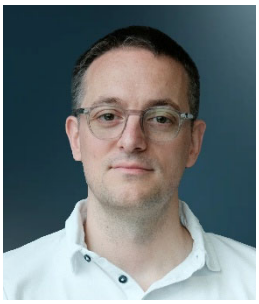
Charles Jouanique
LabV Intelligent Solutions; DE-Selb



FROM DATA CHAOS TO AI-DRIVEN DECISIONS IN FORMULATION DEVELOPMENT

ABSTRACT

Can machine learning predict the performance of a new adhesive formulation before it is tested in the laboratory? Industrial case studies suggest that it can. Yet the biggest challenge is often not the model itself, but the preparation and harmonisation of the underlying data.

The presentation shows an industrial case study that explores the use of machine learning in formulation development. Based on more than 1,000 historical experiments, the project demonstrates both the potential and the practical challenges of applying AI in an industrial R&D environment.

Once the R&D data is structured and connected, the question is no longer whether AI could be applied, but where it could create the greatest value in R&D. The presentation looks at three areas in particular: Generative AI for accessing experiments, documents, and formulation knowledge; Agentic AI for coordinating tasks across data sources and workflows; and AI-driven experimental design, where machine learning and Bayesian optimisation recommend the most promising next experiments.