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Request for Industrial Partners

Blending experimental design and AI for efficient new product development in the chemical industry as part of the sustainability revolution

Acronym: BEDAI

Project ID	
Type	ICON
Period	TBD
Starting date	2024
Total project budget	TBD
Subsidy percentage	According to SBO and O&O regulations
Current industrial partners	Confidential
Catalisti contact	Mathias Jacobs (mjacobs@catalisti.be)

Project description

Introduction

In order to be more sustainable and CO_2-neutral by 2050, producers as well as consumers should be strongly involved. The chemical industry must react fast on the changes in regulation of chemicals and the availability of other sources of raw materials, but also to new demands concerning end-of-life properties of products.

The knowledge that companies have acquired during many years of experimentation is a valuable starting point that helped them to innovate and bring new products to the market. While this experience-based approach has worked out in practice for many years, fast changing trends require a more structured approach that allows to reduce the number of tests as well as the testing time. This would accelerate the time-to-market.

Artificial Intelligence (AI) is a powerful approach to digest complex historical information. However, not all companies have sufficient data to start from, or do have historical information that might not be information-rich. In such cases, the concept of Design of Experiments (DOE) is well-positioned to gain maximal insight from a minimum number of tests. Even more, the concepts of DOE and AI are highly complementary with DOE being excellent to generate small, information rich data, and AI the go-to tool for finding relationships in complex, large data structures.

In this project, we will develop and leverage DOE and AI tools to help the chemical industry to be highly efficient and, thus, sustainable.

The development of a data-driven approach allows to gain insights about the potential of other resources (mixed plastics, bio-based side streams, *etc.*), to be valorised as alternative raw materials in the formulation industry. A relevant description of the alternative raw materials, similar but not identical, can serve as input to better position these alternatives regarding the materials to be replaced. Additionally, special focus will go to how to tackle varying raw material quality when the end product needs to be of a constant quality.

The holistic data-driven approach for efficient new/optimized product or process development will allow to reduce testing time and thus accelerate the time-to-market. Next to the considered use case, the expert system should also be usable for future cases. Additionally, the experimental design will allow efficient comparison of various raw materials, enabling well-thought decisions on which supplier material will fit best for developing the best product for a given customer. Furthermore, the developed expert system can guide the selection of a raw ingredient amongst different suppliers that is sourced from.

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Goals

Performing experiments in a smart, data-driven way, to be more efficient and have more knowledge. This includes the development of Artificial Intelligence (AI) models that can learn from old and/or new data-sets and can provide information on what settings and raw materials to use. In this framework, to make experiments even more efficient, different techniques could be implemented such as the use of optimal experimental design. The common goal is to have computational support when designing your experimental set and to do this more efficient and by gaining statistical knowledge.

The consortium believes that a combination of a proper analysis of historical data combined with efficient experimentation allows chemical companies to improve efficiency and to gain more insight in their products and processes.

- Use of large historical datasets as assistant for efficient experimental planning;
- Prediction of the right formulations in fast changing industrial environments;
- Shorten the time to market by doing smarter and less experiments by use of DoE.

Request

To complete the consortium, Catalisti is searching for additional industrial partners within the formulation industry with a specific case study in which many variables have an effect on the quality of the end product. Companies that do have historical experimental information can bring that information into the project as a starting point.

How to reply to this request

Please send an **email** to Mathias Jacobs (mjacobs@catalisti.be) and Aron Deneyer (adeneyer@catalisti.be), and **briefly describe your interest and potential contribution** to the project. Based on all offers, the current industrial partners will determine together with Catalisti which partners can join the consortium. After submission of your offer, you can be contacted to further elaborate your offer.

Important notice: Partners that wish to participate in Catalisti-supported projects are required to be member of Catalisti. For more information on membership and membership fees, please visit our website or contact Mathias Jacobs (mjacobs@catalisti.be).

Contact

Please contact Mathias Jacobs (mjacobs@catalisti.be) or Aron Deneyer (adeneyer@catalisti.be) if you have questions concerning this RfP.