

Mathematical Optimization at BASF

- A Quarter Century and More... -

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Since the advent of computer, and PCs especially, in the 1970 and 1980, there was a positive climate towards mathematical methods at BASF. Mathematics and mathematical tools were used by various individuals or subgroups in departments to support analytics, the evaluation of experiments, or the description of reaction by differential equations – Mathematics was never strictly centralized at BASF.

The chemical industry is full of problems requiring a mathematical modeling *and* optimization background, *e.g.*, modeling of chemical reactions (parameter estimation in systems of stiff nonlinear ordinary or partial differential equations), the analysis of experimental data in pharmacokinetics, simulations on an atomistic or molecular level in material sciences or the optimal control of biotechnological reactors.

In 1990, the group *Systems for Chemistry* was founded focussing on problems as the ones mentioned above and as new fields of activities at BASF mixed integer mixed integer optimization and later on operations research in the more general sense were added, *e.g.*, blending problems, production planning and scheduling problems, supply network problems. These problems lead to linear programs, mixed-integer problems both linear and nonlinear which brings us also into the field of deterministic global optimization.

Nowadays, mathematical optimization is used in the area of supply chain management (SCM) for a wide range of strategic, tactical, and operational topics encountered at BASF, *e.g.*, to design the structure and size of its rail car fleet.

At BASF we have always followed the idea that in-house groups always keep the ability of solving difficult problems on their own although we also collaborate with research institutions where possible, in order to keep up-to-date with leading edge developments in academia. This independence and competence is important a) for keeping in reasonable contact and collaboration with research institutions in the area of mathematical optimization, but also b) to be able to assess the offerings of such institutions. Finally, there are c) also projects which are confidential and which cannot be communicated to the outside world. An additional advantages of this strategy is that the group as an internal unit can perfectly match its methodological knowledge with the specific application experience of our clients.

Consistent with this basic self-understanding of the group I have, for instance, developed polyhedral modeling and solution approaches useful to solve very difficult or large scale problems, or to compute optimal breakpoint systems to approximate nonlinear terms with a pre-given tolerance in otherwise mixed integer linear problems. When confidentiality aspects allow this, we also publish our solutions.