**Data-driven DoE**

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

## 1. Context

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 datapoints. 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 is developed, which results in the partly replacement of intuition knowledge by data-driven knowledge. Furthermore, the generated insight can serve as prior knowledge when designing new experiments.

Because of the above, we believe 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.

## 2. Goals

The development of 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.

## 3. Call for Interest

Consortium is open to more industrial partners with a specific case study of which a list of (potentially) influencing factors to find the optimal quality can be defined. Companies that do have historical experimental information can bring that information into the project as a starting point.

## 4. Budget estimation, Catalisti innovation program & project type

| Project ID | |
| --- | --- |
| Budget estimation | TBD |
| Catalisti innovation program* | Process Intensification and Transformation |
| Type of cooperation* | ICON |

## How to reply to this call

Please send an email before 5 April 2022 to lfockaert@catalisti.be and briefly describe your interest and potential contribution to the project. Based on all offers, the current industrial partners together with Catalisti will determine which partners can join the consortium. After submission of your offer, you can be contacted to further elaborate your offer. Please contact catalyst Laura-Lynn Fockaert (lfockaert@catalisti.be, +32 476 37 97 64) if you have questions concerning this call.

*Important notice: Partners that wish to participate in Catalisti-supported projects are required to become a member of Catalisti. For more information on membership and membership fees, please visit our website (http://catalisti.be/membership-2/) or contact Laura-Lynn Fockaert.*

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