



AI in Chemistry – An Industry Perspective

Bea Braun

Matthew Malloure, Fabio Aguiere, Sukrit Mukhopadhyay, Dan Christiansen

Seek Together™

This Is Dow



Every answer
starts with asking
the right question.

At Dow, these questions and the pursuit of solutions for the world’s toughest challenges inspire us to collaborate and use our materials science expertise to create innovative solutions that transform our world and deliver a sustainable future.



\$45B
net sales in 2023



~35,900
employees



98
manufacturing sites

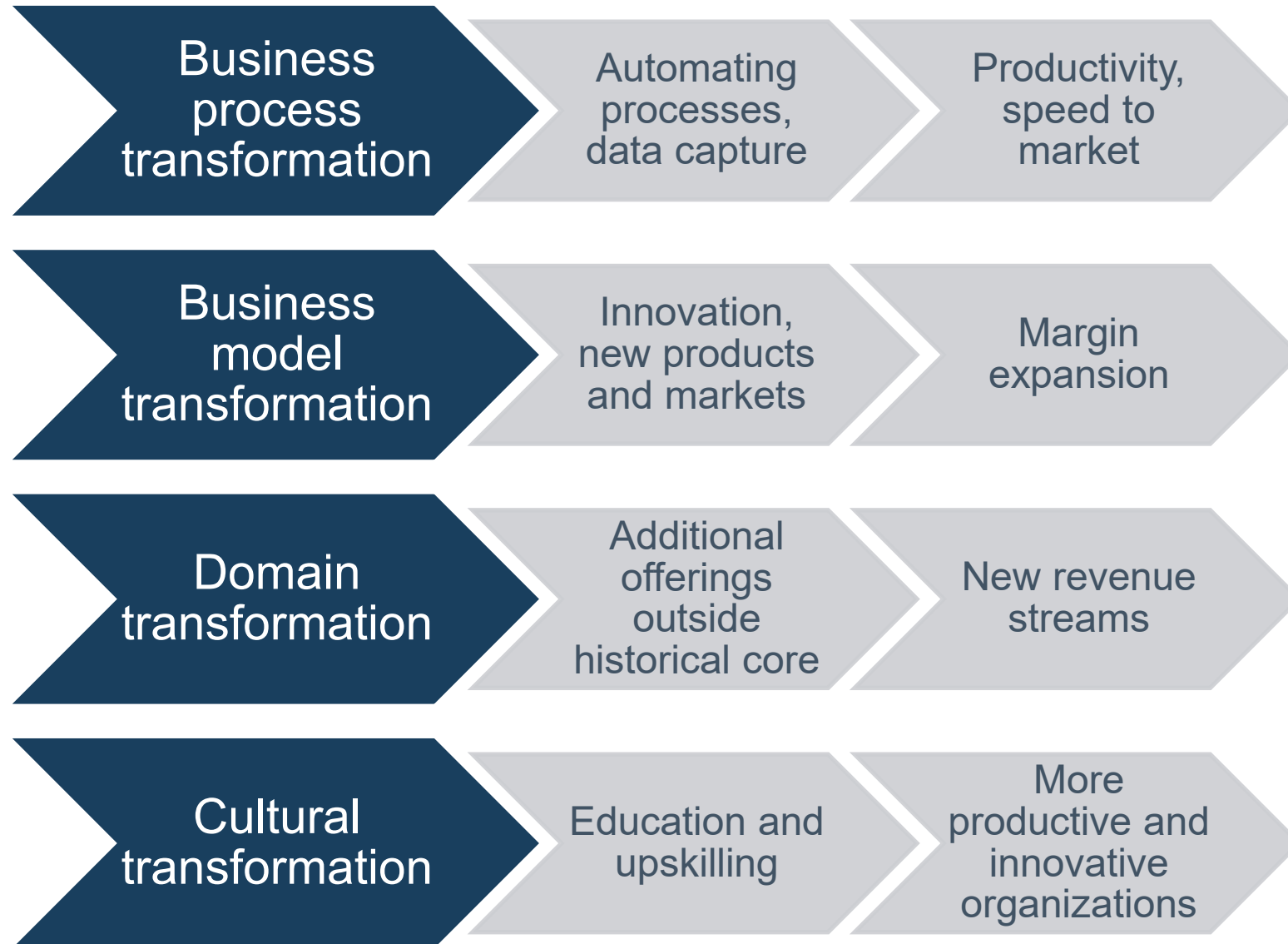


31
countries in which Dow
manufactures products

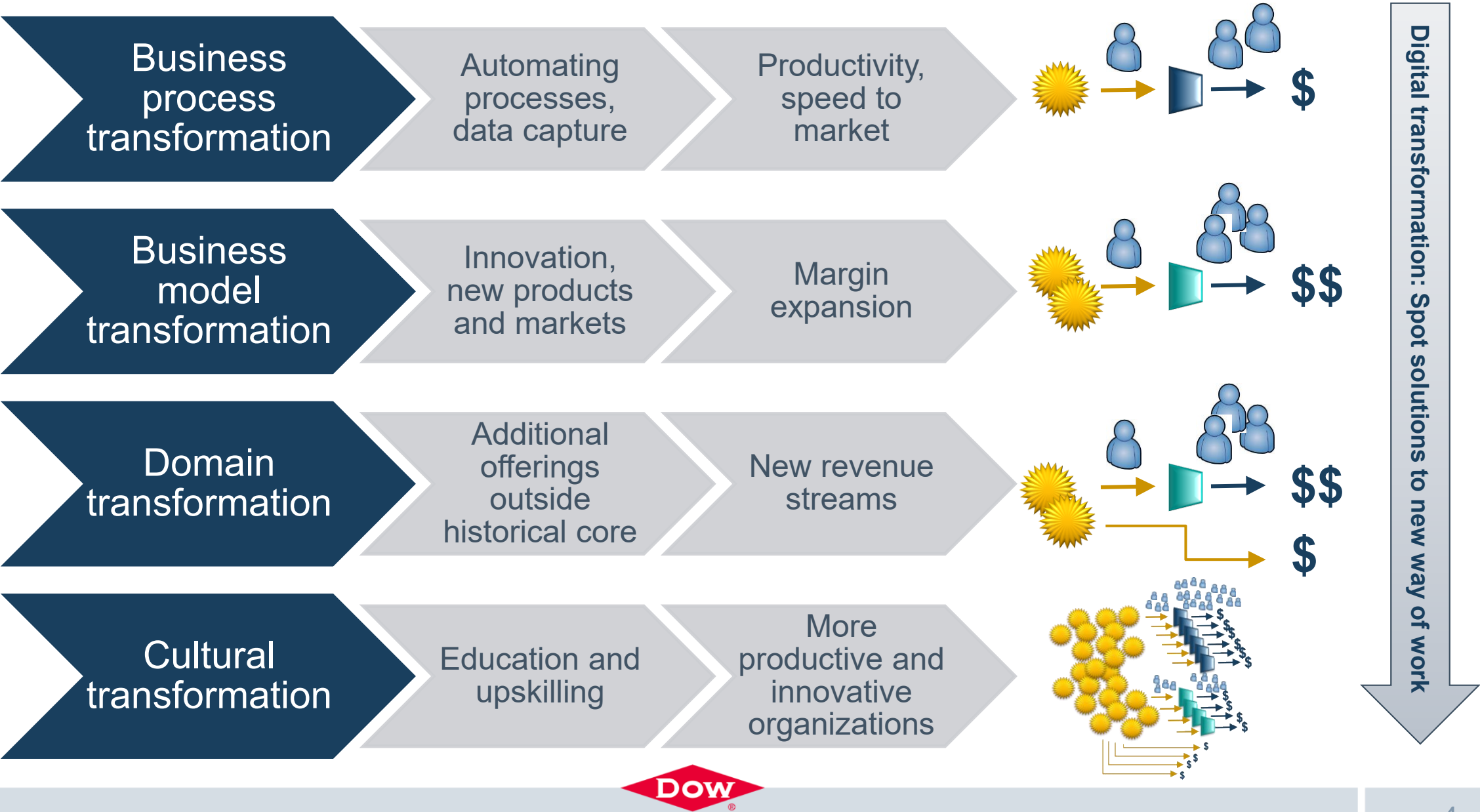
Note: All data as of December 31, 2023



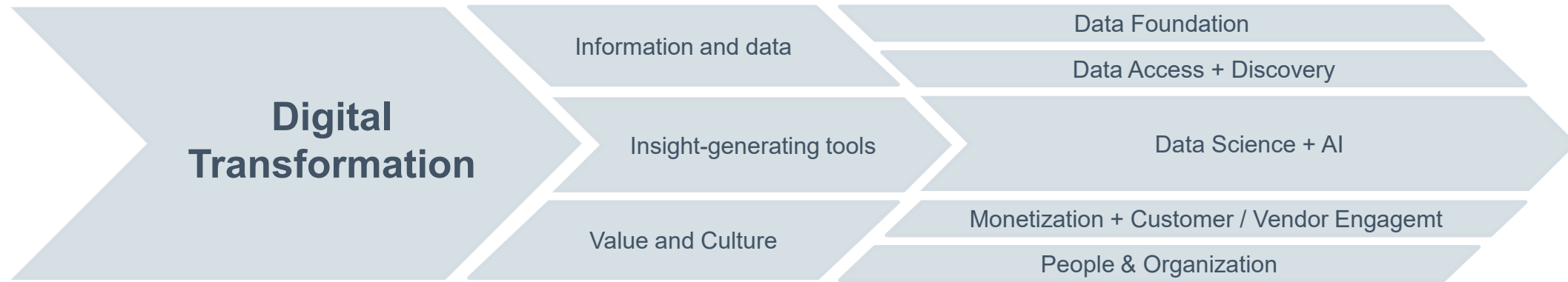
DIGITAL TRANSFORMATION – ESSENTIAL TO ACHIEVING OUR GOALS



DIGITAL TRANSFORMATION – ESSENTIAL TO ACHIEVING OUR GOALS



INGREDIENTS FOR SUCCESS



- Information and data
 - >> data capture and infrastructure
 - >> data access and discovery
 - >> external data
 - >> internal and our competitive advantage
 - >> data catalogs and security
- Insight-generation
 - >> data science & AI
 - >> strong internal expertise in scientific AI/ML
 - >> collaboration with universities*, collaborators, tech companies
- Value and culture
 - >> value generation beyond Dow
 - >> current and new customers
 - >> work process updates, training, upskilling (Citizen Data Science**)

* Toothman, M., Braun, B., Bury, S.J., Moyne, J., Tilbury, D.M., Ye, Y. and Barton, K., 2023. A digital twin framework for prognostics and health management. *Computers in Industry*, 150, p.103948.

* Bilodeau, C., Kazakov, A., Mukhopadhyay, S., Emerson, J., Kalantar, T., Muzny, C. and Jensen, K., 2023. Machine learning for predicting the viscosity of binary liquid mixtures. *Chemical Engineering Journal*, 464, p.142454.

* Strelet, E., Peng, Y., Castillo, I., Rendall, R., Wang, Z., Joswiak, M., Braun, B., Chiang, L. and Reis, M.S., 2023. Multi-source and multimodal data fusion for improved management of a wastewater treatment plant. *Journal of Environmental Chemical Engineering*, 11(6), p.111530.

** Andrews, K., Arturo, S., Benedict, M., Braun, B., Clark, B., Cook, S., Curtis-Fisk, J., D'Ottaviano, F., Licquia, T., Margl, P. and Moore, J., 2025. The Citizen Data Science program at Dow. *Digital Discovery*, 4(5), pp.1124-1133.



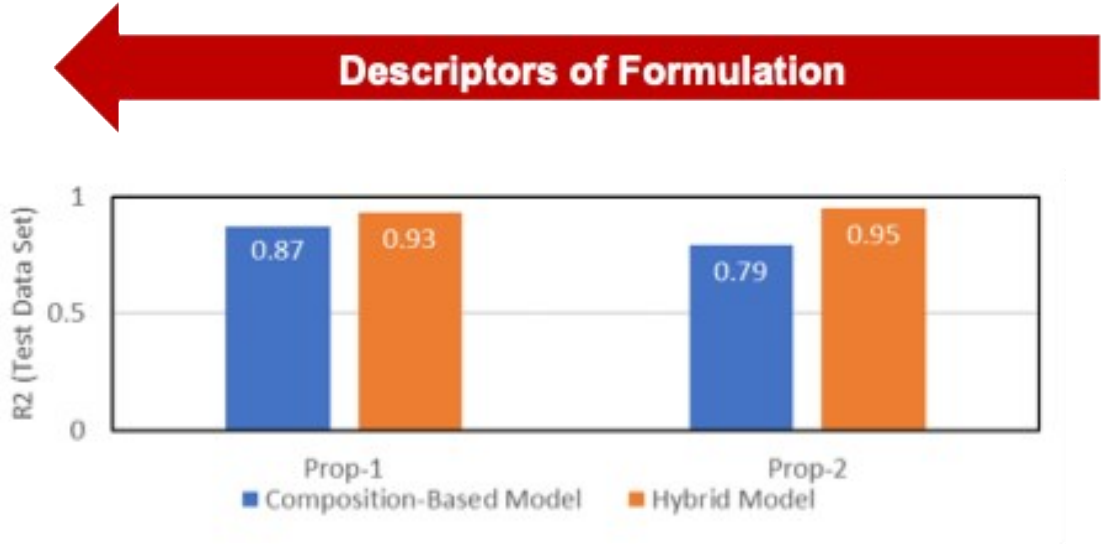
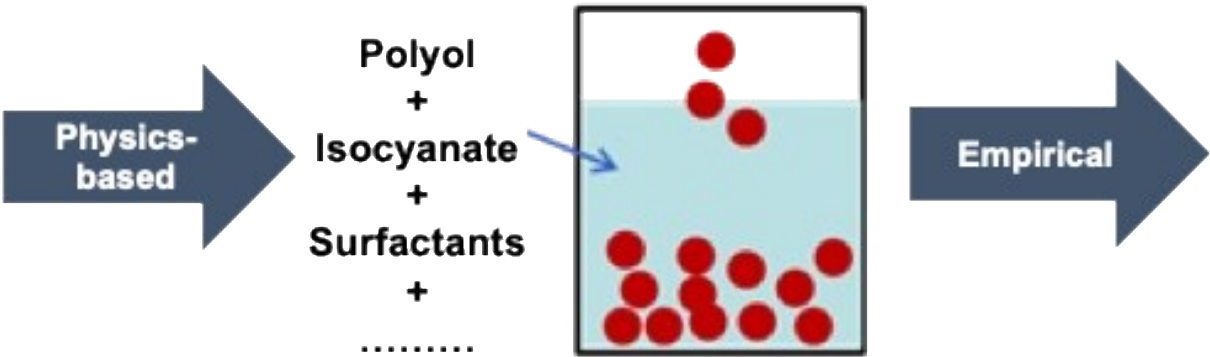
POLYURETHANES PREDICTIVE INTELLIGENCE

Polyol-1 HO~~~~~OH

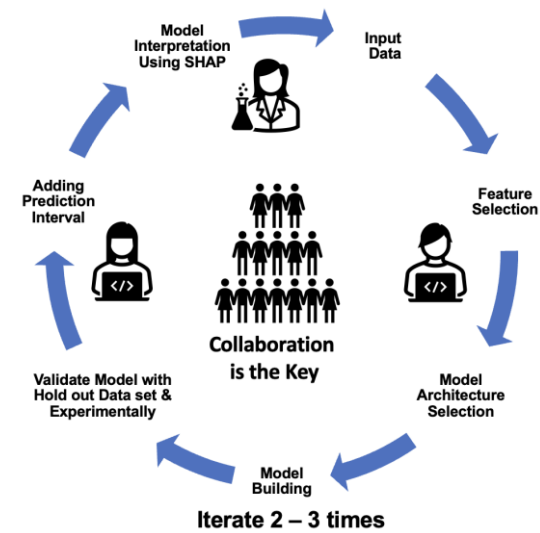
Polyol-2 HO~~~~~OH
 |
 OH

Polyol-3 HO~~~~~OH
 |
                  ~~~~~OH

**Isocyanates**    OCN—NCO



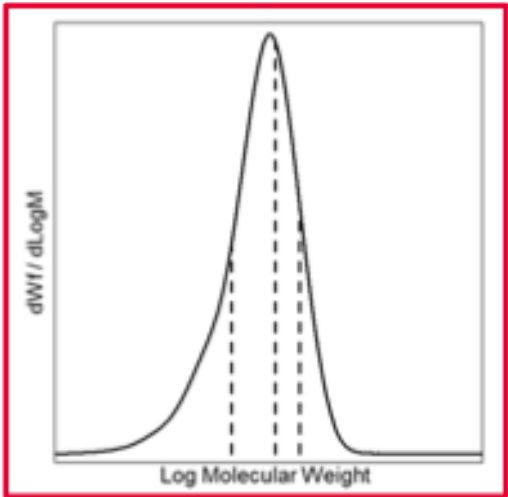
## Performance of Foam



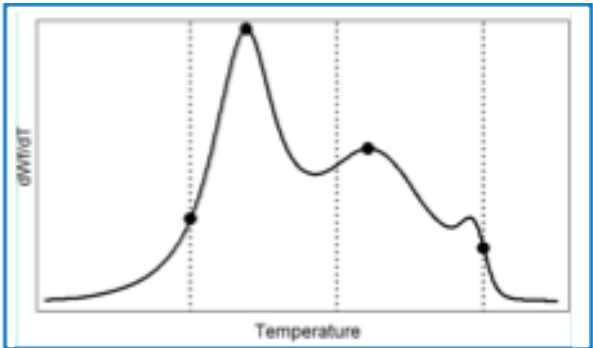
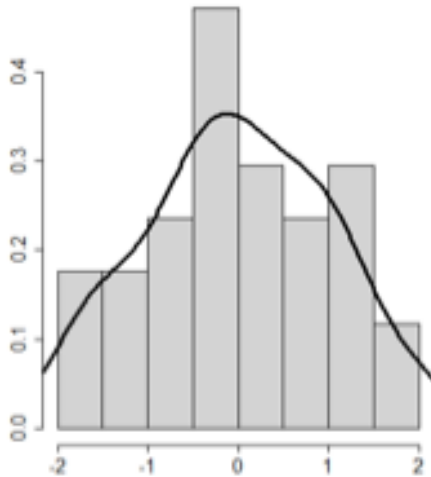
<https://www.dow.com/en-us/product-technology/pt-polyurethanes/harnessing-the-power-of-digitalization.html>



# MODELING FUNCTIONAL DATA



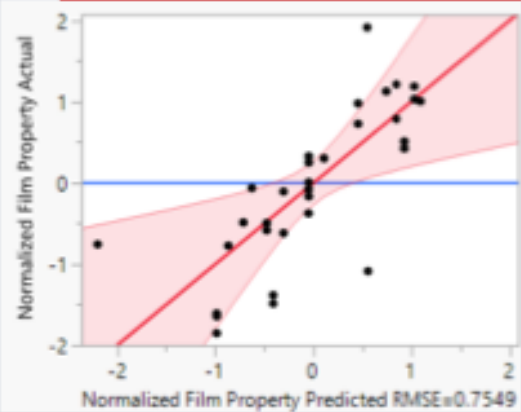
Normalized Performance Property



Compute common molecular weight distribution (MWD) parameters:  $M_w$ ,  $M_n$ ,  $M_z$ ,  $M_w/M_n$

For comonomer content distribution (CCD), compute peak positions and AUCs in subdomains

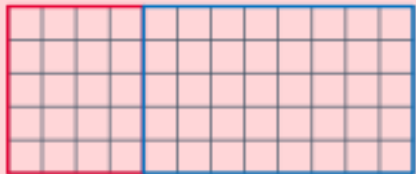
Explain ~40% of the total variability in response



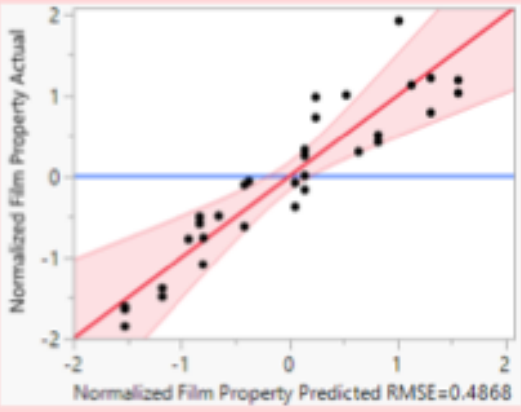
4 FPCs

Join FPC scores to form design matrix

8 FPCs



Explain ~80% of the total variability in response





# OPPORTUNITIES FOR LARGE LANGUAGE MODELS

## EH&S

- Root Cause Identification & Summarization
- Hypothesis Generation for Unplanned Events
- Smart Search of Safety Standards and Training

## Operations

- Leak/Spill Detection (LLVM)
- Equipment/Asset Reliability Estimation from Logs
- Troubleshooting Support

## Business

- Smart Customer Compliant Analysis
- Market Intelligence
- New Application Exploration

## R&D

- Patent and Literature Insight
- Innovation Optimization
- Chatbot for customer intelligence

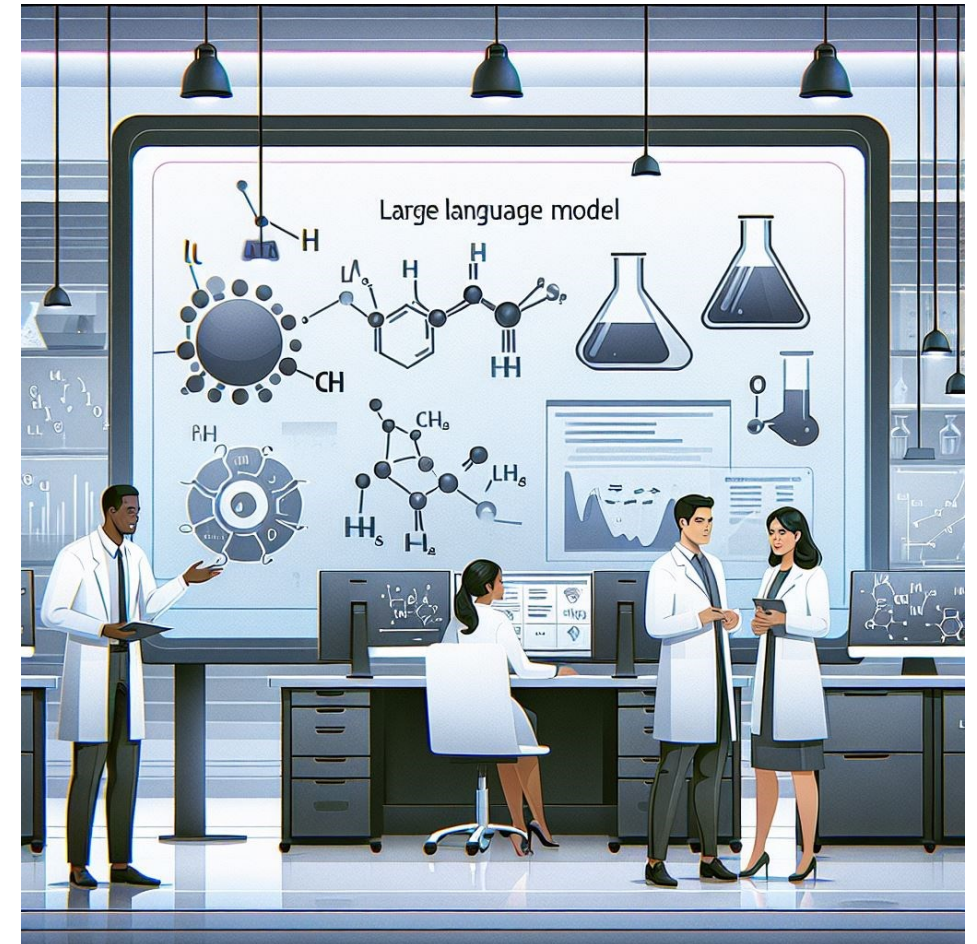
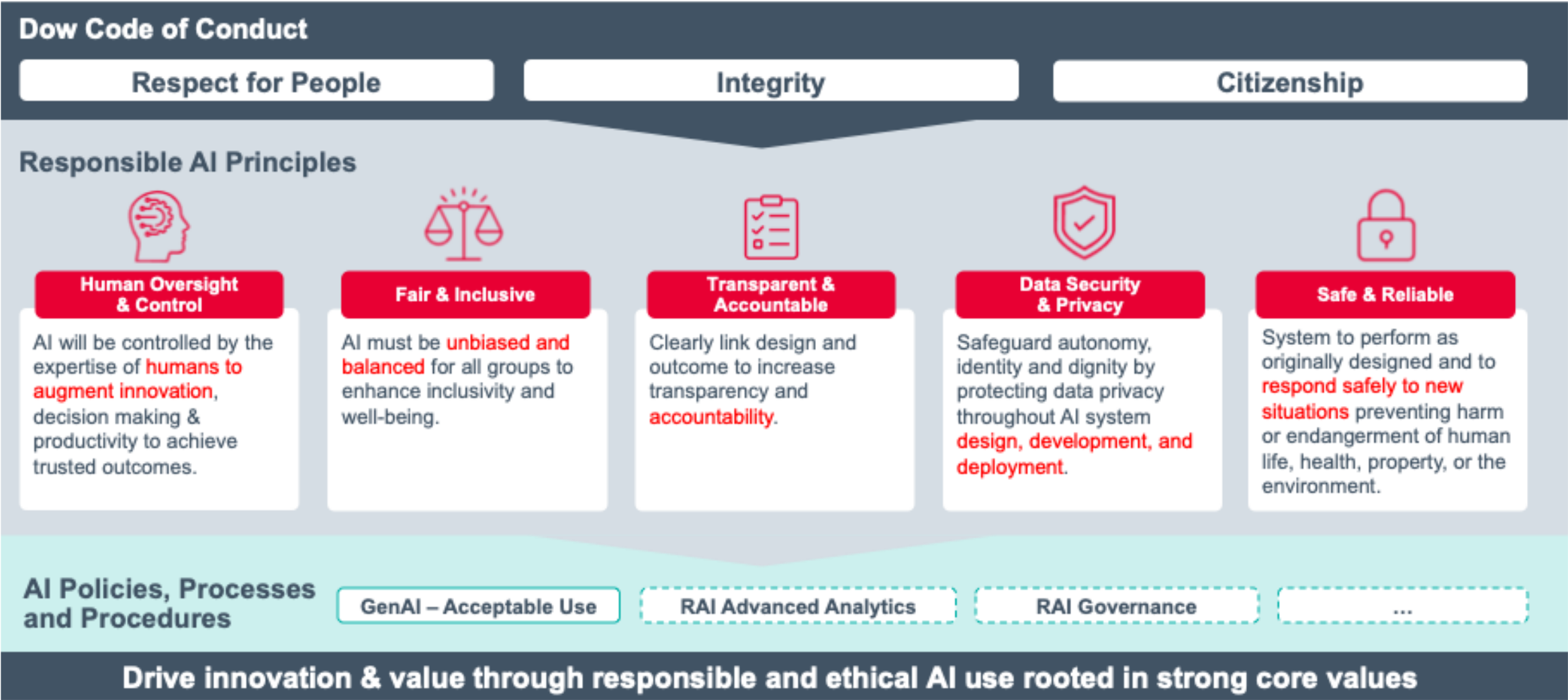


Image generated by Copilot, March 2025



# RESPONSIBLE AI PRINCIPLES





Thank you