

# The Effect of Momentum Loss on Detonation Failure at Very Low Activation Energy

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## Abstract

In this paper, the behavior of detonation waves in a non-ideal environment has been studied. Modeling of detonation has been performed based on one-dimensional Euler equations (momentum conservation) by considering friction as the momentum loss source term in the equation with a single-step Arrhenius law as the chemical kinetics model. Piecewise parabolic method (PPM) has been used to simulate the flow and solve the Euler equations. The shock front conservative tracking algorithm was used to have the finer mesh (Adaptive mesh refinement AMR) at the wave front location. The non-ideal environment is an environment in which external factors, such as friction, cause the detonation behavior to deviate from the ideal behavior. Therefore, the innovation of the present work is modeling detonation in these non-ideal conditions for mixtures with very low activation energy to detect its failure mechanism. The effect of momentum loss on the detonation behavior has been parametrically studied at very low activation energy (in which the detonation behavior is completely regular, here, 8). Depending on the level of mixture activation energy, the detonation has its failure mechanism. It is concluded that the failure mechanisms of the detonation in this study are the mechanisms of pressure drop and chemical reaction rate reduction. The un-burnt packet mechanism is not involved in it. The detonation wave, regardless of the amount of mixture activation energy, fails anyway as the momentum loss exceeds a critical limit.

**Keyword:** Non-Ideal detonation; Detonation stability; Chemical kinetics; Activation energy; Detonation failure.

## 1. Nomenclature

### Latin letters

$e$	total internal energy per mass unit
$E_a$	activation energy
$f$	momentum losses source term
$F$	vector of fluxes
$k_f$	friction coefficient.
$P$	pressure
$S$	vector of source terms
$u$	velocity of the particle
$u_{abs}$	particle velocity
$U$	vector of conservative variables

### Greek letters

$\rho$	density
$\beta$	reaction parameter
$\omega$	reaction rate

### Abbreviations

PPM	Piecewise parabolic method
AMR	Adaptive mesh refinement
hrl	half-reaction length

## 2. Introduction

In the non-ideal environment, external factors such as dissipation mechanisms cause the detonation behavior to deviate from the ideal state. Chapman [1] proposed a theory to calculate the detonation velocity. He found that the unique solution of the one-dimensional conservation equations of the detonation wave is related to the minimum velocity solution, in which the Rayleigh line is tangent to the Hugoniot equilibrium curve. Using this as a criterion, the detonation velocity can be determined from the conservation equations and thermodynamic information of the products. Jouguet [2] proved that the minimum velocity solution is related to establishing the sonic flow condition (relative to the shock wave) at the end of the reaction zone. This is also an independent criterion to determine a unique solution from conservation equations. In this way, the first theory of detonation was proposed by Chapman and Jouguet and became known as the CJ theory. Based on this theory, the detonation wave is assumed to be one-dimensional, stable, and with minimal thickness. CJ theory can only calculate the detonation parameters in thermodynamic

equilibrium. This criterion is not valid for non-ideal detonation, therefore, modified criteria were presented. More improvements to the theory were done by Zeldovich [3], Neumann [4], and Doring [5]. They independently proposed a model for the detonation wave structure, known as the ZND model. In this model, assuming that the detonation is steady state (wave motion with CJ velocity), a thickness for the reaction zone was considered. Most of the numerical simulations performed so far have been based on Arrhenius's single-step reactions. Mazaheri [6] studied the effect of single-step reaction activation energy on instability and its effect on the onset of ideal detonation by numerical simulation of one-dimensional detonation. He studied the shock wave pressure behavior in a mixture with  $\gamma=1.2$  and  $Q/RT_0=50$ , for different activation energies. He showed that at low activation energy ( $E_a/RT_0=25$ ), the detonation behavior is stable and no fluctuations are seen on the detonation front. CJ criterion was in close agreement with the experiment results in smooth tubes.

Non-ideal detonations with velocities lower than CJ involve dissipative mechanisms such as friction and or heat transfer [7]. A new formulation of the governing equations was introduced that eliminates the difficulties with numerical integration across the sonic singularity in the reactive Euler equations. Some numerical simulations were initialized with ZND solution by Li et al [8] for the ideal CJ detonation, and the detonation is allowed to propagate into the explosive layer. The results showed that the detonation in the heterogeneous environment exhibits a three-wave structure of complex shock interactions. Bengoechea et al. [9] presented an experimental and numerical study of a pulsed detonation combustion chamber. Their study reveals the essential aspects of detonation initiation. The results of one of the configurations indicate a deterministic and reliable deflagration-to-detonation transition (DDT) with a short run-up distance, crucial for technical applications. Sun and Wang [10] analyzed the critical characteristics of non-ideal detonation and detonation instability by an analog system. The Steady-state of detonation wave structures was obtained by the analytical method. By changing the value of the sensitivity exponent of reaction rate and the sensitivity coefficient of loss rate, the diagrams of steady detonation velocity and the loss coefficient under the corresponding parameter and detonation failure of linear boundary were obtained. Short et al [11] examined asymptotically the dynamics of two-dimensional, steady detonation wave propagation and failure for a strongly confined high explosive (HE). The asymptotic analysis reveals significant physical insights into how detonation propagation and failure are affected by strong confinement.

Two- and three-dimensional turbulent airflows in a 9-degrees-bent channel were studied numerically by Kuzmin [12]. Solutions of the Reynolds-averaged Navier-Stokes equations are obtained with a finite-volume solver ANSYS CFX. The solutions reveal the instability of formed shock waves and a flow hysteresis in considerable bands of the free-stream Mach number at zero and negative angles of attack. The instability is caused by an interaction of shocks with the expansion flow formed over the convex bend of the lower wall. Debnath and Pandey [13] numerically investigated the detonation combustion wave propagation in pulse detonation combustor with nozzle. The LES turbulence model was used to simulate the combustion wave reacting flows in the combustor with a standard wall function. From these numerical simulations among four acquaint nozzles the highest thrust augmentation could be attained in divergent nozzle geometry and detonation wave propagation velocity eventually reaches 1830 m/s, which is near about C-J velocity. Xiao et al. [14] evaluated the effect of boundary layer losses on two-dimensional cellular detonations obtained in narrow channels. The experiments provide the details of the cellular structure and the detonation speed deficits from the ideal CJ speed. They showed that the dynamics of 2D cellular detonations in narrow channels can be well captured using a quasi-2D approach modeling the lateral boundary layer losses using Mirel's theory.

Very little work has been done in the field of non-ideal detonations. In fact, a non-ideal environment is an environment in which external factors, such as friction, cause the detonation behavior to deviate from the ideal behavior. Therefore, the innovation of the present work is modeling detonation in these non-ideal conditions for mixtures with very low activation energy to detect its failure mechanism. Although the physical mechanisms that cause the abnormal behavior of detonation are quite complex (shock reflection, shock diffraction, transmission, hotspots, etc.), it is possible to model them with suitable sources in terms of momentum and heat losses as a one-dimensional model. There is still a gap for a broader study. In this paper, the governing equations and their solution methods are presented in the form of numerical simulations. To obtain the proper form of the governing equations, some assumptions are considered that are expressed in the following. The numerical solution method is also briefly stated and then the solution of the momentum conservation equation by considering the effects of momentum loss is expressed. The failure mechanisms of detonation and its behaviour in terms of different activation energies are so wide that only very low activation energy (very lower than the limit of detonation stability) have been investigated and studied in this paper. Then the mechanism involved in detonation failure at that activation energy was recognized.

### 3. Modeling

In the simulation of gas detonations, in addition to the equations that model gas-dynamical processes, some equations are needed to simulate the combustion process, called the reaction model or kinetic model. The kinetic models presented so far have followed two different objectives. Some have proposed a reaction model to simulate the mechanism of a particular mixture, such as hydrogen and air, or other mixtures, intending to simulate detonation in a particular mixture. The other group has been looking for a general valid model to study the behaviour of the detonation wave. The most obvious example of this category is the single-step model [15]. In this section, the equations of gas dynamics and chemical kinetics governing the problem and their solution methods for numerical simulation are presented. To obtain the proper form of the governing equations, a series of simplifying assumptions are considered as follows [16]. The analysis is performed based on a one-dimensional model. Terms of diffusion effect are ignored because the velocity is so high that the diffusion mechanism is ineffective and the penetration time scale is much slower than the detonation time scale. With this assumption, Navier-Stokes equations convert to Euler equations. The complete gas state equation is used for raw materials and products. The single-step Arrhenius model is used for chemical kinetics. Total activation energy is assigned to the studied mixture, due to the avoidance of unnecessary simulation complexities, which prolongs the execution time of the numerical solution.

The non-dimensional form of the governing equations of ideal detonation in the framework attached to the wall (Figure 1) is in the form of Equation (1) [6]:

$$\frac{\partial U}{\partial \alpha} + \frac{\partial F}{\partial x} = S \quad (1)$$

where  $U$  is a vector of conservative variables,  $F$  is a vector of fluxes and  $S$  is a representative vector of source terms due to combustion and effects of the reaction zone as follows:

$$U = \begin{bmatrix} \rho \\ \rho u \\ \rho e \\ \rho \beta \end{bmatrix}, F = \begin{bmatrix} \rho u \\ \rho u^2 + p \\ u(\rho e + p) \\ \rho u \beta \end{bmatrix}, S = \begin{bmatrix} 0 \\ 0 \\ 0 \\ -\rho \omega \end{bmatrix} \quad (2)$$

Where  $p$ ,  $\rho$  and  $u$  are respectively the pressure, density and velocity of the particle relative to a laboratory framework.  $e$  is The total internal energy per mass unit and  $\beta$  is the reaction parameter that varies between 1 (for reactants) and 0 (for products).  $\omega$  is the reaction rate which is derived from Arrhenius reaction rate law.

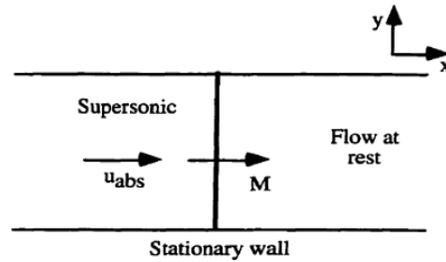


Figure 1. Frame work attached to the wall [6]

The activation energy  $E_a$  is also non-dimensionalized  $RT_0$ , which will no longer be written in order to summarize. To make the spatial variables dimensionless, a characteristic length related to chemical kinetics has been used. That is the length at which the fluid particle moves from the detonation front until half of the reaction has taken place. This length is called the half-reaction length (hrl). Since the conditions in front of the shock wave (unburned area,  $x = 0$ ) are used as the dimensionlessness criteria, the same conditions are selected as the reference. The governing equations considering the effect of friction (non-ideal state) are the same as presented, with the difference that the momentum loss source term  $f$  is entered in the source term vector as Equation (3) and thus its effect is included in the one-dimensional momentum conservation equation.

$$S = \begin{bmatrix} 0 \\ f \\ 0 \\ -\rho \omega \end{bmatrix} \quad (3)$$

Friction loss in pipes is modeled as the momentum source term  $f$  in the momentum conservation equation, for which there are suggestions for its formulation. Zeldovich proposed the form of Equation (4)[3], which is used to develop the code in this research:

$$f = k_f \rho u_{abs} |u_{abs}| \quad (4)$$

where  $u_{abs}$  is the particle velocity in the laboratory frame work and  $k_f$  is the friction coefficient. In this paper, to model the friction loss, a value for  $k_f$  is used which is considered in a laboratory frame work with a negative sign, because the direction of flow and friction force is always opposite.

First, Equation (1) is solved in the form that at first the source terms are removed from the equations[6]. The answers obtained from this equation are used as the initial conditions for Equation (5) which is related to the source term.

$$\frac{\partial U}{\partial \alpha} = S \quad (5)$$

The second step is to solve Equation (5). For the single-step model, this equation is a simple linear differential equation in which its exact solution is easily obtained and after discretization, it is used in the mentioned code.

In this paper, the piecewise parabolic method (PPM) of Colella and Woodward [17] is used to simulate the flow and solve Euler equations, which is one of the higher-order extensions of the Godunov method. The main contribution of Godunov is how the fluxes are computed. Instead of using some averaging between cells values, in the Godunov method the fluxes are computed from an exact solution of the Riemann problem at the interface between two adjacent cells. PPM is a higher-order Godunov method that, instead of using a constant value for the dependent variable at each cell (as in the Godunov method), uses a parabolic profile in each cell. Bourlioux [18] has introduced this method as the best gas-dynamic solution method to track the shock wave front. Mesh independency was checked in each series of calculations and the optimal Mesh was used. Since the reaction becomes complete in the narrow region near the shock wave, it is better to refine the mesh only in this area. This method is a simpler version of the adaptive mesh refinement algorithm.

#### 4. Detonation propagation in a frictional environment

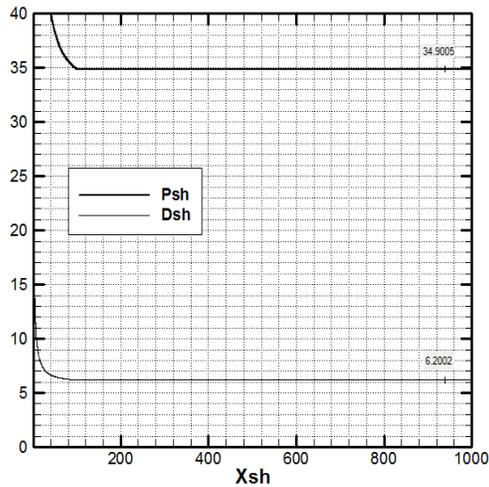
Activation energy is the most important kinetic parameter that controls one-dimensional detonation instability. Detonation instability plays an important role in the dynamic parameters of detonation such as critical initiation energy, etc. By supplying the critical initiation energy, the onset of detonation happens as the pressure pulse progresses between the reaction front and the shock wave front. The compression part of the pressure pulse directs the reaction zone to the shock wave front. Otherwise, the reaction front separates from the shock wave front and the detonation will not be formed due to the subcritical onset. The formation of the pressure pulse is due to the rapid release of energy during the exothermic zone. Friction causes the critical energy required for detonation onset to increase. In the present work, the detonation behavior after the onset stage has been investigated.

For ideal detonations, the activation energy limit for stability is 25. Therefore, with activation energy higher than 25, instability occurs in the form of completely linear or irregular fluctuations. But for detonation in a frictional environment, the stability limit decreases. In the present problem, the activation energy

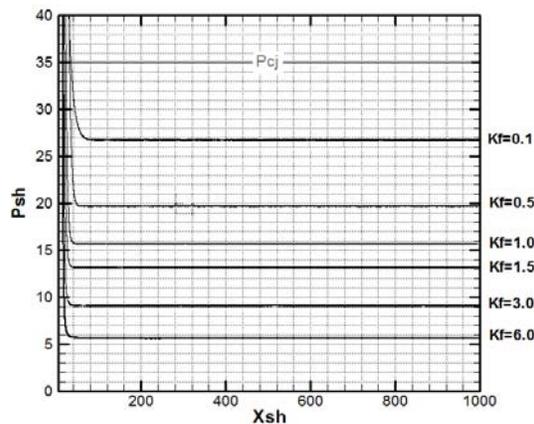
of 8 is considered, which is in a stable range in the ideal state. Other kinetic properties of the mixture are considered as  $Q/RT_0 = 50$ ,  $\gamma = 1.2$ . In order to propagate the stable detonation, the reaction zone and the wave must move together. Consecutively getting away from each other and getting closer to each other in some cases cause instability. The greater the distance between them, the more the detonation decays ([19]-[20]). If the detonation is unstable, numerical errors grow and the detonation instability will be detected. Sometimes disturbance is applied from the outside to the field (such as what has been done in the present study so that friction is a disturbance) and its growth or failure indicates instability or stability of the detonation. In this paper, a detailed study of the detonation behaviour problem and the effect of changing the friction parameter on the detonation behavioural activation energy very lower than the activation energy limit 25 for stability (for example 8) have been done. These values are in the range of low activation energies.

In this section, the detonation behavioural activation energy of 8 is studied. Figure 2 shows the diagram of shock wave pressure ( $P_{sh}$ ) and velocity ( $D_{sh}$ ) versus shock wave location ( $X_{sh}$ ) in the environment with a friction coefficient of  $K_f=0$  (ideal state) at activation energy of 8. This figure shows that in the considered mixture, the detonation wave behaviour is completely stable and it is consistent with the results of the stability analysis. As shown in the figure, the shock wave pressure and velocity are equal to the values of CJ pressure and velocity (34.9 and 6.2), respectively. Then the friction coefficient gradually increases from zero.

In the curves of Figure 3 and Figure 4, the wave behaviour in an environment with roughness, with friction coefficients of 0.1, 0.5, 1.0, 1.5, 3.0, and 6.0 is shown. The shock wave pressure and velocity in all of these cases are still stable, and the only difference is that the detonation has become weaker step by step. Dionne's results [7] also support this claim. When the friction coefficient is such that the local Mach number is close to 1, it means that the energy released from the chemical kinetics is consumed by the friction and is not sufficient for the detonation to be self-sustained. In this way, at a critical friction coefficient, the detonation is so-called failed. As can be seen from these figures, the shock wave pressure and velocity values reached less than CJ values, which is to be expected. In fact, the failure mechanisms in the detonation cause to reduce the shock wave pressure and velocity of the CJ state due to the lateral expansion.



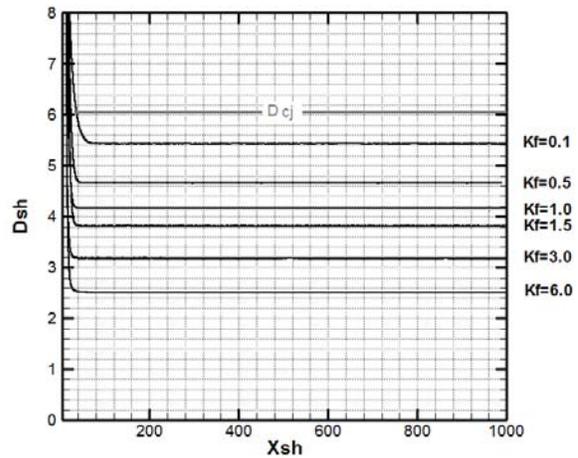
**Figure 2.** The diagram of shock wave pressure (Psh) and velocity (Dsh) versus shock wave location (Xsh) at  $K_f=0$  and  $E_a=8$



**Figure 3.** The diagram of shock wave pressure (Psh) versus shock wave location (Xsh) at  $K_f=0.1$  to  $6.0$  and  $E_a=8$

It should be noted that the detonation initiated with critical  $E_0$  in the frictionless state, by adding friction and applying the same initial blast wave power, was not formed until the blast wave power was slightly increased. After that, with each increase in the friction coefficient, the initial energy is also increased. Due to the wall effects, the flow directs a part of the chemical kinetic energy into the boundary layer. Thus, the competition between the Arrhenius exothermic reaction due to the release of chemical energy and the frictional drag due to the chemical energy loss occurs, and its effect becomes more important as the friction increases [20]. Therefore, the effective energy, which is the chemical kinetic energy minus frictional losses, to maintain, sustain and propagate the detonation wave, reduces causes to decrease the detonation wave pressure and velocity. With one step of increasing the friction

coefficient, the shock wave pressure and velocity reduce but the wave behaviour remains stable. The energy released from the chemical reaction is sufficient for the detonation to be self-sustained, and the frictional force, despite weakening the detonation, has not caused it to become unstable or fail. Therefore frictional forces have decisive effects on the properties of the final flow. The flow would be irreversible due to the existence of friction, therefore in the insulated state, the entropy increases in the direction of the flow. Subsequently with a sufficiently large amount of friction, whether subsonic flow or supersonic flow currently being investigated, the Mach number of the flow reaches 1 and with a further increase in friction, the Mach number remains constant at the same value. The flow is choked due to friction.



**Figure 4.** The diagram of shock wave velocity (Dsh) versus shock wave location (Xsh) at  $K_f=0.1$  to  $6.0$  and  $E_a=8$

Figure 5 and Figure 6 with friction coefficients of 20 show that even though the distance between the reaction front and the shock wave front (which is considered equivalent to the spatial distance from  $\beta$  equal 0.05 to 1) according to Table 1 is almost unchanged rather than the frictionless case, but failure has occurred due to excessive shock wave pressure and velocity drop due to the momentum loss. The pressure level (about 2) and the velocity level (about 1.5) are no longer large enough to refer to this front as the detonation. The detonation behaviour remains stable until fails. It should be noted that the arrows on the pressure profile indicate the distance of the reaction front from the shock wave front. When the shock wave pressure drop begins, the pressure profiles in the known positions in Figure 6 show that there is no pressure pulse sent from the reaction area towards the shock wave, therefore those are not able to increase the shock wave pressure. From the friction coefficient 6 and above, the pressure pulse is still weaker than before until it disappears completely at the friction coefficient equal to 20. Arrows indicate the positions of the reaction front and the shock wave front.

Table 1 shows the distance of the reaction front from the shock wave front (d) in all the cases discussed above. The detonation is fed by the two energy sources, one is the external source, which here is the initiation energy (blast), and the other source is the combustion energy [21]. Moving away from the initiation point causes to reduction the external energy source and slows down the detonation velocity. Since the deceleration is gradual due to the getting away from the initiation point, the sudden detonation pressure drop at the distances away from the initiation point, is due to the sudden decrease in the combustion energy. Thus, the reaction rate decreases due to the shock wave pressure drop such an extent that its energy is not able to sustain the shock wave and the detonation failure starts. The momentum loss causes the reaction to be extinguished.

Figure 7 shows the shock wave pressure and velocity diagram in terms of the friction coefficient parameter. Figure 8 shows the same diagram for several different activation energies from the analytical solution performed by Dionne [7]. To validate the present numerical model Figure 8 was presented, this figure is related to analytical solution performed by Dionne [7]. Dionne [7] predicted the shock behaviour by analytical solution in several activation energies, but in the present study a numerical model was extended to achieve this aim and eventually the two were compared, which matched well. to date, Dionne's [7] study is the most relevant and closest source to the present work to verify. Between the numerical solution results of the current study and analytical solution results, it is observed the similarity of qualitative and behavioural trends.

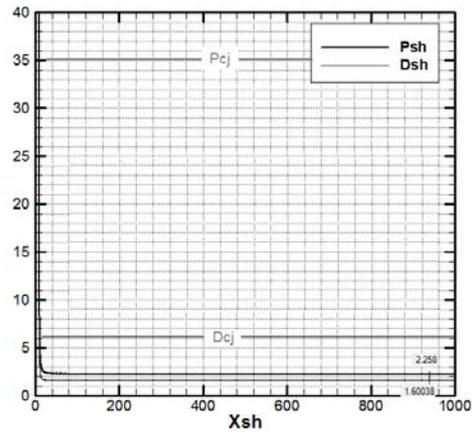


Figure 5. The diagram of shock wave pressure (Psh) and velocity (Dsh) versus shock wave location (Xsh) at Kf=20 and Ea=8

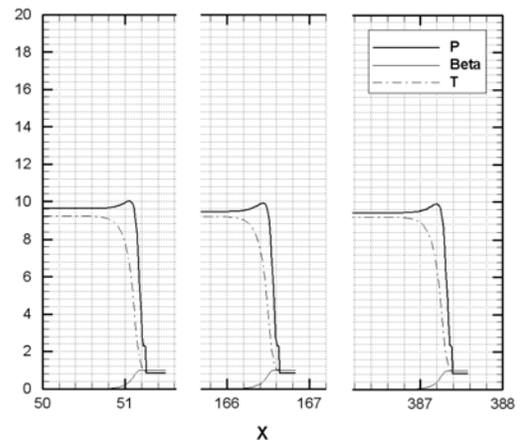


Figure 6. Pressure, reaction parameter and temperature profiles versus shock wave location (Xsh)at Kf=20 and Ea=8

Table 1. Dimensionless distance of the reaction front from the shock wave front (d) in several states with the activation energy of 8

Kf	0	0.05	0.1	0.5	1	1.5	3	6	20	25
d	0.40	0.43	0.46	0.48	0.50	0.50	0.50	0.50	0.50	0.50

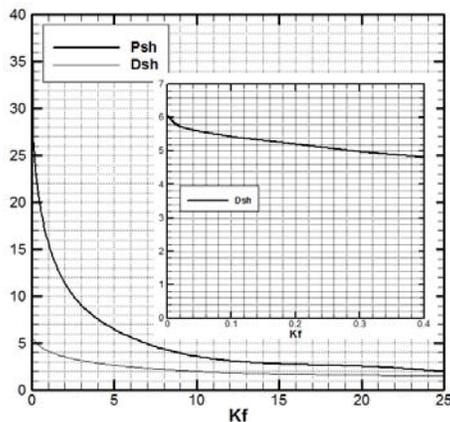


Figure 7. The diagram of shock wave pressure (Psh) and velocity (Dsh) versus friction coefficient (Kf) resulting from numerical simulation with Ea=8

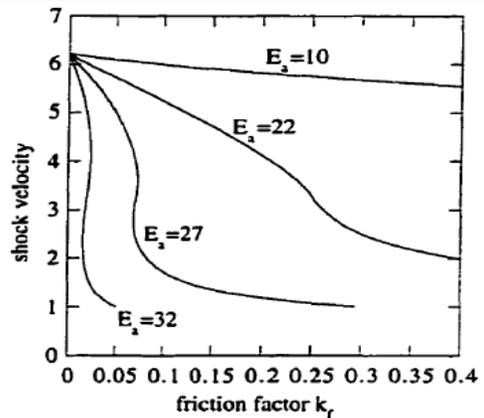


Figure 8. The diagram of shock wave pressure (Psh) and velocity (Dsh) versus friction coefficient (Kf) resulting from analytical solution in several activation energies [7]

Minor quantitative differences are due to the differences in making the equations dimensionless and the activation energy. The important point is that detonation behaviour from stability to failure does not include fluctuations. In fact, due to the pressure drop of the shock wave, the reaction rate behind the shock wave drops sharply, which is the main cause of detonation failure. Therefore, if the activation energy is low, with increasing friction, the detonation is failed without showing any particular unstable behaviour, however, this is not the case with high activation energies.

## 5. CONCLUSION

In this study, the detonation behavior in non-ideal conditions considering friction as a source term in the momentum equation has been modeled. Friction causes the critical energy required to initiate the detonation to increase. The stability limit of detonation in presence of friction decreases. That is, in the same activation energy, the detonation front propagated in the non-ideal environment has higher levels of instability than the ideal state. Friction or momentum loss causes to reduce the detonation pressure and velocity to less than CJ values.

At low activation energy, with increasing friction, there is no significant change in the stable behavior of the detonation front. The detonation gradually decays until it finally fails. At activation energy below the stability limit, the friction causes the shock wave behavior (pressure, velocity, etc.) to fluctuate. As the friction increases, the fluctuation amplitude and its steps become larger. These fluctuations are due to the consecutive getting away and getting closer to the reaction front from the shock wave front so that the farther away they are, the weaker the shock wave becomes. Therefore, higher friction leads to higher levels of instability. As this process continues and the friction coefficient increases further, the detonation will eventually fail. At very low activation energy (equal to 8 in this study), due to the pressure drop of the shock wave, the reaction rate behind the shock wave drops sharply and this drop is the main cause of detonation failure. Therefore, when the activation energy is low, with increasing friction, the detonation fails without exhibiting any particular unstable behavior. Here, the critical friction coefficient to form the detonation activation energy 8 is estimated equal to 20. The failure mechanism of the detonation in this study is the pressure drop mechanism and the un-burnt packet mechanism is not involved in it.

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