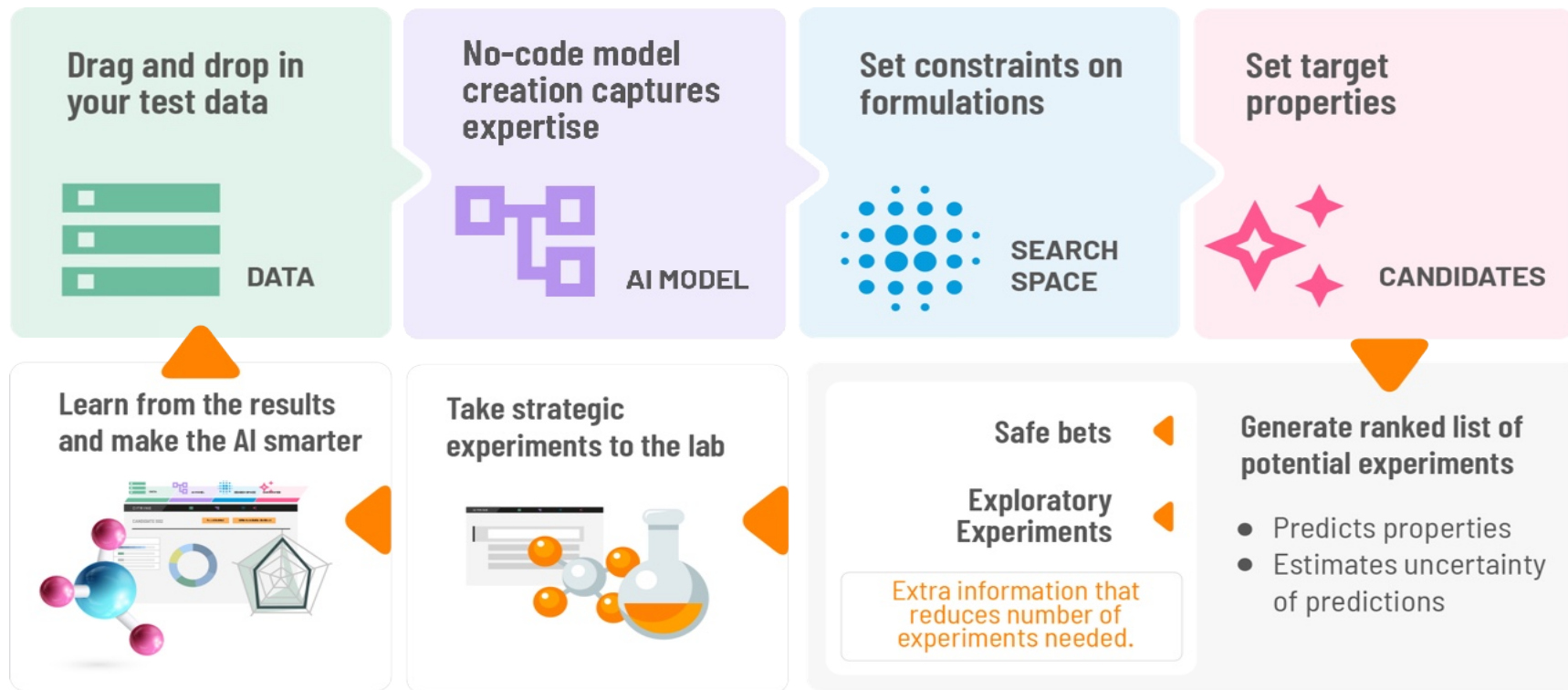
SCORE ↑	NAME		👁	📌
0.028	Candidate 0001	➡	👁	📌
0.022	Candidate 0002	➡	👁	📌
0.020	Candidate 0003	➡	👁	📌
0.018	Candidate 0004	➡	👁	📌
0.018	Candidate 0005	➡	👁	📌
0.018	Candidate 0006	➡	👁	📌

Modified Candidates

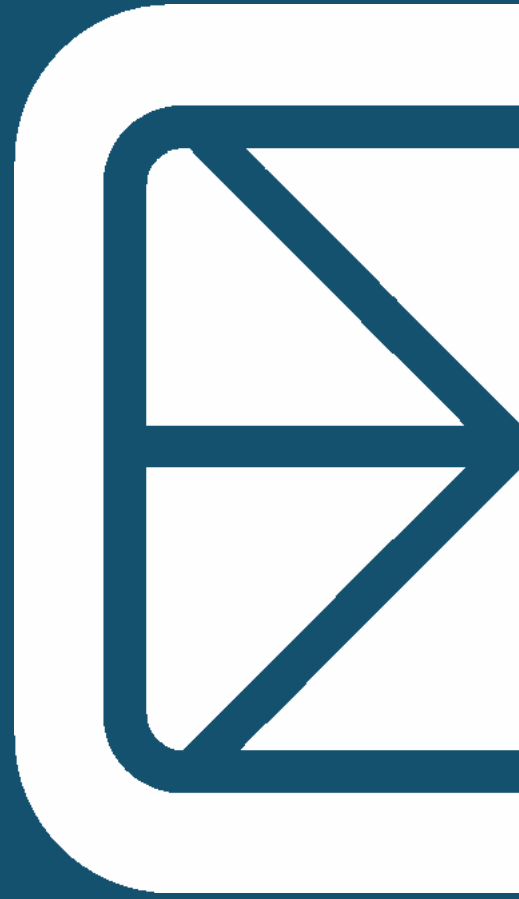
Training Data



# Simple Iterative AI-driven Experimentation Workflow

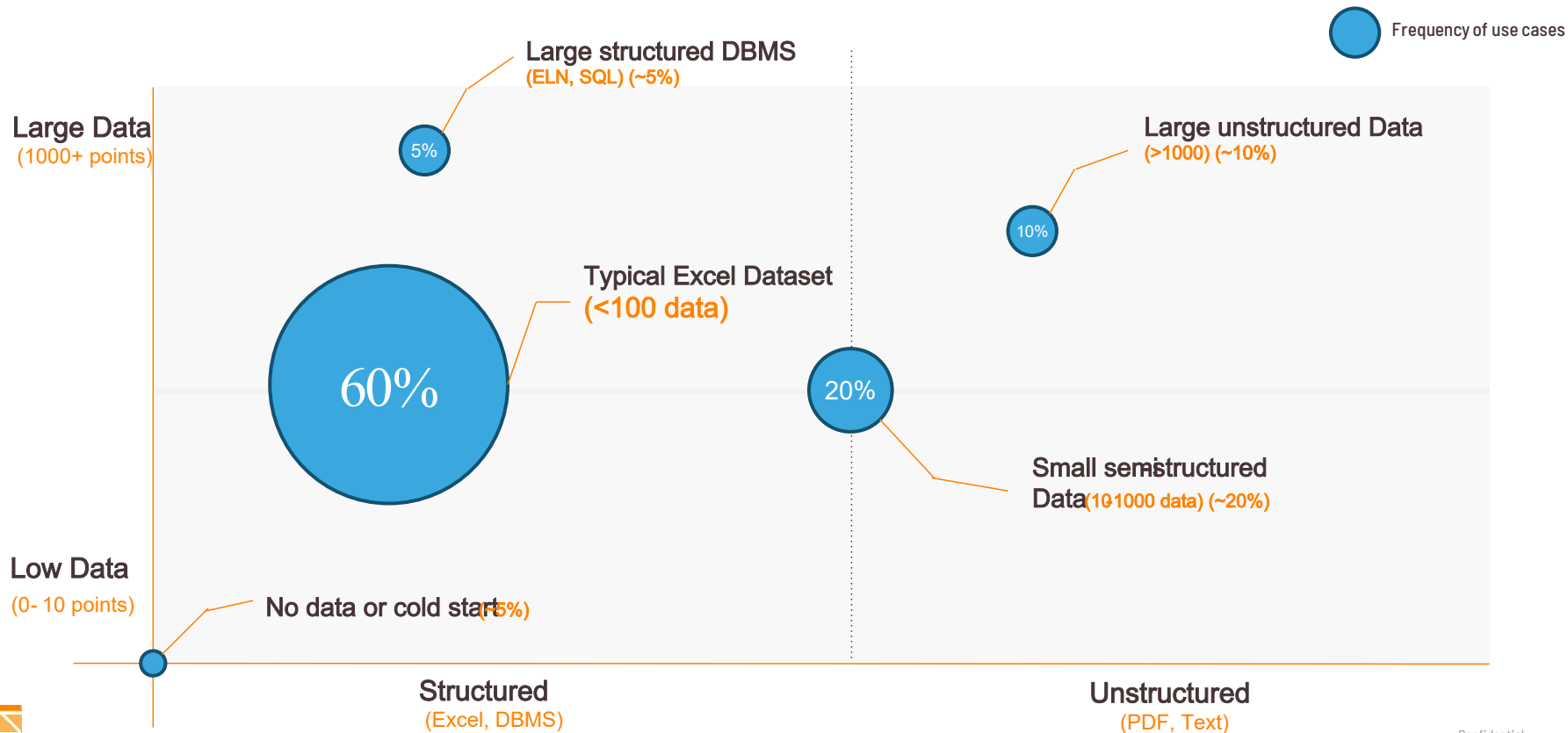


# Our tips



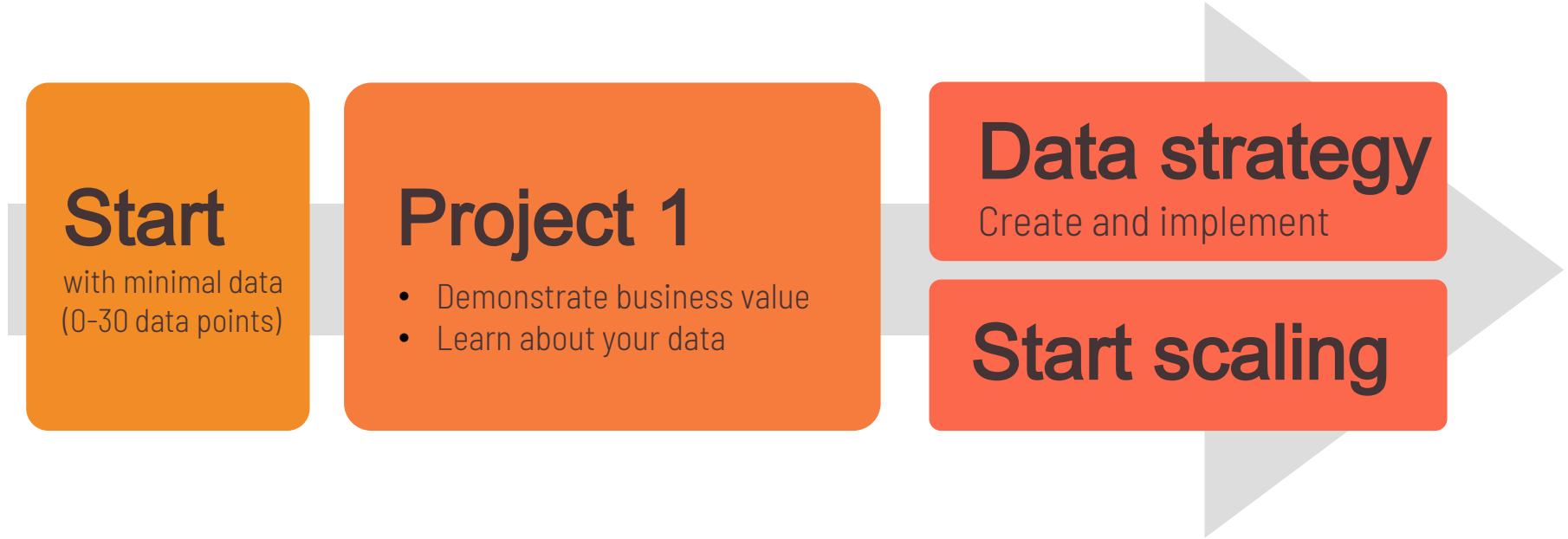
# EVERYTHING STARTS WITH DATA

But you don't need as much as you think

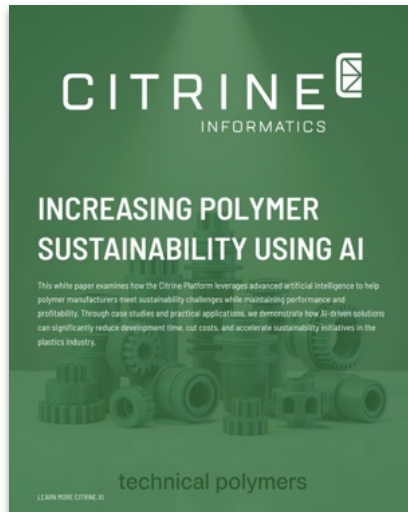


# AI + DATA

## Agile bootstrapping approach



# MORE RESOURCES ON AI AND PLASTICS



### Revolutionizing The Use Of Fire Tests

Reducing time and cost of closed-cell polyurethane foam development

**Customer** **HUNTSMAN**  
BUILDING SOLUTIONS

**Executive Summary**

Huntsman Building Solutions used the Citrine Platform to:

- Reduced reliance on full-scale fire testing
- Shortened development time
- Delivered a high-performing, sprayable, and regulation-compliant foam.

**“ 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. ”**

**Objectives**

Meeting regulations relating to flammability is key for Huntsman, but large scale fire tests (such as ASTM E84) are complex, expensive and time consuming as they are carried out off site by an independent tester. They are an important part of regulatory testing for a product certification and a big milestone in R&D. The are carried out after fine-tuning of the formulation once the team are confident based on small scale fire tests run internally and the testing of other important properties.

**Huntsman wanted to:**

- Establish a development framework that marries deep chemical understanding with rapid data-driven iteration.
- Transform a starting formulation into a formulation capable of passing ASTM E-84.
- Reduce the number of large scale fire tests needed to create a compliant product.
- Deepen materials understanding of the complex chemistry involved.



**Goal: Transform starting formulation A1002 so that it is compliant**

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Contact us to get a copy of the paper [info@citrine.io](mailto:info@citrine.io)



# OUR CUSTOMERS ARE GETTING RESULTS WITH AI TODAY



*Citrine works with...*

7 of the  
top 20

global Specialty Chemicals companies

---

4 of the  
top 10

global Adhesives & Sealants companies

---

2 of the  
top 10

global Surfactant companies



# SUMMARY

## Accelerated Reformulation

AI helps you reformulate products faster, meeting sustainability goals while maintaining performance

## Easy Adoption

The Citrine Platform is designed for product experts

## Proven Expertise

Our team brings a decade of experience implementing AI in companies like yours

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[mhermann@citrine.io](mailto:mhermann@citrine.io)

