Parameter Identification for the Electrical Modeling of Semiconductor Bridges

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Abstract

Semiconductor bridges (SCBs) are commonly used as initiators for explosive and pyrotechnic devices. Their advantages include reduced voltage and energy requirements and exceptional safety features. Moreover, the design of systems which implement SCBs can be expedited using electrical simulation software. Successful use of this software requires that certain parameters be correctly chosen. In this paper, we explain how these parameters can be identified using optimization. We describe the problem focusing on the application of a direct optimization method for its solution, and present some numerical results.
Acknowledgments

Many people contributed to this project. Ken Marx, Rene Bierbaum, and Jason Dimkoff requested the model parameters, provided the SCB models and experimental data, and they patiently supplied the training needed to run Xyce™ and Chile-SPICE. Monica Martinez-Canales provided valuable insight into the optimization problem and committed many hours to producing sensitivity analysis and subsequently trying to make sense of it. Tammy Kolda provided some ideas about the objective function and a code for comparing data points taken at different time intervals.
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1 Introduction

Semiconductor bridges (SCBs) have become a common means of initiating explosive or pyrotechnic devices. Their reduced voltage and energy requirements and their exceptional safety features make them an attractive choice. Furthermore, designing systems which implement SCBs can be accomplished using electrical simulation software. In [12], a model is presented with this purpose in mind. Using this model, the overall goal is to optimally design a SCB firing system with minimal laboratory testing. Moreover, this process may also be used to estimate the effects on the firing system due to failure of components or derivation from component specifications.

This paper is organized as follows: Section 2 describes a typical set of experimental data and two software packages available for producing simulated data. Section 3 includes a general description of simulation-based optimization and how it can be used to solve the parameter identification problem that arises in the computational design of SCB systems. Numerical results are presented in section 4 and some sensitivity analysis and future research directions are discussed in section 5.

2 Semiconductor Bridge

The physics and engineering of an SCB is a complicated and fascinating subject. However, this topic falls outside the scope of this paper. Interested readers are directed to Jason Dimkoff’s SAND report [2] for a complete description of the SCB of interest in this project. His report provides an extensive review of SCB testing and design and covers the following topics: the function of the SCB in the presence of explosive powder, testing anomalies, experiments completed for the determination of model parameters and characteristics, and the development of the electrical model. On the other hand, this paper covers the use of optimization as a tool for identifying the parameters present in an SCB model. In particular, this section covers the characteristics of an SCB relevant to the optimization.
2.1 Experimental Data

An SCB shot is defined by its firing conditions—the initial capacitance and voltage of the system. The resulting data consists of discrete time histories of the voltage and the current of the system. A typical data set is shown in Figure 1. Perhaps the most important point in the data corresponds to vaporization of the bridge. This point is referred to as the \textit{burst point}, and it corresponds to a sudden drop in current and a subsequent rise in voltage. The relevant time frame of an SCB shot ends when both the current and voltage stabilize after the bridge vaporizes.

Experimental data is produced using a wide variety of firing conditions. Each set of capacitance and voltage corresponds to one experiment and numerous experiments may be carried out for each SCB design. As shown in Figure 2, different firing conditions can produce vastly different data. Both the relevant time frame and the burst point are experiment dependent and difficult to define mathematically. Moreover, SCB data obtained via experiment contains a significant amount of noise. In the case of duplicated firing conditions, the resulting data may vary slightly despite using the same initial conditions. Figure 3 gives an example in which the data produced with the same SCB design and the same firing conditions contains noticeable differences. Finally, it should be noted that no-fire results may also be included in any group of experimental data.
Figure 2. Two experimental results produced with the same SCB design and different firing conditions.

Figure 3. Two experimental results produced with the same firing conditions.
2.2 ChileSPICE

One of the software tools available for SCB design is called ChileSPICE. ChileSPICE is Sandia’s enhanced version of Berkeley SPICE 3f5, an electrical simulation software, and it is a tool for complex electrical circuitry that uses a shared memory parallel simulation scheme.

Using this software, an SCB 32B1A model system with 7 parameters was simulated. Below, is a brief explanation of each parameter as well as some bounds over which they can vary.

- $A_{loss}$ is a loss coefficient used in the SCB energy loss model at high charging voltages. ($0 < A_{loss} \leq 3$)

- $\delta$ defines the width of the transition region in the SCB energy loss model at high charging voltages. ($0.5 \leq \delta \leq 1.5$) Note that the model is insensitive to $\delta$ unless it is large.

- $V_{01}$ defines the function splice point for the energy loss function at high charging voltages. In particular, energy loss begins at $V_{01} - \delta$. ($10V \leq V_{01} \leq 60V$)

- $R_{fac}$ is a multiplier for an included table that defines the SCB resistance curve. ($0.25 \leq R_{fac} \leq 4$)

- $E_{ti}$ is the powder ignition energy divided by a constant. It is used to determine the time to powder ignition. ($0.1ns \leq E_{ti} \leq 50ns$)

- $H_{0}$ is a heat transfer coefficient for energy transfer back to the SCB after the powder has ignited. ($0.05MHz \leq H_{0} \leq 5MHz$)

- $E_{p}$ is the energy transferred to the powder. ($0.001mJ \leq E_{p} \leq 0.1mJ$)

With the exception of $R_{fac}$, each of the above parameters is described in detail in the derivation of the SCB model included in [12].

The parameter bounds given here were determined by the SCB design engineers and are based on experimental results and observations. It should be noted that the parameters $E_{ti}$, $H_{0}$, and $E_{p}$ are all part of the thermal feedback mechanism in the low energy regime, and their quantitative effects on the overall SCB system are not well understood. Thus, their bounds are looser than those of the other four parameters. Moreover, because of the uncertainties on the bounds of the thermal parameters, we began our optimization computations by varying them on a logarithmic scale. Computational experiment proved this to be unnecessary, and so the results presented in Section 4 were produced by allowing $E_{ti}$ to vary between 1 and 50, $H_{0}$ to vary between 0.05 and 5, and $E_{p}$ to vary between 0.001 and 0.1.
After an initial set of computational experiments was completed, we opted to hold $R_{\text{fac}}$ constant at 1 and to replace the parameters $A_{\text{loss}}$, $\delta$, and $V_{01}$ with a table. This table replaces the loss function in the SCB model and represents a linear interpolation of points for the loss plot. The coefficients in this table are functions of the voltage and should take values between 0 and 1. If any of the parameters go above 1, this might indicate that a loss mechanism is missing. This table consists of 8 parameters, bringing the total number of parameters for this SCB model to 11.

### 2.3 Xyce

As the project progressed, the development of a newer Sandia circuit modeling tool called Xyce\textsuperscript{TM} also progressed. Xyce\textsuperscript{TM} was designed to run efficiently on high performance parallel computers and eventually, the capabilities necessary to model a SCB were added. Thus, the decision was made to transfer the SCB design to Xyce\textsuperscript{TM} from ChileSPICE. The development and use of the Xyce\textsuperscript{TM} code is explained in detail in [8]. Xyce\textsuperscript{TM} was successfully used to study the SCB 32B1A model discussed in the previous section. In addition, it was used to study the model 50B1A SCB with less than 20 model parameters.

### 3 Parameter Identification via Optimization

In order to design the SCB systems using the electrical simulation software described in the previous section, we must identify appropriate parameter values. Recall that, given an initial capacitance and voltage, experimental data is produced in the laboratory. Moreover, given the same initial capacitance and voltage and a specified set of input parameters, the simulator computes comparable simulated data. Then, the problem of SCB design parameter identification can be stated as follows: What set of simulator input parameters produces simulated data that is most like the corresponding experimental data?. Finding this set of parameters will allow the SCB design to be tested and improved.

#### 3.1 Simulation-Based Optimization

The SCB parameter identification problem is merely a simulation-based optimization problem. Such problems are characterized by a relatively small number of variables and an objective function whose evaluation requires the results of a complex simulation. In the case of parameter estimation problems, the goal is always to identify the set of simulator input parameters that produces output that most closely matches some given observed data. For this problem, the objective function might be of the
form
\[ f(x) = \sum_{i=1}^{N} (s_i(x) - o_i)^2. \]

Here, \( N \) denotes the number of data points to be compared; for example, the points could correspond to times or spatial locations. The values \( o_i \) for \( i = 1, \ldots, N \) are the given observed data values at these points, and the values \( s_i(x) \) for \( i = 1, \ldots, N \) are the simulator outputs at the same points, depending on the input \( x \). Note that in order to discover the \( x \) that yields the best fit to the observed data, multiple simulations are required. In the case of the SCB problem, \( x \) refers to the parameters discussed in Section 2.

For the SCB parameter identification problem, there is an added level of complexity. First, there are multiple starting conditions. Hence, one set of parameters must be identified to satisfy a variety of experiments. Second, some experiments are duplicated. Third, the data includes both a current and a voltage reading at each time interval. To incorporate these characteristics, we use the modified objective function

\[ f(x) = \sum_{i=1}^{N} w_i \sum_{t=1}^{T_i} \left[ \alpha_t \| Sc_i(t; x) - Ec_i(t) \|^2 + \beta_t \| Sv_i(t; x) - Ev_i(t) \|^2 \right]. \quad (3.1) \]

Here, \( N \) is the number of experiments, \( T_i \) is the total time for experiment \( i \), \( Sc_i(t; x) \) and \( Sv_i(t; x) \) are the simulated current and voltage data points, respectively, for experiment \( i \) at time \( t \) with SCB parameters \( x \), and \( Ec_i(t) \) and \( Ev_i(t) \) are the experimental current and voltage data points for experiment \( i \) at time \( t \). The multiplier \( w_i \) is used as a weight to prevent placing higher importance on experiments that have been repeated. We use \( w_i = 1/n_i \) where \( n_i \) is the number experiments in the set that have the same firing conditions as experiment \( i \). The multipliers \( \alpha_t \) and \( \beta_t \) are necessary to account for differences in the measurement units of the current and voltage values. In our computations, the voltages are given in volts (V) and the currents are given in amps (A). Hence, they are of the same order of magnitude, and we can set \( \alpha_t, \beta_t = 1 \) for all \( t \).

As stated, objective function (3.1) assumes that the experimental and simulated data points are available at the same time intervals. In reality, this is not the case. We are estimating and comparing the voltage and current curves. Hence, each simulated data point is compared to the experimental data point closest to it. Moreover, this comparison is unimportant after the voltage and current curves stagnate. Hence, \( T_i \) reflects the relevant time interval for experiment \( i \). In the future, we would like to automate the process of determining an appropriate \( T_i \), but for this project, it was set by observation of the experimental data.

Finally, we note that this version of the objective function is not the only appropriate option for this problem. In fact, because of the importance of vaporization
in the SCB model, incorporating the burst point in the objective function should be beneficial. Unfortunately, the lack of a mathematical description of this point prevented us from including it.

The SCB parameter identification problem can be stated as the following optimization problem:

\[
\begin{align*}
\text{min} & \quad f(x) \\
\text{s.t.} & \quad \mathcal{L} \leq x \leq \mathcal{U},
\end{align*}
\]

where \( f : \mathbb{R}^n \rightarrow \mathbb{R} \) is the function defined in (3.1), \( x, \mathcal{L}, \mathcal{U} \in \mathbb{R}^n \); and \( \mathcal{L} \) and \( \mathcal{U} \) are given lower and upper bounds on \( x \) respectively. The method for solving this problem as follows:

1. A trial set of parameters is produced either using the initial guess or the optimization algorithm.
2. The trial parameters are used to prepare the appropriate simulator input file.
3. Simulated data is produced. For the SCB parameter identification, this step is repeated up to \( N \) times, once for each unique pair of firing conditions.
4. The simulated data and experimental data are compared using (3.1).
5. The objective function value is returned to the optimization method. Step 1 and all subsequent steps are repeated until convergence.

This process is illustrated in Figure 4.

### 3.2 APPSPACK

To solve (3.2), an optimization algorithm is required. We apply APPSPACK [5], an software appropriate for solving unconstrained and bound constrained optimization problems. In particular, it was specifically designed for simulation-based optimization and problems characterized by expensive function evaluations. APPSPACK implements asynchronous parallel pattern search (APPS) [7,9]. Pattern search methods use a predetermined pattern of points to sample the given function domain. When certain requirements on the form of the points in the pattern are imposed, it can be shown that if the objective function is smooth, global convergence to a stationary point is guaranteed [3,11,16].

The majority of the computational cost of pattern search methods is the function evaluations, so parallel pattern search (PPS) techniques have been derived to reduce the overall computational time. Specifically, PPS exploits the fact that once the
points in the search pattern have been defined, the function values at these points can be computed simultaneously [1, 15]. The particular implementation of PPS that we use is asynchronous. Asynchronous parallel pattern search (APPS) retains the positive features of PPS, but it does not assume that the amount of time required for an objective function evaluation is constant or that the processors are homogeneous. It does not have any required synchronizations and thus requires less total time than PPS to return results [6]. Furthermore, it has been shown that APPS is globally convergent under the standard assumptions for PPS [10].

Using APPSPACK to solve optimization problems has several advantages: No derivative information is needed; the procedure for evaluating the objective function can be executed via a separate program or script; the code can be run in serial or parallel, regardless of whether or not the function evaluation itself is parallel; and the software is freely available.

The script used to calculate the objective function (3.1) for the SCB parameter identification problem included the following steps:

1. Prepare the simulator library to include the parameters suggested by APPSPACK
2. For \( i = 1 \) to \( N \)
   (a) Create the circuit file for experiment \( i \)
   (b) Run the simulator
   (c) Convert the simulator output to correct format

Figure 4. Illustration of the simulation-based optimization process.
Figure 5. A comparison of the experimental (dashed lines) and simulated (solid lines) data for two different experiments. The voltage curves are blue, and the current curves are red. Results produced with the same SCB design parameters and different firing conditions. The results on the left, which are for a high-energy system, show a better correspondence between data types than the low-energy system on the right.

(d) Compare output with experimental results

3. Sum results of (d) and return answer to APPSPACK

4 Numerical Results

In solving optimization problem (3.2) with objective function (3.1), the goal is to identify only one set of SCB model parameters regardless of the number of experimental data sets. In other words, the parameters should be such that simulating each data set requires only a change in the firing conditions. The results presented below illustrate the difficulties in finding one definitive set of parameters. Within one group of data, the simulated data for some experiments is an excellent match to the observed data while the match for others is merely acceptable and for still others, it is completely inconsistent.

The simulated 32B1A SCB model was originally created using the ChileSPICE software described in Section 2.2. For this model, 18 sets of experimental data are available with 15 different firing conditions and 3 sets resulting from repeated firing conditions. Initially, 7 model SCB parameters were determined by APPSPACK. To illustrate the results, the experimental data and the simulated data generated using the parameters suggested by the optimization solution were compared. As the examples in Figure 5 show, the results were mixed. For some experiments, the
simulated and experimental data were remarkably similar while for others, there was almost no similarity. Analysis of these initial results showed that similarities between the experimental data and the simulated data were related to the firing conditions. In fact, the energy $E$, defined as

$$E = \frac{1}{2}CV^2,$$

where $C$ is the capacitance ($\mu$F) and $V$ is the voltage (V), could be used to classify this relationship. The experimental and simulated data were most alike for those experiments that with energies more than 40mJ and least alike for those with energies less than 8mJ. These results suggest that three sets of parameters may be more appropriate for this SCB model. In other words, a different set should be sought for systems with low, intermediate, and high energy. To avoid this, the loss parameters $A_{\text{loss}}$, $\delta$, and $V_{01}$ were replaced with a table as described in Section 2.

The new SCB model contains 11 parameters which were subsequently determined using APPSPACK. Again, the experimental data and the resulting simulated data were compared. Figure 6 gives two examples of the most promising results. In contrast, Figure 7 gives two examples of the least promising. It is interesting to note that all four experiments have energies between 8 and 25 mJ and can be classified as intermediate in terms of system energy.

The 50B1A SCB model was incorporated using the Xyce™ software. For this model, 23 sets of experimental data were generated using 10 different firing conditions. Some of the experiments were repeated up to 6 times. This group included a
Figure 7. A comparison of the experimental (dashed lines) and simulated (solid lines) data with voltage curves in blue, and the current curve is in red. These results are representative of the worst obtained from a group 18 experiments with the same SCB model and parameters and different firing conditions.

large number of no fire data sets. As Figure 8 shows, the SCB model had difficulty simulating this behavior. Therefore, it was decided this model needed to be studied and refined before any more simulations would be completed.

5 Sensitivity Analysis

This project demonstrates the usefulness of optimization in the design of the SCB models needed by electrical simulation software. However, initial results showed that the model design process would also likely benefit from sensitivity analysis, an investigation into how the resulting simulation output response varies with changes in the model parameters. To this end, a main effects analysis was completed using Sandia’s Distributed Design and Analysis of Computer Experiments (DDACE) code. A complete description of DDACE is available in the DAKOTA user manual [4].

The purpose of a main effects analysis is to quantify the “input uncertainty” of a model. In other words, it measures how much the output of a model changes with respect to changes in its input parameters. The DDACE software expresses this measure as a non-normalized McKay correlation ratio [13]. This ratio places a numerical value on the importance of one parameter relative to the whole set of tracked parameters. A McKay correlation ratio close to 0 indicates that the parameter value has little effect on the output of the model while a larger ratio implies that the parameter is an important contributor in the model and that determining the correct parameter value(s) is critical to the usefulness of the model. Calculation of
Figure 8. A comparison of the experimental (dashed lines) and simulated (solid lines) data where the voltage curves are blue, and the current curves are red. This experiment did not fire, but the simulation is unable to capture that behavior.

The McKay correlation ratio requires sampling the parameter design space. DDACE includes a variety of sampling methods, and for this project, Latin hypercube sampling (LHS)[14] was used. Table 1 shows the non-normalized McKay correlation ratios associated with the SCB model parameters. They were calculated using 94 LHS samples with 2 replications. Note that none of the correlation ratios are close to 0 indicating that all 7 SCB model parameters are important to the overall model design, and their correct identification is key to successful simulations.

After examining the sensitivity results and presenting them to the Sandia Validation Metrics group, the following feedback was given:

- The repeated experiments should be used to study the variability in the data. Because no model should be more accurate than the data it represents, this variability should be incorporated in both the SCB model design and the optimization of the model parameters.

- The weighting scheme in the objective function could be used to represent the importance of the experimental data. Currently, each experiment is considered with equal importance and the parameters are optimized accordingly. It might be more effective to focus on the more representative experiments. Note that this may also require an alternative objective function.

- The nonlinear relationships between parameters needs to be explored in order to obtain a better understanding of their overall effect on the SCB model. This can be ascertained by analyzing interaction effects.

Future work in the area of SCB model design and the optimization of its parameters
Table 1. The non-normalized McKay correlation ratios of the SCB parameters. This ratio is a measure of the effect of the individual parameter on the overall system.

<table>
<thead>
<tr>
<th>Parameter</th>
<th>$\rho_M$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$A_{loss}$</td>
<td>0.455</td>
</tr>
<tr>
<td>$\delta$</td>
<td>0.504</td>
</tr>
<tr>
<td>$V_{01}$</td>
<td>0.545</td>
</tr>
<tr>
<td>$R_{fac}$</td>
<td>0.582</td>
</tr>
<tr>
<td>$E_{ti}$</td>
<td>0.421</td>
</tr>
<tr>
<td>$H_0$</td>
<td>0.688</td>
</tr>
<tr>
<td>$E_p$</td>
<td>0.532</td>
</tr>
</tbody>
</table>

would investigate these suggested measures. We would explore the entire SCB model parameter space to confirm if the most important parameters do, in fact, correspond to the parameters tracked in this paper. Recall that the parameters studied in this paper were singled out as important to study based on engineering experiments and judgment. The purpose of the optimization and sensitivity analysis studies is to quantify this engineering judgment and to lend a mathematical perspective on the design process. Our hope is that the results of our mathematical studies will help improve the overall usefulness of computer simulations.
References


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