

Development of a sophisticated framework for complex single- and multi-objective optimization tasks

Matthias Leipold,^a Sven Gruetzmann,^a Georg Fieg,^a Dietrich Maschmeyer,^b Jörg Sauer,^c Holger Wiederhold^c

^aHamburg University of Technology, Schwarzenbergstr. 95, 21073 Hamburg, Germany

^bEvonik Oxeno GmbH, Paul-Baumann-Straße 1, 45772 Marl, Germany

^cEvonik Degussa GmbH, Paul-Baumann-Straße 1, 45772 Marl, Germany

Abstract

This work introduces a general framework for the global optimization of arbitrary single- and multi-objective optimization tasks. The framework covers the industrial demand on a user-friendly toolkit uniting arbitrary optimizations in one graphical user interface. The framework includes a stand-alone solver communicating over a free programmable interface with one or multiple instances of any simulation tool. The functionality of the framework is shown by two highly differing case studies. The first concerns the determination of intrinsic kinetics, carried out at our industrial partners the Evonik Degussa GmbH and Evonik Oxeno GmbH. The second addresses the multi-objective mixed-integer dynamic optimization of a middle vessel batch distillation including the startup. In both case studies the high flexibility of the framework, its easy setup and its robust optimization capabilities will be shown.

Keywords: robust optimization, evolutionary algorithm, industrial application, intrinsic kinetics, middle vessel batch distillation.

1. Introduction

In the last decade optimization tasks have become a crucial technology in industry. They are one of the main challenges in chemical and process engineering today since they bear an important part to save competitiveness of industrial companies [1].

Optimizations are important in all stages of product and plant life cycles. That means on the one hand regularly occurring optimization tasks e.g. concerning data regression for reaction kinetics, pressure loss correlations or thermodynamic properties like vapor pressure curves. On the other hand there arise extensive optimization problems concerning the modeling and design of whole processes. All these tasks imply complex optimizations including non-linearity, mixed integer problems, dynamic optimizations, structural complexities, boundary conditions or multiple objective functions.

In general there are solution methods available for all kinds of optimization problems. These were mainly developed for academic purposes. Today many common engineering programs utilize these developments with user-friendly graphical user interfaces (GUI). However, integrated solution methods often are limited to few optimization tasks with a fixed structure. They lack the possibility to freely setup more complex jobs. By contrast there are comprehensive mathematical toolkits available offering a great freedom to setup models and optimization tasks. Anyway, these programs usually are missing a user-friendly GUI.

The objective of this contribution is to provide a sophisticated framework for all kinds of single- and multi-objective optimization tasks including an easy to use GUI and usage of arbitrary simulation toolkits.

2. Optimization framework

The framework consists of four major elements as shown in Figure 1. The first one covers an evolutionary algorithm (EA) as solver that is provided in a single-objective and a multi-objective implementation. As second element an arbitrary simulation tool with the possibility of remote access is applied. The third element comprises a suitable communication interface for the formulated problem. Finally the fourth element is a GUI covering all other parts in an optimization.

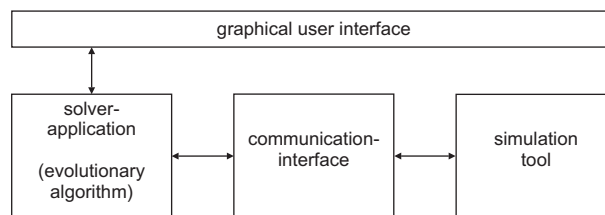


Figure 1: Communication structure of the optimization framework

2.1. Solver algorithm

For the solver algorithm an evolutionary algorithm (EA) was chosen. This is for two reasons. First and most important, an EA is not specialized on any kind of problem (e.g. NLP, MINLP or MIDO) [2]. Furthermore, it can perform global optimizations while it is independent of initial values [2]. For single-objective optimizations the Modified Differential Evolution (MDE) algorithm by Angira and Babu is applied and for multi-objective optimizations the non-constrain-dominated sorting MDE presented by Gruetzmann et al. was chosen [3-5].

Besides the EA other more specialized and thus faster solvers can be implemented. Main restriction is that the only information available about the used simulation are input and output values. Accordingly the mathematics of the optimization is fully unknown to the solver.

The chosen EA as a general solver is implemented in Visual Basic for Applications (VBA) with the GUI realized in MS Excel. This platform was chosen for two reasons. First, MS Excel is a well known and accepted standard in industry and research. Moreover, most commercial and free simulation tools available comprise communication protocols to VBA or MS Excel.

2.2. Simulation tool

Within the framework any simulation tool can be applied. Although it is part of the framework, it is independent of the solver and the frameworks GUI to maintain a standardized working flow within the tool. Precondition for the usage of a software as “simulation tool” in the sense of the framework is a suitable remote access. The given minimum requirements are that at least the necessary input parameters may be changed externally (e.g. by manipulation of a project file), a simulation can be automatically

started and run without any user input (e.g. run by a shell command) and the solution parameters can be read from the finished simulation (e.g. read from an output file).

2.3. Interface

The communication interface is the main part of the framework. It establishes the high flexibility for the setup of simulations since any required external program call supported by the simulation tool is executable. There are no restrictions concerning the type of variables. Even parameters changing the simulation structure are possible.

The communication interface, like the solver-algorithm, is implemented in VBA. It is completely freely programmable. This assembly offers a wide range of possibilities. Besides optimizations of a single process it is quite easy to set up more complex scenarios. For example the sequential usage of different simulation programs is imaginable to combine separately developed process elements in a plant wide optimization. Another example is the simultaneous optimization of more than one simulation dependent on the same input parameters as shown in case study one.

To fulfill the request of a user-friendly GUI it is possible to build graphical communication interfaces for different programs without the loss of flexibility. For the industrial standard process engineering programs Aspen Plus and Aspen Custom Modeler suitable graphical communication interfaces were developed and can be used for a fast and easy setup of optimizations. For usage of the chemical engineering program Presto Kinetics a similar interface was set up.

3. Case studies – examples of successful application

The optimization framework has already been successfully applied to multiple optimization tasks. In this contribution two of them will be presented. First is a single-objective optimization from our industrial partners (Evonik Degussa GmbH and Evonik Oxeno GmbH) for the determination of complex intrinsic kinetics. The second one concerns a multi-objective optimization of a multi-vessel batch distillation.

3.1. Determination of intrinsic kinetics

The first case study considers a single-objective non-linear global optimization for the determination of complex intrinsic oligomerization and isomerization kinetics based on a multitude of measurements at different process parameters. It was performed in a survey of our industrial partners the Evonik Degussa GmbH and Evonik Oxeno GmbH. For simulations a steady-state model realized in Presto Kinetics was applied. Next to the actual intrinsic kinetics it incorporates the description of several physicochemical mechanisms as for example catalyst activity, inhibition or different reaction pathways.

The optimization task was set up using a least square formulation as objective function, validating the model versus measurements. In one run measurements of up to ten different operating conditions varying in temperature, pressure, reactant concentration and the properties of the catalyst fixed-bed were optimized simultaneously. The objective function is directly dependent on the measured ($w_{M,i}$) and calculated (w_i) mass fractions. Whereas, the calculated mass fractions are dependent on activation energy, pre-exponential factor, inhibition constants, distribution constants etc. which will be summarized in the mathematical formulations by \underline{x} . Additionally the set up task is

constrained by boundary conditions g , the reaction model, and h , parameter boundaries, to a priori exclude physicochemical improper model parameterizations. The optimization problem can be formulated as follows:

$$\text{Min: } F(\underline{x}) = \sum_n \left[\sum_i \left[(w_{M,i} - w_i(\underline{x}))^2 \right] \right] \quad (1)$$

subject to:

$$\underline{g}(\underline{x}) = 0 \quad (2)$$

$$\underline{h}(\underline{x}) > 0 \quad (3)$$

where n is the number of simultaneously optimized operation conditions and i the number of measured data points at each operation condition. For the optimization task a communication interface was set up. It is based on an application object provided by Presto Kinetics offering routines to read and write parameters and to run the model. To automatically assign the measured data to Presto Kinetics, the communication interface includes routines to create the required data files for the model. Additionally the capability for the sequential run of a predefined number of simulations was implemented.

The result of the optimization is a set of model parameters independent of the process conditions. With these parameters a multitude of measured data can be described reliably. In Figure 2 an example of measured data and the appropriate calculated profiles along the fixed bed length is shown. It can be seen that the optimization setup in the framework is well capable of finding a sufficient set of model parameters, incorporating the boundary condition of a physicochemical acceptable model.

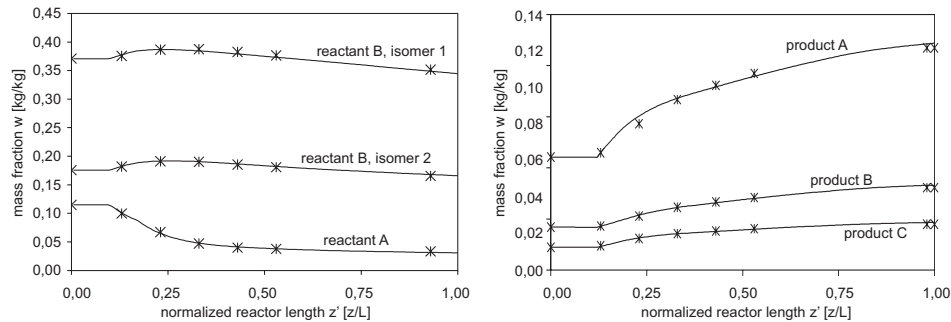


Figure 2: Reactant and product mass fraction profiles along the fixed-bed.
measured data point: X; calculated profile: —

3.2. Design and control of multivessel batch distillation

The second case study discusses the multi-objective mixed-integer dynamic optimization of a middle vessel batch distillation column. For that purpose a rigorous process model in Aspen Custom Modeler by Gruetzmann and Fieg considering the start-up phase of the process was used [6].

The objective was to perform an optimization of investment (IC) and operation costs (OC) for an investment decision. To overcome the problem of an a priori decision for the tradeoff between IC and OC a multi-objective optimization was performed. Whereas, OC is a function of time dependent operation parameters \underline{u}_O while IC is a function of design parameters \underline{u}_D . The simulation is additionally constrained by a given demand of purity. A mathematical formulation of the optimization task can be written as follows:

$$\text{Min: } OC = f_1(\underline{u}_O, t) \wedge IC = f_2(\underline{u}_D) \quad (4)$$

subject to:

$$g(\dot{\underline{x}}, \underline{x}, t, \underline{u}_D, \underline{u}_O) = 0 \quad (5)$$

$$w_i \geq w_{\min} \quad \forall i = 1, 2, 3 \quad (6)$$

$$h(w_i) = \sum_{j=1}^{N_{\Delta t}} \Delta w_{i,j} \geq 0 \quad \forall i = 1, 2, 3 \wedge j = 1, \dots, N_{\Delta t} \quad (7)$$

where g is the dynamic process-model, $\dot{\underline{x}}$ and \underline{x} are the time dependent and independent state variables and w is the mass fraction of a component.

For the optimization a communication interface based on the Aspen Custom Modeler application object was implemented. The interface incorporates reading and writing of parameters, remote control for running the simulations including full error handling and routines for the manipulation of the simulation structure (e.g. creation of additional internal tasks). An interaction structure of the framework including the Aspen custom Modeler communication interface is given in Figure 3.

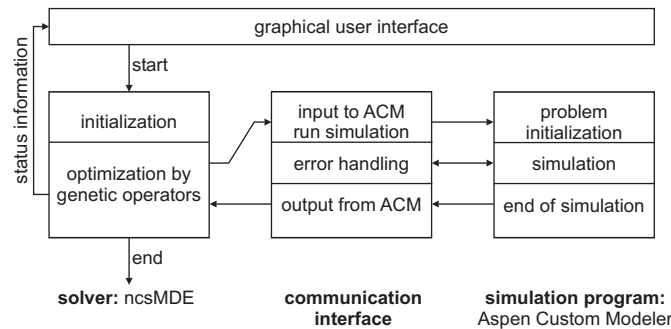


Figure 3: Interaction structure of the optimization framework including ncsMDE-Aspen Custom Modeler communication interface

In the case study an industrial scale distillation column for the separation of a mixture of 400 kg each of hexanol, octanol and decanol subject of product purity of at least 99 % was performed. In order to assure a reasonable vapor load, the reboiler duties has been set to 200 kW.

Illustrated in Figure 4 are the pareto-optimal solutions, that are the best tradeoffs between OC and IC. Shown is generation 2163 this is when the optimization was aborted since no further improvements could be achieved. Also shown are second best (2. Front) and third best (3. Front) tradeoff solutions along with a front of reference points calculated using a temperature control. In the second diagram of Figure 4 the solver efficiency is shown by means of mean violation of constraints. Started at high constraint violations due to the randomly chosen initial values, constraint violation is rapidly decreasing. This once again shows the effectiveness of the solver and the framework.

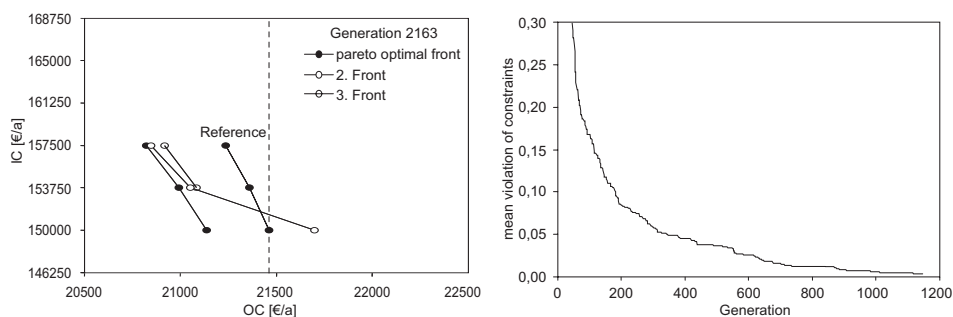


Figure 4: pareto-optimal solutions of case study two and efficiency of optimization

4. Summary and Conclusions

In this contribution, for the first time, a sophisticated framework incorporating a user-friendly graphical user interface combined with a robust solver for arbitrary optimization tasks has been presented. In two highly differing case studies the efficiency of the framework could be shown. The framework or more precisely the communication interface was easily adapted for different programs and various structural setups. The used evolutionary algorithm was shown to reliably solve single- and multi-objective optimization tasks including mixed integer non-linear tasks as well as mixed integer dynamic optimizations. The presented framework is a reliable and easy to handle tool for the application on further optimization tasks.

References

- [1] L.T. Biegler and I.E. Grossmann, *Comp. Chem. Eng.*, 28 (2004) 1169
- [2] K. Deb, *Multi-Objective Optimization Using Evolutionary Algorithms*, Wiley, Chichester, 2004
- [3] R. Angira and B.V. Babu, *Proc. ICAI-07*, (2005) 911
- [4] S. Gruetzmann, M. Leipold, G. Fieg, *Proc. ESCAPE17*, (2007)
- [5] M. Leipold, S. Gruetzmann, G. Fieg, *Comp. Chem. Eng.*, (2007) (submitted)
- [6] S. Gruetzmann and G. Fieg, *Ind. Eng. Chem. Res.*, (2007) (accepted)