Journal of Energetic Materials
Publication details, including instructions for authors and subscription information:
http://www.informaworld.com/smpp/title~content=t713770432

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Boyd D. Schimel[a]; Ernest L. Baker[b]; Walter J. Grantham[a]
[a] School of Mechanical and Materials Engineering Washington State University, Pullman, WA [b] U. S. Army, ARDEC Picatinny Arsenal, NJ

To cite this Article Schimel, Boyd D. , Baker, Ernest L. and Grantham, Walter J.(1997) 'A method for parameter optimization of reactive flow continuum models by sequential quadratic programming', Journal of Energetic Materials, 15: 4, 289 — 311
To link to this Article: DOI: 10.1080/07370659708216089
URL: http://dx.doi.org/10.1080/07370659708216089

A METHOD FOR PARAMETER OPTIMIZATION OF REACTIVE FLOW CONTINUUM MODELS BY SEQUENTIAL QUADRATIC PROGRAMMING

Boyd D. Schimel*, Ernest L. Baker**, and Walter J. Grantham*

*School of Mechanical and Materials Engineering
Washington State University
Pullman, WA 99164-2920

**U.S. Army, ARDEC
Picatinny Arsenal, NJ 07806-5000

ABSTRACT

This paper presents a procedure for performing parameter optimization of ignition and growth continuum models for high explosive systems. Continuum modeling of reactive flow in high explosive systems can yield highly accurate predictions of experimental observations. However, the numerical parameter optimization that is needed to establish these predictions generally requires many evaluations of a model, and in the case of continuum reactive flow models, each evaluation requires long run times. In terms of keeping the total number of function evaluations low, the variable metric sequential quadratic programming approach is at present the most efficient general nonlinear local optimization method available. In this investigation, the variable metric sequential quadratic programming code NLQPEB is coupled to the two-dimensional high rate continuum modeling programs CALE and DYNA2D. An example parameter optimization of an

Journal of Energetic Materials Vol. 15, 289-311 (1997)
Published in 1997 by Dowden, Brodman & Devine, Inc.

ignition and growth model for the HMX-based high explosive PAX2A is presented. The optimization procedure adjusts the ignition and growth reaction rate model parameters in order to locally minimize the difference between calculated and experimental pressure histories from Manganin gauge experiments.

INTRODUCTION

Sequential quadratic programming methods have been successfully applied in previous investigations to the optimization of explosive product equation of state parameters[1], shaped charge analytic design models[2], and explosively formed projectile (EFP) models[3,4,5]. These efforts have not only demonstrated the utility of modern nonlinear optimization methods, but they have also resulted in significant advancements in high explosives technology and have prompted broader application of sequential quadratic programming methods to other areas of munitions modeling. However, to date almost no attention has been placed on the application of optimization to reactive flow modeling for the prediction of high explosive initiation. The primary reasons for this are twofold. Firstly, the reactive flow continuum modeling of these systems requires both fine meshing and small time step sizes to preserve accuracy. These factors contribute to long run times. Secondly, numerical instability associated with the computational aspects of reactive flow modeling have also contributed to making parametric investigations difficult. However, advances in reactive flow modeling technology for high explosive systems[6,7], and dramatic increases in computing speed and availability are, at present, offsetting these difficulties. For example, one-dimensional reactive flow modeling of initiation can be performed in a relatively short time; on the order of five minutes on a personal computer. These relatively short run times make parameter optimization by the sequential quadratic programming method highly practical.

MANGANIN GAUGE EXPERIMENTATION

A series of impact initiation tests were conducted on the HMX-based high explosive PAX2A at the Lawrence Livermore National Laboratory (LLNL) High Explosives Applications Facility (HEAF). The tests were conducted to supply data for the parameterization of the high explosive ignition and growth model. Manganin gauge transducers were employed to read pressure at various positions within the explosive material. The apparatus, shown schematically in Figure 1, was designed to simulate a linear one-dimensional test for measuring the pressures during the ignition and growth phases of a explosive reaction. In an actual one-dimensional test, the presence of the Manganin gauges may interfere with the detonation front. Therefore, the wedge-shaped configuration shown was used for testing.

The apparatus consisted of two main parts: a projectile donor assembly and an explosive wedge acceptor assembly. The donor assembly consisted of a plastic sabot that housed either a steel or aluminum impactor. The acceptor assembly consisted of an aluminum buffer plate and two sections of the explosive PAX2A. One section of the explosive was cut in the shape of a cylindrical wedge, where one end face remained orthogonal to the cylinder axes, and the opposite end face was cut on a plane 15 degrees from orthogonal. The remaining section of PAX2A was disk shaped. Two Manganin gauges were placed between the buffer plate and the orthogonal end face of the explosive wedge, and a six gauge packet was sandwiched between the 15 degree end face of the wedge and the explosive disk. The dimensions of the explosive wedge acceptor assembly were such that side rarefaction into the PAX2A components would not interfere with the Manganin gauge measurements within the experimental time frame.

An experiment was initiated by propelling the donor apparatus into the explosive wedge acceptor assembly. The velocity of the projectile donor assembly

was measured just prior to impact. The Manganin gauge measurement points A and B in Figure 1 were used to determine the pressure verses time histories on the initial impact plane of the explosive, and hence, were used to help ensure that the initial shock front was coplanar with the interface. As the shock front propagates, the Manganin gauges C through H are encountered in sequence. The spacing between gauges in the axial dimension is constant. Therefore, the test simulates a one-dimensional experiment where gauges have been spaced at constant intervals, but without any interference from the preceding gauges.

CONTINUUM MODELING

The high rate continuum modeling software CALE[6] and DYNA2D[7] were interfaced with the optimization software in this investigation. These computer programs model the reactive flow through explicit time integration of the conservation equations for mass, momementum and energy, as well as a reactant to product reaction rate. The materials state, including reacted fraction, are discretized on a computational mesh. DYNA2D is a Lagrangian description finite element code and CALE is an arbitrary Lagrangian-Eularian finite difference code. An example of the computational mesh used in this investigation is shown in Figure 2. Due to the one-dimensional nature of the model, each mesh area is one cell in height by the stated number of cells in length. The constitutive models, equations of state and reaction rate models are described in the following paragraph.

Constitutive models and equations of state for the nonexplosive materials shown in Figure 2 are as follows. The Lexan sabot utilized a Mie-Gruneisen equation of state which models pressure as a function of material density and energy. The sabot was assigned a strength of zero in the constitutive model. The bullet and buffer plate materials were modeled with the Mie-Gruneisen equation of

state, and the Steinberg-Guinan constitutive equations[8] which model shear modulus and yield strength as functions of strain, temperature, and pressure.

The Jones-Wilkens-Lee (JWL) thermodynamic equation of state model[9] was used for the unreacted explosive and reaction products. The equation is equivalent in form for the reactants and products and is given by:

$$P = Ae^{-R_1 V} + Be^{-R_2 V} + \frac{\omega C_v T}{V} \tag{1}$$

where P = pressure, V = relative volume, T = temperature, C_v = heat capacity, ω = Grunesen parameter, and A, B, R_1, R_2 = constants. Separate sets of variables and constants were defined for the reactant and product equations of state.

The ignition and growth reaction rate is given by the Tarver burn rate equation:

$$\frac{dF}{dt} = I(1-F)^b(\rho/\rho_o - 1 - a)^x + G_1(1-F)^c F^d P^y + G_2(1-F)^e F^g P^z \tag{2}$$

where F = fraction reacted, t = time, ρ = density, ρ_0 = initial density, P = pressure, and I, b, a, x, G_1, c, d, y, G_2, e, g, and z are constants. The reaction rate equation is used to model different behavioral regimes of the detonation through assignment set of constant limits. Limits F_{Imax}, F_{G1max}, and F_{G2min}, are placed on the burn fraction to control the active range of the constants I, G_1, and, G_2, respectively. Particularly, if $F > F_{Imax}$ then I = 0, if $F > F_{G1max}$ then $G_1 = 0$, and if $F < F_{G1max}$ then $G_1 = 0$. As the reacted fraction increases, internal energy is liberated at the rate

$$\frac{dE}{dt} = (E_o / \rho_o)\frac{dF}{dt}, \tag{3}$$

where E_o has units of specific internal energy times density.

VARIABLE METRIC SEQUENTIAL QUADRATIC PROGRAMMING

The objective of optimization is to minimize (or maximize) a function of one or more parameters. A set of equality and/or inequality constraints that are also functions of the parameter set, and which confine the parameter values to specified regions of the search space, may also be imposed as part of the optimization problem. A minimization problem may be stated more formally in the following mathematical format:

$$\begin{aligned} &\text{minimize } F(x) \\ &\text{subject to: } g(x) = 0 \\ &\qquad\qquad h(x) \geq 0 \end{aligned} \tag{4}$$

where x is a real-valued vector of variable parameters, $F(x)$ is a scalar-valued cost function, and $g(x)$ and $h(x)$ are vectors of constraint functions.

The solution to the general optimization problem is obtained by Lagrange Multiplier analysis. The Lagrangian for the standard optimization problem may be written as

$$L(x,\lambda,\mu) = F(x) - \lambda^T g(x) - \mu^T h(x), \tag{5}$$

where λ and μ are Lagrange multiplier vectors. The following Kuhn-Tucker necessary[10,11] conditions for a local minimum may be applied to gain potential solutions to this problem:

$$\frac{\partial L}{\partial x_i} = \frac{\partial F}{\partial x_i} - \lambda^T \frac{\partial g}{\partial x_i} - \mu^T \frac{\partial h}{\partial x_i} = 0$$
$$\mu^T h(x) = 0 \qquad (6)$$
$$\mu_j \geq 0.$$

In cases where it is unclear if a point satisfying the necessary conditions is a minimum, maximum, or otherwise, a set of second-order sufficient conditions may be applied for clarification[10].

If the analytical representation of $F(x)$ or the constraint set is not available, or not tractable, then numerical methods may be applied to find an approximation to the solution of (4). At present, the most efficient numerical approach to solving nonlinear optimization problems is the Sequential Quadratic Programming (SQP) method[12]. The SQP method produces iterative estimates of the of the optimal parameter values and the Lagrange multipliers. As the numerical algorithm converges, these iterative estimates approach the optimal parameter values and Lagrange multipliers that would result from the analytical method (6), if it were applied.

The primary computational components of a sequential quadratic program are responsible for the formation of an iterative locally quadratic approximation to the Lagrangian function, and a sufficient decrease line search of an augmented Lagrangian merit function. An iterative quadratic approximation to the Lagrangian is given by,

$$L_q(x_k, \lambda_k, \mu_k) = L_q(x_{k-1}, \lambda_{k-1}, \mu_{k-1}) + d_k^T \nabla L_q(x_{k-1}, \lambda_{k-1}, \mu_{k-1}) + \frac{1}{2} d_k{}^T B_k d_k \qquad (7)$$

where ∇ is the gradient operator (with respect to x),

$$d_x = x_k - x_{k-1} \qquad (8)$$

and x_k and x_{k-1} are the values of the parameter vector x at the current iteration and the previous iteration, respectively. The second-order partial derivative, or Hessian, approximation matrix, B_k in (7), is generated by variable metric update equations. The update that is typically applied is the Broyden-Fletcher-Goldfarb-Shanno (BFGS) update[13,14,15,16], which was modified by Powel[17]:

$$B_k = B_{k-1} - \frac{B_{k-1} s s^T B_{k-1}}{s^T B_{k-1} s} + \frac{\eta \eta^T}{\eta^T s}, \tag{9}$$

where

$$\begin{aligned} s &= x_{k-1} - x_{k-2} \\ \eta &= \theta\psi + (1-\theta) B_{k-1} s \\ \psi &= \nabla L_q(x_{k-1}, \lambda_{k-1}, \mu_{k-1}) - \nabla L_q(x_{k-2}, \lambda_{k-1}, \mu_{k-1}), \end{aligned} \tag{10}$$

and

$$\theta = \begin{cases} 1 & \text{if } s^T\psi \geq 0.2 s^T B_{k-1} s, \\ \dfrac{0.8 s^T B_{k-1} s}{s^T B_{k-1} s - s^T \psi} & \text{otherwise.} \end{cases} \tag{11}$$

The quadratic approximation to the Lagrangian function is solved for the direction, d_k, in parameter space that points in a minimizing direction of the quadratic. The variable metric matrix, B_k, must remain positive definite to ensure a bounded solution for the search direction, d_k. In practice, a positive definite B_k is maintained by the Levenberg-Marquardt method or by storing the variable metric updates in

Cholesky decomposed form[18,19]. The positive definite state of B_k enables (7) to be solved as a minimization problem.

In a numerical setting, the quadratic approximation to the Lagrangian may be recast, through primal-dual relationships[19], into the following quadratic subproblem with linearized constraints:

$$\begin{aligned} \min_{d_k} \quad & F(x_{k-1}) + d_k^T \nabla F(x_{k-1}) + d_k^T B_k d_k \\ \text{subject to:} \quad & g(x_{k-1}) + d_k^T \nabla g(x_{k-1}) = 0 \\ & h(x_{k-1}) + d_k^T \nabla h(x_{k-1}) \geq 0. \end{aligned} \tag{12}$$

The maintenance of a positive definite B_k ensures that the local approximation given in (12) can be readily solved for the search direction, d_k, through standard convex quadratic programming methods[20]. In practice, other numerical techniques may be applied to prevent the linearized constraint approximations from completely closing off the feasible region[11,12]. An active sets strategy[18,21] is also employed so that only the inequality constraints that are satisfied to within some small tolerance of an equality are included in the quadratic model, thereby reducing the overall computational effort.

Following solution of the quadratic subproblem, a one-dimensional line search along the minimizing direction, d_k, is conducted. Another class of approximations to the Lagrangian (augmented Lagrangian merit functions) are typically used for this phase of the analysis. The following merit function[22] was used for this analysis:

$$W(x_k, \lambda_k, \mu_k) = F(x_k) + \left|\lambda_k^T g(x_k)\right| + \left|\mu_k^T h(x_k)\right|. \tag{13}$$

The iteration point, x_k, is determined by evaluating (13) at successive candidate points, $\bar{x}_k$, until a sufficient decrease in the value of (13) is found. The candidate points are generated from the line search update equation

$$\bar{x}_k = x_{k-1} + \alpha d_k. \tag{14}$$

The variable α is a scalar-valued step length parameter that is iteratively adjusted by a step-length algorithm. In program NLQPEB[18], α is initialized to one at the beginning of each line search and the candidate point, $\bar{x}_k$, from (14) is tested for a sufficient decrease in (13) by applying Armijo's step-length criteria[19,21,23]. If the criteria are satisfied then the value of the candidate point generated by (13) is assigned to x_k and this value is passed to the next overall iteration of the SQP algorithm. However, if the criteria are not satisfied, a two-point-slope quadratic approximation[11] of (13) is solved for a minimizing α. The quadratic approximation utilizes function and gradient values of (13) from iteration point x_{k-1} and the function value of (13) for the candidate point $\bar{x}_k$. The step-length criteria and the minimization of the quadratic approximation are applied in an interpolative manner until a sufficient decrease or some termination criterion is reached.

The SQP algorithm proceeds by solving the quadratic subproblem and line search problem at each Newton iteration, defined by (7). Successive Newton iterations are applied until one or more termination criteria are achieved. Termination criteria include: a maximum number of Newton iterations, a maximum number of line search iterations, the norm of the difference between successive iteration points less than some upper bound, or the norm of the gradient of the Lagrangian in (7) less than some upper bound. Any of the first three termination criteria may be equivalent to a failure of the algorithm, either by nonconvergence or premature convergence to a nonoptimal value. The last termination criterion constitutes a

successful termination of the algorithm, where the conditions stated in (6) have been satisfied to within a defined numerical tolerance.

For this investigation, the general purpose variable metric sequential quadratic program NLQPEB[18] was used to perform the parameter optimizations. NLQPEB is similar to the algorithm defined in[12], but it has the added feature that the update of the variable metric matrix, B_k, is not performed until after completion of the line search, as opposed to directly preceding solution of the quadratic subproblem. The initialization process was observed to aid in the convergence of parameters with small cost function sensitivities in this study.

COST FUNCTION DEFINITION

The cost function defines, subject to any constraints, what is to be minimized by the optimization program. The form of the cost function selected can greatly influence how the theoretical predictions and the experimental data correspond to one another. Hence, the process of selecting a cost function is in part determined by the scientists perception of how a good quality fit between the data and theoretical predictions should look.

The experimental Manganin gauge data produced by the explosive wedge tests was marked by rapid changes in pressure as the detonation front passed. If the wrong type of cost function were selected, then the predictions might be almost entirely dominated by the behavior in a close neighborhood of the detonation front. It was observed that minor differences between measured and predicted arrival times of the detonation front resulted in large contributions to some types of cost functions. For instance, the end result of applying an error-squared cost function to the optimization of ignition and growth parameters were reasonably accurate predictions of the detonation front arrival times at each Manganin gauge

location, but relatively poor predictions of the observed experimental behavior that occurred afterwards. Hence, this type of cost function was deemed too sensitive to the portion of the data associated with the shock wave, and the following weighted absolute difference cost function was applied:

$$F = \frac{1}{n}\sum_{i} c_i \left| P_{cal\,i} - P_{exp\,i} \right|, \tag{15}$$

where c_i = i^{th} the weight factor, $P_{cal\,i}$ = the i^{th} calculated pressure history data point, $P_{exp\,i}$ = the i^{th} experimental pressure history data point, n = data point count, and i ranges from 1 to n. A maximum allowed difference of 0.5 Mbar between experimental and calculated pressures was applied at each data point in order to further soften the ignition over-sensitivity effects associated with the shock wave.

OPTIMIZATION OF THE EQUATIONS OF STATE AND BURN RATE PARAMETERS

The NLQPEB optimization program was coupled, as shown in Figure 3, to the LLNL developed two-dimensional high rate continuum modeling programs DYNA2D and CALE. The resulting program has the ability to optimize initial modeling parameters using either DYNA2D, CALE, or both. The combined codes were used to optimally parameterize the thermodynamic equations of state and the ignition and growth model to experimental records.

Prior to this investigation, the NLQPEB nonlinear optimization program was used to parameterize a JWL detonation products equation of state (1), in order to closely reproduce experimental cylinder test wall velocities[1]. A test cylinder con-

sisted of a 10-inch long, by 1-inch outside diameter, by 3/4-inch inside diameter precision machined oxygen free copper tube filled with PAX2A explosive material. The explosive charge was detonated from one end and the cylinder wall expansion was recorded with an ultrahigh speed smear camera. The film record of the cylinder wall expansion was then digitized and wall velocities were determined at various levels of expansion. Program NLQPEB was then applied to an analytic cylinder test model to optimize experimental and calculated cylinder wall velocities using an error squared cost function. Equality constraints were added to produce a chosen detonation energy and measured Chapman-Jouguet detonation velocity. The resulting JWL equation of state was verified using DYNA2D modeling of the same experiment.

An unreacted JWL equation of state was similarly parameterized[1] using NLQPEB to closely reproduce an unreacted Hugoniot[24] based on initial shock behavior from wedge test and Lagrange gauge experimentation. Equality constraints were added to produce an initial unpressurized state (P = 0.) and chosen Von Neumann spike pressure[24]. The resuting JWL constants and material strength parameters are presented in Table 1.

Program NLQPEB was used to parameterize the Tarver burn rate model (2), using the cost function defined in (15). The reaction rate constants used for the initial values of the optimization variables were based on LX-10 ignition andgrowth constants[25]. A number of optimizations were performed investigating different optimization variable initial values, cost functions, and optimization parameter set effects. Table 2 presents the initial and final optimization cost function values, along with the initial and final optimized ignition and growth constants. The results presented in Table 2 used six of the Ignition and Growth constants as

optimization variables and resulted in 38 iterations requiring about 3 1/2 hours of CPU time.

TABLE 1. PAX2A JWL Constants

	Unreacted	Product
ρ_0 (g/cc)	1.770	
A (Mbar)	319.010	65.3959
B (Mbar)	-0.0959833	1.76944
R_1	10.4816	9.22529
R_2	1.77660	2.66610
ω	0.88	0.369892
Cv (Mbar/°K)	2.7813e-5	1.e-5
T_0 (°K)	298.	
E_0 (Mbar)		0.0907976
Y (Mbar)	0.0018	
G (Mbar)	0.0454	

A large reduction in the optimization cost function value indicates a large improvement in agreement between the calculated pressure histories and the experimental pressure histories. Figure 4 presents a comparison of the initial calculated pressure histories to the experimental pressure histories. Figure 5 presents a comparison of the final optimized calculated pressure histories to the experimental pressure histories. A dramatic improvement in agreement to the data is evident for the optimized parameter set. Figures 4 and 5 were generated from the output of DYNA2D; CALE produces similar results. Note that the optimization results in Table 2 only used a subset of the available model parameters. While this optimization gives good agreement with experimental results, a more complete optimization including more model parameters may give even better agreement.

TABLE 2. PAX2A Ignition and Growth Constants

	Initial	Optimized
Z (COST)	0.0303 Mbar	0.0169 Mbar
I	7.43e11	7.5380e11
b^*	0.667	0.667
a^*	0.001	0.001
x	20.0	23.069
G_1	90.	90.395
c^*	0.667	0.667
d^*	0.333	0.333
y	2.0	1.9939
G_2	400.0	403.20
e^*	0.333	0.333
g^*	1.0	1.0
z	2.0	3.2328
F_{1max}*	0.3	0.3
F_{G1max}*	0.5	0.5
F_{G2min}*	0.5	0.5
* = not used as an optimization variable		

CONCLUSIONS

Optimization by the variable metric sequential quadratic programming method has been successfully applied to Lagrangian and Arbitrary Lagrangian Eulerian codes for reactive flow continuum modeling of high explosive initiation. The final calculated pressure histories are observed to agree well with the experimental ones. Application of the variable metric SQP method greatly reduces the model parameterization time and successfully improves the quantitative agreement in comparison with manual efforts. Additionally, the optimization methods should

be extendible to more complex initiation models, providing improved initiation prediction for the computational design of safer munitions systems. Parametric optimization of increased complexity high explosive behavior and models continues to be investigated. Ongoing efforts are concentrating on improvement of global optimization strategies and optimization using distributed and scaleable parallel computer structures.

ACKNOWLEDGMENTS

This Research was supported by the US Army Armament Research, Development, and Engineering Center, under the auspices of the US Army Research Office Scientific Services Program. Portions of the research were administered by Battelle (Delivery Order 1484, Contract No. DAAL03-91-C-0034).

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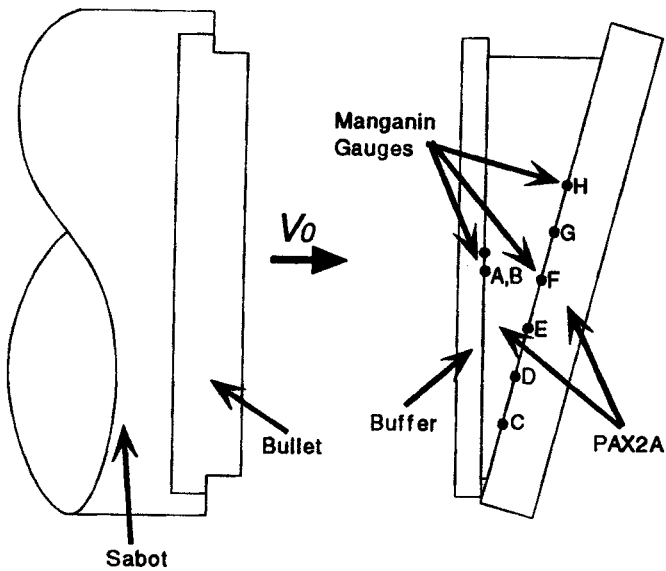

FIGURE 1. Manganin gauge experimental apparatus.

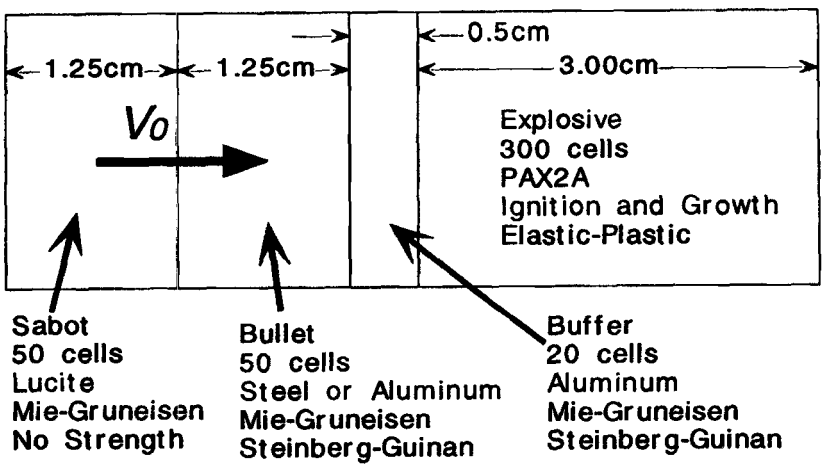

FIGURE 2. Schematic of DYNA2D meshing and material setup.

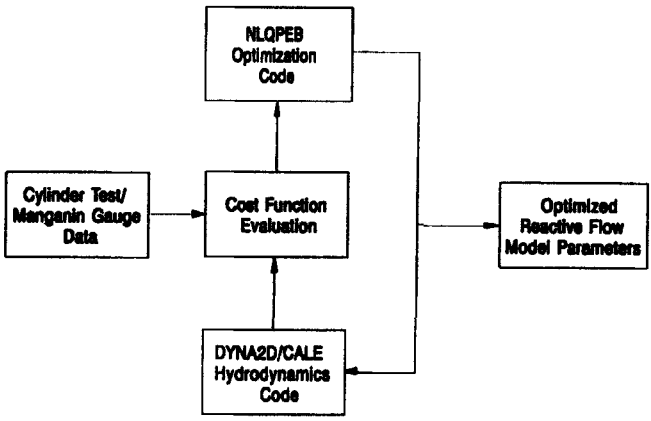

FIGURE 3. Flow chart for the reactive flow continuum model parameter optimizations.

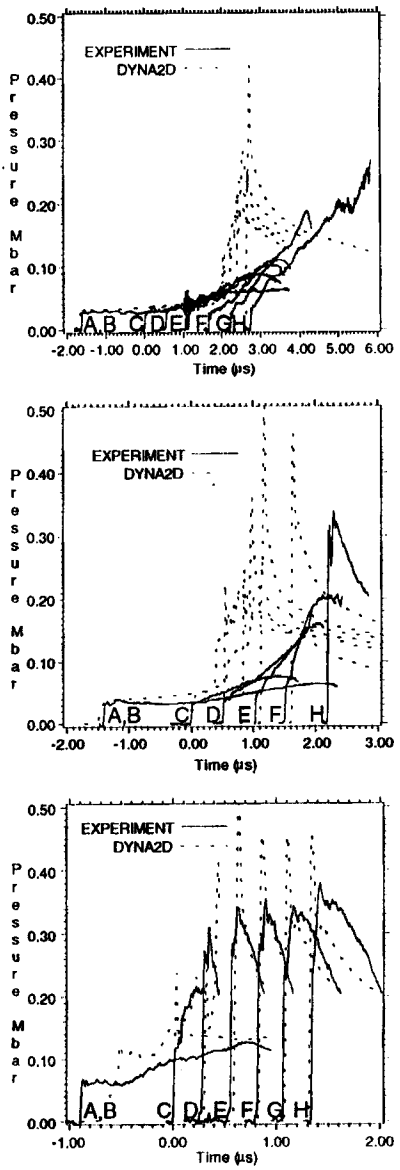

FIGURE 4. Initial calculated pressure histories versus experimental pressure histories.

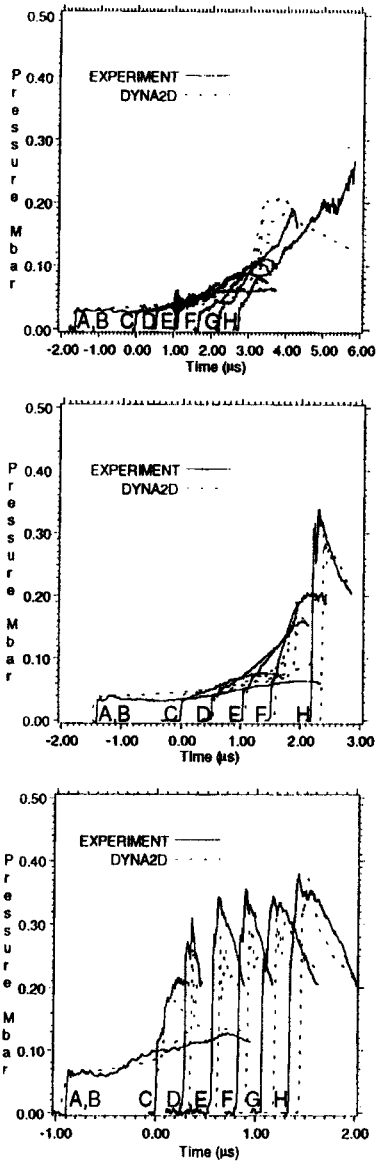

FIGURE 5. Final optimized calculated pressure histories versus experimental pressure histories.