Single and double shock initiation modelling for high explosive materials in last three decades

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Abstract. The explosives materials are normally in an energetically metastable state. These can undergo rapid chemical decomposition only if sufficient energy has first been added to get the process started. Such energy can be provided by shocks. To predict the response of these materials under impacts of shocks of different strengths and durations and at various conditions, mathematical models are used. During the last three decades, a lot of research has been carried out and several shock initiation models have been presented. The models can be divided into continuum based and physics based models. In this study the single and double shock initiation models presented in last three decades have been reviewed and the ranges of their application has been discussed.

1. Introduction
Keeping in view the high costs of experiments, the demand to develop the analytical and computational models for shock initiation of explosives materials to provide both an understanding and predictive capability has always been present. In last three decades, a large number of shock initiation models, also known as reactive burn models, have been developed. The development of a large number of initiation models points out, on one hand the importance and necessity of the modeling of shock initiation process, while on the other hand reflects the difficulty in modeling the process. These models make use of concept of hotspots, that take roots from the experimental findings that the initiation mechanism of both Homogeneous and heterogeneous explosives are entirely different [1-2]. Bowden and Yoffe [3] first introduced the concept of hot-spot generation during initiation of heterogeneous explosives. However only few experimental evidences [4-5] could be found. The shock initiation process is usually described as having two phases: (i) an ignition phase where ‘hot-spots’ are generated due to shock compression heats up the explosive at the discontinuities and the subsequent chemical reactions further raise the temperature of these localized heated regions or hot spots, and (ii) a growth phase where the ‘hot-spots’ grow and coalesce to consume the remainder of the explosive material. In spite of little knowledge regarding the evolution of ‘hot-spots’ behind a shock wave, Field in his two landmark papers [6-7] summarized ten possible mechanisms for ‘hot-spot’ generation. However in a typical shock initiation problem any one or more than one mechanism may be responsible for producing of hot spots, and no universal agreement exist among the research community about the mechanism(s) responsible to produce ‘hot-spots’. Pore collapse [8], shear banding [9-12] and frictional heating [13] are the three relatively more plausible mechanisms.
responsible for shock initiation. The reactive burn model must also model the effects of the factors significantly affecting the shock initiation and sensitivity of explosives such as initial density (initial porosity)\cite{14-16}, crystal or grain size distribution\cite{17}, crystal orientation, some microstructure effects\cite{18-21} and initial temperature\cite{22-23} of the explosive.

In the present paper we will review the models which are well known and widely used in shock initiation studies and have been key developments in the field. These models can be classified into two types: (i) continuum-based models, and (ii) physics-based or mesoscale models. There is yet another class of models which may be called hybrid models will also be reviewed.

2. Continuum-based reactive burn models

These models are phenomenological in nature. The reactive Euler equations are widely used for modeling the initiation of explosives. For engineering simulations the cell size is much greater than the scale of material heterogeneities. The limited resolution necessitates using a homogenized constitutive relation for the explosive. These models have been in use for calculations for practical engineering application because of their realistic requirement of the computational resources. Since the assumption of homogenization eliminates the temperature fluctuations at the discontinuities, burn models have to account for the effect of hot spots on the reaction rate.

2.1. Forest fire model

The Forest Fire model\cite{24-26} assumes that the reaction rate depends only on the pressure. The pressure dependence is determined such that the lead reactive shock follows the buildup curve derived from the Pop plot\cite{27}. In addition to the Pop plot, the Forest Fire rate requires the reactive shock Hugoniot. It is determined from the initial particle velocity and shock velocity measured in a series of wedge experiments. The reaction rate equation is given as

\[
\frac{d\lambda}{dt} = (1-\lambda) G(P)
\]

where \( \lambda \) is the reaction progress variable and \( t \) in above equation denotes time, \( \lambda = 0 \) corresponds to the unreacted explosive while \( \lambda=1 \) corresponds to the fully reacted explosive. \( G(P) \) is assumed to be an exponential power series in local pressure variables and is of the form:

\[
G(P) = \sum_{i=1}^{n} C_i P^i
\]

where \( C_i \) are determined by using the reactant’s equation of state, reactive Hugoniot and equation of state of detonation products using square wave assumption.

2.2. Lee-tarver ignition and growth model

The Lee-Tarver model\cite{28-29} uses two Jones-Wilkins-Lee (JWL) equations of state, one for the unreacted solid explosive and the other for reaction products, in the temperature dependent form:

\[
P = A e^{-b V} + B e^{-R_1 V} + \omega C_v T/V
\]

where \( P \) is pressure, \( V \) is relative volume, \( T \) is temperature, \( \omega \) is the Grüneisen coefficient, \( C_v \) is the average heat capacity, and \( A, B, R_1 \) and \( R_2 \) are constants. The ignition and growth concept is represented by a reaction rate equation which was originally divided into an ignition term and a single growth term\cite{29}, but was later modified\cite{30} to model the short pulse duration shock initiation experiments by the addition of an extra growth term. The reaction rate (RR) equation\cite{30} is given as

\[
\frac{d\lambda}{dt} = I(1-\lambda)^x (\rho/\rho_0 - 1 - a)^y + G_1 (1-\lambda)^x \lambda^d P^e + G_2 (1-\lambda)^x \lambda^g P^z
\]

where \( \rho \) is the current density, \( \rho_0 \) is the initial density and the parameter \( a \) is a critical compression that is used to inhibit ignition, and hence reaction, until a certain degree of compression has been reached. \( I, b, x, G_1, G_2, c, d, y, e, g \) and \( z \) are constants. The ignition term runs from \( 0 < \lambda < \lambda_{\text{igmax}} \), the first
growth term from \(0 < \lambda < \lambda_{G1\text{max}}\) while the second growth term works from \(\lambda_{G2\text{min}} < \lambda < 1\). The form factors \((1 - \lambda)^c \lambda^d\) and \((1 - \lambda)^e \lambda^f\) are in accordance with the grain burning topology [31] for spherical grains burning from inside and outside.

This model [30] has been applied to many experimental shock initiation and detonation studies of solid explosives [16, 32-37] and propellants and embedded in several hydrocodes, making it the most popular reactive burn model in use today in spite of its short comings in some cases [38, 39]. The parameters of reaction rate equation for quite a large number of explosives have been determined [40] at different conditions. Various shock induced phenomena have successfully been predicted, including run-distance to detonation (Pop-Plot) data [29], short pulse shock initiation data [30], in-material pressure gauge measurements examining growth of reaction in shock initiated explosives [28], detonation propagation and failure [36], and corner turning data [28]. Lee-Tarver model has also been used to explore the shock initiation criteria of explosives subject to the flyer impact [41].

Murphy [42] proposed an improved reaction rate equation with less parameters, making it easier to parameterize and optimize. The main problem with the model is that the parameters are empirical fit to some particular experimental data. Thus, there are doubts over the ability of the model to predict a wide range of phenomena with a single set of parameters, or to predict outside its fitting regime.

2.3. Johnson-Tang-Forest model
The Johnson-Tang-Forest (JTF) model [43] is a kind of ignition and growth model elaborating the contribution of the ‘hot-spot’ ignition phase in describing the shock initiation of heterogeneous explosives. It introduces internal degree of freedom for mass fraction of hot spots \(f\), the incident shock pressure \(P_s\) and the hot spot temperature \(T_{hs}\). The average burn rate if given by

\[
\frac{d\lambda}{dt} = \mu \frac{df}{dt} + \left[1 - \lambda - \mu(1 - f)\right]\left(\frac{f - f_o}{1 - f_e}\right) + G(P, P_s)
\]

where \(\mu\) is the mass fraction of explosive turned into hot spots, \(f_o\) is the threshold value for mass fraction of hot spots \(f\) and \(G(P, P_s)\) is an empirical function which is constrained to approach the Forest Fire rate at high pressures, and is given as

\[
G(P, P_s) = G_o(P) \left[1 + \frac{F(P_s)}{G_o(P_s)}\right]
\]

where \(F(P_s)\) is the Forest Fire rate and \(G_o\) is a fitting parameter. In this model the ignition process includes average ‘hot-spot’ temperature as an explicit parameter. The ignition phase is based upon a thermal explosion where the induction time is a function of average ‘hot-spot’ temperature and the growth phase is represented by a polynomial in pressure that is similar to the Forest Fire reaction rate.

2.4. CREST reactive burn model
The CREST reactive burn model [44] is an entropy-dependent reactive burn model based on the analysis [45] of high quality, in-material gauge results of velocity histories in shock to detonation transition experiments carried out by Gustavsen et al. [46] for two HMX based explosives and one TATB based explosive. CREST uses a finite strain form of equation of state [47] for the unreacted explosive, JWL equation of state for the reaction products and isentropic solid equation of state [48] model is used for the reacting mixture. Pressure equilibrium assumption is used for the solid and the gaseous components during the reaction. The unreacted explosive equation of state is porosity dependent. The snow plough porosity model [47] is used [49] to account for the effect of porosity and initial temperature [50] on the solid unreacted explosive response. The reaction model utilizes two reaction rates: (i) a fast reaction rate \(d\lambda_1/dt\) which encompasses all primary sources of reactions such hot spot, and (ii) a slower reaction rate \(d\lambda_2/dt\) corresponding to the bulk burn of the explosive. The overall reaction rate \(d\lambda/dt\) is the weighted sum of the two rates, as given by
where $m_1$ and $m_2$ are the weighting factors. The description of the individual reaction rate can be seen in reference [44, 51]. CREST model has been successfully used in predicting the effect of porosity [52], initial temperature [50, 53] on shock sensitivity of explosives effects, corner turning experiments at different initial temperatures [53, 54], desensitization phenomena [53] and failure diameters [55]. Since CREST does not explicitly model the microstructure of explosives, it cannot predict the effect of particle size on shock sensitivity of the explosives [55].

2.5. Wescott-Stewart-Davis (WSD) model

The WSD model [56] utilizes a wide-ranging equation of state and a reaction rate law. The equation of state is calibrated to fit the shock and product Hugoniot curves that fit experimental data. The reaction law model is calibrated to fit detonation shock dynamics [57] relations ($D_n-\kappa$) and shock initiation data. The reaction rate similar to Lee-Tarver model is given by

$$\frac{d\lambda}{dt} = m_1 \frac{d\lambda}{dt} + m_2 \frac{d\lambda}{dt}$$

where $m_1$ and $m_2$ refer to the ignition and growth terms respectively. The details of the variables can be found in reference [56]. The reaction rate equation differs from Lee-Tarver model in that there are two different pressure sensitivities in the growth term, one for shock initiation and another for full detonation, thus allowing the matching of a wide variety of experiments with one set of parameters. This also allows the simulation of problems with both shock initiation and highly curved detonation waves. The application of this model to detonation diffraction and detonation-material interaction problems was encouraging.

3. Physics-based shock initiation models

Physics-based or mesoscale models for shock initiation of explosives can be classified into mainly two categories: (i) statistical ‘hot-spot’ models, and (ii) explicit ‘hot-spot’ models where some physical phenomena are used to model the hot spots.

3.1. The statistical ‘hot-spot’ models

Because of random distribution in sizes an orientation of the constituent particles of a typical heterogeneous explosive, the exact position and mechanism of hot spots formation is hard to predict. Even the so called explicit hot spot models elaborating some specific mechanism such as pore collapse for shock initiation take and average distribution of hot spots. The statistical hot spot models such as in reference [58] rely on an assumption of the size and number density of ‘hot-spots’ in shocked compressed material as the starting point for their calculations. Such information is usually obtained from the results of large scale mesoscale simulations of an ensemble of the explosive. The microstructure of the explosive consisting of the pore size distribution, grain size distribution, binder, and other solid inclusions is given as input to large scale, direct numerical simulations codes [59-61] and the size and distribution of ‘hot-spots’ as the initial conditions for a statistical hot spot model calculation. However, the computational resources requirement is pretty high to perform the direct numerical simulations of typical problems [62]. Moreover the task of extracting data from the direct numerical simulation codes to input the statistical hot spot modelling codes is complex. In the model of Hamates et al. [63], rather than keeping track of distributed ‘hot-spots’ (as in reference [58]), an aggregated ‘hot-spot’ concept is used representing the overall contribution of the distributed ‘hot-spots’. An approach [64] to computationally predict and quantify the stochasticity of the ignition process in polymer-bonded explosives (PBXs) under impact loading is a recent development in statistical modeling of ignition.
3.2. Mechanism-based explicit hot spot models

Most of the physical based models take one particular mechanism for shock initiation. To date, no theory of hot-spots has attempted to cover all of the different possible ‘hot-spot’ phenomena, and most of the models have modeled ‘hot-spot’ ignition from this perspective. Numerous experimental studies e.g. [15] as well as experimental results e.g. [16] have shown that increasing porosity can make an explosive material more sensitive to shock initiation. This emphasizes the idea that the pores are prime candidates as potential ‘hot-spot’ sites. A large number of models based on pore collapse theories have been presented during last three decades. The new models and their applications reported are AMORC [65], the Cook-Haskin’s CHARM model [66], the model of Bennett [67], the model of Khasainov et al. [68], Belmas et al. [65], Frey [69], Kang et al. [70], Bonnett and Butler [71], Massoni et al. [72], Whitworth[73], Bouma et al. [74], Brundage et al. [75], Springer et al. [76], Cheng et al.[77] and recently Akiki et al. [78]. Khasainov et al. [68] were the pioneer to build a viscoplastic pore collapse model and apply it to ‘hot-spot’ formation in explosives. The model of Khasainov [68] has since been implemented into the Autodyn hydrocode, and the two-dimensional Eulerian code EDEN [79]. Nonetheless, there are some models which simultaneously model more than one phenomenon for shock initiation of explosives. Example is the model by Shaw et al. [80] and Howe et al. [81].

4. Hybrid models

This class of models which may be called hybrid models, because in such models the ignition is modelled by some mesoscopic process such as pore collapse while the growth is modelled by using some empirical relations similar to continuum based models. Two of them are discussed below.

4.1. Kim’s model

Kim’s model [82, 83] is a kind of an ignition and growth model where the elastic viscoplastic pore collapse mechanism similar to Carroll and Holt [84] is assumed to be responsible for the ignition of explosives. After ignition, the growth of reaction is modeled by using the empirical relations somewhat similar to those of Lee-Tarver’s model. The reaction rate is given as

$$\frac{d\lambda}{dt} = \left( \frac{d\lambda}{dt} \right)_{\text{ignition}} + \frac{F}{r_o} \lambda^{2/3} p^{-y} + \frac{G}{r_o} p^z (1 - \lambda)^{2/5} \frac{d\lambda}{dt} = \left( \frac{d\lambda}{dt} \right)_{\text{ignition}} + A \left( \frac{p}{r_o} \right)^{y/2} + B \left( \frac{p}{r_o} \right)^{z/2}$$

where $r_o$ is average particle radius in micrometers, $F$, $G$, $y$ and $z$ are growth constants. Kim [82] used his model to study the SDT experiments for a specific particle size formulation of only one explosive (PBX9404) to achieve good agreement.

4.2. DZK model

Duan’s ignition model (later named as DZK hot-spot model [85]) is also a kind of ignition and growth model, where the ignition term is based on the collapsing of the pores while the growth terms are based on the burning topology of pores. It has been implemented in DYNA2D software [86] and has been used to predict the effects of the particle size [87], the porosity of the explosive [88], the strength and content of the binder in a PBX explosive [88] and recently the effect of initial temperature on the shock initiation [85]. The DZK reaction rate equation is a sum of three terms: i) the ignition term by DZK hot spot model [89], ii) the slow growth term suggested by Kim [83], and iii) the fast growth term proposed by Zhang [90], and is of the form [89]:

$$\frac{d\lambda}{dt} = \left( \frac{d\lambda}{dt} \right)_{\text{ignition}} + \frac{3\lambda^{2/3}}{r_o} aP^n + GP^z (1 - \lambda)^x,$$

where the empirical parameters $a$, $G$, $n$, $z$, $\lambda$ and $x$ are determined by experiments.
5. Double shock initiation and desensitization phenomena

The models described in previous sections usually address single shock initiation. The double shock initiation phenomena is little more complex. The most interesting phenomena arising due to double or multiple shocking of an explosive is desensitization. It is now an established fact that passage of a weak shock desensitizes the explosive for the succeeding stronger shock. This phenomenon is either a desirable phenomenon for safety scenarios or, on the other hand, a highly undesirable phenomenon for design of explosive applications where the performance and yield of the device is of primary concern. A number of experimental findings [38-39, 91-98] have been reported confirming that the preshocks cause the desensitization effects in heterogeneous explosives. The SC jet initiation tests [99-105] for heterogeneous explosives also indicate the occurrence of desensitization phenomena.

5.1. Modeling desensitization using continuum based models

Unfortunately, most of the phenomenological models are unable to simulate the situations involving the preshock desensitization. Therefore separate desensitization procedures have to be annexed with them to enable such models to account for the desensitization effects. For example, the JTF model [43] accounts for the preshock desensitization phenomena by restricting creation of hot spots to the first shock only, and allowing a second shock to provide only adiabatic heating. Wescott-Stewart-Davis (WSD) model [56] has been improved [106] to a temperature dependent form WSD (T) for such calculations. Mader [25] used multiple shock Forest-Fire model to simulate the shock desensitization experiments [105]. However a reactive burn model CREST [44] that uses entropy-dependent reaction rates, has been successful [53] in simulating the persistent dead zones in corner turning experiments [107] on PBX 9502 explosive. However the model is still being improved at Atomic Weapon Establishment (AWE) of UK [51].

The standard Lee-Tarver model [29] cannot reproduce the desensitization effects. Several attempts have been made to modify it. Long ago, Tarver [38] added a condition in the reaction rate equation to account for desensitization of LX-17 by reflected shocks. The condition was that if a critical range of pressures is applied to the explosive, the reaction rate was forced to zero. The calculated growth histories using the modified reaction rate equation agreed well for the reflected shock experiments, except for few exceptions. Whitworth [108] described a simple model to predict shock desensitization effect by modifying the reaction rate equation by making it dependent on the preshock pressure \( P_{shk} \). In place of local pressure \( P \) in reaction rate equation, \( P = \min (P, P_{shk}) \) was used to find the reaction rate. A qualitative agreement was reported for the calculations of Mulford’s precursor shock experiment [92] using the modified reaction rate equation. Whitworth also applied his modified reaction rate equation for detonation quenching experiments. However, contrary to the experimental results [109], the rate of quenching increased with decreasing pressure of the precursor shock.

In order to model the qualitative features of the corner-turning failure in LX-17, Sours [107] presented a failure model that cut off the reaction rate below certain detonation velocities. A single reaction rate equation was used which was a stripped down version of Lee-Tarver model, and the coefficients of this rate equation were different in different regions of the explosive. In a more recent approach, Sours [110] later refined his model by employing a single reaction rate format which varied for different pressure regimes in explosive to simultaneously model dead zone, failure region and the detonation region in corner turning experiments. This model could reproduce various experimental features including detonation failure region in corner turning experiments of LX-17.

Oliveira [111] proposed a modification in Lee-Tarver model by introducing the desensitization rate \( S \) as \( S = MP(1 - \phi)(\phi + \epsilon) \), where \( \phi \) is the degree of desensitization, which equals 1 for virgin state while 0 for completely desensitized explosive. \( M \) is rate constant and \( \epsilon \) is a small positive number to ensure some desensitization at \( \phi = 0 \) when \( P > 0 \). Thus the Ignition term in reaction rate equation becomes as \( R_i = (1 - \phi)^{\eta}(1 - a(\phi) \phi) \), where the modified critical compression \( a(\phi) \) is defined as \( a(\phi) = a_0 + a_1(1 - \phi) + a_2(\phi) \), where \( 1 + a_0 \) is critical compression for ignition of the virgin material and \( 1 + a_1 \) is the...
same for the completely desensitized material. The second change proposed [111] was to change the switching limit of the growth term from 0 to \( \lambda_{G1\text{min}}(\phi) \), defined by \( \lambda_{G1\text{min}}(\phi) = \lambda_c \phi \), where \( \lambda_c > 0 \).

This modification requires four additional empirical constants to enable the ignition and growth model to account for the desensitization effect. Using the augmented model, Oliveira [111] qualitatively reproduced the main features of the corner turning experiments including dead zones. It has been used by Tarver et al. [37] for simulation various experiments [112] involving desensitization. The form factor \((1 - \phi) \phi\) for desensitization rate equation seems similar to the form factor \((1 - \lambda) \lambda^d\) of the growth terms in original Lee-Tarver reaction rate equation, with \( \lambda \) replaced by \( \phi \). However we find no logic behind this similarity. Moreover the form factor also implies that the desensitization rate is maximum when the material is 50% desensitized, again without any experimental evidence. To improve the Oliveira’s model, the authors have developed a modification in Lee-Tarver model and successfully applied [113] to simulate the shaped charge jet initiation of covered explosives.

5.2. Modeling desensitization using physics based models

The pores in explosives are considered as the potential hot spot sites. The preshock compresses some of the pores creating the hotspots while most of the remaining unreacted pores are squeezed, thus making it almost impossible for the second (stronger) shock to find additional potential hot spot sites. Unlike for the phenomenological reactive flow models discussed in the previous section the mesoscopic reactive flow models based on pore collapse are ideal candidates to simulate the situations involving the preshock desensitization of the solid explosives. Since the desensitization is believed to occur due to closure of pores, the reactive flow models based on pore collapse mechanisms should be able to account for the desensitization phenomena induced by preshocking of the heterogeneous explosives, without any special treatment such as annexation of a separate desensitization model.

During the preshocking process, the pores are either fully or partially collapsed depending upon the preshock pressure and the burn fraction is very low to lead to the growth of reactions. Obviously it can be thought that once a pore is closed/shrunk by the preshock, the preceding stronger shock will hardly find any pore to compress, inhibiting the ignition and growth. The explosive will behave as an inert material until the preceding stronger shock overtakes the weaker shock, after that explosive could be ignited depending upon the shock strength. Hence it is obvious that such models should be able to simulate multiple shock experiments, where desensitization effects play an important role. The AMORC model [65] has been shown to be able to describe the phenomenon of desensitization by preshocking in HMX, TATB, and HMX/TATB compositions [114]. In an unpublished work, the authors have demonstrated the use of the DZK model for simulation of desensitization experiments.

6. References

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