Multi-dimensional detonation stability: Recent theoretical advances.

Mark Short
Theoretical and Applied Mechanics, University of Illinois
104 South Wright St, Urbana, IL 61801, USA
e-mail short1@uiuc.edu

Introduction

The recent interest in using detonation waves to drive high-speed propulsion devices such as the pulsed detonation wave engine has stimulated renewed interest in the problem of detonation wave stability. Detonation waves propagating in a rectangular tube reveal a well-known cellular instability, patterns induced by vorticity associated with triple-shock interaction points, which etch their locus on soot-covered foil on the channel walls. Although the problem of detonation stability was extensively studied by Erpenbeck in the 1960's, only in the last decade has progress been made in this important topic through analytical modelling. Notable contributions include those by Abouseif & Toong (1982, 1986) using a model of a large-activation energy induction zone coupled with a finite rate heat-release-zone, Boulioux, Majda and Roytburd (1991, 1992) with weakly nonlinear analyses about neutral stability points, Yao & Stewart (1996), Short (1996, 1997) and Short & Stewart (1997) based on low to moderate frequency, weak curvature, dynamics of the instability mechanism, and Clavin, Williams & He (1997) and Short & Stewart (1999) based on limits of large overdrive and/or weak-heat-release. In this article we explain two of these models that have advanced our undertanding of the dynamics of detonation instability.

Model

For the most part we will be concerned with a detonation model that consists of the inviscid reactive Euler equations, an ideal thermal equation of state and either a one-step Arrhenius reaction, or a three-step chain-branching reaction.

Detonation parameters

Central to the problem of detonation stability is a recognition of the four fundamental parameters underlying the structure of the steady wave, parameters which play a critical role in the detonation stability problem. These are (i) the ratio of specific heats γ, (ii) the activation energy of the reaction, $E = \gamma\widetilde{E}/\widetilde{T}_0$ or $\theta = \gamma\widetilde{E}/\widetilde{T}_s$, (iii) the heat release of reaction, $Q = \gamma\widetilde{Q}/\widetilde{T}_0$ or $\beta = \gamma\widetilde{Q}/\widetilde{T}_s$, and (iv) the detonation overdrive $f = (D/D_{CJ})^2$, where $\widetilde{T}_0$ and $\widetilde{T}_s$ are the ambient and post-shock shock temperatures, the latter being a function of the Mach number D^*. The many advances that have been made in understanding detonation stability employ one or all of these parameters in some type of asymptotic limit, the number of plausibly interesting combinations being large (as indicated in the experimental literature), providing a wide scope for investigation.

The effective weak-heat-release model

A major simplication of the steady detonation structure occurs when the heat release by reaction relative to the post-shock detonation temperature is small. The basic thermodynamic structure is then that of a reactionless shock wave (fig 1), which for finite Mach numbers in an ideal gas is stable. An analytical study of detonation stability (restricting our attention to a one-step Arrhenius rate model in this case) can then be made through a regular perturbation analysis (an idea first suggested by Erpenbeck 1964) by expanding both the steady structure and the small, time-dependent, perturbation quantities about the uniform shock state (see Short & Stewart 1999 for details), in which the reactant mass fraction is a simple exponentially decaying function ($= 1 - (1/2)^X$). The conclusions of this analysis are as follows:

For a finite D^*, and a finite $f > 1$, such that

$$f = \mathrm{ord}(1) > 1, \quad D^{*\,2} = \mathrm{ord}(1), \quad \beta = \mathrm{ord}(Q), \quad \theta = \mathrm{ord}(E), \tag{1}$$

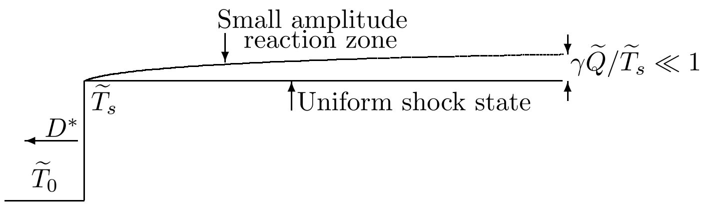

Figure 1: The structure of an effective weak-heat-release detonation.

the detonation is found to be stable under the following two conditions,

$$(\gamma-1)\beta \ll 1, \quad \frac{1}{\theta} \gg (\gamma-1)\beta. \tag{2}$$

This includes the two important cases where $(\gamma-1)=\mathrm{ord}(1)$, $Q \ll 1$, and $(\gamma-1) \ll 1$, $Q = \mathrm{ord}(1)$.

On the other hand, for large Mach numbers the reactionless shock in an ideal gas becomes neutrally stable. Weak exothermicity can then render the detonation unstable. The precise degree of exothermicity required to achieve this was revealed in Short & Stewart (1999). Specifically, the presence of a neutral stability boundary was identified in the following parameter regime

$$f \gg 1, \quad D^{*2} \gg 1, \quad (\gamma-1)=\mathrm{ord}(1), \quad \theta=\mathrm{ord}(1), \quad E=\mathrm{ord}(D^{*2}) \tag{3}$$

and

$$(\gamma-1)\beta \ll 1, \quad \beta=\mathrm{ord}(1/D^{*2}), \quad Q=\mathrm{ord}(1). \tag{4}$$

Above the neutral stability boundary, instability is characterised by a single unstable mode present over a finite range of wavenumbers. Alternatively for a parameter regime again represented by (3), but with

$$(\gamma-1)\beta \ll 1, \quad \beta \gg \mathrm{ord}(1/D^{*2}), \quad Q \gg 1, \tag{5}$$

the detonation is always unstable, again characterized by the presence of a single mode over a finite range of wavenumbers.

The remaining problem concerns how a finite Mach number, overdriven detonation can be rendered unstable in the limit of weak-heat-release $Q \ll 1$. Clearly, the only option is a reaction rate having a sufficiently large activation energy. The precise order of the activation energy required was identified in Short & Blythe (1999), where it turns out that when $(\gamma-1)QE = \mathrm{ord}(1)$, $(\gamma-1)Q \ll 1$, and $(\gamma-1)=\mathrm{ord}(1)$, the finite Mach number detonation can become unstable. In this limit, perturbations in the reaction rate are sufficiently strong that they have the same importance as terms which would otherwise govern inert shock stability.

In summary, (i) *finite Mach number detonations having a heat release due to reaction* $\ll$ *ambient temperature, with activation energies* $E \ll 1/Q$, *where* $Q \ll 1$, *are stable.* (ii) *Finite Mach number detonations having a heat release* $\ll$ *ambient temperature and sufficently large activation energies* $E = ord(1/Q)$ *can be unstable.* (iii) *Large Mach number overdriven detonations having a heat release of the order of the ambient temperature with activation energies possible as large as* $E = ord(D^{*2})$ *can be stable or unstable.* (iv) *Large Mach number overdriven detonations having a heat release due to reaction much greater than the ambient temperature are always unstable.* In closing we mention another recent study by Clavin, He and Williams (1997) who predict in the limit of large overdrives, the detonation is unconditionally unstable. Our analysis identifies a range of distinguished limits between the four fundamental detonation parameters where neutral stability boundaries can lie, and illustrates that one must be careful in how one chooses between the many choices of distinguished limits (also see the summary paragraph).

Large-activation-energy induction zone model

One of the first investigations of detonation stability was Zaidel's treatment of the square-wave detonation. The square-wave model is an ad-hoc structure consisting of a shock wave followed by an induction zone with no heat release, the length of which is controlled by a one-step Arrhenius reaction rate, and a discontinous main reaction layer *with no spatial structure.* A stability analysis reveals an infinite number of unstable modes whose growth rates increase with increasing frequency.

In contrast, a rational modification of the square-wave model is possible, which reproduces many of the features of the actual dynamics of detonation instability. Fig 2 depicts a detonation consisting of a shock wave followed by a weak-heat-release induction zone whose length is governed by a one-step Arrhenius reaction with a large activation activation energy θ. Following the induction zone is the main reaction layer, which in contrast to Zaidel's model, has a finite thickness l_R, with $l_R \ll l_i$. Such a structure is reminiscent of that associated with a three-step chain-branching reaction model, $F \to Y$, $F + Y \to 2Y$, $Y \to P$ (Short & Quirk 1997) for moderately large values of the chain-branching cross-over temperature.

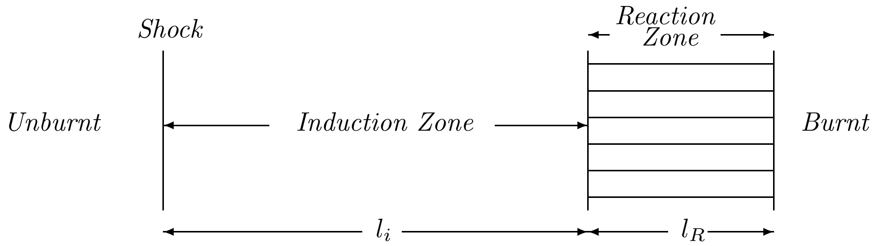

Figure 2:

Within this model, Short (1996, 1997b) and Short & Stewart (1997) have successfully described the behaviour of all modes having a frequency (t_w^{-1}) of the order of the inverse particle transit time through the induction zone (t_i^{-1}), including the low-frequency waves where (t_w^{-1}) $\ll$ (t_i^{-1}), and corresponding wavelengths of transverse perturbations to the front having $l_w \sim O(l_i)$. On these frequencies and wavelengths the reaction zone may be legitimately treated as a discontinuity within an asymptotic framework. Note, however, this analysis cannot be used the predict the behaviour of modes having a frequency $>$ (t_i^{-1}) for two reasons; the reaction zone cannot be treated as a discontinuity for such high-frequency disturbances: it's spatial structure must be accounted for (Clavin, He & Williams 1997). Secondly, the analysis of the relative motion of the reaction zone relative to the shock must be modified. However, it is well-known that high-frequency disturbances having (t_w^{-1}) $\sim$ (t_R^{-1}), where t_R is the partical transit time through the reaction zone, are stable (Short 1997a). Our model does not suffer the same pathology as Zaidel's work for this very reason. Our aim was purely to obtain a description of only the lowest frequency modes that are present. So what of the higher frequency modes, some of which may be linearly unstable ? It transpires that in the majority of numerical calculations presented to date, the higher-frequency modes are damped out as nonlinear dynamics begin to influence the detonation behaviour. The only mode that survives is the lowest frequency unstable mode. Thus although within the context of a linear analysis, some of the higher frequency modes may have a larger growth rate, the only ones that are important for the nonlinear dynamics are the lowest frequency modes. This is why one observes the final detonation cell spacing typically having a both a characteristic wavelength and thickness much greater than scales defined by the induction zone (Linan & Williams 1992). Hence our attempt to accurately model only the low frequency modes, i.e. the important ones in respect of the nonlinear dynamics.

In order to obtain an analytical dispersion relation for the stability behaviour, Short (1996, 1997) and Short & Stewart (1997) also invoked an additional assumption of a ratio of specific heats close to unity, i.e. $\gamma - 1 \ll 1$, a limit first introduced in the context of combustion theory by Blythe & Crighton (1989). In this case, the dynamics of the detonation instability are as follows: for disturbances which evolve on induction zone time-scales, an $O(\epsilon')$ perturbation of the shock front leads to $O(\theta(\gamma - 1)\epsilon')$ changes in the induction zone length due to the large activation energy sensitivity of the Arrhenius rate model. When $(\gamma - 1) \gg \theta^{-1}$, this generates $O(\theta(\gamma - 1)\epsilon')$ fluctuations in the burnt zone. Suppression of such disturbances (due to an incompatability with the appropriate boundary condition in the burnt zone) leads to a multi-dimensional dispersion relation, which has some of the features of the actual detonation behaviour, although growth rates are found to decrease monotonically with increasing wavenumber. On the other hand, when $\theta(\gamma - 1) = O(1)$, $O(\epsilon')$ perturbations are generated in the burnt zone, which leads to a dispersion relation where the growth rate has a maximum as the wavenumber varies (Short 1996). Such a maximum corresponds to the initial cell sizing one typically observes in detonation calculations. Moreover, the dispersion relation is a function of the four fundamental detonation parameters γ, Q, E and f. It turns out that the dispersion relation has all the features associated with detonation stability. For example, increasing f implies greater stability. Increasing Q or E implies greater instability.

When disturbances evolve on time scales slower than those defined by induction zone time scales, disturbances are propagated through the induction zone in a quasi-steady manner to a first approximation. Again, there is a dramatic response of the variation in the reaction front location to the pertubations. Although such an analysis does not predict pulsating detonation waves (Buckmaster & Ludford 1996), accounting for the additional effects of acoustic wave propagation in the induction zone in a first approximation does lead to a dispersion relation which predicts the onset of pulsating detonation wave behaviour. Comparisions with numerical evaluated stability relations are found to be excellent (Short & Stewart 1998). In addition, accounting for curvature effects of the detonation front, such that $\partial h/\partial t \sim O(\partial^2 h/\partial y^2)$, where $h(y,t)$ represents a linear pertubation of the detonation front with a transverse coordinate y, leads to a third-order in time, sixth-order in space parabolic linear evolution equation, which can predict the initial onset of detonation cells (Short 1997b). *In this case, and for these parameter regimes, we find the mechanism of detonation instability to be driven by an intricate coupling between acoustic wave disturbances in the induction zone, the temperature sensitivity of the reaction rate and the presence of weak-heat-release within the induction zone.*

Summary

Experiments on detonation stability demonstrate a wide range of behaviour based on variations in the four fundamental detonation parameters. We have uncovered the mechanisms underlying the detonation stability for some combinations of these parameters. We also recognise, and stress, that just because we have found the stability mechanisms for a few sets of distinguished limits between these parameters, we acknowledge that this mechanism may not play a central role for other interesting combinations of limits, but simply we have the stability mechanism for our chosen set of distinguished limits. Other researchers are under the impression that having discovered the the mechanisms leading to instability for one set of detonation parameters, this mechanism applies to all sets of limits, but this is clearly untrue. A wide range of mechanisms are possible, depending on the choice of limits. It also seems that most limits that have been investigated can be reproduced on a laboratory scale.

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References

G. Abouseif & T.Y. Toong, 1982 Theory of unstable one-dimensional detonations. *Comb. Flame* **45** 64–94.

G. Abouseif & T.Y. Toong, 1986 Theory of unstable two-dimensional detonations: Genesis of the transverse waves, *Combust. Flame* **63** 191–207.

A. Bourlioux, A.J. Majda & V. Roytburd, 1991 Theoretical and numerical structure for unstable one-dimensional detonations. *SIAM J. Appl. Math.* **51** 303–343.

A. Bourlioux & A.J. Majda, 1992 Theoretical and numerical structure for unstable two-dimensional detonations, *Comb. and Flame* **90** 211–229.

Buckmaster, J.D. & Ludford, G.S.S. 1986 The effect of structure on the stability of detonations I. Role of the induction zone. In *Twenty-first Symposium (International) on Combustion,* The Combustion Institute. pp. 1669–1676.

Clavin, P., He, L. & Williams, F.A. 1997 Multidimensional stability analysis of overdriven gaseous detonations. *Phys. Fluids* **9**, 3764–3785.

Short, M. 1996 An asymptotic derivation of the linear stability of the square wave detonation using the Newtonian limit. *Proc. Roy. Soc. A* **452**, 2203–2224.

Short, M. & Quirk, J.J. 1997 On the nonlinear stability and detonability limit of a detonation wave for a model three-step chain-branching reaction. *J. Fluid Mech.* **339**, 89–119.

Short, M. 1997 Multi-dimensional linear stability of a detonation wave at high-activation energy.*SIAM J. Appl. Math.* **57**, 307–326.

Short, M. 1997 A parabolic linear evolution equation for cellular detonation instability. *Combust. Theory Modell.* **1** 313–346.

Short, M. & Stewart, D.S. 1997 Low-frequency two-dimensional linear instability of plane detonation. *J. Fluid Mech.* **340** 249–295.

Short, M. & Stewart, D.S. 1998 Cellular detonation stability. I: A normal-mode linear analysis. *J. Fluid Mech.* **368**, 229–262.

Short, M. & Stewart, D.S. 1999 Multi-dimensional stability of weak-heat-release detonations. *J. Fluid Mech.* **382**, 109–136.

Short, M. & Blythe, P.A. 1999 Structure and stability of weak-heat-release detonations for finite Mach numbers. To appear.

J. Yao and D.S. Stewart. On the dynamics of multi-dimensional detonation waves. *J. Fluid Mech.* **309** 225-275.