

TITLE STORY // MODEL CALIBRATION

CALIBRATION OF FIELD DATA AND SIMULATION AS AN OPTIMIZATION TASK WITH SIGNALS

Methods of sensitivity analysis and optimization with optiSLang can be used to improve a system design by understanding and validating its characteristic signal responses.

Introduction

Signals are characteristic system responses that are critical in helping to understand, validate and improve the physical model of the system, as well as the system design itself by understanding the important parameters. Here, calibration means using field observations and simulation runs in order to estimate simulation model parameters or to update the uncertainty regarding these parameters. This can be formulated as an optimization task where the output parameters are signals and the target function is, for example, the sum of the square deviations of the signal from the testing and the signal from the simulation. The optimization task of identifying the right input parameters can then be formulated, for instance, to minimize the value of the target function by selecting the appropriate values for the input parameters. A simple example, however, shows that this can lead to a non-unique solution for the input parameters. Therefore, additional boundary conditions for the calibration can be very useful.

Knowing from the calibration the significance and sensitivity of input parameters, further optimization can be used to improve the system or product design. With the informa-

tion from the calibration, the design space can be adapted and appropriate surrogate models can be used that also respect nonlinear system behaviour.

In the case of strong scattering of test and/or simulation results, the identification task must be enhanced by stochastic analysis as the fit of single signals by design variables are no longer sufficient. Then, a parameter space has to be used where the input variables also have stochastic elements, like a stochastic distribution.

The technique of identifying the input parameters within an optimization task for the calibration of field data including measured signals and signals generated from the simulation can be used across all industries where virtual prototyping is important.

This article will give a first introduction and discusses some methods and measures used for sensitivity analysis and optimizations. The parameter identification as a special optimization task will be also shown by using two theoretical examples followed by three industrial applications. One of them will be explained in detail.

Model Validation and Calibration with the Parameter Identification as an Optimization Task

Optimization using numerical simulations can, in general, be classified into two different categories: the first category is associated with the target to improve the functionalities of the product and the second category is to test and improve the model to more appropriately fit with the reality (Fig. 0).

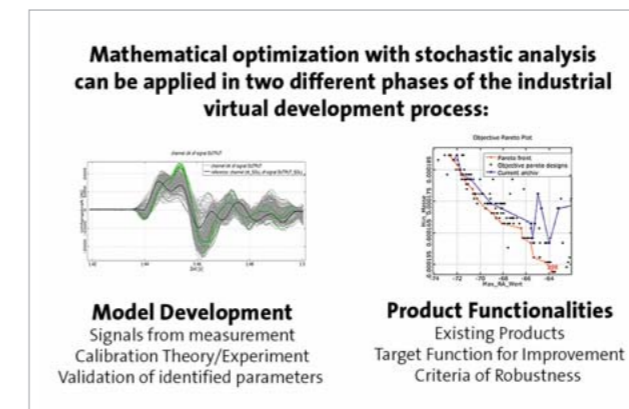


Fig. 0: Model calibration and improvement of product functionalities

While optimization has been already in wide spread usage for the improvement of product functionalities, the potential for the usage of similar optimization techniques to improve the quality of the model, typically with parameterization and calibration, is often not exploited.

The workflows that are used for the calibration of a model are similar to those used for the improvement of functionalities of the product. In both cases, it is recommended to start with a sensitivity analysis, especially when handling with a large number of parameters. A sensitivity analysis is used to study which input parameters have significant importance for which output parameters. These studies are also used to establish a meta model that approximates the output parameters as functions of the input parameters. This step can help to reduce the design space to the important parameters. For the criteria of importance of parameters and quality of the meta model, different statistical measures have been established. It is important that these meta models also include nonlinear dependencies of the parameters and that the prognosis quality is quantified. For the quantification of the quality of prognosis of such a model, the Coefficient of Prognosis, CoP, is introduced. With these CoPs, a nonlinear meta model can be selected that provides not only the best fit for the data but also the best model with respect to the ability for the best prognosis. Trying to only provide a model that best fits the data can lead easily to an overfitting and incapability of explaining further data. The model, based on the best CoPs, is the Metamodel of Optimal Prognosis, MOP. A typical workflow for the optimization of product functionalities is shown in Fig. 1. After the definition of the Design Space

X (the parameterization) and during the design of experiment (DOE), designs with different input parameters X_i are created. These different designs are solved, generating the values for the output parameter Y_i . These data samples can be used to establish the MOP, that can significantly reduce the design space to the important variables X_{red} , including nonlinear dependencies. Also, from the sensitivity analysis

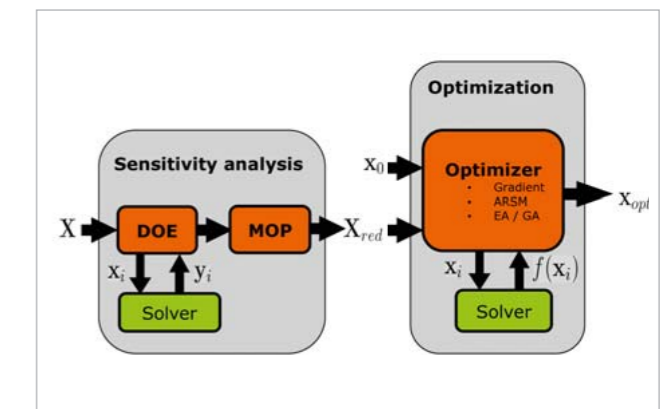


Fig. 1: A typical workflow for an optimization, starting with a sensitivity analysis for selecting the important parameters, followed by the optimization

a sufficient initial parameter set X_0 is selected for optimization. Here, it is necessary to define at least one optimization function $f(X_i)$. Several optimization methods are available like gradient based, adaptive response surface, or evolutionary and genetic methods. Finally, an optimized set of input parameters X_{opt} is found.

The workflow for the calibration can be similar. A difference to the measurements, i.e. the sum of squared deviations of measured and calculated data for the corresponding time steps, is used as an optimization function. The identified parameter set is then the optimized set of input parameters X_{opt} .

Two theoretical examples

There are not many optimization tools available that can handle different field measurements, i.e. time series for a pressure. Also, in general, they do not have the ability to include signals efficiently from the real test environment which is necessary for the target function of optimization. This is one of the main reasons that the potential of using optimization for parameter identification has not yet been fully exploited.

During the development of such a simulation model, the parameterization is the key to ensure its realistic behavior. The first example is a simple damped harmonic oscillator. This can be used to understand how signals can be handled. The example also illustrates that different optimization runs can lead to quite different parameter values. This is due to the fact that the solution can be realized with different values of the input parameters.

The basic input parameters for the calibration of the damped oscillator are the mass m , the initial kinetic energy E_{kin} , the damping c and the stiffness k (Fig. 2).

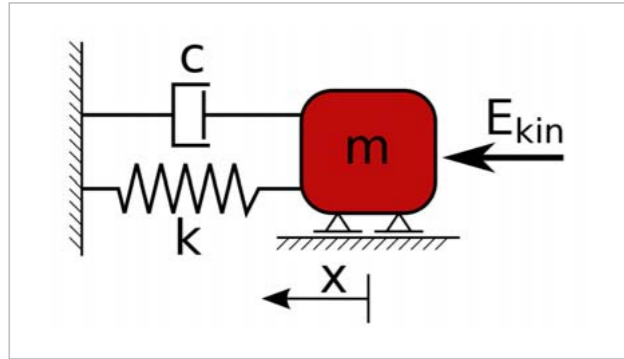


Fig. 2: Damped harmonic oscillator

The reference signal is taken from the displacement x over time for some parameters that are unknown in this example (Fig.3, red curve).

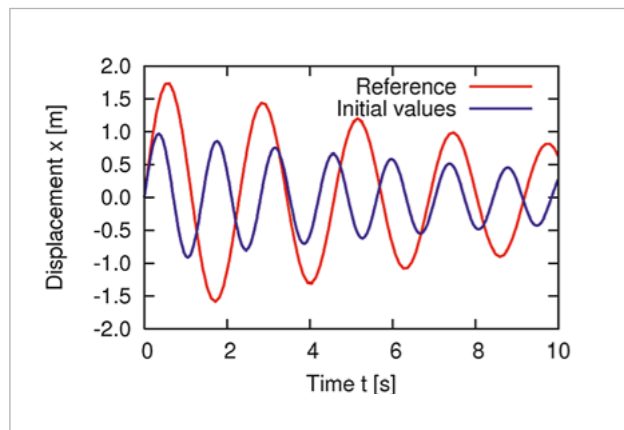


Fig. 3: The reference signal and the signal calculated from the initial values

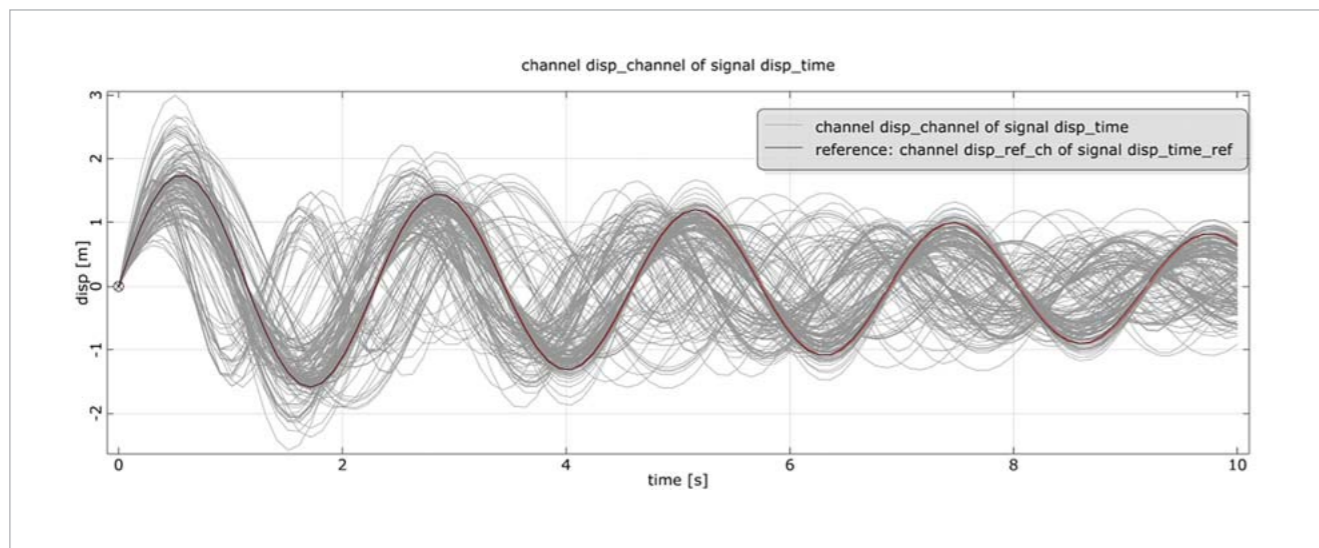


Fig. 4: The reference signal together with all signals from the sensitivity analysis

Equations for the damped oscillator:

$$m\ddot{x} + c\dot{x} + kx = 0$$

$$\ddot{x} + \frac{c}{m}\dot{x} + \frac{k}{m}x = 0$$

$$\ddot{x} + 2D\omega_0\dot{x} + \omega_0^2x = 0$$

Analytic solution for the displacement:

$$x(t) = e^{-D\omega_0 t} \sqrt{\frac{2E_{kin}}{m}} \frac{1}{\omega} \sin(\omega t)$$

Undamped eigen-frequency ω_0 :

$$\omega_0 = \sqrt{\frac{k}{m}}$$

Lehr's damping ratio D :

$$2D\omega_0 = \frac{c}{m}$$

Damped eigen-frequency ω :

$$\omega = \omega_0 \sqrt{1 - D^2}$$

The target for the optimization is to identify input parameters that generate a signal very close to the reference signal. Therefore, the objective function is the sum of squared differences between the displacement of the reference x^* and the displacement of the calculated solution x at n discrete time steps. Signals are generally discretized due to the measurement.

$$f(m, k, D, E_{kin}) = \sum_{i=1}^n (x_i^* - x_i)^2$$

The sensitivity study for this case shows that all input variables are significant. Thus, all signals from the designs of the design of experiment were processed during the sensitivity study. Illustrating the solutions for all these initial parameters, as shown in Fig. 4, often already provides an understanding of interesting frequency ranges for real world applications. Furthermore, some information are given about the feasibility of the parameter identification itself.

Running different optimizations lead to different sets of initial parameters as shown in Fig. 5.

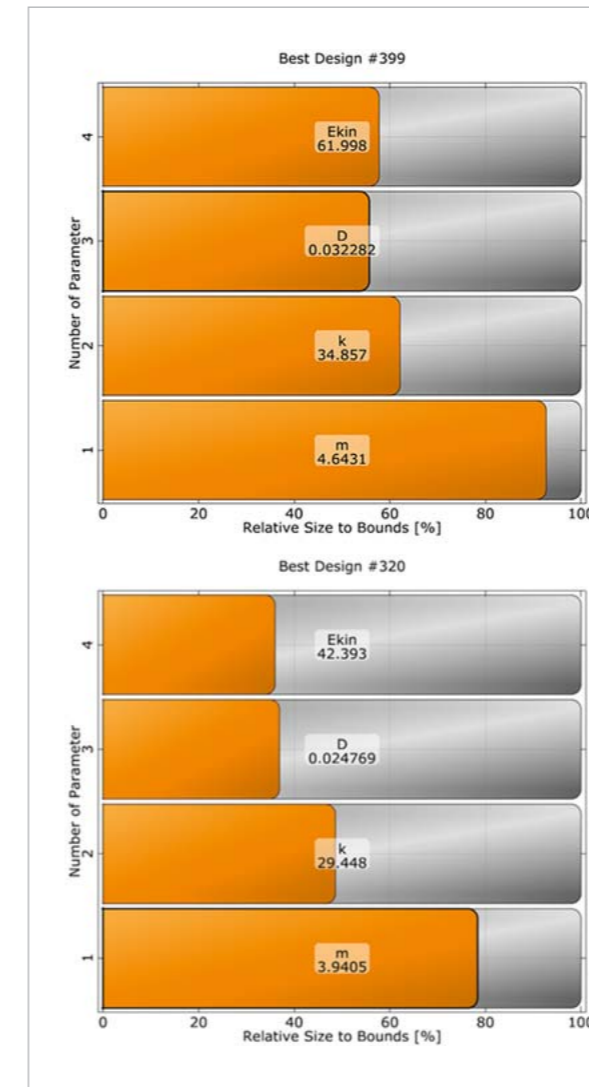


Fig. 5: Two different optimizations lead to rather different identified parameter values

Here, despite the different values for the parameters, both optimization runs lead to sufficient results showing only small differences compared to the reference signal (Fig. 6).

This non-unique solution for the identified parameters is due to the fact that the parameters E_{kin} and m , as well as m and k appear only pairwise in the solution for the displacement. It is only their ratio that matters for the solution.

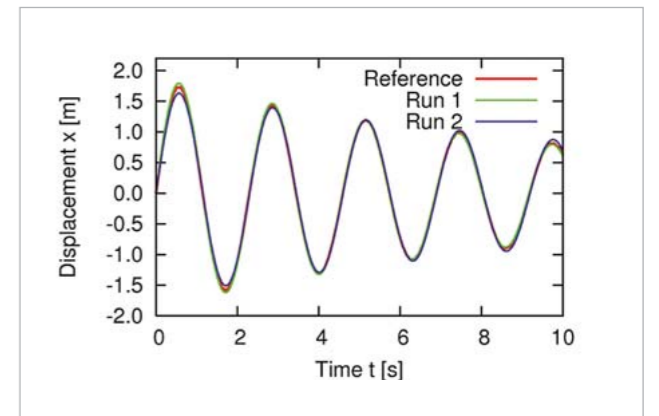


Fig. 6: The identified parameter values from both optimizations lead to a sufficient approximation of the reference signal

Therefore, a unique solution can be generated by having, for example, a constant mass value for the optimization. This example is shown in more detail also for training purposes with signals in an optiSlang tutorial available from Dynardo and currently included in the software delivery. The second example is a simplified CFD test model where a reference vector of the 12 outflow velocities exists. The optimization task is to find the set of 10 input parameters for the pressures (Press_1 ... Press_10) that come close to the outflow velocities (Fig.7).

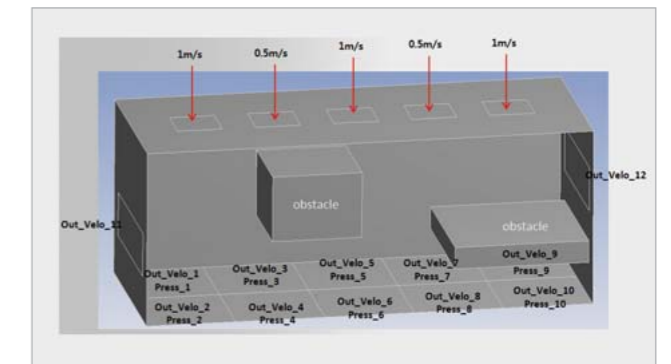


Fig. 7: A CFD example of a box with two obstacles

The optimization function to minimize, similar to the signal function for the damped harmonic oscillator case, is the squared deviation of the reference velocities Ref_Velo_i and the velocities Out_Velo_i from the calculated solution:

$$\sum_{i=1}^{12} (Ref_Velo_i - Out_Velo_i)^2$$

Also, in this case it is important to have additional constraints. It was chosen that each output parameter is close enough within 10% of the corresponding reference output parameter:

$$abs((Ref_Velo_i / Out_Velo_i) * 100 - 100) < 10$$

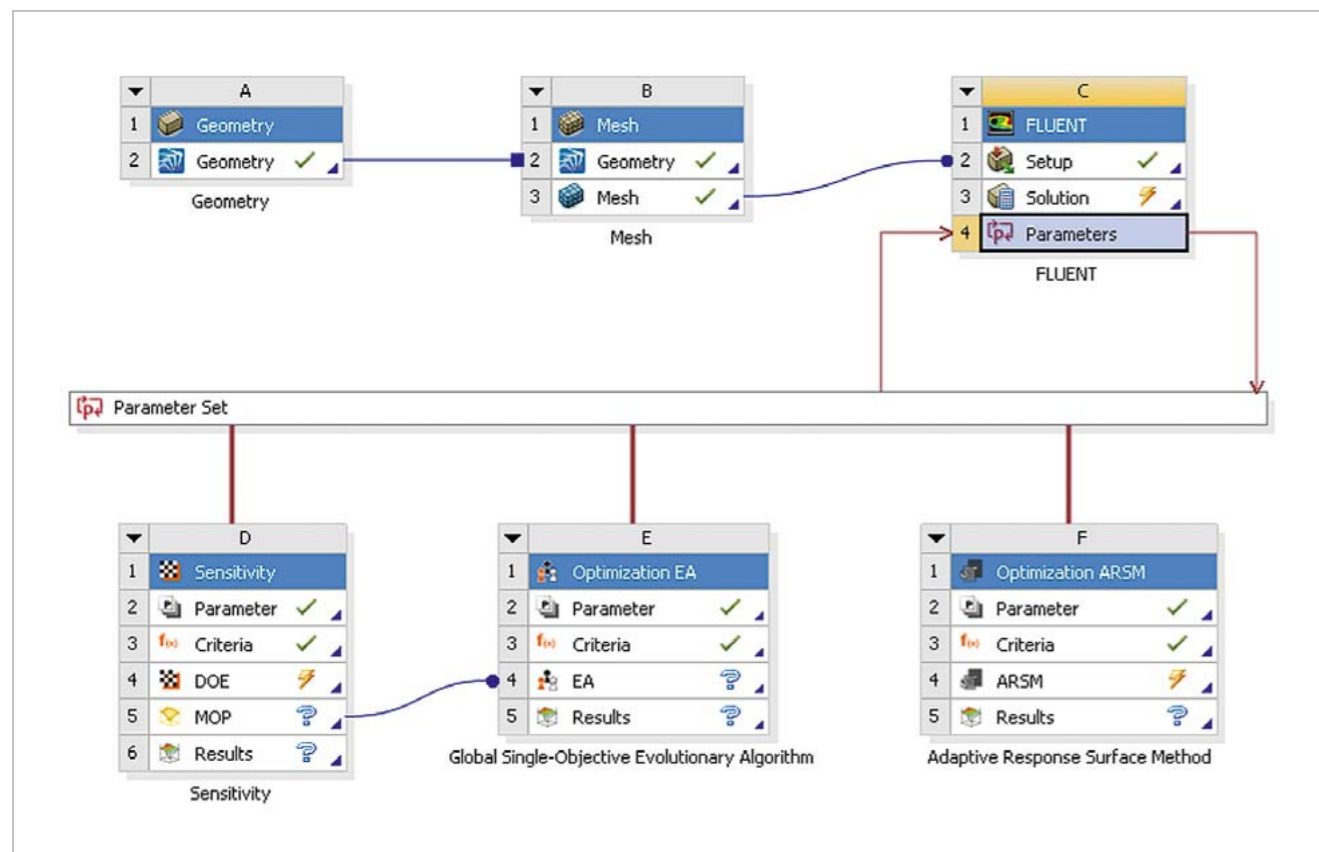


Fig. 8: The ANSYS Workbench set up with optiSlang inside ANSYS Workbench for the CFD example of a box with two obstacles

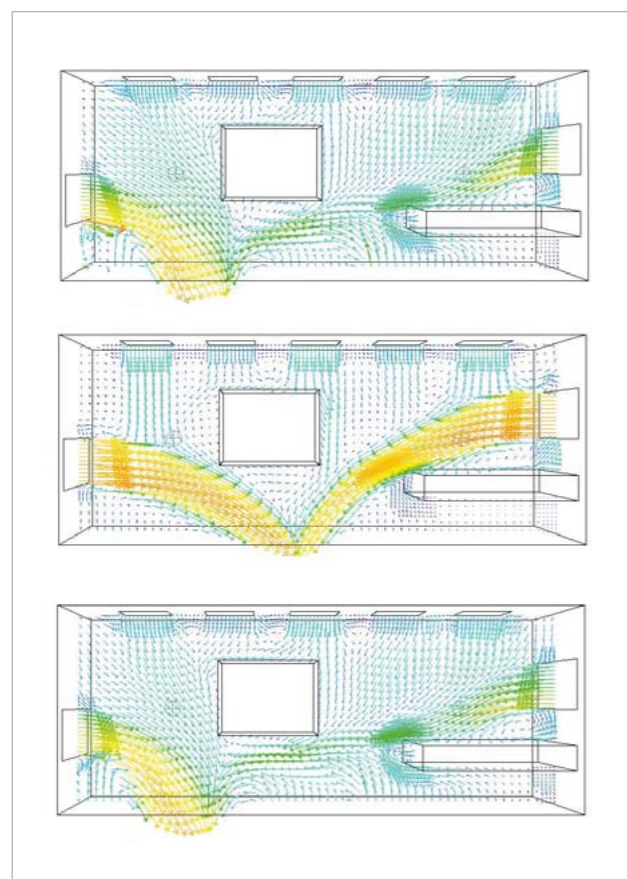


Fig. 9: Reference solution (top), initial solution (middle) and optimized solution (bottom) showing the velocity vectors colored by velocity magnitude

This problem was solved with optiSlang inside of ANSYS Workbench. The complete workflow is shown in Fig. 8. The solution was found with an Adaptive Response Surface Method. In general, this method is recommended for a small number of continuous input parameters (Fig. 9).

Practical Applications

The field of practical applications for model calibration by parameter identification cover a broad range. Some publications are available from the online library of Dynardo, showing applications from different industrial areas like civil engineering (Zabel and Brehm, 2008), automotive (Will, 2006) and oil & gas (Will, 2010). In this article, the focus will only be on two applications with signals, some progresses we have made for an NVH automotive application and a new model calibration for a nuclear waste depository analysis.

Calibration and Optimization of Driving Comfort Behaviour

In product development of luxury cars, Noise Vibration Harshness (NVH) plays a very important role. Driver, co-pilot and passenger on the back seats should feel very comfortable during any driving conditions. Therefore, the calibration of virtual models to available test data and the reduction of noise levels inside the car cabin is an important task of the virtual prototyping. For the formulation of a successful calibration design space as well as a successful objective function, two challenges need to be met. First, a very large

number of variables may have an influence on the passenger car air vibration. Second, the frequency signals show a very large number of vibration modes. As a result, the selection of the main influencing parameters and the signal processing to extract response values which belong to one vibration mode are a very important part of the calibration process. In the example, we start with a variation space of 485 sheet metal thicknesses of all body parts which might have an influence. Fig. 10 shows the variation of one of the sound pressure signals of 200 Latin Hypercube samples of the sensitivity analysis (Fig. 10).

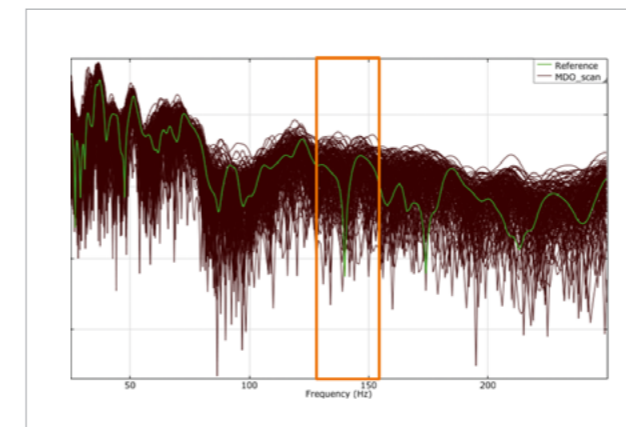


Fig. 10: Variation of sound level, green – reference, black – 200 samples of the sensitivity analysis

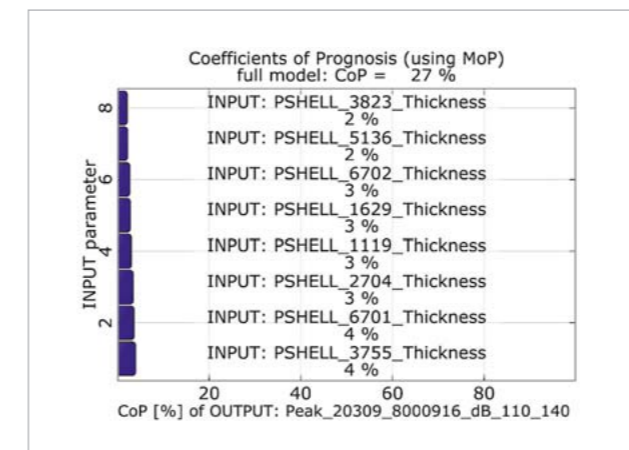


Fig. 11: CoP value of the peak sound level in the frequency window 110 to 140 Hz, sensitivity study using 485 variables

Having the signal variation window, the frequency window was defined to extract the peak sound values which correspond to the vibration mode of interest. Note that because of stiffness variation, the frequency and the sound value are varying at the same time and we need to adjust the extraction windows to avoid mode switch of important vibration modes within one extraction window.

Unfortunately, the CoPs for the variation of the peak sound level are below 30%, which indicate that only the impor-

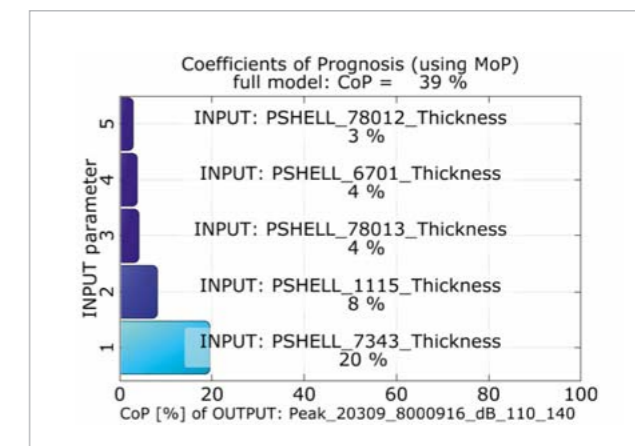


Fig. 12: CoP values of the peak sound level in the frequency window 110 to 140 Hz, sensitivity study using 37 variables

tant variables for less than 30% of the total variation were identified. It is our experience for this kind of identification task, that increasing of sampling to 300 or 400 designs or alternative extraction windows does not increase the CoP levels significantly. The main reason for the small CoP levels is that the pressure sound levels are influenced by mechanisms of 10 to 20 variables. To identify these mechanisms out of 500 variables, a very large number of sample points will be necessary (Fig. 11).

Therefore, the CoP values from the first sensitivity analysis were used to reduce the design space manually. Those 37 variables were selected which showed significant CoPs for any of the response values of interest and repeated the sensitivity study in the reduced design space. At the second sensitivity study using 37 variables, the variation interval of the peak value within the frequency window 110 to 140 Hz is 80% compared to the first sensitivity study using 485 variables. That approved the CoP based selection of important parameters. In the reduced space, higher CoP values of the full model are close to 40% and higher CoP values of single variables are identified (Fig.12).

Within the reduced design space of 37 important variables, the main contributors could also be identified for the other important frequencies and positions. Furthermore, the calibration to the reference signal was performed successfully. Of course, after having a model which shows sufficient forecast quality to measurements, the next step in the virtual prototyping will be the optimization. Here, the minimization of peak sound pressure levels is shown in Fig. 13 (see next page).

Calibration of a Nuclear Waste Depository Model

During the research for the safeness of nuclear waste depositories, heating experiments are performed in underground laboratories in order to understand the thermal-hydraulic-mechanical (T-H-M) interactions. In these experiments, the change due to the heat energy input over time of temperature, pore water pressure and stress fields are measured.

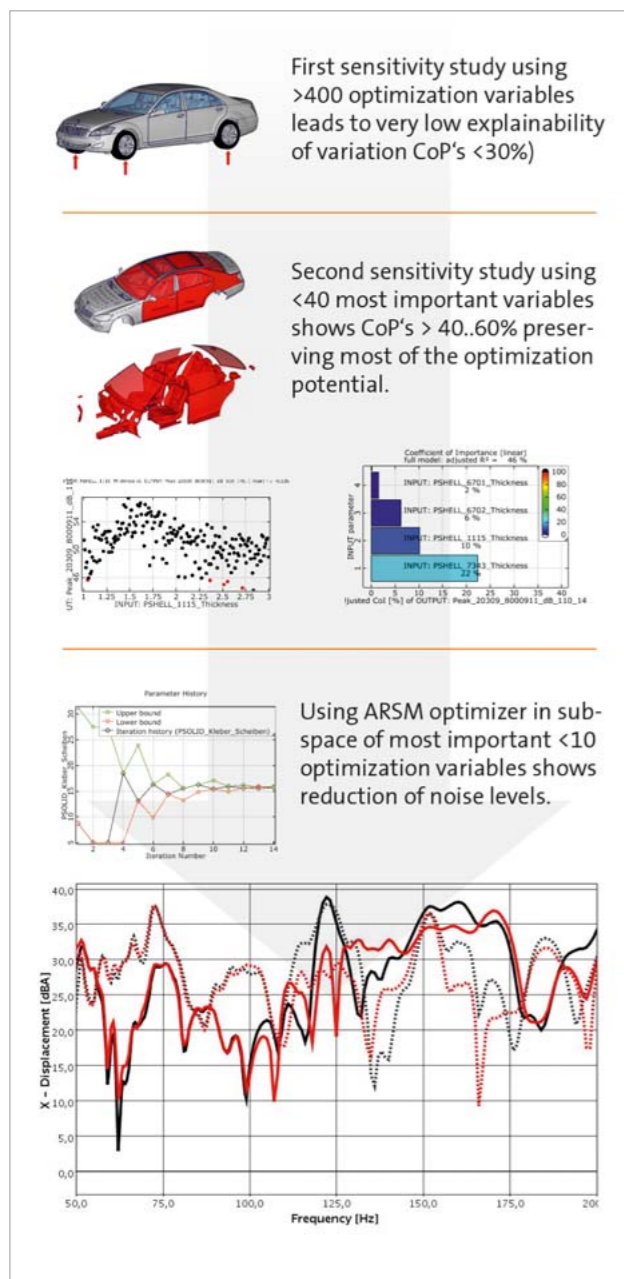


Fig. 13: Overview of the process for an optimization using the same sensitivity study but selecting only the eight most important variables for the optimization (by courtesy of DAIMLER AG)

The DBE TECHNOLOGIE GmbH develops, in cooperation with the Dynardo GmbH, simulation models that are able to comprehend these interactions in claystone. An important component of these developments is the calibration of the models with respect to the results of the measurements. The heating experiment has been simulated with a T-H-M coupled 3-dimensional finite element analysis with ANSYS and multiPlas. Therefore, special routines from the poro-elasticity theory, thermal-hydraulic coupling and thermal-mechanical coupling in isotropic and anisotropic claystone formations were developed and implemented in ANSYS. For the sensitivity analysis and for the parameter identification, optiSLang was used. Due to the complexity of the T-H-M phenomena, about 30 model parameters were

used. In this case, it was essential for the successful calibration of measurement and simulation to use the powerful algorithms and filter strategies for large parameter spaces of optiSLang and the achieved short calculation times due to efficient numerical algorithms of ANSYS with multiPlas. In the sensitivity analysis, the material parameters (including parameters for the coupling) have been varied within physical possible boundaries.

From the experiment temperature and pore water pressure data are available for 17 measurement points during the heating, as well as before the heating. Due to uncertainties in the process before the heating, the calibration and parameter identification was restricted to the heating process itself. For the evaluation of the sensitivities, the relative pore water pressures discrete time values were used. By the selection of these output values, statements became possible for the sensitivity at the beginning and at the end of the heating, as well as for the time when the pore pressure reached the maximum.

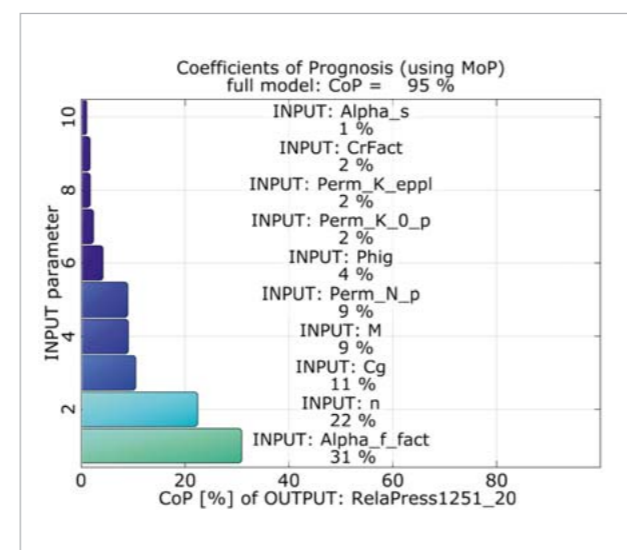


Fig. 14: High CoPs are an indicator for the sufficient quality of the model

The total Coefficients of Prognosis (CoP) show high values of above 85% (Fig. 14). This underlines that the physical phenomena are very well explainable through the identi-

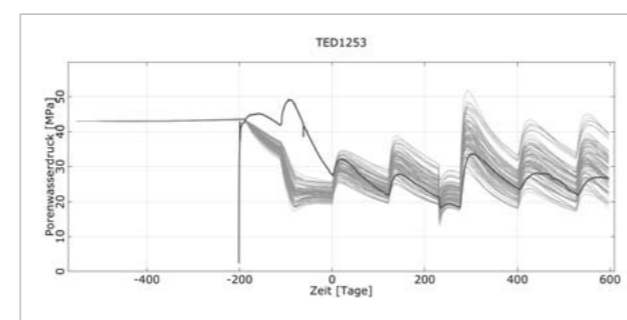


Fig. 15: Pore water pressure at measurement point TED1253, as a signal over time, compared with the simulated signals of the sensitivity analysis

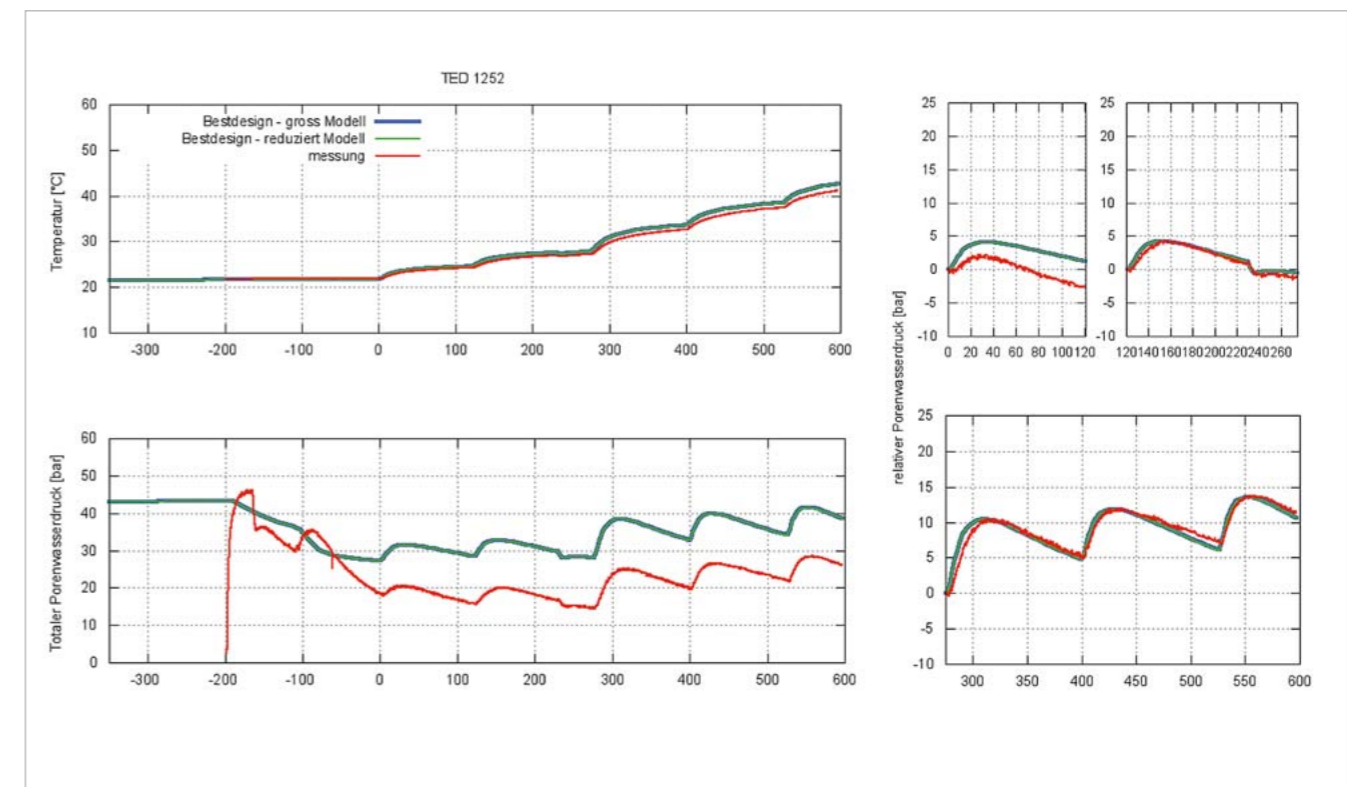


Fig. 16: Comparison of measurement vs. simulation at measurement point TED1252 after parameter identification. Top left: temperature over time, bottom left: total pore water pressure, right: relative water pressure for the three phases of heating.

fied correlations and also indicates that the correct important parameters for establishing the model were used.

By comparison of the scatter range of the calculated signals with the signals from the measurement (Fig. 15), statements about the quality of the model and the possible calibration of the model with the measurement are possible. If the scatter range of the calculated values is surrounding the measured values, then a successful calibration within the selected boundaries of the parameters can be possible. The figure shows that this is possible from the start of the heating experiment ($t=0$).

For the parameter identification, the optimization selected a set of input parameters leading to a good approximation of the measured signals of the temperature and the pore water pressure over time. Parameters that only showed a negligible sensitivity have not been varied through the optimization for the parameter identification. They have been set to their reference values.

The comparison of the measured and calculated time signals of temperature and pore water pressure (s. figure 16) shows that with the identified parameter for the model the physical phenomena could be simulated very plausibly and a very good calibration with temperature and pore water pressure was reached.

Outlook

This article explained, using theoretical and practical cases, how the calibration of a model with parameter identification can be treated as an optimization problem including signals. These techniques will become most probably an important standard technology for the development of more accurate models for the simulation.

In the following article we present a more detailed example for model calibration and parameter identification where also the varying influences of the parameters for the different stages of an experiment are analyzed. Additionally, in this example, the parallel coordinate plot of optiSLang is used to understand which parameters are really good identifiable.

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Example: Identification of concrete fracture parameters from a wedge splitting test

The following example will explain the basic procedure using a wedge splitting test regarding Trunk [Trunk1999]. During this experiment, a pre-slotted specimen was loaded vertically along a predefined crack edge. With this setup, the experimental measurement of the post-cracking behavior was possible.

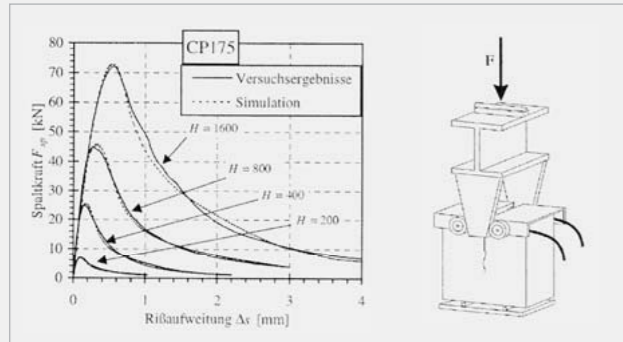


Fig. 1: Wedge splitting test regarding Trunk, experimental setup and measured load-displacement curves for different specimen

The simulation model represents the specimen as a linear elastic continuum containing 2D plane-stress elements. The theoretical crack evolution was represented by 2D interface elements, whereby the softening behavior was modeled using a common bilinear softening law. The tensile strength f_t and the specific fracture energy G_f as well as the two shape parameters α_{ft} and α_{wc} describing the kink of the bilinear curve, serve as fracture parameters. The simulation was conducted path-controlled causing a steadily increased crack opening width. In the first step, a sensitivity analysis was performed. Here, the Young's modulus E , the Poisson's ratio ν and the four fracture parameters were varied. As a design-of-experiment-scheme, a correlation-optimized Latin Hypercube Sampling was used. The simulation curves were

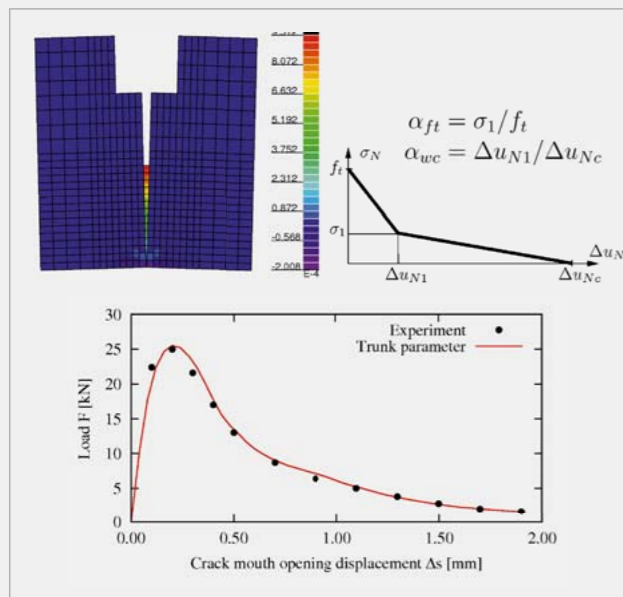


Fig. 2: 2D simulation model (top left) with stress history vertical to the crack surface, bilinear softening model (top right) and simulative load-crack opening curve (bottom)

calculated and imported in optiSlang via a signal module for each of the 100 samples. The curves showed a good adoption of the estimated range of values according to the reference signals (Fig. 3). An identification with the estimated parameter ranges was possible. Furthermore, the influence of the model parameters on the response variables was analyzed using the Metamodel of Optimal Prognosis.

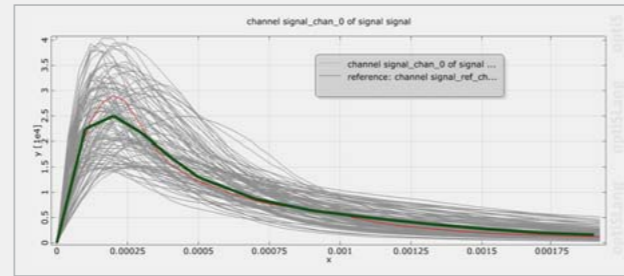


Fig. 3: The range of 100 simulation curves from the Latin Hypercube Sampling covers the reference signal from the measurements sufficiently.

Fig. 4 shows the meta-model and Fig. 5 the parameter influence concerning the sum squared errors. It can be seen that the Poisson's ratio and one of the form parameters most likely cause no effect. However, the approximation quality was not satisfying and less important factors were not identified due to insufficient sampling points. To ensure that only parameters without influence were excluded from the

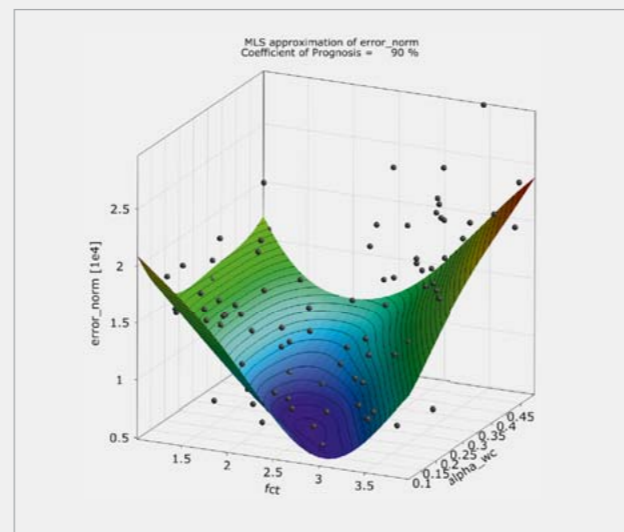


Fig. 4: Approximation of the sum of squared errors using Moving Least Squares

identification, effects appearing during the softening process were analyzed more detailed. The loads at the reference points (Fig. 2) were extracted from the signals of the simulation model and, for each value, a sensitivity analysis was conducted. This could be done without any further simulation runs because the additional scalar values were just extracted from the calculated response signals. The displacement dependent sensitivity indices are shown in Fig. 6. It illustrates that the Poisson's ratio had no influence. Apart from that, all parameters caused at least a partial effect during the simulation. The conclusion can be drawn that all parameters except the Poisson's ratio were identifiable from the measurement data.

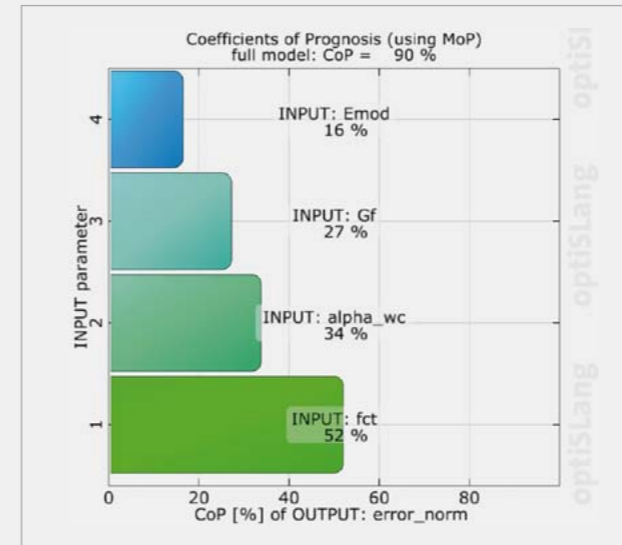


Fig. 5: Variance-based sensitivity indices of the parameters to be identified (right)

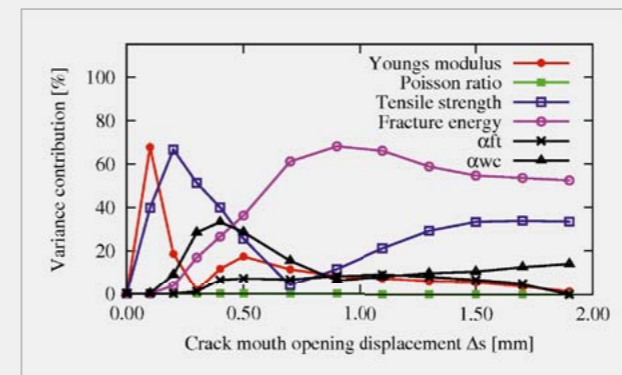


Fig. 6: Sensitivity indices for all input parameters depending on the crack opening width

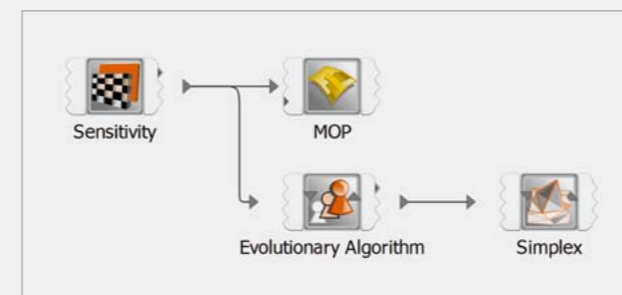


Fig. 7: Flow chart of identification: the sensitivity analysis generated the DoE designs as well as a response surface model using the Metamodel of Optimal Prognosis. For global search, the best designs served as a start population for the Evolutionary Algorithm. The resulting best design was then used as the starting point of the local search using simplex Nelder-Mead.

The next step was the conduction of a global optimization using an Evolutionary Algorithm with the 10 best designs of the sensitivity study as a start population. This improved the convergence of the optimization process significantly. The best design was then used as a start design for a local optimization. For the local search, the Simplex-Nelder-Mead method was used (Fig. 7). Finally, the issue of ambiguity was verified in detail. For this purpose, the designs of the local optimization were depicted as a parallel coordinates plot. The range of the sum of squared errors was restricted. Thus, only

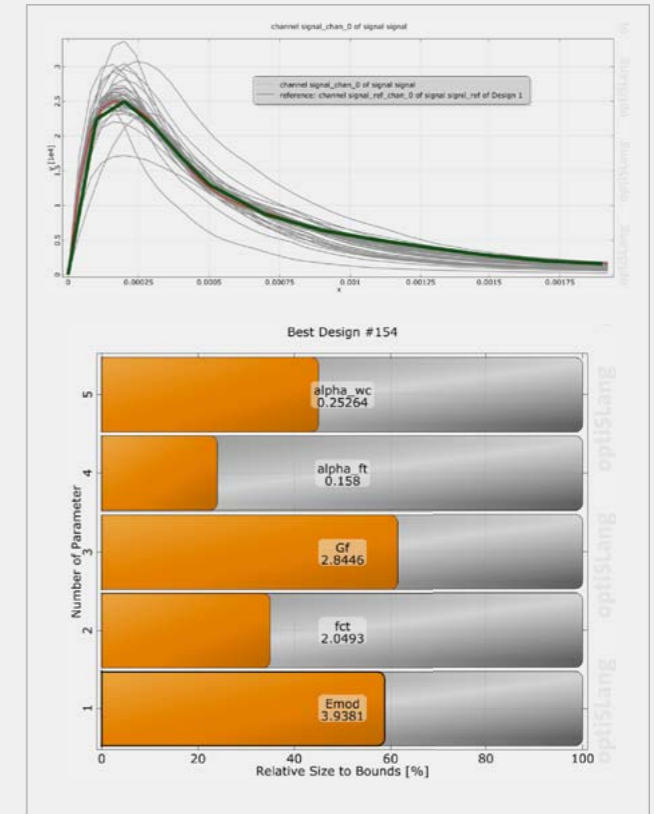


Fig. 8: Optimized simulation curves and optimal parameters showing a very good correlation between measurement and simulation

simulation curves with a very similar course were shown. In reference to the accompanying parameter ranges, it was illustrated that the modulus of elasticity, the tensile strength as well as the fracture energy show very small intervals and were sufficiently identi-

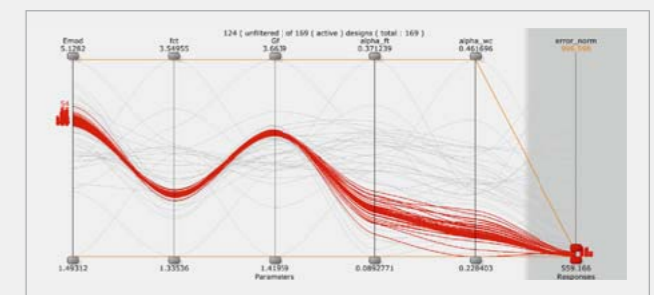


Fig. 9: Parallel coordinate plot of the best optimization designs for all considered material parameters and the sum of the least squares.

fiable. The two shape parameters showed very similar result diagrams applied with a larger deviation margin. Therefore, they were not sufficiently identifiable from using the available measurement points. Here, the consideration of further experimental data would certainly improve the validity.

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[Trunk 1999] Trunk, B., "Einfluss der Bauteilgröße auf die Bruchenergie von Beton", Dissertation, Eidgenössische Technische Hochschule, Zürich, 1999