Using TEMPER's Genetic Algorithm and MSIAC Databases to fit SDT Model Parameters

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TEMPER is a toolbox of simple (empirical, analytical, 1D numerical …) models used for ammunition safety. Many models are dedicated to shock to detonation transitions (SDT) : Held's criterion expressed either as v²d or u²d, Jacobs-Roslund original and modified threshold velocity models, several approaches based on the "critical energy" concept (Walker-Wasley, James, Peugeot), Yactor's model, and $P^n.\tau$ criterion. These models range from purely empirical to analytical (impedance matching, 1D shock duration, a.s.o.) and can be applied either to only bare energetic materials or bare as well as covered ones.

A quick assessment of ammunition safety or mitigation concepts could take advantage of these models, provided that we are able to find model parameters for the high explosives studied. Unfortunately, there are only scarce data in the literature, for few formulations and a limited number of models. On the other hand, explosive formulations have been extensively tested and test results have been gathered by MSIAC in several databases, including FraID (fragment impacts), BIRD (bullet impacts), HEAT (cook off), DARTS (shape charge jet impacts) and NEWGATES (gap test results). It would then be extremely interesting to find model parameters by analyzing experimental results.

This could be done by two approaches:
- Sometimes a direct relationship between experimental results and model parameters can be found. It has been exemplified by P-F PÉRON during the IMEMTS 2009[5] through the correlation of Gap Test results and Jacobs-Roslund parameters;
- An alternative technique is to ask the model to replicate experimental results and to use optimization routines to fit model parameters in order to minimize the discrepancies between model and experiments.

The present paper aims at illustrating the second approach through the use of TEMPER and its built-in genetic algorithm feature, the MSIAC Fragment Impact Database (FraiD) being the source of experimental results.

1 Introduction

1.1 TEMPER

TEMPER[1] [Toolbox of Engineering Models for the Prediction of Explosive Reactions] is a toolbox of simple (empirical, analytical, 1D numerical …) models dedicated to ammunition safety. Its main features have already been described in several symposia[2,3,4,5]. TEMPER has originally been developed at CEA/Gramat (formerly CEG) and has then been made available to other countries through MSIAC (NATO Munition Safety Information and Analysis Center). TEMPER's development is shared between CEA/Gramat and MSIAC, other potential developers being warmly invited to contribute.

Many models are dedicated to mechanical insults, and especially shock to detonation transitions (SDT). They range from purely empirical ones (Held's criterion) to more scientific and analytical ones (including impedance matching, 1D shock duration, a.s.o.) and can be applied either to only bare energetic materials or to bare as well as covered configurations.

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1.2 MSIAC Databases

On the other hand, explosive formulations have been extensively tested and test results have been gathered by MSIAC in several databases, including FraID (fragment impacts), BIRD (bullet impacts), HEAT (cook off), DARTS (shape charge jet impacts) and NEWGATES (gap test results). It would then be extremely interesting to find model parameters by analyzing experimental results.

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1.3 Optimization techniques

Optimization techniques are mathematical routines used to minimize or maximize a function. They have a wide range of applications, from finding zeros of functions to heuristic problems, for which no algorithms exist (the Travelling Salesman Problem for instance).

In the present application, we assume that we have an experimental threshold curve as well as a computed threshold curve, the latter being given by TEMPER through a model depending on a set of parameters $(P_1, …, P_N)$. The function of interest should be a measure of the discrepancy between the two curves. If the function tends to a minimum (usually 0) when the two curves match perfectly, it is called a "cost function" which has to be minimized during the optimization algorithm. On the opposite, if it tends to a maximum (usually 1 for a normalized function) for a perfect match, the function is called a "fitness function" and should be maximized during the optimization process. For both cases, an optimization technique is required to find an optimal set of parameters, i.e. a set $(P_1^{opt}, …, P_N^{opt})$ for which the computed threshold curves matches best the experimental one.

There are many optimization procedures, for instance gradient descent algorithms, simulated annealing techniques, Simplex methods, neural networks, etc. For instance, the solver add-on in Microsoft Excel™ uses a gradient-based search. The choice of an optimization technique for TEMPER relied on three main points:

- the computational burden,
- the ability to find the global optimum, without being stuck in local optima (see Figure 1),
- the robustness, i.e. the ability to solve many different problems without changing the parameterization of the technique itself.
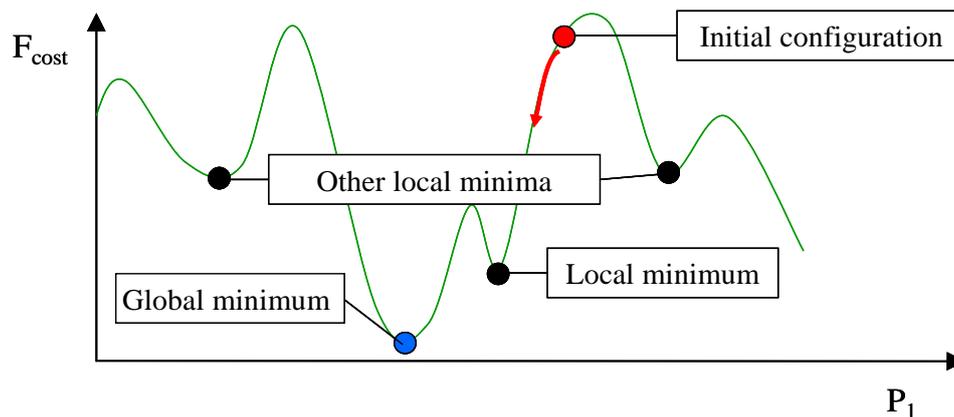
Figure 1: Optimization: the problem of local minima

A genetic algorithm has been chosen and implemented in TEMPER since version 2.0: this technique is a relatively all-purpose one, is not very computationally expensive, and succeeds most of the time in finding the global optimum.

1.4 Genetic Algorithms (GA)

The purpose here is not to enter into a detailed description of genetic algorithms, but since the "advanced" option in TEMPER allows modifying the parameters of the technique, it is worth understanding how it works.

Contrary to many optimization techniques, a genetic algorithm begins with not only a single "first guess" [i.e. a set of initial model parameters, which has to be optimized], but rather a "population" of sets of parameters, called "individuals". Each parameter is coded on one or several "genes" and the method follows the evolution of the population of individuals, as if is was a "real" population of animals.

The population is supposed to obey Darwin's laws of adaptation to the environment. The adaptation of a given individual is measured by its fitness function (from the viewpoint of SDT models, recall that the fitness is the ability for a given set of model parameters to reproduce as close as possible experimental results).

To mimic the evolution of a real population, each successive "generation" of individuals goes through several steps, namely:

- Selection of the "best" individuals (generally those with the highest fitness values, which is called "elitist" selection),
- Reproduction of the selected individuals and creation of a new generation by "cross-over" of parent genes to produce child genes (the very best individual of a generation is kept as is in the new generation, to avoid losing the highest fitness),
- Random mutations (to avoid an early freezing in local optima),

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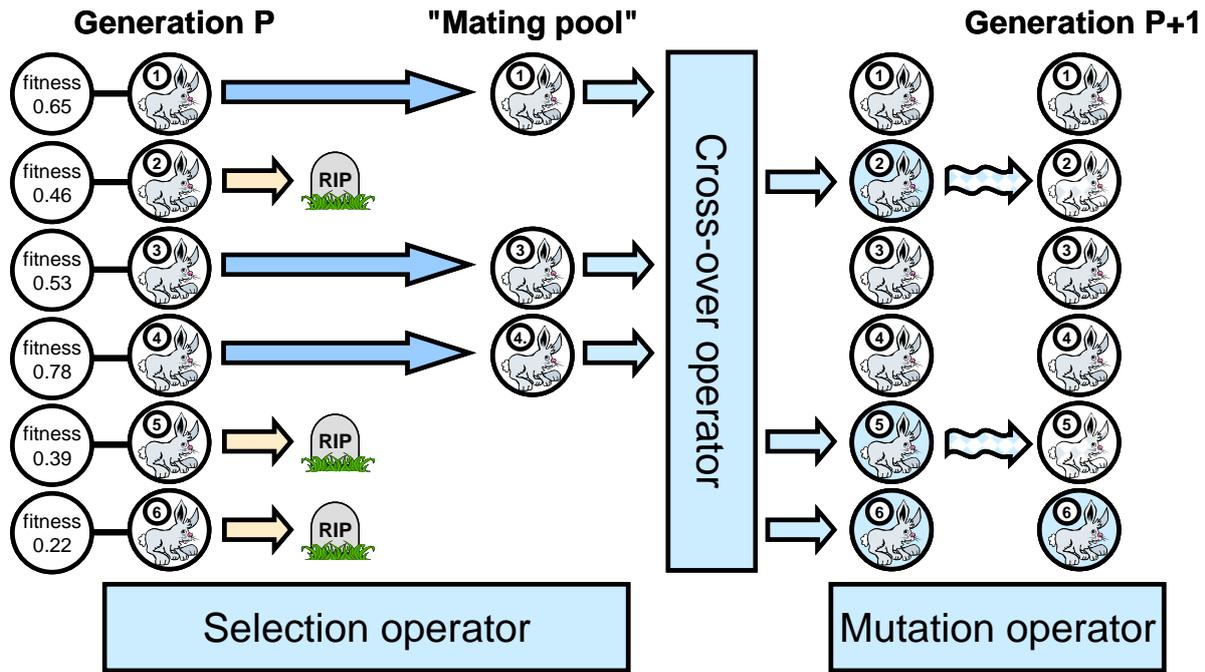
Figure 2: Illustration of genetic algorithms for a population of 6 individuals

When genes are binary-coded, defining a cross-over operator and a mutation operator is relatively straightforward (for instance, a mutation operator changes a random gene from 0 to 1 or from 1 to 0 through a boolean NOT operator). Moreover, it has been proved for the binary case that both the current best individual and the population as a whole tend towards the global optimum, i.e. the global best fitness. In our application however, genes are real number, encoding model parameters. The choice of a real number representation is important, because the different operators should respect the variation range of each model parameter, which is defined initially.

TEMPER uses the following trick to make sure that variation ranges are respected. A given parameter P_i is coded in two half-genes G_{2i-1} and G_{2i}, such as:

$G_{2i-1} \in [0,1]$
$G_{2i} \in [0,1]$
$P_i = P_{i,min} + (G_{2i-1} \times G_{2i})^{1/2} \times (P_{i,max} - P_{i,min})$

The fitness assessment is performed by comparing experimental and computed threshold curves in a given threshold plane. Threshold curves are defined by each model as Y=f(X) functions (for instance threshold projectile velocity as a function of projectile diameter, or threshold pressure as a function of pressure duration).

If the model does not implement a reverse function $X=f^{-1}(Y)$ then the fitness is computed through the distances in Y coordinates for each experimental X data points. If the reverse function is implemented, a more sophisticated evaluation of distances between experimental results and threshold curve is used.

In both cases, the distances in Y and, eventually, in X are respectively scaled by DeltaY and DeltaX, maximum differences in Y and X found in the set of experimental data points, in order to avoid problems with X and Y units.

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2 Determining parameters of SDT Models

2.1 Available SDT Models

The SDT models available in TEMPER are:
- the Held's criterion expressed either as v²d or u²d,
- the Jacobs-Roslund original and MSIAC-modified threshold velocity models,
- several approaches based on the "critical energy" concept (Walker-Wasley, James, Peugeot),
- the Yactor's model, based on pop-plot results,
- the generic $P^n.\tau$ criterion.

The two former classes of models are purely empirical and make only use of the projectile diameter and velocity (from a TEMPER Stimulus), as well as the cover thickness for Jacobs-Roslund models (from a TEMPER Structure). The three latter classes of SDT models rely on impedance-matching computations, and require the knowledge of material Hugoniots.

Table 1 summarizes a brief description of models and their list of parameters (V, u, d, t, d_{crit}, P, τ:, U_{HE}, $\rho_{0,HE}$ being respectively projectile velocity, cratering or material velocity, projectile diameter, cover thickness, critical diameter, impact pressure, impact duration, shock velocity in the explosive and explosive initial density). Several models could have had slightly different formulations (for instance the Yactor's model could have taken into account d_{crit} in the computation of the catch-up distance) but Table 1 only shows the current implementations in TEMPER and the corresponding parameters.

Model	Formulation	Parameters
Held's criteria	$V^2.d = K$ or $u^2.d = K'$	1: K or K'
Jacobs-Roslund (original)	$V_{threshold} = A/d^\beta.(1+B).(1+C.t/d)$ $(d>d_{crit})$ $V_{threshold} = E/d^\alpha$ $(d<d_{crit})$ Usually B is considered as a parameter, but depends also on projectile shape, taking B=0 for flat projectiles.	7: d_{crit}, A, B, C, E, α, β. C also depends on projectile shape, but $C_{round} = 1/3.C_{flat}$, so only C_{flat} is required. It also depends on projectile and cover materials.
Jacobs-Roslund (MSIAC)	Same as above for $d>d_{crit}$, except that parameters are computed from the LSGT threshold pressure.	1: P_{LSGT}
Walker-Wasley's Critical Energy	$P.u.\tau = E_{crit}$ Since τ is computed as the time giving the maximum volume of 1D shock, this model is, strictly speaking, James' reformulation of the original Walker-Wasley's model.	1: E_{crit}
James' Critical Energy	$P.u.\tau > E_{crit}+\Sigma_{crit}.(2.\rho_{0,HE}.U_{HE}.\tau)$ This is the two-parameter version of James' Critical Energy model.	2: E_{crit}, Σ_{crit}
Peugeot's Threshold Energy	$P.u.\tau > F.Exp(d_{crit}/(2.d)-1)+K.P^{2-n}/(\rho_{0,HE}.U_{HE})$ F is not a parameter but a dimensional factor whose value depends on the units used.	3: d_{crit}, n, K
$P^n.\tau$ criterion	$P^n.\tau = K$	2: n, K
Yactor's criterion	Compares the catch-up distance of lateral rarefaction waves to the run-to-detonation distance given by the pop-plot curve : $X_{run} = Exp((lnb - Ln(P)) / a)$	2: a, lnb

Table 1 : Models descriptions and parameters

2.2 Source of Experimental Data

Since we focused on SDT results, our reference of experimental data is the MSIAC Fragment Impact Database (FraID) v1.8[6]. FraID presents more than 1700 impact results on 90 high explosives formulations, giving details on the high explosive under study, its covering and/or casing, and the projectile characteristics as well as the result in terms of type of reaction.

For many formulations however, only a few results are listed, which will hinder the optimization process from finding a good fit, especially for multi-parameter models. On the other hand, for some formulations several tens of results are available, which should be more than sufficient to fit parameters!

2.3 Optimization Procedure

The Excel™ format used in FraID cannot be read directly by TEMPER. An example of HE workbook is given in Figure 3 for PBX 9404. It can be seen that results for both bare and covered situations are available. Preparing a TEMPER fit requires extracting data corresponding to one single TEMPER scenario, so there is no possibility for the moment to try fitting all results at the same time.

Figure 3: FraID's workbook for PBX 9404

If we are working for instance on the flat steel projectile / bare PBX 9404 scenario, the following steps should be performed before launching the optimization process:

- Creation of a txt file with the corresponding experimental results (one result per line), converting the figures in international units and ordering the columns in the following format "X value; Y value; results" as shown in Figure 4 (X and Y being the coordinates of a threshold curve for the model under study).
- Creation of the corresponding scenario in TEMPER, including the proper definition of materials (i.e. Steel projectile in our example), and selection of a single model for which we want to fit parameters (Figure 5),
- Creation (if not already done) of a new energetic material through the "Material Editor" window,
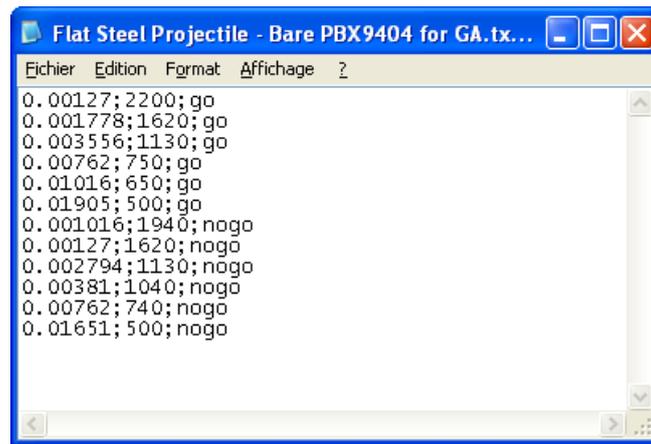
Figure 4: Experimental points for bare PBX 9404 impacted by flat steel projectiles
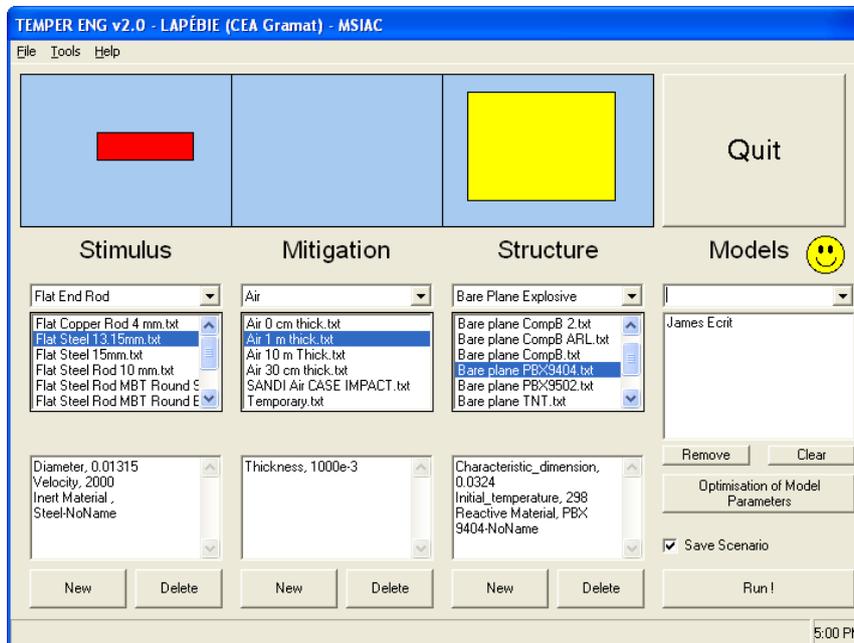
Figure 5: TEMPER's scenario in preparation

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Instead of clicking on the "Run !" button, the user has to click on the "Optimization of Model Parameters" button, and is then redirected to the genetic algorithm interface (see Figure 6 for the interface with "advanced" settings).

The user should then select a reasonable minimum and maximum value for each model parameters, and click on the "Open points file" to select the experimental data file previously prepared (making sure that the proper index of model curve is selected: the name of the corresponding X and Y variables as well as the required units appear on the interface to help the user).

It is either possible to click on "Start" directly or to change the genetic algorithm settings (number of individuals, maximum number of generations, type of selection, cross-over and mutation probabilities, a.s.o.). We strongly suggest keeping the default options, at least for a first run. During the optimization, the current generation number and the current best fitness appear on the bottom right of the interface.
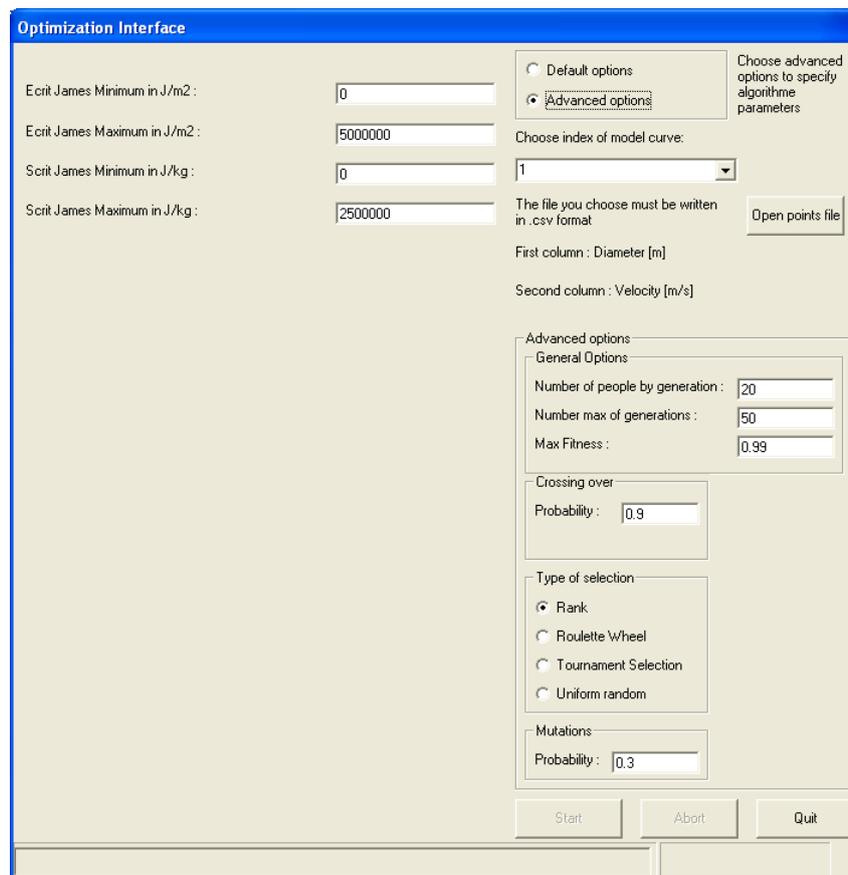
Figure 6: "Advanced" genetic algorithm interface

At the end of the optimization, the fitted value of each parameter is displayed in pop-up windows, and also appears on the genetic algorithm interface as both "min" and "max" values (see Figure 7). In our example, James parameters E_{crit} and S_{crit} are respectively fitted to 672 080 and 24 281, for a global fitness of 0.978. No direct link to the material editor exists for the moment, but we plan to paste these fitted parameters directly into the energetic material file.

At the same time, Excel™ results are displayed in a new window: a first graph shows the evolution of the minimum, mean and maximum fitness as a function of generation number and a second graph shows the fitted threshold curve, superimposed with experimental results (Figure 8).
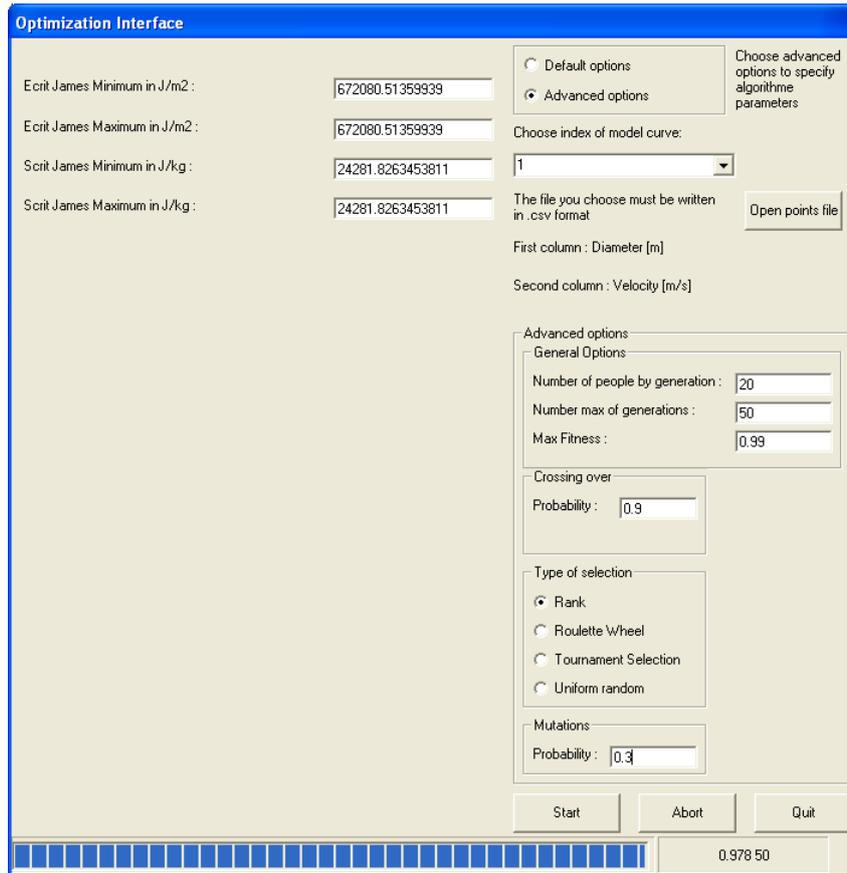
Figure 7: Optimization results (genetic algorithm window)
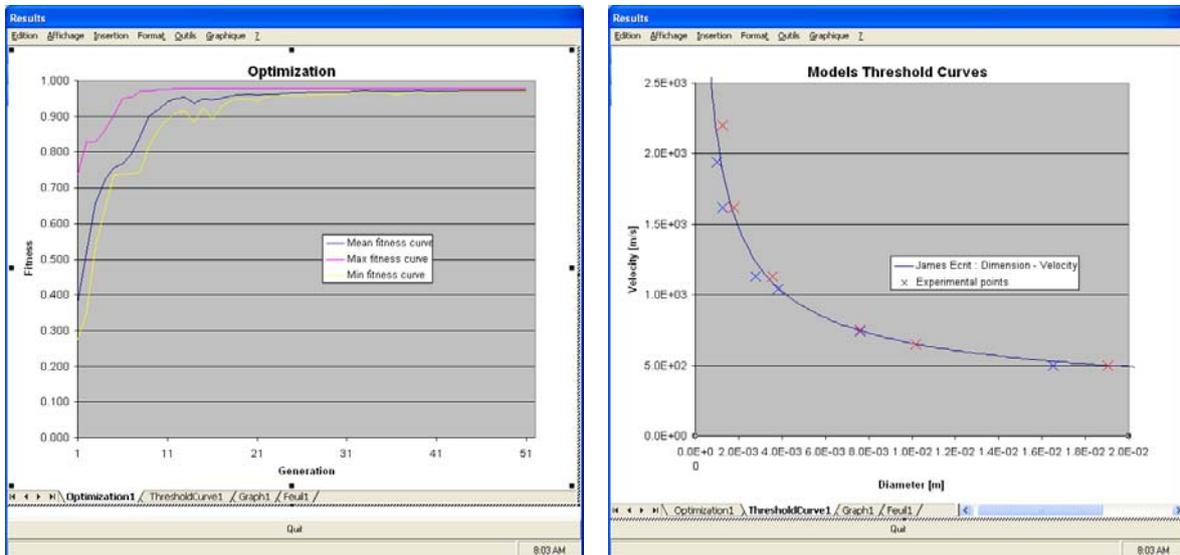

Figure 8: Optimization results (Excel™ window)

If the results are not satisfactory enough, the user may run the genetic algorithm several times, modifying either the optimization settings or the variation range of parameters. We want to point out that GA optimization is a stochastic process, which means that different runs will lead to (slightly) different parameter values.

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3   Results

3.1   Overview

The work has been performed at CEA/Gramat by H. Vigié during her one-month training period[7]. She focused on the following models: Held, Walker-Wasley, James, Yactor, $P^n\tau$ and Jacobs-Roslund. The following high explosives have been extensively studied: CompB, B2141, PBX 9404, PE4, PETN, Tetryl, and TNT. Some high explosives have only been fitted for a subset of models: B2203A, B2214, NM. There were too little results in FraID for the others HE.

For one-parameter models, using a genetic algorithm is not mandatory, since other less computer-expensive techniques could have been used. Only GA is available in TEMPER, but since the coding of optimization is also object-oriented, we could easily add alternative techniques, such as gradient descent for simpler problems.

It is clearly out of scope of this article to provide a detailed list of results for all the fitted models and all FraID high explosives under study. This will however be done in a future MSIAC report. In the following paragraphs, we will focus on several results, showing comparisons with already published parameters. We will also point out the limitations of this optimization process and propose solutions to overcome them.

3.2   James' model for PBX 9404

James published[8] several E_{crit} and S_{crit} (Σ_{crit} in his paper) values, and illustrates the results for both flat and round steel projectiles impacting PBX9404. Experimental data are available in FraID as well, albeit not exactly the same than James' ones for round impacts.
James' values for PBX9404, fitting both flat and round impacts, are E_{crit}=450 000 J/m² and S_{crit}=50 000 J/kg, whereas TEMPER's values fitting flat impacts are E_{crit}=672 080 J/m² and S_{crit}=24 281 J/kg.

For flat impacts, the corresponding fitness is 0.935 for James' parameters and 0.978 for TEMPER's parameters. A look at the corresponding threshold curves in Figure 9 clearly shows that the genetic algorithms values fit better the experiments. However, it is impossible to fit flat and round impacts at the same time using TEMPER. Using parameters fitted for flat impacts to model round impacts, TEMPER parameters give a fitness of 0.923, which is still better than the fitness value using James parameters (0.895). If a new optimization is ran for round impacts, TEMPER values change to E_{crit}=623 883 J/m² and S_{crit}=0 J/kg, giving a fitness of 0.953. Using these new parameters to model flat impacts gives a fitness of 0.928.

These results show that the build-in optimization feature in TEMPER works well and is perfectly able to find a best set of parameters for a given scenario. However, a limitation of TEMPER is its inability to work on more than one scenario at the same time. An evolution is required to fit parameters on several scenarios, each scenario having its own data file.
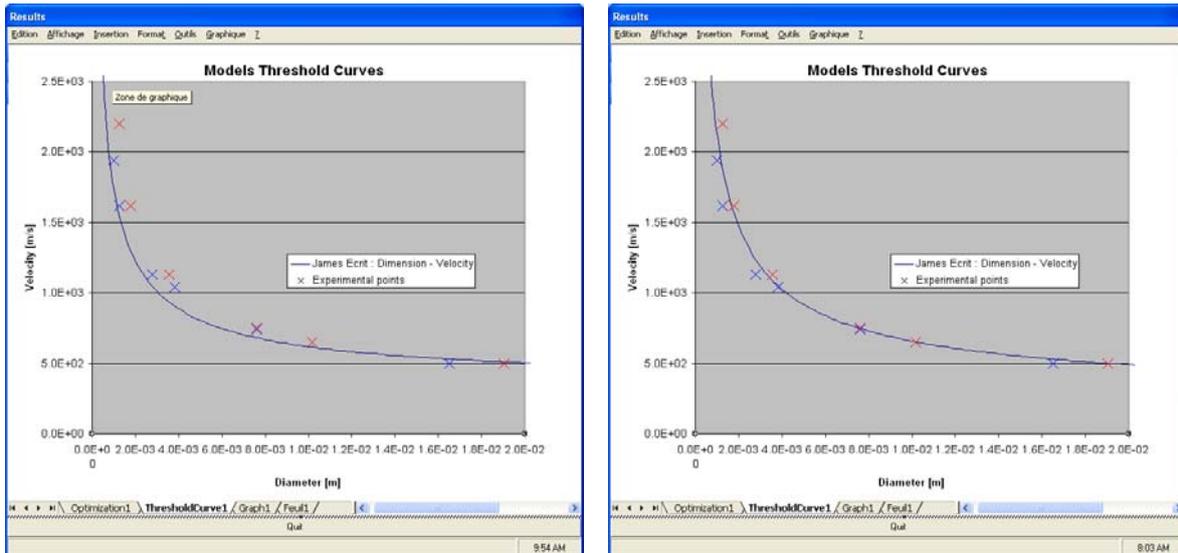
**Figure 9: Flat steel projectile on bare PBX9404
two sets of parameters: James (Right) and TEMPER (Left)**

3.3 Yactor's model and pop-plots

This model, available for both bare and confined energetic materials, is based on pop-plot results in terms of run-to-detonation distance as a function of impact pressure. For many high explosives, the following empirical relation[9] holds true:

$\log_{10}(P \text{ [GPa]}) = c_1 - c_2.\log_{10}(X_{run} \text{ [mm]})$

In TEMPER, the implementation is as follows

$X_{run} \text{ [m]} = \text{Exp}((\text{lnb} - \ln(P \text{ [Pa]})) / a)$

Equating both expressions leads to the following determination of Yactor's parameters from experimental pop-plots:

$a = c_2$
$\text{lnb} = \ln(10).(c_1 - 3.c_2 + 9)$

For porous Tetryl at 1 500 kg/m³ density, $c_1 = 0.75$ and $c_2 = 0.81$, or as required by TEMPER lnb=16.855 and a=0.81. In FraID, we find four detonation threshold points for bare porous Tetryl at 1 500 to 1 540 kg/m³. The pop-plot values give a fitness of 0.927, whereas the TEMPER fit gives lnb=17.1911 and a=0.73 ($c_1 = 0.74$ and $c_2 = 0.73$) with an excellent fitness value of 0.983.

The fitted values seem to differ notably from the experimental pop-plot, but Figure 10 shows that the discrepancy is not that important. The difference is mainly due to the shock velocity / particle velocity relation (U_s/U_p), refitted from LASL data as linear in TEMPER [$U_s = 0.8774 + 2.5973.U_p$; U_p and U_s in mm/µs], but in fact strongly diverging from linearity as shown by the fit proposed in the LASL Handbook[9] [$U_s = 2.1714 + 1.6225.U_p - 0.3411/U_p$; U_p and U_s in mm/µs] (see Figure 11). We notice however that the LASL fit is not valid for low U_p.
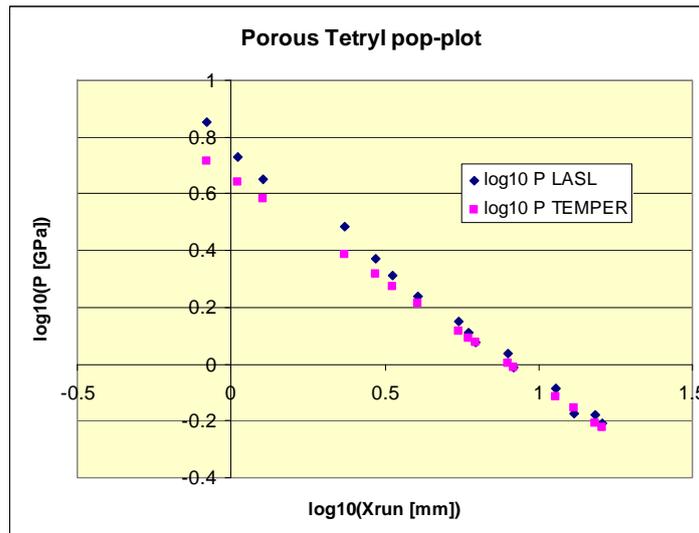
Figure 10: Pop-plot of porous Tetryl (density = 1 500 kg/m3)
Experimental pop-plot (dark blue) and values from a fitted Yactor's model (pink)
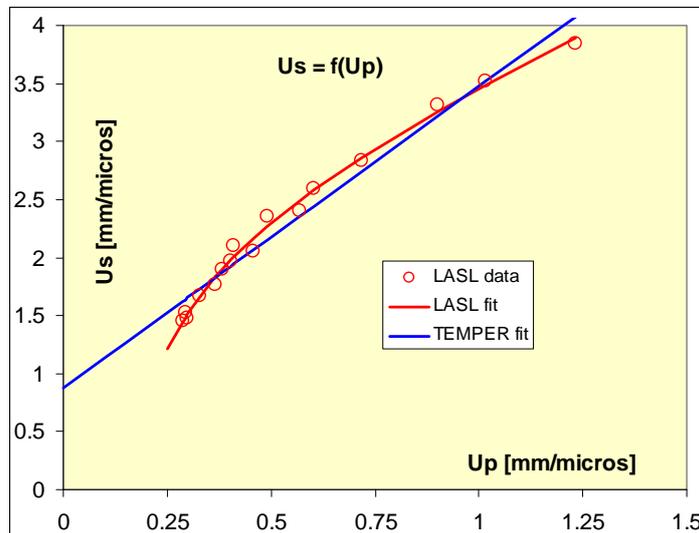

Figure 11: Us/Up relation: LASL and TEMPER

3.4 Jacobs-Roslund's model

It has been extremely difficult to find good fits for the original Jacobs-Roslund evaluation of threshold velocity (see Table 1). The underlying problem is that (for $d>d_{crit}$), the threshold velocity is expressed as $V=f(d,t/d)$ to account for both bare and covered explosives. An appropriate global optimization would thus require working with experimental data points having variations in both d and t/d and fit a threshold surface $V=f(d,t/d)$.

Unfortunately, TEMPER handles only threshold curves in 2D, that is variation of a variable expressed as a function of a single other variable. When performing parametric simulations with variations of t, TEMPER displays a set of $V=f(d)$ curves, but this cannot be used directly in the optimization procedure.

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Other problems with this model are that:
- It cannot be continuous at d=d$_{crit}$ for both bare and covered HE.
- The number of parameters requires having many experimental points to ensure a good fit, which was not the case for most of the formulations.
- The "C" parameter depends on the nature of projectile and cover materials. Since it's an empirical model, no direct dependence on material Hugoniots can be written, so it is impossible to estimate a C value for couples of materials that have not already been tested.

The solution we suggest for the moment is:
- To ignore results for diameters under d$_{crit}$,
- To focus first on flat impacts on bare HE (assuming B=0, this step leads to A and β values)
- To study flat impacts results with a fixed t/d ratio (leading to a value for C)
- To check if this preliminary C value also works for others t/d ratios (with the same materials)
- To test on round projectiles or spheres in order to determine a B value.

This step-by-step procedure does not require any powerful optimization technique, and could be done either using TEMPER or Excel™. It is certainly a strong limitation for the moment, since genetic algorithms are mainly useful for multi-parameter situations, but could not be used to perform the overall optimization of such models. In our case, each cover thickness corresponds to a different scenario, thus making a global optimization very difficult to handle.

Another alternative is to use the MSIAC modification of this model, which only requires one parameter[5].

4   Conclusions and Future Work

4.1 Summary

TEMPER has been used in order to derive SDT model parameters from experiments. The experiments are summarized in the MSIAC FraID database. It has been shown that the built-in optimization technique (genetic algorithm) allows a quick and reliable estimation of model parameters, provided that a sufficient amount of experimental data is available (the more parameters in the model, the more data we need).

The main limitation of this work is that the fitting procedure requires experimental results to be expressed in one of the threshold planes (for instance duration/pressure or diameter/velocity) handled by the model. Consequently, the user can only optimize one scenario at a time, which forbids any attempt to perform a "global" optimization on all available results.

4.2 Future work

A collaborative MSIAC-CEA Gramat report will be made available in 2011 with the proposed SDT model parameters for a number of energetic materials and configurations.

TEMPER will be modified to let the used paste optimization results directly into the energetic material file.

An attempt will be made to include in TEMPER the ability to perform optimization on multiple scenarios at once. It should raise the current limitation on complex, multi-parameter models.

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