# **Detonation Transmission Across an Inert Gap**

Kelsey C. Tang-Yuk, John H.S. Lee McGill University Montreal, QC, Canada

> Hoi Dick Ng Concordia University Montreal, QC, Canada

XiaoCheng Mi University of Cambridge Cambridge, United Kingdom

## 1 Introduction

In this study the transmission of a gaseous detonation wave across an inert layer is simulated. Both onedimensional Zeldovich-von Neumann-Döring detonations and two dimensional cellular detonations are considered. The problem is of interest in detonation propagation in a non-uniform mixture where there are 'pockets' of inert or mixture outside the detonation limits. This problem is also relevant as it is equivalent to the gap test of condensed phase explosives. Previous experimental work on this problem includes those of Bull *et al.* [1] and Bjerketvedt *et al.* [2]. They concluded that the key parameters governing this problem are the CJ properties of the initial detonation, the width of the inert section and the sensitivity of the downstream mixture.

# **2** Computational Details

The problem is illustrated in figure 1 for an incident cellular detonation. The detonation is initiated by a high pressure region with a sinusoidal perturbation in two-dimensions and initiation is sufficiently far



Figure 1: Problem illustration.

upstream such that a steady CJ wave is obtained prior to encountering the inert layer of thickness,  $\delta_i$ .

The system is governed by the reactive Euler equations with heat release described by chain branching kinetics. The present study uses a two step induction-reaction kinetic model (given by equation 1) where possible, and a three step chain-branching kinetic model (given by equation 2) to obtain a more complete range of mixtures. This approach also allows the model dependence of the results to be scrutinized.

$$\frac{d(\rho\xi)}{dt} = H(1-\xi)\rho k_{\rm I} \exp\left[E_{\rm I}\left(\frac{1}{T_{\rm s}} - \frac{1}{T}\right)\right]$$

$$\frac{d(\rho\lambda)}{dt} = (1-H(1-\xi))\rho k_{\rm R}(1-\lambda) \exp\left[\frac{-E_{\rm R}}{T}\right], \quad H(1-\xi) = \begin{cases} 1 & \xi < 1\\ 0 & \xi \ge 1 \end{cases}$$
(1)

$$\frac{d(\rho f)}{dt} = -\rho(\omega_{\rm I} + \omega_{\rm B}), \quad \frac{d(\rho y)}{dt} = \rho(\omega_{\rm I} + \omega_{\rm B} - \omega_{\rm C})$$

$$\omega_{\rm I} = f \exp\left[E_{\rm I}\left(\frac{1}{T_{\rm I}} - \frac{1}{T}\right)\right], \quad \omega_{\rm B} = \rho f y \exp\left[E_{\rm B}\left(\frac{1}{T_{\rm B}} - \frac{1}{T}\right)\right], \quad \omega_{\rm C} = y$$
(2)

The models are fully described by Ng *et al.* in [5] and [4], respectively. The non-dimensionalization of state and flow variables and the scaling of rate constants also follow these studies.

The simulation is based upon a uniform Cartesian grid. The MUSCL-Hancock scheme with the van Leer nonsmooth slope limiter and a Harten-Lax-van Leer-contact (HLLC) approximate solver for the Riemann problem are used, described by Toro [6]. In one-dimension a minimum resolution of 100 cells per unit length is used and the convergence of the critical thickness  $\delta_{i,cr}$  has been verified with resolutions of 200-400 cells. In two-dimensions the resolution is 10 grid points per induction length,  $\Delta_I$ . The domain width, W in figure 1, is defined to be 300 times  $\Delta_I$  and a periodic boundary condition is applied to the top and bottom of the domain.

## **3** Results and Discussion

### 3.1 1D

We first discuss the case of an incident ZND detonation. Figure 2 shows a selected typical case. In this figure the shock front pressure of the detonation is plotted with distance. The inert layer begins at begins at x = 0 (dashed black line). Its thickness is varied, and the coloured dashed lines indicate the end of the layer for the different cases.

Upstream of the inert layer, the shock pressure corresponds to that of the ZND detonation. After entering the inert layer, it begins to decay at around x = 4. Thus, the longer the inert layer, the weaker the shock transmitted into the reactive mixture downstream. For  $\delta_i \leq 7$ , downstream of the inert layer, the detonation drops below the CJ pressure but ultimately recovers and re-accelerates to an overdriven detonation before asymptotically decaying. A detonation wave with the original shock pressure is reformed downstream. However, for  $\delta_i \geq 8$ , the detonation fails to re-accelerate and decays continuously as it propagates downstream. A non-reacting shock wave is formed. Therefore, there exists a critical thickness  $\delta_{i,cr} = 7.5 \pm 0.5$  for the detonation to be reformed downstream.

In figure 3, profiles of pressure and heat release are plotted with distance for the sub-critical ( $\delta_i = 7$ ) and critical ( $\delta_i = 8$ ) cases. In both cases, at the time that the wave exits the inert layer, most of the reactive mixture from upstream has finished reacting. The decay is caused by a decoupling of the reaction front from the leading shock. At sub-critical, there is eventually a build up of pressure in the reaction zone,



Figure 2: Shock pressure history for  $\delta_i = 6, 7, 8, 10$ . Result is for the three step kinetic model with  $E_I = 37.5, T_I = 3, E_B = 20, T_B = 0.89$  and where  $Q = 41.67, \gamma = 1.2$ 

which allows the reaction to ultimately re-couple with the shock front. At failure the detonation continues to decelerate and eventually fails because the reaction becomes increasingly decoupled from the leading shock. The failure and re-initiation process is found to be analogous to others in detonation physics [3], for example blast initiation. Here the thickness of the inert layer is analogous to the blast energy. Similar results are obtained for the two step induction-reaction kinetic model.

#### **3.2** 1D: Variation of parameters

For the two step model, the kinetic parameters that can be independently varied are the activation energies of the induction and reaction zones,  $E_{\rm I}$  and  $E_{\rm R}$  and the pre-exponential constant of the reaction zone,  $k_{\rm R}$ . For the three step model, they are the chain initiating and chain branching activation energies,  $E_{\rm I}$  and  $E_{\rm B}$ and cross-over temperatures,  $T_{\rm I}$  and  $T_{\rm B}$ . Additionally, the CJ properties are set by the dimensionless heat release Q and specific heat ratio  $\gamma$ . It should be noted that the parameters are restricted in order to obtain a stable ZND detonation.

The parameters were varied and the critical thickness  $\delta_{i,cr}$  was found for each combination. These results were found collapse onto curves when plotted in the  $\frac{\delta_{i,cr}}{\Delta_R}$  against  $E_{a,e}$  plane. Here  $\Delta_R$  is a characteristic reaction length scale. Taken from [5], it was defined as follows,

$$\Delta_{\rm R} = \frac{u_{\rm CJ}}{\dot{\sigma}_{\rm max}}, \qquad \dot{\sigma} = (\gamma - 1) \frac{Q}{c^2} \frac{d\lambda}{dt}$$
(3)

where  $u_{\rm CJ}$  is the CJ particle velocity in the shock frame. The thermicity  $\dot{\sigma}$  is a normalized heat release rate where  $\lambda$  is the product mass fraction for both reaction models. The parameter  $E_{\rm a,e}$  is an effective activation energy that attempts to quantify the temperature sensitivity of the induction process. In dimensional terms, it is defined as follows,

$$E_{\rm a,e} = \frac{\tilde{E}_{\rm a}}{\gamma \tilde{R} \tilde{T}_0} = \frac{\tilde{E}_{\rm a}}{\tilde{c_0}^2} \tag{4}$$

where  $T_0$  is the temperature and  $\tilde{c_0}$  the sound speed of the unburnt mixture. For the two step model it is given by  $E_{a,e} = \frac{E_I}{\gamma}$ , consistent with previous non-dimensionalization. For the three step model it has to be estimated. To do this two adiabatic, constant volume explosion simulations are performed with slightly

 $27^{\rm th}$  ICDERS – July  $28^{\rm th}$  –August  $2^{\rm nd}, 2019$  – Beijing, China



(b) Inert layer thickness,  $\delta_i = 8$ 

Figure 3: Profiles of pressure and the heat release rate for  $E_{\rm I} = 37.5$ ,  $T_{\rm I} = 3$ ,  $E_{\rm B} = 20$ ,  $T_{\rm B} = 0.89$  and where Q = 41.67,  $\gamma = 1.2$ .

different initial temperatures. The shock temperatures for  $\pm 1\% M_{\rm CJ}$  are used as was tested by Schultz and Shepherd [7]. Assuming an Arrhenius form of the induction time, the activation energy can be calculated. For details see [7].

The result is given in figure 4. Each value of  $M_{\rm CJ}$  is plotted in a different colour, and results using the two step and three step models are indicated by the circle and triangle markers respectively. A few things are readily apparent. Firstly, the critical inert thickness  $\delta_{\rm i,cr}$  can range from the order of magnitude of the ZND wave thickness (i.e.  $\frac{\delta_{\rm i,cr}}{\Delta_{\rm R}} \sim 1$  for high activation energy), to more than 15 times it's thickness. Additionally, the results of the two and three step models are directly compared in purple, where  $M_{\rm CJ}$ ,  $\gamma$ and Q are held constant. The results are coherent, implying that the results are independent of the kinetic model used.

The curves are dependent on  $M_{\rm CJ}$ . However, there is an overlap of the results for  $M_{\rm CJ} = 3.0$  and  $M_{\rm CJ} = 4.2$ , where  $\gamma$  has been varied but Q is constant. This may suggest that each curve is dependent on the more specific value of Q as opposed to  $M_{\rm CJ}$ . It should be noted that Q has been normalized by  $\gamma \tilde{R}\tilde{T}_0 = c_0^2$  and so  $\gamma$  is included in it's definition. Finally, the overall trend indicates that the inert layer thickness that a detonation can withstand relative to it's size (i.e. the ratio  $\frac{\delta_{i,cr}}{\Delta_{\rm R}}$ ) is dependent on an effective activation energy parameter,  $E_{\rm a,e}$  here. The higher  $E_{\rm a,e}$  the easier the detonation fails, and the lower  $E_{\rm a,e}$  the easier the detonation fails, and the lower  $E_{\rm a,e}$  the easier the detonation of failure for direct initiation given by Eckett *et al.* [8], in that unsteadiness in the induction zone was shown to be the defining factor. It also seems to be consistent with the conclusions of Bjerketvedt *et al.* [2]. They found the key parameters to be the CJ properties of the upstream mixture ( $M_{\rm CJ}$  here) and the sensitivity of the downstream mixture. The exact relationship between activation energy and sensitivity is unclear, however it's evident that the specifics of the kinetics is important.



Figure 4: Variation of the critical inert thickness  $\delta_{i,cr}$  normalized by the ZND length  $\Delta_R$  with an effective activation energy  $E_{a,e}$  for the two step and three step kinetic models.



(b) Inert layer thickness,  $\delta_i = 50$ 

Figure 5: Numerical soot foils for  $\epsilon_{I} = 8.0$  and  $k_{R} = 0.9$ .

## 3.3 2D: Determination of critical thickness

Preliminary simulations were also performed in two-dimensions for the two step kinetic model. Numerical soot foils are generated by tracking the maximum pressure obtained at each point in the domain. A subcritical case where the thickness of the inert layer  $\delta_i = 48$  is shown in figure 5a. The dotted lines indicate the initial inert layer boundaries. Before the inert layer the detonation in this mixture has a mildly unstable cellular pattern. Then, after the inert layer the detonation is weakened, and some triple points disappear creating larger cells. However it is ultimately re-initiated downstream via a localized explosion near the center-line of the domain. Then,  $\delta_i$  is increased to 50 in figure 5b. In this case, the detonation continues to weaken downstream, the transverse waves are damped out and ultimately a transmitted shock wave is obtained. Therefore,  $\delta_{i,cr} = 49.0 \pm 1.0$ . This is an order of magnitude larger than it is for the 1D case, where for the same kinetic parameters  $\delta_{i,cr} = 4.5 \pm 0.5$ . This indicates that cellular instabilities play an important role and the survival of these instabilities (triple points) aid the re-initiation downstream.

#### Tang-Yuk, K.C.

However, it should be noted that this value of  $\delta_{i,cr}$  corresponds to the resolution used. The resolution is known to affect the amount of numerical diffusion in simulations based on the Euler equations, with higher resolution decreasing the numerical diffusion [9]. How the critical thickness is affected by the number of computational grids will be the subject of further study.

## 4 Concluding Remarks

The transmission of a detonation wave across a layer of inert material has been numerically simulated. When the inert layer is less than some critical thickness,  $\delta_i < \delta_{i,cr}$ , the detonation first decays downstream but then is ultimately re-accelerated and re-initiated. Conversely, when the inert layer thickness  $\delta_i > \delta_{i,cr}$ , the detonation fails to be transmitted downstream. The wave amplification and failure process closely resembles other detonation initiation phenomenon such as blast initiation. The critical thickness  $\delta_{i,cr}$  is highly dependent on and decreases with the temperature sensitivity of the induction process, quantified as the effective activation energy  $E_{a,e}$ . This is consistent with the results of both Bjerketvedt *et al.* [2] and of Eckett *et al.* [8]. Preliminary two-dimensional simulations indicate that the critical thickness is an order of magnitude larger than in one-dimension.

Future work will include a more complete parametric and resolution study in two dimensions. It will also consider the effect of non-planar reactive-inert interfaces and different upstream and downstream reactive mixtures.

## References

- [1] Bull DC, Elsworth JE, McLeod MA. (1981). Initiation of unconfined gas detonations in hydrocarbonair mixtures by a sympathetic mechanism. Progress in Astronautics and Aeronautics, 75: 61-72.
- [2] Bjerketvedt D, Sonju OK, Moen IO. (1986). The influence of experimental condition on the reinitiation of detonation across an inert region. Progress in Astronautics and Aeronautics, 106: 109-130.
- [3] Lee JHS. (1977). Initiation of gaseous detonation. Annual Review of Physical Chemistry, 28: 75-104.
- [4] Ng HD, Lee JHS. (2003). Direct initiation of detonation with a multi-step reaction scheme. Journal of Fluid Mechanics, 476: 179-211.
- [5] Ng HD, Radulescu MI, Higgins AJ, Nikiforakis N, Lee JHS. (2005). Numerical investigation of the instability for one-dimensional ChapmanJouguet detonations with chain-branching kinetics. Combustion Theory and Modelling, 9(3): 385-401.
- [6] Toro EF. (1999) Riemann Solvers and Numerical Methods for Fluid Dynamics. Springer-Verlag.
- [7] Schultz E, Shepherd J. (2000). Validation of detailed reaction mechanisms for detonation simulation. GALCIT Technical Report FM99-5.
- [8] Eckett C, Quirk J, Shepherd J. (2000). The role of unsteadiness in direct initiation of gaseous detonations. Journal of Fluid Mechanics, 421: 147-183.
- [9] Radulescu, MI. (2018). A detonation paradox: Why inviscid detonation simulations predict the incorrect trend for the role of instability in gaseous cellular detonations?. Combustion and Flame, 195: 151-162.