OPTIMIZATION

Production plant for colored gemstones in the Optimization department: Colored gemstones are produced in a highly individual process, which considers aesthetic principles while working with absolute precisions of 10 – 15 micrometers even at maximal production volume. The design is modular and scalable.

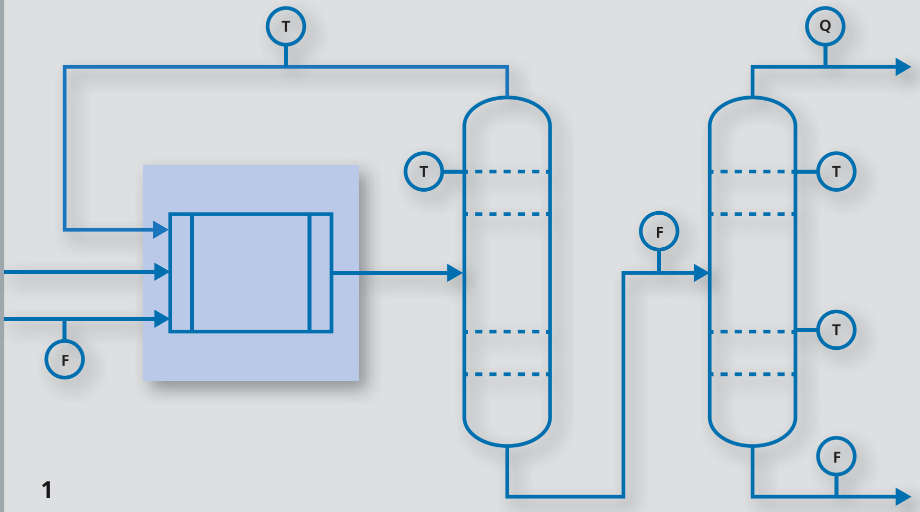
PROF. DR. KARL-HEINZ KÜFER
HEAD OF DEPARTMENT

Working in close cooperation with partners in research and industry, the department's main focus is to develop custom solutions for planning and decision making problems encountered in the logistic, engineering, and life science sectors. The work is characterized by a methodical approach to the interrelationships among simulation, optimization, and decision support. Simulation in this context refers to the construction of mathematical models while taking into account the design parameters, restrictions, and optimization of the quality and cost. The division's core competencies include the development and implementation of application and customer-specific optimization methods to calculate the best possible process and product designs. In the development and implementation of interactive decision support tools, we give special consideration to multiple criteria approaches and to the integration of simulation and optimization algorithms. In general, optimization is viewed not so much as a mathematical problem to be solved, but rather as a continuous process supported by the department's development of suitable tools. Our cooperation with customers in various industrial sectors ranges from consulting projects to the restructuring of decision making processes, but may also include the development of custom software for the optimization of complex processes and the creation of unique features.

MAIN TOPICS

- Medical therapy planning
- Arrangement and cutting problems
- Production planning and resource efficiency
- Process engineering
- Model learning and smart data
- Supply Chain Networks

Contact
karl-heinz.kuefer@itwm.fraunhofer.de
www.itwm.fraunhofer.de/en/opt



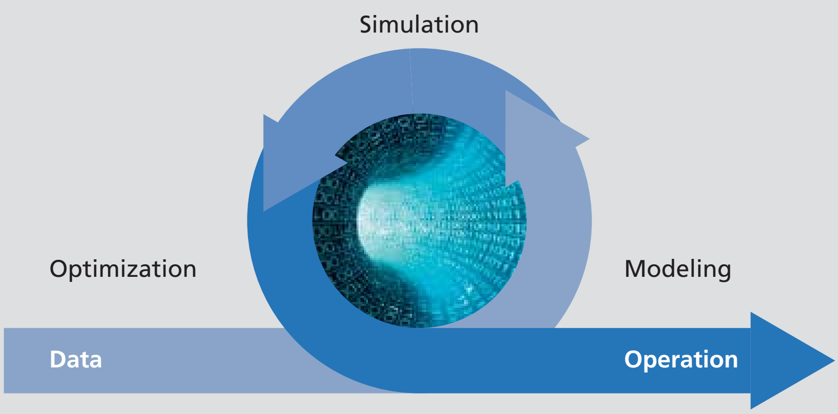
1

GREY BOX MODEL FOR COMPLETE PROCESS OPTIMIZATION

1 Schematic shows a flowsheet with a reaction unit for material transformation and two distillation columns for purification; the circles symbolize measuring points (T: Temperature reading, F: Flow measurement, Q: Measured cooling capacity)

The virtualization of chemical manufacturing plants in a model and the subsequent, model-based optimization are key steps towards innovation, as well as for efficiency and quality improvements. The success of this approach crucially depends on the reliability of the models. ITWM and BASF SE are developing, in a bilateral cooperation project, hybrid modeling methods that integrate physical-chemical know-how ("white") with data-driven approaches ("black"). The methods are used at the BASF flowsheet simulator so as to be available for the everyday work of the process engineers.

A typical chemical production process includes a chemical reactor for material transformations, with the educt from the reaction being fed into a purification process, for example, distillation. To model this process in a flowsheet simulator, not only is knowledge of the chemical reactions required, but also the thermodynamics to describe the distillation must be known. The situation where knowledge of the stoichiometries and reaction constants is incomplete is quite typical in industrial practice, whereas the distillation processes are well known. Besides this physical White Box knowledge, historical process data is available for a variety of measured operating points. The goal of the project is to generate information from the process data that can be used to close the gaps of the physical models. To this end, the first step is to replace the reactor with a simplified short-cut model, which contains – together with the purification model – all existing physical equations. The reconciliation performed using the model enable predictions that are as close as possible to the observed measurements for the real plant. A reconciliation consists of the minimization of a sum of squares, where the squared difference between model predictions and observed measurement points is as low as possible. Each term is weighted with the inverse variance of the measurement point. Since the variances are often vague and the adjustments to the various measurement variables are conflicting, this step includes not just one, but a set of reconciliation problems with optional user interaction. The result of this step is reliable soft sensor data about the inputs and outputs of the reactor. The second step consists of the identification of a model for the insufficiently modeled apparatus – in this case, the reactor – on the basis of the soft sensor data. Various methods are available, for example, regression methods with predefined functions, but also artificial neural networks with back propagation training. Quantitative statements about the confidence intervals and prediction errors are possible using statistical methods. In addition, the parameters for which only unreliable estimates exist can be separated from those that are identifiable with high accuracy. In a third step, the data-driven model from step 2 is inserted in the flowsheet to generate a complete model of the process. This is by no means a trivial step for several reasons: Besides ensuring the solvability of the whole system, the extrapolability for a complete process



2

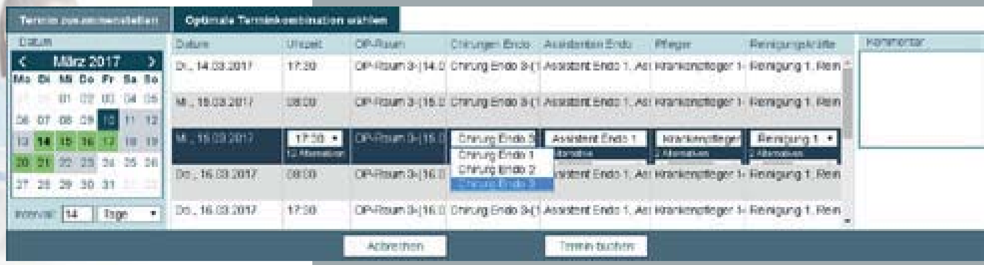
© www.istockphoto.de/Mike_Kiev

optimization must also be assured. This is carried out using optimization processes that not only account for the multi-criteria nature of the problem, but are also able to deal with uncertainties. These methods include robust and stochastic optimization.

The generally continuous uncertainty of the model parameters is described by a discrete selection of scenarios. The selection of the scenarios ensures the greatest possible representation of the uncertainties; strategies for statistical experimental design are available as are randomized approaches. The impact of these scenarios on the target function is calculated and quantified by means of sensitivity measures. The aim of robust optimization is the best possible design of the worst possible scenario. This optimization strategy is performed on a multi-criteria basis, taking into account the many competing objectives. Furthermore, the above mentioned sensitivity measures can be defined as target functions – in addition to those already provided – and minimized (for minimized sensitivity to uncertainties) or maximized (for maximized sensitivity, for example, when experimental design is important). In this way, it is possible to study the cost of a more or less sensitive process design relative to other business targets. Practical experience shows, in many cases, a relatively small adjustment to the process design is sufficient to achieve a significant improvement in robustness. If the uncertainty in the model's predictions is still too great after preparing the Grey Box model, a model-based, multi-criteria experimental design is developed where the data generated from the experiment is maximized while meeting other business targets to the fullest extent possible. An important next step is the fine tuning of the data-based methods to facilitate the integration of limiting conditions such as balance equations. This effects, for example, the topology of the artificial neural network being used. It is also interesting to see to what extent the White Box environment can ensure the reduction of confidence intervals that result from the data-driven model identification. This is especially important for process optimization under uncertain model parameters.

2 *Learning from data: Typical workflow with modeling, simulation, optimization, including data for near reality models*

© www.istockphoto.de/skynesher



1

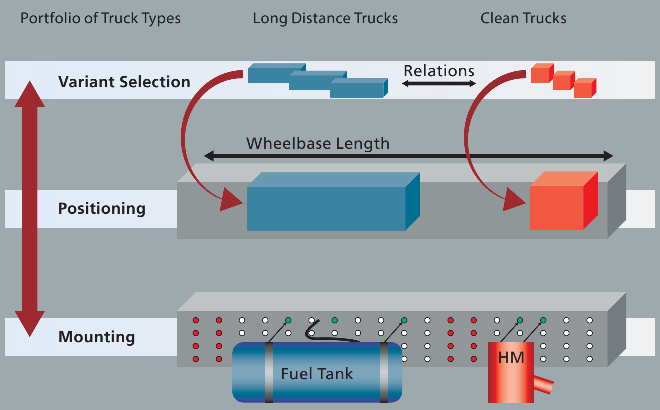
INTERACTIVE SURGICAL OP PLANNING ASSISTANCE

1 *Optimal schedules with subsequent corrections possible*

Modern operating rooms are a key factor, perhaps the dominant factor, in the cost calculation of a surgical intervention because of the increasingly expensive technical equipment. To economically operate a hospital with its own OR equipment, the goal is to maximize the utilization of the OR. From this perspective, a plan should be filled in with scheduled OPs in such a way that they span the whole day without any break inbetween.

On the other hand, OP planners face conditions and dependencies that make planning significantly more complicated. Surgeries may require special equipment that may not be available in every OR or is available only in limited quantities. Surgeons, nurses, and the patients themselves are limited by other appointments, vacations, or shift schedules, medical considerations may restrict the time of day, and after each surgery there has to be a free bed for the patient. One special challenge is the variation in the duration of surgeries: Even when an appendix operation is normally completed in 10 minutes, it can take much longer in case of unexpected complications. When planning on the basis of simple average values, substantial waiting times may occur, in the worst case operations may even be postponed to the next day.

As part of a European Fund for Regional Development project, the Optimization department is developing a software component for interactive assistance in operation scheduleplanning in cooperation with the software company Imilia from Berlin, which offers in its portfolio the software “Timerbee,” a planning and schedulingsoftware for the healthcare sector. The “OP Planner” toolcalculates smart planning suggestions for long term planning and the allocation of individual patient appointments, as well as a detailed schedule for the next day that takes into account all of the dependencies mentioned above, in addition to addressing the risk of delay by means of optimized sequences and a clever distribution of high risk surgeries to different operating rooms. An appointment request made in the OP Planner software is sent directly to the planning component developed at ITWM, which creates a mathematical model of the planning problem using the master data supplied by Timerbee. By Constraint Programming the solution space is explored and a manageable number of optimized and structurally different suggestions are presented to the user for selection and further interactive adjustment. Fast data connections and efficient implementation of the constraint search ensure user friendly behavior without any significant delays in the software.



1

2

VOLVO GTT CHASSISPACK: COMPLEXITY REDUCTION IN TRUCK CHASSIS PACKAGING

Volvo Group Trucks Technology (GTT) offer their customers tailor-made trucks specified by a combination of numerous truck design features (called variants) from which the customer can choose. All possible product configurations can potentially be manufactured, unless there is a documented reason explicitly forbidding it. On the one hand, this enables Volvo to offer trucks for varying customer needs; on the other hand, it results in a very large amount of potential truck configurations that has to be maintained.

Many combinations of variants that are not allowed together are documented explicitly with so-called restrictions in an engineering knowledge database. However, much of the knowledge required by engineers is documented only implicitly in the database, particularly since the set of explicit restrictions leads to new hidden rules. This makes it difficult to solve numerous truck design problems occurring frequently in practice. Whenever there is a change in the product, for example when a new technology has to be included, the engineers are responsible for ensuring that the change is valid for all of the implicitly defined truck configurations. To find engineering solutions to all possible, highly varying truck specifications at the same time makes this a complicated and tedious task. In the long-lasting cooperation between Volvo GTT and the department Optimization, a lot of case studies have been done yielding a suite of algorithms and Software tools for facilitating the work of the engineers. Currently, the algorithms are being developed as services that will be integrated into numerous tools used by engineers routinely.

For example, the latest service is designed for automatically inferring knowledge from Volvo's database that is hard to gain without the help of advanced algorithms. Hidden rules make it hard to find appropriate solutions if engineers can only rely on their experience. This algorithm is successfully used in the ChassisPack Hole Explorer that helps engineers to understand, which mounting holes on the chassis are used by which items. In one case study the tool made it easier to find vacant holes for an additional ground stud that was needed in a certain area of the chassis for new electrical function. A large portion of the total complexity of the truck development is related to the chassis. Therefore, several case studies resulted in a tool called ChassisPack Analyzer focusing on the chassis. This tool helps to conduct what-if-studies, for example for finding a reduced variant selection that approximates the "ideal" Pareto set of truck layouts. The chassis packaging is modeled as a 1.5D packing problem that uses a constraint programming solver for generating non-overlapping positions for truck items and maximizes fuel volume by choosing the largest feasible fuel tank variant.

1 *Parameterization of the truck chassis on different levels*

2 *Analyzing truck layouts with ChassisPack Analyzer*

TRIDEFF: SIMULATION OF TRIBOLOGIC PROPERTIES OF COMPOSITE MATERIALS

1 *Gearbox components: The heat generated at the surfaces from friction, in combination with a strong temperature dependent properties of thin, tribologically active films on these surfaces leads to a complex interaction of load spectra and material properties, which can hardly be analyzed using conventional experimental methods.*

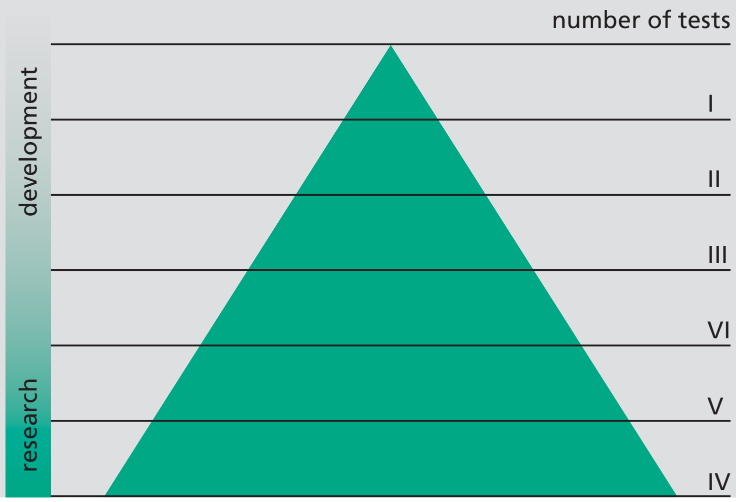
The energy transition and the constant price increases for raw materials create challenges for sustainable R&D focusing more and more on energy and raw material efficiency . This is especially true for components that are subject to friction and wear. For example, a typical vehicle experiences an energy loss of up to 35 percent because of friction. The branch of science that studies such systems is called Tribology.

Tribologic properties are generally system properties as load spectra and thermal balances of components are of critical importance. Generally, a large number of parameters can affect the behavior of tribologic systems. In material and component development, this makes it all the more challenging to draw conclusions about the actual behavior of the real tribological system based on tribological lab tests using standard component geometries.

The current practice, based on simple test setups like "pin-on-disc" or "block-on-ring," is to choose a material or preselected materials and, in the further course of development, refine the test setup in six categories, becoming ever more practice-focused down to field testing. At the same time, the selection of materials is further restricted and the number of required experiments is reduced, category by category.

TriDeff is a DFG sponsored project being carried out in cooperation with the Chair of Composite Engineering at TU Kaiserslautern. ITWM develops new optimization methods for a faster, targeted selection of friction reducing composite materials. The material class being studied is based on a polymer matrix material (PEEK), applied as a thin coating to the component surface. Dispersed throughout such matrix materials are fibers (for example, carbon or fiberglass), as well as micro- and nano particles. Since these inclusions are very small, the overall external surface of the material has homogeneous properties, which are strongly dependent on the distribution and orientation of the film and, correspondingly, the coating process. This is the reason why a model of the properties of the new composite must first be prepared so they can be characterized more quickly and their behavior under tribological stress can be predicted from their composition. The main focus is initially on mechanical strength (durability), thermal properties (conductivity and expansion) and other tribological characteristics.

In many cases, a targeted optimization of material properties is possible for specific application scenarios because of the high degree of flexibility in the composition and properties of the composite materials. However, in spite of this great flexibility, this optimization potential can hardly be explored by purely experimental methods. This is all the more true when the starting



material itself is complicated. The plastic (PEEK) used as the basic material in this project exhibits very strong temperature dependent properties, so the temperature balance in the overall system – being one of the key system properties – must be described with great accuracy.

One of the main aims of the ongoing development at ITWM in the TriDeff project is to "virtualize" the selection of the composition of a composite by means of the mathematical theory of homogenization, whereby combining the simple properties of all the individual materials that are aggregated in the composite can be used to predict the more complex behavior of possible variants of the composite material and optimize them for application-specific purpose. The overriding scientific objective of the project is a full description of the correlation between different categories of tribological testing with particular attention on the thermal balance, specifically, the relationships between Categories VI and V (Fig. 2). Finally, an FE model will be developed as a sort of digital demonstrator for Category V and experimentally validated at TU Kaiserslautern.

2 *Reducing the number of possible variants of a tribosystem by test category: Field testing on real systems, for example, long term studies in the automobile sector are used in Category I. Categories II, III, and IV (test bench with complete system, component, assembly) systematically applies requirements to Category I for the parts being tested. The actual material development takes place in Categories IV, V, and VI in the lab with simulated component surfaces or using simple test specimens.*