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57-MM WARHEAD COOKOFF SIMULATIONS USING TOPAZ2D

by

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Approved by/approuvé par

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19/3/96
Date

ABSTRACT

The finite element program for thermal analysis, TOPAZ2D, was used to model the slow cookoff of a new 57-mm shell filled with the plastic-bonded explosive CX-84A. In spite of some gross approximations for the thermal parameters and reaction kinetics, a good estimate of the time to reaction was obtained.

RÉSUMÉ

Le programme d'éléments finis pour analyse thermique, TOPAZ2D, a été utilisé pour simuler le chauffage progressif lent d'un nouvel obus de 57 mm rempli avec l'explosif composite CX-84A. Malgré des approximations grossières utilisées pour les caractéristiques thermiques des composantes et la cinétique de réaction, on a obtenu une bonne estimation du temps de réaction.

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EXECUTIVE SUMMARY

The Canadian Forces have a possible capability deficiency in the safety of the storage, transportation, handling and use of munitions in that the present munitions are subject to initiation by unplanned stimuli such as fires. A fire in a magazine on board a ship, for example, could lead to a mass detonation with the loss of the ship and its personnel. Newer, insensitive explosives would lower the risk of such an accident. The definition of "insensitive" means, in the case of a fire, no reaction of the explosive other than burning.

In anticipation of future needs of the CF, DREV started a long-term program to develop explosives which are less likely to react violently to unexpected events. In particular, DREV recently had a task to develop a prototype 57-mm warhead for use aboard Navy vessels. This warhead has been tested experimentally in a slow cookoff situation and the present document attempts a post-experiment simulation of this test using the finite element computer program TOPAZ2D. A simplified model of a fuseless 57-mm shell was set up and its outer temperature was raised at the same rate as in the experiment. The explosive filling (the DREV explosive CX-84A) was assumed to react according to one-step, first-order Arrhenius reaction kinetics. The reaction parameters were varied until good agreement was obtained between the simulated and experimental times to reaction. These fitted parameters were then used to successfully model another experiment.

As a consequence of this work, the results of the 57-mm cookoff test are better understood and, more importantly, the explosive CX-84A's thermal properties are now better characterized. This means that the time-to-reaction of this explosive in other warheads subjected to cookoffs can be better simulated. This will lead to savings of time and money in the development of new warheads and shorten the time required to introduce them into service.

LIST OF SYMBOLS

E	activation energy
kT	temperature in energy units
q	internal energy density
Q	heat of reaction
ln(Z)	(logarithm of) the preexponential factor
ρ	mass density

1.0 INTRODUCTION

The Canadian Forces are facing increased demands for weapons systems which cost less and are safer to use. Costs and risks which were acceptable years ago no longer are. This is especially true for munitions where policies requiring less sensitive ones are being introduced. DREV has anticipated this and has been developing less sensitive explosives for use in such munitions for a number of years now.

Among the potential hazards a munition could face is a fire in a magazine or on a weapons platform. With present munitions (often filled with the explosive Composition B), a fire leads to detonations. One of the goals of DREV's research is to develop an explosive which does not detonate in a fire. One of the explosives DREV developed, called CX-84A, meets this requirement. DREV received a task to develop a 57-mm shell for the Canadian Navy and CX-84A was used as the explosive in it.

The object of this report is to perform a post-experiment simulation of the slow cookoff of the 57-mm warhead using the recently acquired finite element computer program called TOPAZ2D (Ref. 1). With this program, the heating process of the warhead can be simulated and the time to reaction can be found and compared to the experimental results. Agreement between simulation and experiment leads to greater confidence in the computer results. The program can then be used to simulate other situations where time, money or technical difficulties do not permit live trials or experiments to be performed.

This work was performed at DREV between August 1994 and July 1995 under PSC 31C, Energetic Materials.

2.0 SIMULATION DETAILS

The details of the simulations will now be outlined. This section begins with a short description of the computer program used. This is followed by details of how the problem was set up and solved for this work.

2.1 The Program TOPAZ2D

TOPAZ2D is a two-dimensional finite element computer program for heat transfer analysis originating from Lawrence Livermore National Laboratory in the United States. As such, it can solve for steady-state or transient temperature fields in planar or axisymmetric geometries subject to a wide variety of time- and temperature-dependent boundary conditions. A limited thermally controlled chemical reaction capability is included. The version used for this report is dated 07/02/92. A few minor changes (mostly to operating system calls) were made to the program at DREV so that it would execute on an IBM PC computer.

TABLE I

Thermal parameters of materials used

Material	Density ($kg\ m^{-3}$)	Heat Capacity ($J\ kg^{-1}\ K^{-1}$)	Thermal Conductivity ($W\ m^{-1}\ K^{-1}$)
Steel	7870.	502.	50.
Aluminum	2700.	886.	201.
Tungsten	19300.	142.	147.
CX-84A	1573.	1360.45	0.185

2.2 The Model Used

In a finite element simulation, a problem is set up in three phases: description of the geometry, specification of the materials's thermal properties and application of the appropriate boundary conditions.

The geometry of the shell is now described. The mesh and materials used are shown in Fig. 1. Two simplifying approximations were made. Firstly, the fuse was replaced by a plug made of aluminum. Secondly, the section of thin steel wall lined with a rubber belt loaded with tungsten beads was replaced by a solid wall of tungsten. The error introduced by these assumptions should be small provided that the heat capacities and especially the thermal conductivities of the true components are compatible with the approximations.

The thermal properties of the various materials which make up the warhead are given in Table I (Refs. 2 and 3). These are assumed to be constant although TOPAZ2D does have provision for temperature-dependent properties.

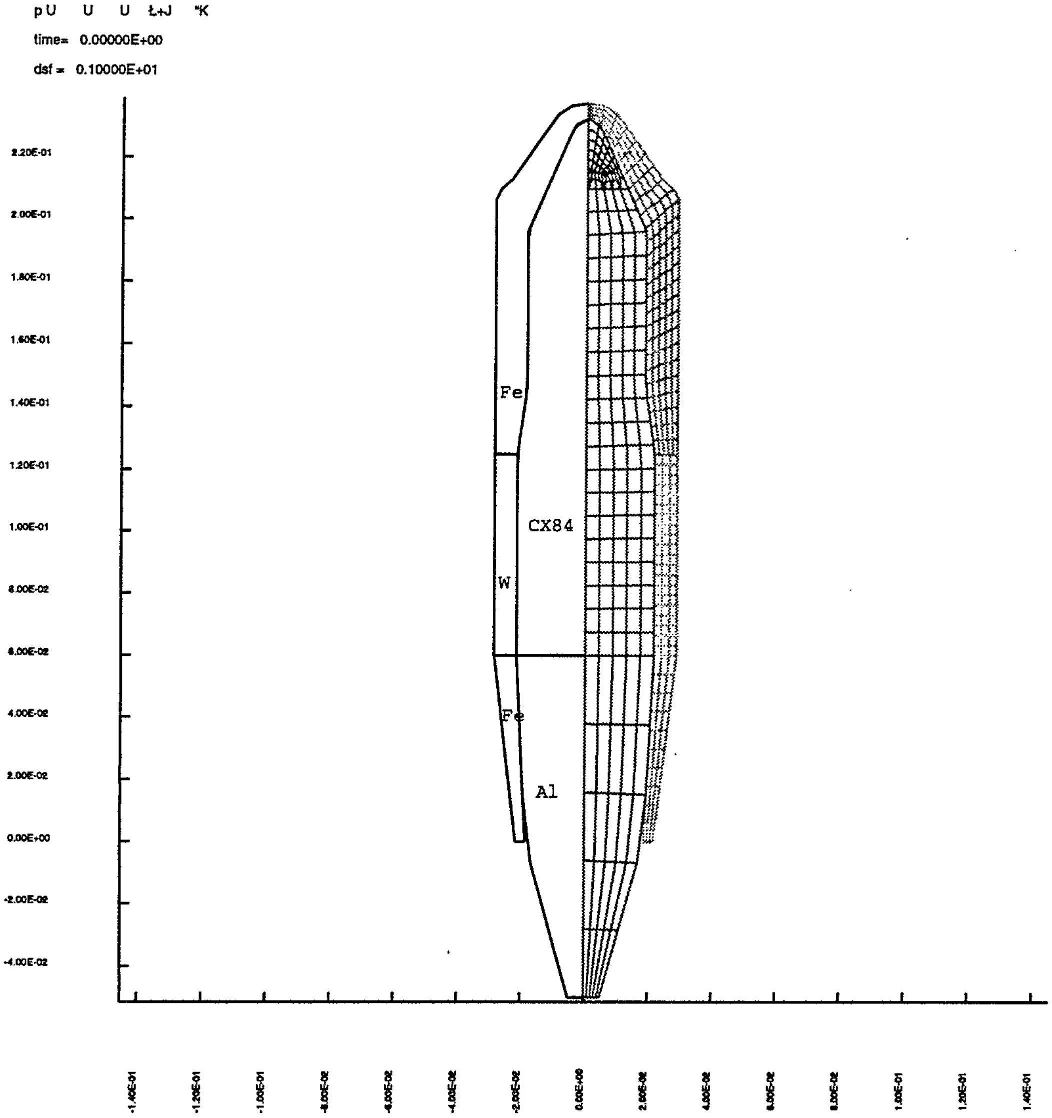

FIGURE 1 – Mesh used to model 57-mm shell

TABLE II

Reaction parameters for RDX (from literature)

Parameter	Value
Q	$2.093\ 10^6$ J kg^{-1}
$\ln(Z(s^{-1}))$	42.14175
E	197160.6 J mol^{-1}

The reaction of the explosive is described by a simple, first-order Arrhenius reaction kinetics, namely,

$$\frac{dq}{dt} = \rho Q Z e^{-\frac{E}{kT}}.$$

The choice of Q, Z and E are fixed, more or less, by the chemical composition of the explosive. Since CX-84A is 84% RDX, a first approximation for the calculations is that it is 100% RDX and the parameters for pure RDX (Ref. 4) are then used. These are given in Table II and are the default parameters referred to in later sections.

The boundary condition which was used mimics the experimental situation. The temperature of the outer wall of the shell is raised at a rate of 100 K h^{-1} for the first hour and 3.3 K h^{-1} thereafter. Also, as an initial condition, the entire shell was initially at 293 K.

3.0 RESULTS AND DISCUSSION

The evolution of the heating process in the 57-mm shell can be followed using the program TOPAZ2D. As the surface is heated, the outer metallic layer of the shell rapidly reaches thermal equilibrium with the surroundings. The heat flows more slowly into the explosive due to the explosive's much lower thermal conductivity. After several hours (for the default reaction parameters, around 34000 s), there is a point where all the shell has reached the same temperature, which would be a surprising result if the interior material were inert as the shell is being heated continuously. The explosive, of course, is not inert and is in fact reacting, generating heat and raising its own temperature. The interior temperature continues to rise and soon rises very rapidly. At this point, the simulation sometimes stops due to numerical difficulties. The temperature contours shortly before this time in the explosive (presented in Fig. 2) show that the reaction starts one to two centimeters behind the fuse. In Fig. 3, the temperature of an interior point in the center of the hottest region (on the axis of symmetry about 2 cm into the explosive from the explosive-fuse interface) is shown as a function of time. This clearly shows a slow rise in temperature, followed by a rapid increase as the reaction takes off. After this time, the composition of the explosive will certainly be different (due to a production of reaction products) and the thermal parameters will no longer be valid. It is assumed that in the real world, an explosion would occur about this time.

The heat generation by the reacting explosive has been assumed to be simple, first-order Arrhenius kinetics for a pure mass of RDX. The literature parameters for this reaction were determined by previous cookoff experiments. When these parameters are used, the time to explosion is underestimated (49000 s versus the experimental 72000 s (Ref. 5)).

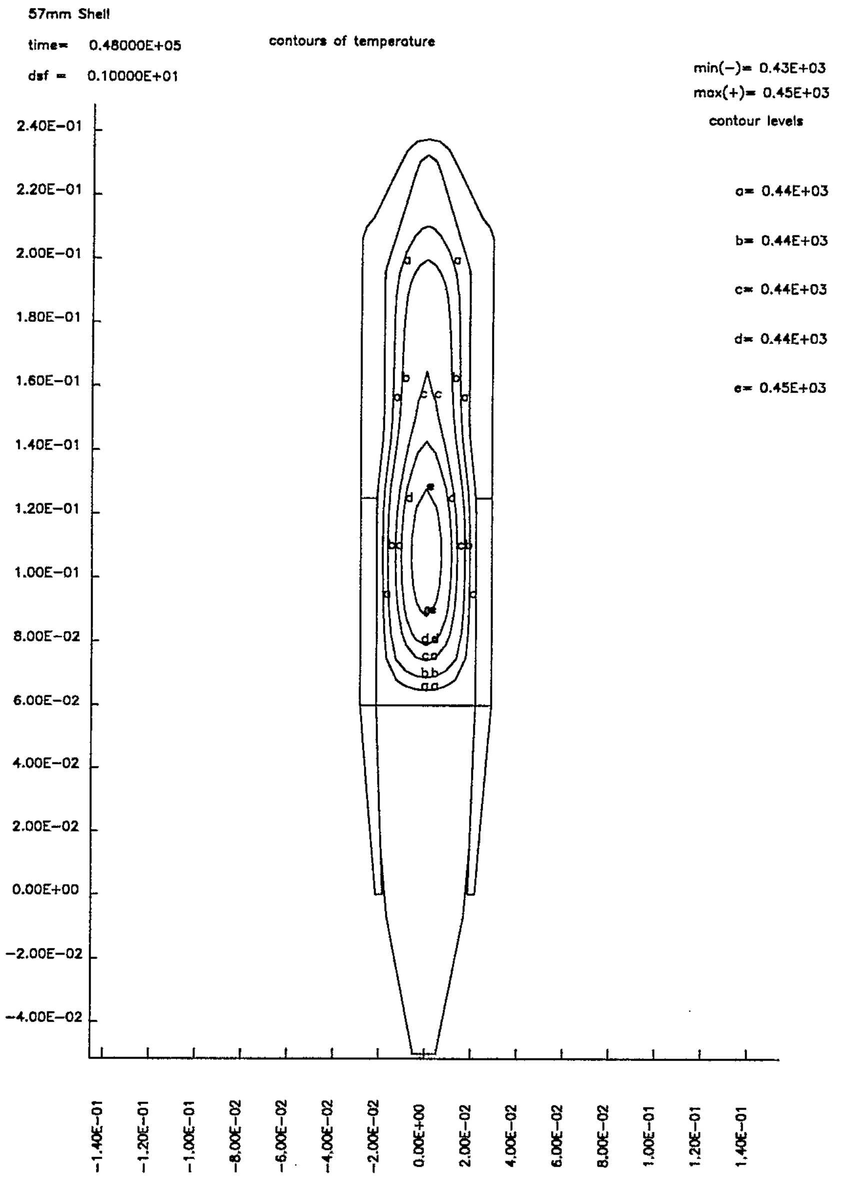

FIGURE 2 – Temperature contours in the explosive after 48000 s. Default reaction parameters were used.

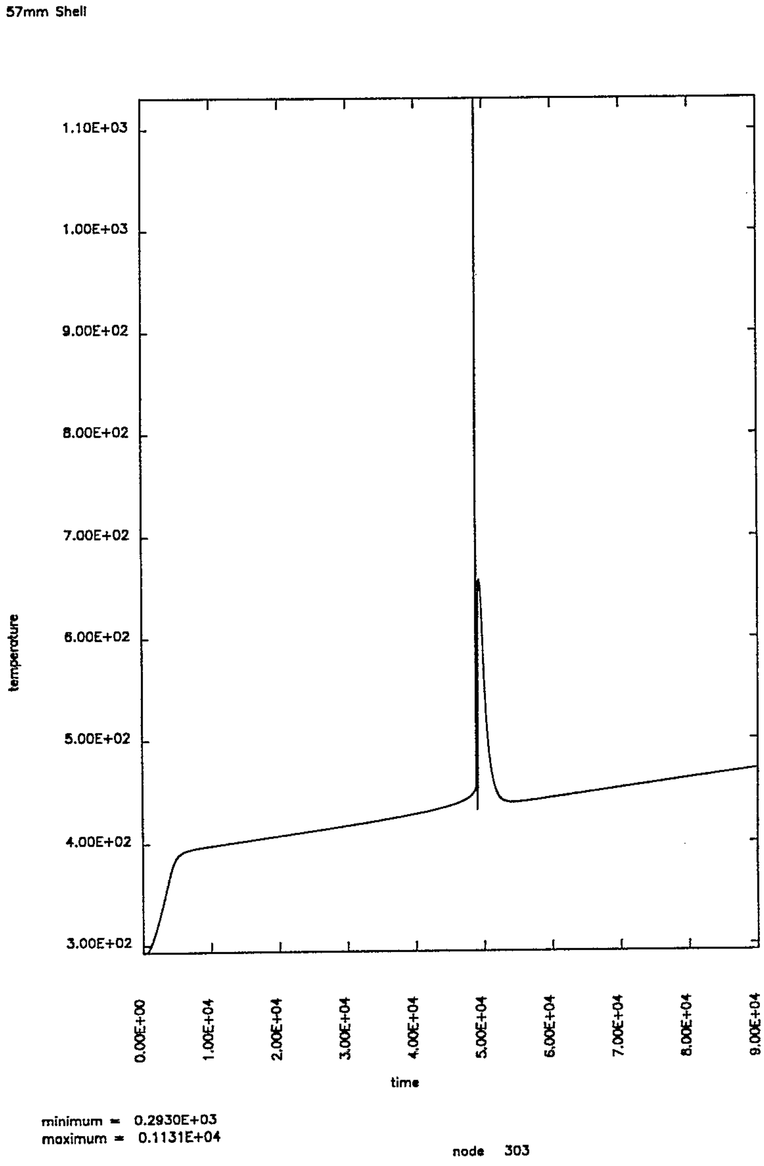

FIGURE 3 – Temperature on the axis of symmetry, 2 cm from the explosive-aluminum interface. Default reaction parameters were used.

A parametric study was undertaken to see if the experimental time could be better reproduced by varying the parameters for the reaction. There are three parameters which can be varied. These are ln(Z), Q and E, which correspond to the preexponential factor, the heat of reaction and the activation energy, respectively. Each of these was varied over a limited range and the times to rapid heating were observed. In Figs. 4-6, the effect of varying these parameters is shown. In general, varying Q does not greatly affect the time, whereas changing ln(Z) or E by a small percentage (say, by 5 %) changes the time to reaction a great deal (say, by a factor of 2).

To best reproduce the experimentally observed time of reaction (approximately 72000 s), one could simply use a ln(Z) of about 40 (where Z is in s^{-1}) or a E of about 207000 J mol^{-1}, otherwise keeping the default values. Another approach is to vary two or three parameters and attempt to reproduce the experimental time to reaction. To do this, Q was kept at the default value since the time to reaction varies the least with changes in it and ln(Z) and E were varied. The results, presented in Fig. 7, show a smooth variation of the time to reaction with variations in ln(Z) and E. No definitive set of parameters can be selected a priori as the "best". Rather, a choice of self-consistent sets exists and ultimately it is an arbitrary preference of the modeller which governs the situation.

As a further example, simulations were performed to see the effect of the heating rate on the cookoff times for a cylinder of explosive. A steel cylinder 5.813 inches in diameter and 11.169 inches long is filled with CX-84A and heated at 3.3, 9, 25 or 75 K h^{-1} after

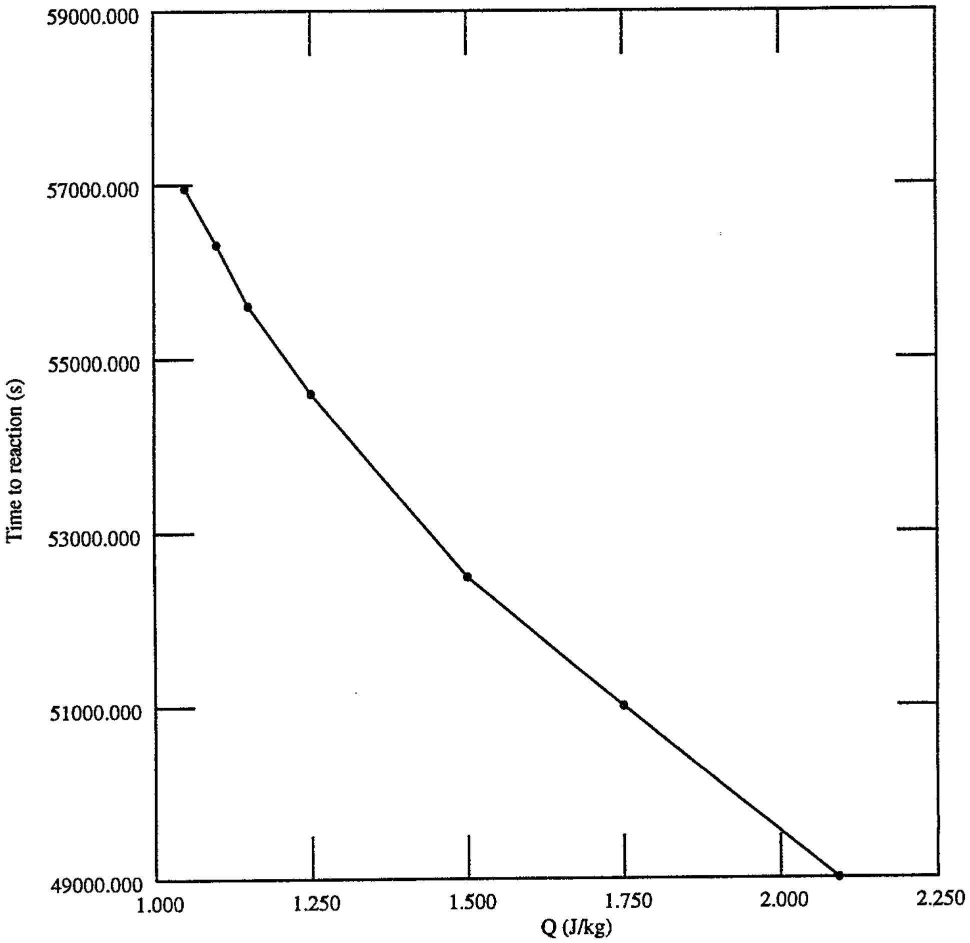

FIGURE 4 – Effect of varying the heat of reaction, Q

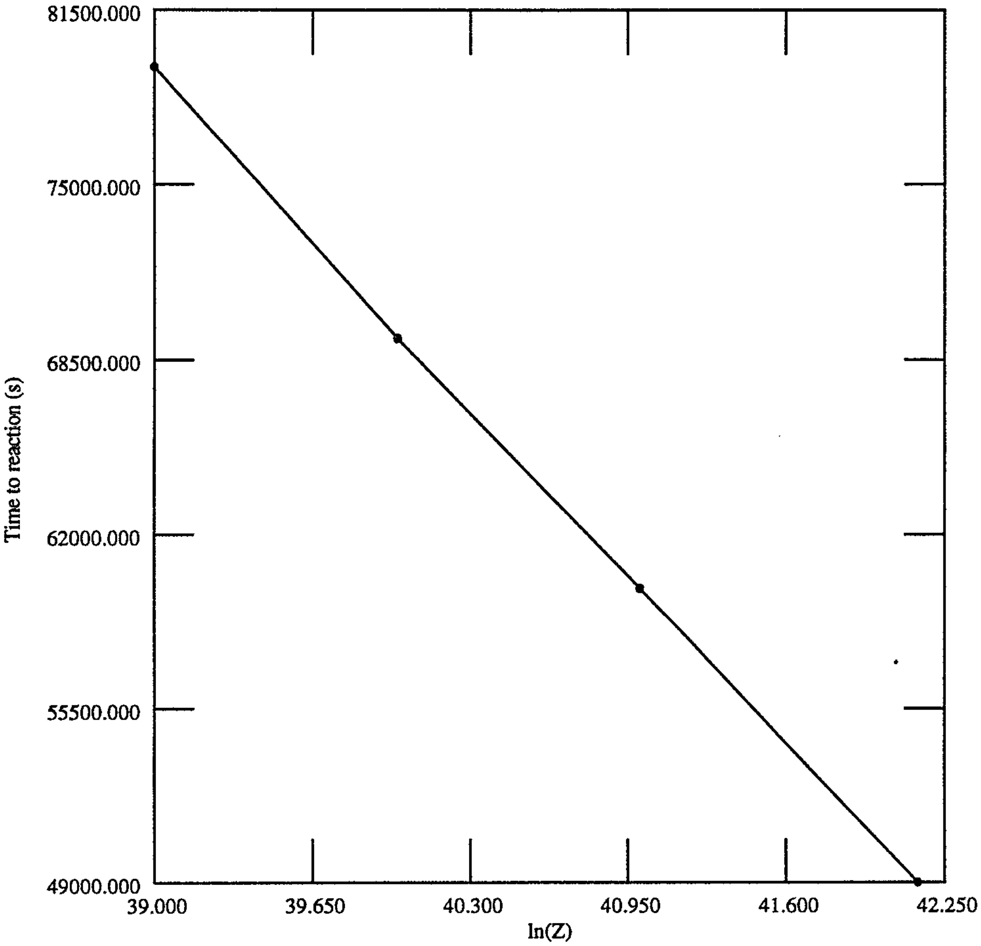

FIGURE 5 – Effect of varying the preexponential factor, ln(Z), where Z is in s^{-1}.

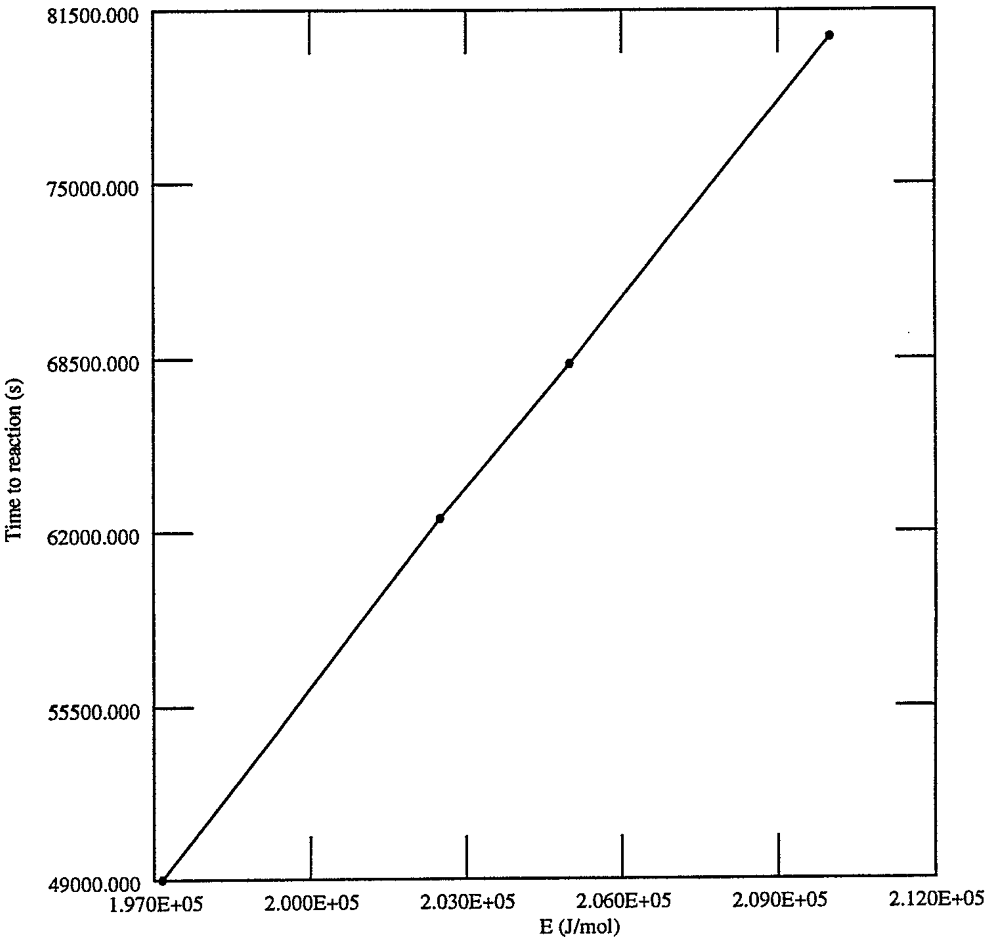

FIGURE 6 – Effect of varying the activation energy, E

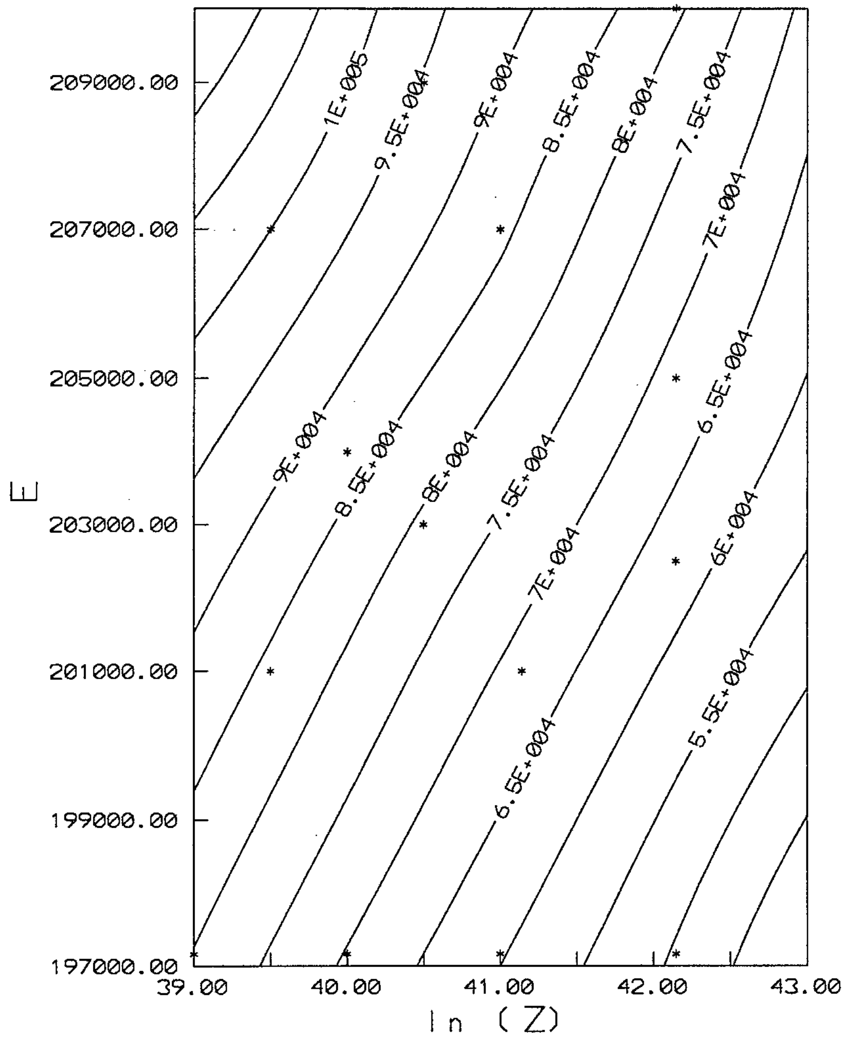

FIGURE 7 – Time to reaction obtained by varying both E and ln(Z) for the default Q where E is in J mol^{-1} and Z is in s^{-1}. The *'s represent the points used for the contouring.

being heated to 100 C according to the method described in Ref. 6. A ln(Z) of 40.14175 (where Z is in s^{-1}) was used, while Q and E were set at the default values. The times to reaction from the present simulations and experiments of Ref. 6 are compared in Fig. 8. There is quite good agreement between them if one realizes that there is a certain amount of variability in the experimental time to reaction. At 3.3 K h^{-1}, the time to reaction varied between about 65000 s (18 h) and 97000 s (27 h). For each of the other rates, only one test was described in Ref. 6.

In spite of the success above, it is worthwhile to end this section with a few comments on the limitations of the present model and possibilities for future work. Better thermal parameters, especially temperature-dependent ones, could be used but this should have a relatively small effect on the final results. Different reaction kinetics could be used. The problem here is to choose them correctly. The reactions involved leading to a detonation are not completely known and many are currently being studied around the world. Finally, the occurrence of an explosion does not depend solely on the reaction kinetics. Rather, there is an interaction between the reaction, which generates large volumes of high pressure gases, and the mechanical confinement of the explosive. For example, if the shell casing cracks and gases or explosive escape, the danger of a detonation will be reduced. To model this, the reaction and its products must be coupled to the mechanical effects caused by the pressure buildup, but this is not normally done in a single program and is certainly not in TOPAZ.

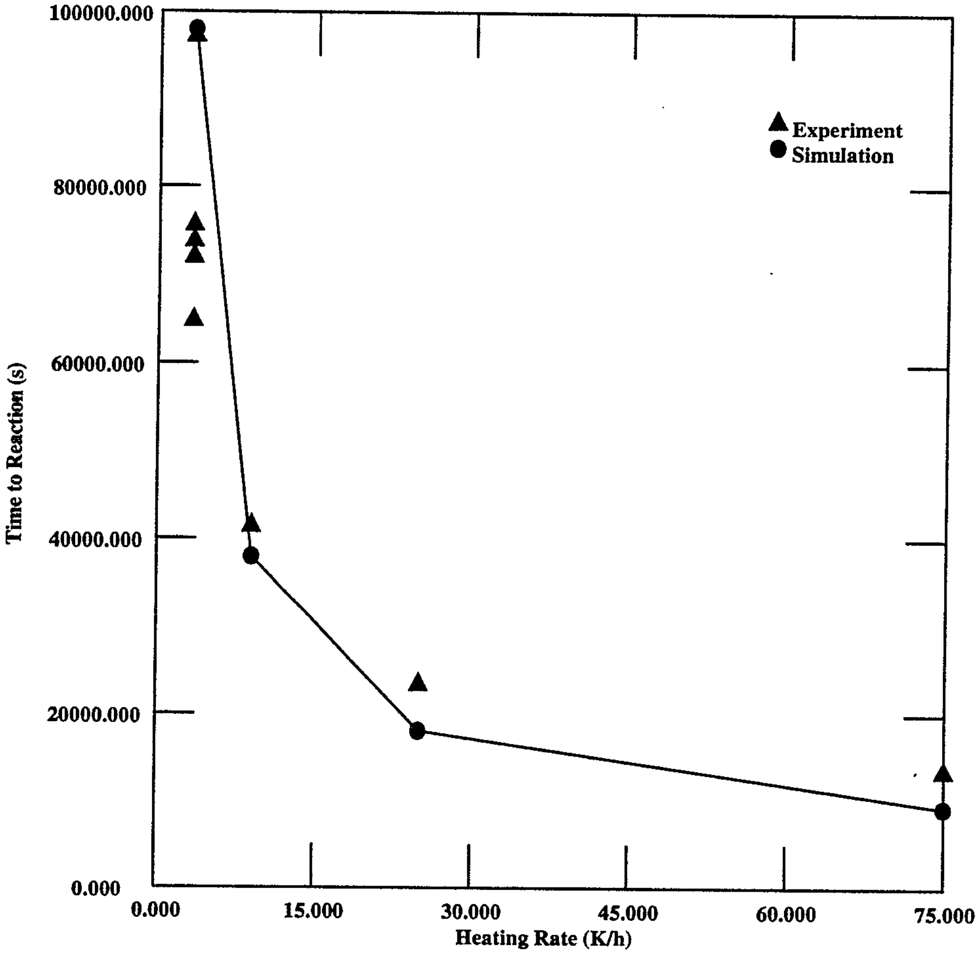

FIGURE 8 – Effect of heating rate on time to reaction for a cylinder of CX-84A

4.0 CONCLUSIONS

TOPAZ has great potential for calculating the cookoff times for a practical munition provided the thermal and chemical reaction properties of the major components and explosives are known. Even a crude model with gross approximations can reproduce almost quantitatively the observed experimental results. As a result, a consistent set of thermal properties for CX-84A has been obtained and can be used to predict the cookoff behaviour of this explosive in other configurations.

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