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Request for Industrial Partners

Data-Driven Experimental Design for Efficient New Product Development in the Chemical Industries

Acronym: DOE

Project ID	
Type	ICON
Period	2 years
Starting date	TBD
Total project budget	TBD
Subsidy percentage	according to SBO and O&O regulations
Current industrial partners	confidential
Catalisti contact	Laura-Lynn Fockaert (lfockaert@catalisi.be)

Project description

Introduction

Providing customers the best possible quality is central to any business. In a world where both the customer's requirements as well as the raw materials to start from are constant, this is a one-time exercise. However, in practice this simplified situation hardly never holds and companies need to constantly experiment and re-optimize their products and processes to fulfil the customers high and challenging requirements. The knowledge that companies have acquired during many years of – performing experiments is a valuable starting point and allows them to answer the changing needs of customers with potentially changing raw material properties, shortages & legislation. While this experience-based approach has worked out in practice for many years, fast changing trends towards renewable feedstock, scarcity of raw materials and more severe legislation, require a more structured approach that would reduce testing time and thus would accelerate the time-to-market. Moreover, the knowledge gained through experiments needs to be secured in a solid way. The field of the Design of Experiments (DOE) exactly aims at gaining maximal information from a limited number of well-chosen experiments.

During the last decade, the DOE knowledge has substantially increased, and has come to a point where tailor-made experimental designs that take into account all possible constraints can be generated.

Additionally, most companies have performed extensive testing in the past, and the data generated can provide valuable insight if properly analysed. This analysis is not always straightforward, e.g. because data are stored in different data silos or are complex in nature due to the combination of continuous as well as discrete data points. Machine Learning algorithms tailored to the typical setting of the industry would allow companies to valorise these historical datasets. As such, a data-driven expert can lead to the partly replacement of intuition knowledge by data-driven knowledge. Furthermore, the generated insight can serve as prior knowledge when designing new experiments.

As such, we believe that the combination of a proper analysis of historical data combined with efficient experimentation will allow chemical companies to improve efficiency and will result in gaining more insight in products and processes.

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Goals

The goal of the project is to develop novel experimental plans that are tailored to the specific needs of the chemical industries (mixture of components, multi-stage, varying / different suppliers, changing ingredients (e.g. from petrochemical to biobased, …). This includes the development of modelling software that can learn from old and/or new data-sets as well as modelled data via group contribution techniques and can provide information on what settings and raw materials to use. In this framework, a deep analysis of historical data is combined with optimal experimental design and analysis tools that are tailored to the typical needs of the sector.

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.

The development of such a data-driven approach allows us to gain insights on the variables in feedstock, raw materials or process conditions on process/ formulation optimums for maximum product quality.

The transition to circular economy brings challenges. With the development of a custom-made data-driven approach, this project aims to prepare formulating and processing companies to these challenges. Special focus will go to how to tackle varying input parameters (for example raw material quality) when the end product needs to be of a constant quality. A possible formulation-related case-study is the examination of the potential of waste streams (e.g. mixed plastics, bio-based side streams, etc.), to be valorised as alternative raw materials in the formulation industry. An example of a more process-related case-study is solvent recovery, examining the required purity profiles to obtain high quality distilled-products.

Request
To complete the consortium, Catalisti is searching for additional industrial partners with a specific case study of which a list of (potentially) influencing factors can be defined to find optimal (process or product-related) quality. 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 Laura-Lynn Fockaert (lfockaert@catalisti.be) with Peggy Fredrickx (pfredrickx@catalisti.be) in CC, 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 Laura-Lynn Fockaert (lfockaert@catalisti.be).

> Gewijzigde veldcode

Contact
Please contact Laura-Lynn Fockaert (lfockaert@catalisti.be, +32 476 379 764) if you have questions concerning this RfP.