

Experimental $D(\kappa)$ Relationships for Unstable Detonations

Q. Xiao, M.I. Radulescu

Department of Mechanical Engineering, University of Ottawa
Ottawa, Ontario, Canada

1 Introduction

Real detonations in gases have been experimentally observed to travel at a speed with velocity deficit, with respect to the ideal Chapman-Jouguet (CJ) speed, in the presence of non-ideal effects, such as lateral mass divergence, unsteadiness, and momentum and heat losses [1]. A significant question arises that, can the classical one-dimensional (1D) Zeldovichvon Neumann-Doering (ZND) model, which neglects the multi-dimensional, time-varying cellular structures, be able to model the real detonation dynamics at the macro-scale? Despite the fact that this question has been attempted extensively in the past in narrow tubes and tubes with porous walls, e.g., see Refs. [2, 3], these works adopted a number of assumptions and matching constants in modeling the dynamics of detonations [4], by applying the steady ZND model with extensions, which probably significantly impacted the comparisons between the calculated predictions and the experiments.

Recently, Nakayama et al. [5] experimentally conducted a pioneering work investigating stable curved detonations in rectangular-cross-section curved channels and obtained the characteristic $D(\kappa)$ relationships of detonations in mixtures of $C_2H_4/3O_2$, $2H_2/O_2$, and $2C_2H_2/5O_2/5Ar$ in curved channels. A universal $D(\kappa)$ curve was found. More recently, Radulescu and Borzou [4] experimentally proposed two exponentially shaped channels (exponential horns), which allowed detonations to propagate with a constant mean mass divergence in quasi-steady state. By constructing the characteristic $D(\kappa)$ relationships, they were able to directly evaluate the boundary layer induced mass divergence, and moreover, make a meaningful comparison of the experimental results with theoretical models. In their experiments, only two mixtures of different stability were tested, i.e., the highly unstable one of $C_3H_8/5O_2$ with very irregular cellular structures, and the weakly unstable one of $2C_2H_2/5O_2/21Ar$ with regular cells. Therefore, the objective of this work is to apply this novel strategy to unstable detonations in other mixtures of $CH_4/2O_2$, $C_2H_4/3O_2$, and $C_2H_6/3.5O_2$, for the purpose of constructing the characteristic curves and comparing them with the generalized ZND model with lateral mass divergence.

2 Experimental Setup

The experiments were conducted in a 3.4 m long aluminium rectangular channel with an internal height and width of 203 mm and 19 mm, respectively. The experimental set-up is the same as that adopted by Radulescu and Borzou [4]. The shock tube comprises three sections, a detonation initiation section, a propagation section, and a test section. The mixture was ignited in the initiation section by a high voltage igniter (HVI), which could store up to 1000 J with the deposition time of 2 μs . Two different polyvinyl-chloride (PVC) ramps, which enabled the cross-sectional area $A(x)$ of the channel to diverge exponentially

with a constant logarithmic area divergence rate ($K = \frac{d(\ln A(x))}{dx}$), were adopted in the test section. The large ramp had the logarithmic area divergence rate of 2.17 m^{-1} , while for the small one such rate was 4.34 m^{-1} . The mixtures presently studied were $\text{CH}_4/2\text{O}_2$, $\text{C}_2\text{H}_4/3\text{O}_2$, and $\text{C}_2\text{H}_6/3.5\text{O}_2$. Eight high frequency piezoelectric PCB pressure sensors were adopted for recording the pressure signals and a Z-type schlieren technique was utilized for visualizing the detonation evolution process.

3 Results and Discussion

3.1 Quasi-steady Detonations with a Constant Mean Mass Divergence

Figure 1 demonstrates the evolution of detonation fronts near the end of the large ramp, for the investigated mixtures in the present study under different initial pressures well above the limit. Detonations propagated from left towards right. As a result of the lateral flow divergence, detonation fronts are evidently curved. One can also observe the formation of unreacted gas pockets in the mixture of $\text{CH}_4/2\text{O}_2$ due to the incomplete consumption of the fuels in the thick induction zone by the non-reactive transverse shocks, as shown in Fig.1(a) and (b). The visualized reaction zone structure appears to be highly turbulent. While for mixtures of $\text{C}_2\text{H}_4/3\text{O}_2$ and $\text{C}_2\text{H}_6/3.5\text{O}_2$ in Fig.1(c) and (d), detonation fronts are much more smooth with very fine scale cellular structures. More importantly, it can be observed that detonation fronts acquired a constant characteristic global curvature, which agrees quite well with that of the dashed red lines denoting the arcs of circles of the expected curvature from the quasi-1D approximation, whose radius equals the reciprocal of the logarithmic area divergence rate $K = 2.17 \text{ m}^{-1}$. This has also been numerically shown by Radulescu and Borzou [4]. The very good agreement between the real curved detonation fronts and the theoretically expected arcs demonstrates the independence of detonation front's global curvature on mixture compositions and initial pressures, suggesting the appropriateness of assuming quasi-steady detonations in the present work.

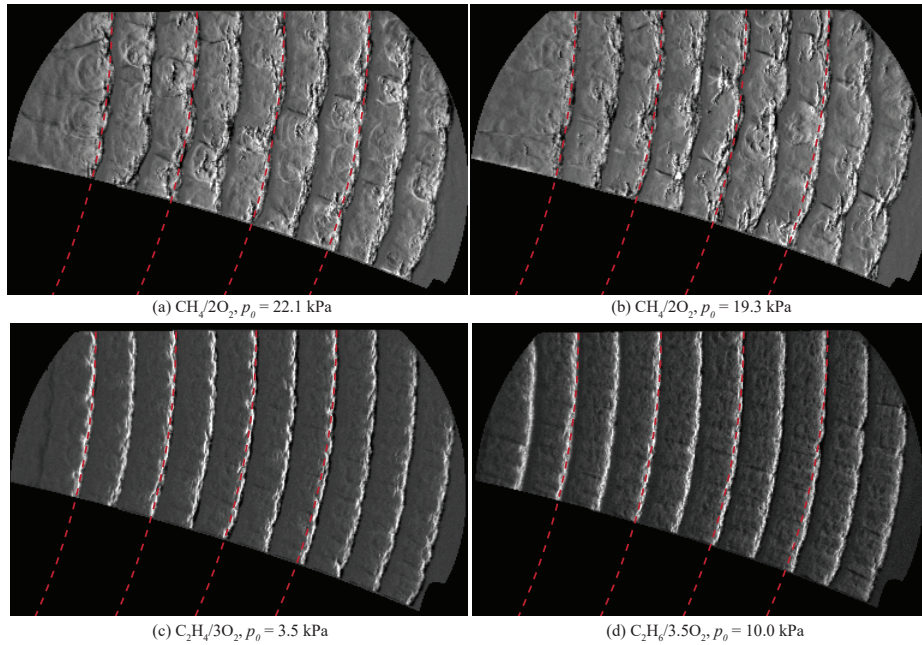


Figure 1: Superimposed detonation fronts near the end of the large ramp in different mixtures. Note that the red dashed lines represent arcs of circles with the expected curvature from the quasi-1D approximation.

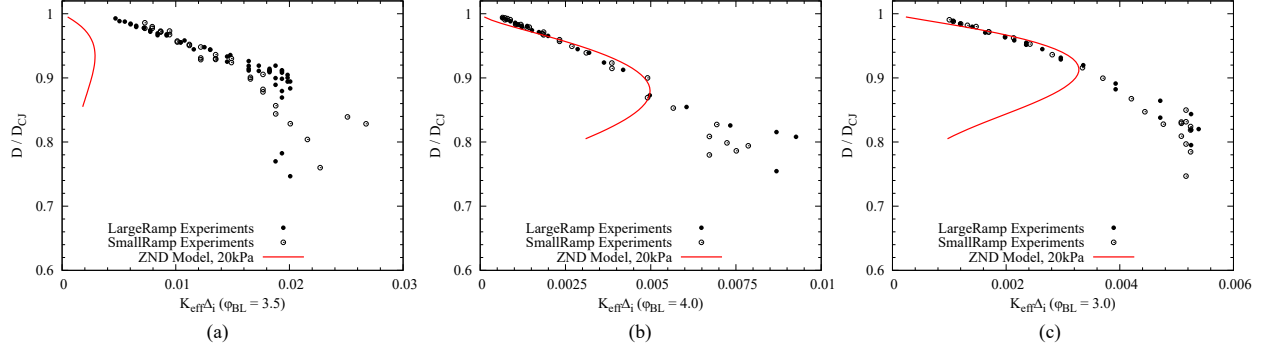


Figure 2: Experimentally obtained characteristic $D/D_{CJ} - K_{eff}\Delta_i$ relationships of (a) $\text{CH}_4/2\text{O}_2$, (b) $\text{C}_2\text{H}_4/3\text{O}_2$, and (c) $\text{C}_2\text{H}_6/3.5\text{O}_2$ in comparison with the generalized ZND model predictions.

3.2 The Characteristic $D(\kappa)$ Relationships

The total mass divergence rate experienced by detonations propagating along ramps in this study includes two parts, the one due to the physical area divergence of the exponentially diverging channel and the other due to divergence of the flow rendered by the boundary layer growth on the channel walls. The effective lateral flow divergence rate can thus be expressed as:

$$K_{eff} = \underbrace{\frac{1}{A} \frac{dA}{dx}}_K + \phi_{BL} \quad (1)$$

where ϕ_{BL} represents the contribution of the boundary layer losses. Instead of modelling the equivalent mass divergence rate ϕ_{BL} of boundary layers, Radulescu and Borzou [4] directly evaluated this loss rate from experiments by analytically comparing the experimental data of two ramps with two underlying assumptions: (1) detonations propagating inside the exponentially diverging channel of different expansion ratios have the same constant ϕ_{BL} since the channel's dimension of the width is unchanged; (2) for the same mixture, it has a unique relation between the velocity deficits and its losses. As a result, the effective rate of total mass divergence can be calibrated by collapsing together the experimental $D(\kappa)$ curves of detonations in the large and small ramp experiments, and then the loss rate ϕ_{BL} due to boundary layers can be derived [4]. The finally obtained constant boundary layer loss rates ϕ_{BL} for $\text{CH}_4/2\text{O}_2$, $\text{C}_2\text{H}_4/3\text{O}_2$, and $\text{C}_2\text{H}_6/3.5\text{O}_2$ are 3.5 m^{-1} , 4.0 m^{-1} , and 3.0 m^{-1} , respectively. Figure 2 shows the experimentally collapsed $D/D_{CJ} - K_{eff}\Delta_i$ curves characterizing relationships between velocity deficits and losses for the mixtures involved in this study, in comparison with the generalized ZND model predictions. The abscissa is the non-dimensional loss obtained by multiplying the mass divergence rate with the CJ detonation induction zone length Δ_i , which was calculated under the framework of SDToolbox [6] by using the San Diego chemical mechanism (Williams 2014) [7]. The computational details of the ZND model predicted curve could refer to that of Radulescu and Borzou [4]. It can be seen that the steady ZND model predictions depart far away from the experimental results of $\text{CH}_4/2\text{O}_2$, while appear to capture well those of $\text{C}_2\text{H}_4/3\text{O}_2$ and $\text{C}_2\text{H}_6/3.5\text{O}_2$ for the small mass divergence and velocity deficits.

Nakayama et al. [5] proposed the cell width λ as the length scale non-dimensionalizing the mass divergence, and obtained the characteristic $D/D_{CJ} - \kappa\lambda$ relationships. In the subsequent analysis of the present work, the cell width λ is also adopted as a characteristic length scale for normalization, which was obtained

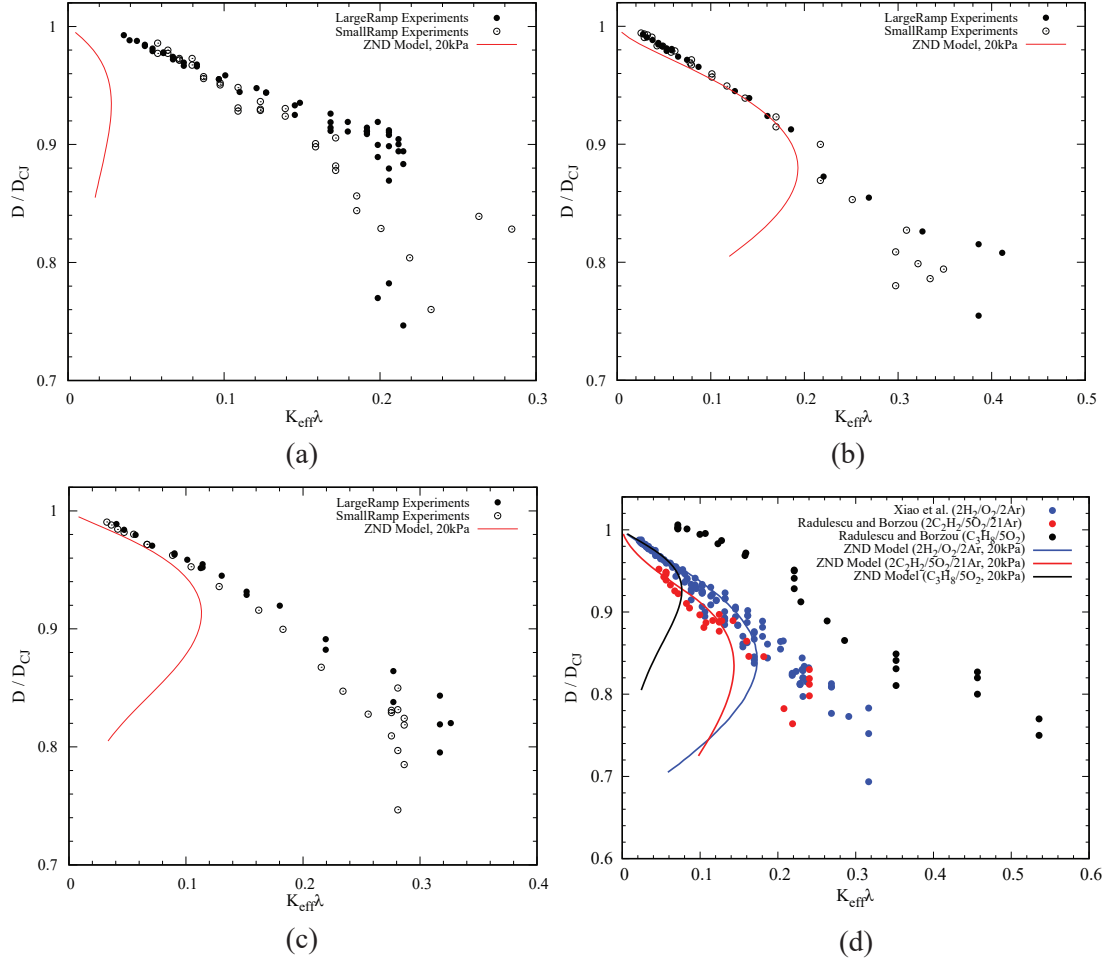


Figure 3: Characteristic $D/D_{CJ} - K_{eff}\lambda$ relationships for various mixtures: (a) $\text{CH}_4/2\text{O}_2$, (b) $\text{C}_2\text{H}_4/3\text{O}_2$, (c) $\text{C}_2\text{H}_6/3.5\text{O}_2$, and (d) $2\text{H}_2/\text{O}_2/2\text{Ar}$ adapted from Xiao et al. [9], $\text{C}_3\text{H}_8/5\text{O}_2$ and $2\text{C}_2\text{H}_2/5\text{O}_2/21\text{Ar}$ adapted from Radulescu and Borzou [4].

by fitting the corresponding data given in the Detonation Database of Caltech [8]. Figure 3 shows the characteristic $D/D_{CJ} - K_{eff}\lambda$ relationships for various mixtures. It can be clearly seen that the constant boundary layer induced mass divergence rates ϕ_{BL} , directly obtained from the above calibration, were able to collapse the $D(\kappa)$ relationships, normalized by the cell width, of both the large ramp and small ramp, as illustrated in Fig.3(a)-(c) for detonations in mixtures of $\text{CH}_4/2\text{O}_2$, $\text{C}_2\text{H}_4/3\text{O}_2$, and $\text{C}_2\text{H}_6/3.5\text{O}_2$. It thus suggests the independence of obtaining the loss rates due to boundary layers on the normalization length scales. Again, the comparison of the experimentally obtained $D/D_{CJ} - K_{eff}\lambda$ curves with the theoretical predictions showed that the generalized ZND model can predict very well the dynamics of detonations in mixtures of $\text{C}_2\text{H}_4/3\text{O}_2$ and $\text{C}_2\text{H}_6/3.5\text{O}_2$, however, very poorly for $\text{CH}_4/2\text{O}_2$ detonations. These comparisons demonstrate that the experimentally observed unstable detonations can propagate with much larger lateral mass divergence and velocity deficits than predicted by the extended ZND model.

Additionally, $D/D_{CJ} - K_{eff}\lambda$ relationships for the other mixtures of $2\text{H}_2/\text{O}_2/2\text{Ar}$, and $\text{C}_3\text{H}_8/5\text{O}_2$ and

$2\text{C}_2\text{H}_2/5\text{O}_2/21\text{Ar}$ have also been obtained by adapting the experimental data in Xiao et al. [9] and Radulescu and Borzou [4], respectively, as shown in Fig.3(d). The corresponding ZND model predictions were again made with the San Diego chemical mechanism (Williams 2014). The results in Fig.3(d) show that the predictions made with the ZND model are in excellent agreement with the experimental values for the weakly unstable detonations in mixtures of $2\text{H}_2/\text{O}_2/2\text{Ar}$ and $2\text{C}_2\text{H}_2/5\text{O}_2/21\text{Ar}$, despite its failure of underpredicting the near-limit dynamics. On the other hand, for $\text{C}_3\text{H}_8/5\text{O}_2$ detonations, the ZND model obviously fails to predict the experiments.

Figure 4 summarizes the characteristic $D/D_{CJ} - K_{eff}\lambda$ relationships for various mixtures. It appears that for detonations in mixtures of $\text{CH}_4/2\text{O}_2$, $\text{C}_2\text{H}_4/3\text{O}_2$, and $\text{C}_2\text{H}_6/3.5\text{O}_2$, they share the same $D/D_{CJ} - K_{eff}\lambda$ relationship, which differs from the universal curve found by Nakayama et al.. Moreover, for detonations in other mixtures of $\text{C}_3\text{H}_8/5\text{O}_2$, $2\text{H}_2/\text{O}_2/2\text{Ar}$ and $2\text{C}_2\text{H}_2/5\text{O}_2/21\text{Ar}$, they do not occupy such a unique relationship.

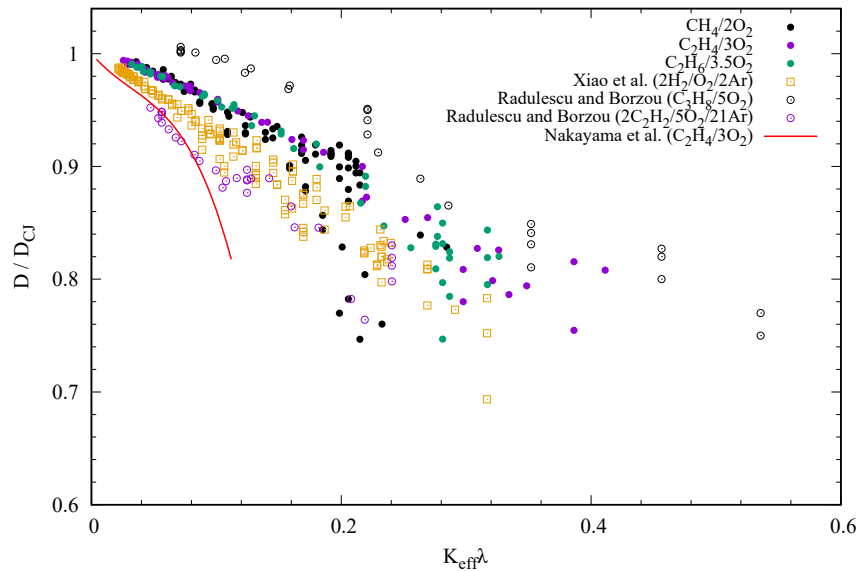


Figure 4: The characteristic $D/D_{CJ} - K_{eff}\lambda$ relationships for various mixtures.

4 Conclusion

In the present study, experiments of unstable detonations in three different mixtures propagating inside the exponentially diverging channels with varied constant exponential area divergence rates were conducted. The results showed that, well above the limit, quasi-steady detonations can be reasonably assumed with a constant mean mass divergence. Comparisons between the experimentally obtained characteristic $D/D_{CJ} - K_{eff}\Delta_i$ and $D/D_{CJ} - K_{eff}\lambda$ relationships and ZND model predictions demonstrated that the ZND model can predict the dynamics quite well for detonations in most mixtures except $\text{CH}_4/2\text{O}_2$ and $\text{C}_3\text{H}_8/5\text{O}_2$. For detonations in mixtures of $\text{CH}_4/2\text{O}_2$, $\text{C}_2\text{H}_4/3\text{O}_2$, and $\text{C}_2\text{H}_6/3.5\text{O}_2$, they share the same $D/D_{CJ} - K_{eff}\lambda$ relationship, while for detonations in other mixtures of $\text{C}_3\text{H}_8/5\text{O}_2$, $2\text{H}_2/\text{O}_2/2\text{Ar}$ and $2\text{C}_2\text{H}_2/5\text{O}_2/21\text{Ar}$, they do not occupy such a unique relationship.

References

- [1] Lee, John H. S. (2008). The Detonation Phenomenon. Cambridge University Press.
- [2] Radulescu, Matei I. and Lee, John H. S. (2002). The Failure Mechanism of Gaseous Detonations: Experiments in Porous Wall Tubes. Combust. Flame.
- [3] Chao, J., Ng, H.D., Lee, J.H.S. (2009). Detonability limits in thin annular channels. Proc. Combust. Inst.
- [4] Radulescu, Matei I. and Borzou, Bijan. (2018). Dynamics of detonations with a constant mean flow divergence. Journal of Fluid Mechanics.
- [5] Nakayama, H., Kasahara, J., Lee, Matuso, A., Funaki, I. (2013). Front shock behavior of stable curved detonation waves in rectangular-cross-section curved channels. Proc. Combust. Inst.
- [6] <http://shepherd.caltech.edu/EDL/public/cantera/html/SDToolbox>
- [7] Williams, F. A. (2014). 2014 Chemical-Kinetic Mechanisms for Combustion Applications, San Diego Mechanism web page, Mechanical and Aerospace Engineering (Combustion Research).
- [8] <http://shepherd.caltech.edu/detnodb/html/db12.html>.
- [9] Q. Xiao, M. Radulescu, Wang Y., Chang J., M. La Fleche. Propagation characteristics of $2\text{H}_2/\text{O}_2/2\text{Ar}$ detonations in channels with constant area divergence. 26th International Colloquium on Dynamics of Explosions and Reactive Systems, Boston, MA (2017)