

### WP3 Industrial Implementation

WP3 aims at providing the digital tools required for unlocking investment decisions. The chemical industry can be rather conservative and risk-averse when it comes to investment into disruptive flow technology. Having the capability of quantifying and communicating the commercial values and risks that will convince management to profit from innovation. In order to do so, it needs to be able to compare different value and supply chain scenarios that depend on many discrete and variable input parameters, whilst meeting the need to satisfy a range of criteria/desired outcomes. In WP3, we will also develop tools and concepts to support the implementation of modular flow reactors to allow greater flexibility in pilot and production facilities, and subsequent automation facilitated through AI.

Once R&D is completed and before the results of mini-pilot studies can be translated into commercial investment, a transparent decision-making process is required, based on *technoeconomic & sustainability benchmarking (OF7a)*, as well as considerations of industrial value and supply chains (*OF8*). This will require the integration of several aspects of a manufacturing process: technological (including yield and selectivity, solvent, safety), economic (including capital and operating expenditures), sustainability (including the carbon footprints, the raw material) and environmental aspects (e.g. solvent use and circular economy).

In WP3, we will develop *Digital Twins (OF7b)* to assess these criteria at various stages of the innovation chain, aiming to provide guidance at the many decision points throughout the entire R&D workflow, in which way to take forward research from the first synthetic lab experiments through engineering a pilot plant to the final decision of investing into a production plant. For example, a bench chemist would be advised on the implications of alternative synthetic routes on engineering a large-scale process, on implications on the cost of goods and sustainability, and on the impact on a future value and supply chain. The digital twin will calculate scenarios for different routes by combining the experimental data acquired in WP1 and 2, with reasonable approximations of missing data. A holistically informed R&D workflow will translate into reduced R&D cost and time-to-market and help in deciding early on, which process options for a desired product are best suited, e. g. batch vs. flow or world-scale vs. distributed scale. In the early stages of a R&D project the industrial innovation workflow must be carefully assessed to focus on relevant aspects. At the late stages of development, when sufficient information is available, we will apply these tools for benchmarking alternative processing options with the aim of providing a comprehensive package for an informed investment decision. Therefore, we will build on BASF's unique capabilities in sustainability benchmarking and combine it with academic know-how on Life Cycle Analysis (LCA) and technoeconomic analysis, providing opportunities for genuinely novel research.

*Value & supply chain optimization (OF8)*. The overall economic value and risk of a new production process requires a compelling business case to justify the deployment of an innovative processing concept. Supply chains must be optimized to find a globally attractive and resilient concept of providing a product, when and where it is needed, by considering the logistics of energy and feedstock to the production site as well as the logistics of the product to the customer. OF8 creates a graph-based digital twin of the value and supply chain. It will explore how machine learning can be used to suggest optimal decisions on future value and supply chains, and develop novel ways of transferring historic insight from other value and supply chains, e. g. through vector-based technology. It will consider risk management by placing a particular focus on the rigorous implementation of uncertainty in the models. When these methods have been demonstrated to work on a use-case, they will be applied to evaluate a novel concept to be developed in close interaction with OF 7b. In this way we could create a new business that would help in overcoming the "investment trap" and support the widespread implementation flow technology in a conservative industry.