A thermochemical code to model detonations in condensed energetic materials using genetic algorithms

A. Zayer, U. Riedel, and J. Warnatz
IWR, University of Heidelberg, Im Neuenheimer Feld 368
D-69120 Heidelberg, Germany

Corresponding author: A. Zayer: zayer@iwr.uni-heidelberg.de

Introduction

We discuss the implementation of genetic algorithms for modeling chemical equilibrium and detonation parameters at the Chapman Jouguet state. Our strategy has the advantage that no initial estimate of the equilibrium product distribution needs to be made. It is also an efficient strategy for finding the global minimum, since for highly non-ideal condensed energetic materials, the calculation of the chemical equilibrium through free energy minimization, using deterministic algorithms, can lead to a local minimum being found instead of a global minimum. This can result in an incorrect prediction of the chemical products distribution.

Fundamental Issues

To handle gaseous products, The JCZS equation of state was chosen for the implementation in the code because for this equation of state data is available. The Sandia database [1] lists more than 700 species.
The relationship between the pressure, the volume, and the temperature [2] is

$$P = P_0(V) + G(V,T)\frac{nRT}{V}$$

where $P_0\ (V)$ is the volume-dependent pressure along the zero degree isotherm and $G\ (V, T)$ is a term accounting for the thermal contribution to the pressure arising from intermolecular forces. The variables P_0 and G depend on the parameters ε/k and r^* of the exponential-6 potential function [1]:

$$\varphi(r) = \varepsilon\left[\left(\frac{6}{\eta-6}\right)\exp\left[\eta\left(1-\frac{r}{r^*}\right)\right]-\left(\frac{\eta}{\eta-6}\right)\left(\frac{r^*}{r}\right)^6\right]$$

The chemical equilibrium is calculated through free energy minimization. The chemical potential for gaseous species is defined by

$$\mu_i = \frac{\partial A_{ideal}}{\partial n_i} + \frac{\partial E_o(V)}{\partial n_i} + \frac{\partial(nRT\ln f(V,T)}{\partial n_i}$$

and for solid products, such as graphite and aluminum, the Cowan equation of state was implemented in the code. The chemical potential [3] is defined by

$$\frac{\mu_s}{RT} = \frac{\left(F^0 - H_0^0\right)_s}{RT} + \frac{\left(H_0^0\right)}{RT} + \frac{F_s'}{RT}$$

where F_s' is given by

$$F_s^{'} = M_r\left(PV_s - P_0V_0 - [a_sV + b_s \ln V - \frac{c_s}{V} - \frac{d_s}{2V^2} - \frac{e_s}{3V^3}\right)$$
$$+ M_r\left((A_1V + A_2 \ln V)T_V + \left(C_1V + \frac{C_2V^2}{2} + \frac{C_3V^3}{3}\right)T_V^2\right)$$

For gaseous products, the internal energy is equivalent to

$$E(T,V,n) = E_{ideal} + \int_{\infty}^{V}\left(\frac{\partial E_0}{\partial V} - nRT^2\left[\frac{\partial^2 \ln(f)}{\partial V \partial T}\right]\right)dV$$

and for the solid component [3], it is equivalent to

$$E_s(T,V) = (H_T^0 - H_0^0)_s + (H_0^0)_s - P^0V^0 + \int_{V_s^0}^{V_s}[T^2b(V) - p_1(V)]dV$$

In our approach to improve the efficiency and accelerate the convergence of the algorithm, a hybrid scheme combining a genetic algorithm and the method of feasible direction is used. The way in which this scheme functions is that the genetic algorithm first gives us an approximate global optimum and the method of feasible direction is then applied for descending the last steps to the global minimum.

To provide calculations, an initial population of chromosomes is chosen randomly in the search space, and the fittest chromosomes are then selected on the basis of the percentage that their fitness contributes to the cumulative fitness of the whole population; a roulette wheel selection is used for this purpose. Crossover and mutation operations are applied to the population to generate the fittest chromosomes with a mutation probability of p_m = 0.005 and a crossover probability of p_c = 0.6.

Handling constraints in genetic algorithms is a difficult task that is currently being researched. In the program Method K [4] is used. This method has proven to provide better results in comparison to other methods. The purpose of this method is to define a penalty function as follows:

$$P(\bar{x}) = \begin{cases} \left(K - \sum_{i=1}^{s} \frac{k}{p}\right) - f(\bar{x}) & s \neq p \\ 0 & otherwise \end{cases}$$

The penalty function equals zero and if no violations occur, the penalty function is positive. k is a large constant [O (10^9)], p the number of constraints, and s the number of constraints that have been satisfied.

The values obtained from the genetic algorithm are now used to start the feasible directions method [5, 6], which is a modification of the steepest descend algorithm. This method takes into account the gradients of the objective function and the active violated constraints, as well as the search direction in the previous iteration. The procedure is updated according to the following equation:

$$N^{q+1} = N^q + \lambda S^q$$

where N^0 is the initial vector, S^q is the search direction, and λ is a scalar whose value is determined using a one-dimensional search. The search direction S^q is determined using the Fletcher-Reeves conjugate direction method when no active or violated constraints exist.

$$S^q = -\nabla F(N^{q-1}) + \beta S^{q-1}$$

where

$$\beta = \frac{\left|\nabla F\left(N^{q-1}\right)\right|^2}{\left|\nabla F\left(N^{q-2}\right)\right|^2}.$$

Results and Discussion

To validate the predictions of our approach, the results obtained have been compared against different experimental and computed results from different references [7, 3, 8, and 1].

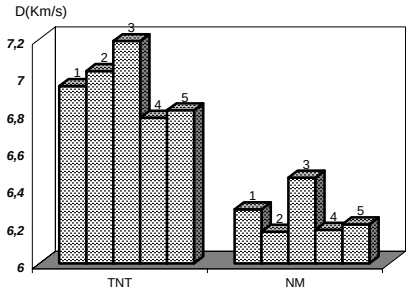

Figure 1. Experimental and calculated CJ detonation velocity for 2, 4, 6-Trinitrotoluene (TNT) and Nitromethan (NM).

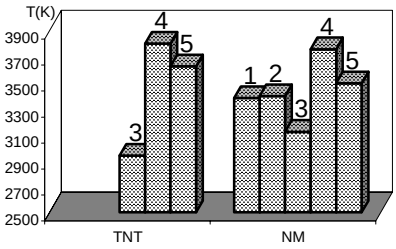

Figure 2. Experimental and calculated detonation Temperature for 2, 4, 6-Trinitrotoluene (TNT) and Nitromethan (NM).

In figures 1 and 2, the numbers 1, 2, 3, 4 successively represent results published in the literature, namely experimental data [1] and the results obtained using the CHEETAH [1], BKW [7], and AMRL [8] codes. Our own results are denoted by the number 5.
In figures 3, 4, and 5, we present the experimental CJ pressure for RDX, TNT, and PETN at various load densities and compare our results to the experimental data [1]. Open symbols designate the results of calculations, closed symbols the experimental results [1], and solid lines denote regressions.

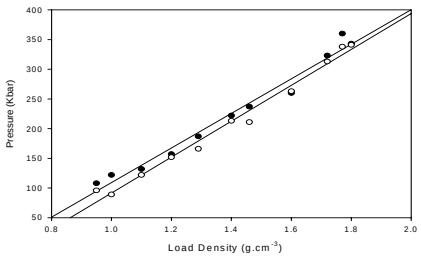

Figure 3. Detonation pressure for RDX as a function of loading density.

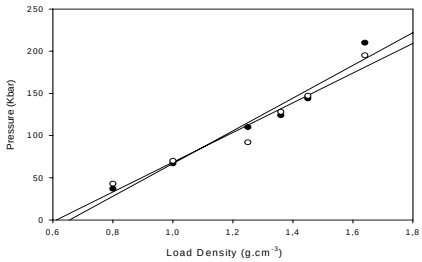

Figure 4. Detonation pressure for TNT as a function of loading density.

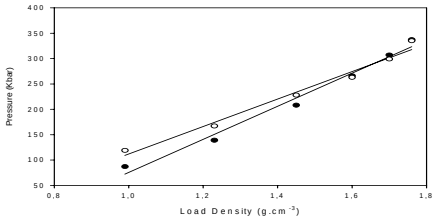

Figure 5. Detonation pressure for PETN as a function of loading density.

As can be seen, the computed results are in reasonably good agreement with the experimental data. The pressure deviation for TNT, RDX, and PETN are to within 3%, 5%, and 6% respectively to the experimental data.
The comparison of the computed detonation velocities for TNT and NM to the experimental data values gives a deviation no larger than 3%. Our calculated detonation velocities are within the range of the values calculated by other authors. The difference of the temperature predicted for NM is also within 2%.
The differences in the calculated detonation parameters observed between our code and the CHEETAH and AMRL codes can be explained by the fact that different values are used for the potential well depth ε_i, the equilibrium distance r_i, and for the thermodynamic data, or because the internal error control of the other computation methods are different.

Acknowledgements

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