

# Optimizing Chemical Formulations With Low Risk



Changing a successful product requires a certain amount of courage. Costs and benefits have to be weighed up against each other in order to make a sound decision. In the FORCE (Formulations and Computational Engineering) project, researchers at Fraunhofer ITWM are developing a system that supports such decisions.

Good decision-making is the objective of FORCE.

People are creatures of habit. If their favorite shampoo suddenly feels different, many people find this annoying and may switch products the next time they buy. “Companies do not easily change chemical formulations of successful products, whether that is in the cosmetics sector or in other industries,” says Dr. Peter Klein, a scientist in the “Optimization” field who is leading the FORCE project.

## Assessing consequences – making decisions

The objective of FORCE is to develop a Business Decision Support System (BDSS) specifically tailored to the optimization of chemical formulations. The software-based optimization and decision support system will cover the business processes of product optimization,

The FORCE project started in January 2017 and ended in March 2021 after extension. It is funded under the Leadership in Enabling Industrial Technologies LEIT pillar of the EU H2020 program.





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*Left: Ten international project partners were involved in FORCE – the entire team came together for the launch. Right: New scent, different feel? Changes in the production process must be well considered.*

development and quality control. In order to be as close as possible to the needs of the industry, case studies from three different companies with their specific products will be used: project partners are Dow Benelux (PU foams for thermal insulation), Megara Resins SA (PU-based liquids for paints, coatings or printer inks) and Unilever UK Central Resource Ltd. (shampoos).

“Production processes are complex. Anyone who intervenes in them has to take a great many parameters into account,” says Klein.

“Our platform is therefore designed to reveal to the user what which adjusting screws do and to show different options.” “Ultimately,” he says, “it is always a matter of finding the best possible compromises between goals that are in conflict with each other.” The system shows its users the best possible compromises on the basis of Pareto fronts.

### Interactive decision-making

For a decision strategy, you compare, for example, which substances can be changed in their concentration ratios and then receive results that need to be evaluated: “Then you have to weigh things up. For example, you compare production costs with quality,” says Klein, describing a typical dilemma. “We can support this process with interactive decision-making, for example, by simulating that the consistency of a shampoo changes due to the modification of attributes from the chemical process. On this basis, it is possible to decide whether the product will continue to meet the expectations of its target group and whether the production costs saved should be accepted for the noticeable change to the product.”

In addition, the BDSS also incorporates constraints, such as legislation or certain standard values that must also be changeable: If a regulation changes, the performance indicators in the formula must be renewed. For the software users, this means that they can repeatedly check an optimization problem including new constraints. “The same is true for price, when you match production and material costs with technical requirements: We can simulate different ingredients for the same result while checking the cost issue.”

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