Nonlinear Stability of Square Wave Detonations and the Zaidel Paradox

Annamaris Olmo-Velázquez & Luc Bauwens
University of Calgary,
Calgary AB, Canada

1 Introduction

The Zaidel paradox [1] remains a controversial topic, the community being divided between those convinced Zaidel's analysis is unphysical and meaningless [2], and those who see at least some value in his results [3]. Zaidel analyzed the linear stability of square wave detonations based upon an arbitrary induction zone length, obtaining a spectrum in which growth rate increases with frequency, which is either unphysical or points to the higher frequencies associated with the thin reaction zone as being the most unstable. This was quickly followed by Erpenbeck's analysis for single step kinetics with finite activation energy [4]. Subsequent studies also resolved the reaction zone, for instance [5]. While it is easy to dismiss Zaidel's analysis and to point to Erpenbeck's as being clearly superior, realistic kinetic models invariably include a broad range of rates, hence a detonation structure including zones of very different magnitudes. As a result it is difficult or impossible to analyze stability assuming finite rates for all steps; in many cases of realistic kinetics [6, 7], such as for instance oxygen-oxygen, the square wave model is actually realistic, because initiation is typically much slower than the main reaction with [8], for hydrogen, rate ratios of the order of 10^{-6}. It is not just the structure obtained for single step Arrhenius kinetics and high activation energy [9], but also for all situation where initiation is slow compared with the main reaction. This makes it worthwhile to revisit the Zaidel pathology, and to identify its physical explanation.

In contrast with shocks, detonation waves are usually unstable, yet there are nowhere near as many results available for single discontinuity Rankine-Hugoniot (RH) waves, either for transverse linear [10] or non-linear stability [11]. The former focused only upon marginal stability limits, with regimes of stability, instability and marginal stability. Following [12] they express limits as functions of a Grüneisen parameter, for which the Chapman-Jouguet limit depends upon the equation of state. [11] appears to be the only study of detonation break up, showing that, at least for ideal gases, thin, single discontinuity detonation waves are unconditionally susceptible to break up into a non-reactive solution consisting of a weaker shock, a contact discontinuity and an expansion wave.

Crucially, Erpenbeck [9] noted that neither Zaidel's normal mode or equivalently his Laplace transform approach could yield a solution to the stability initial boundary value problem, since given the features of the Zaidel spectrum, the inverse transform does not exist. For single step Arrhenius and high activation energy, [13] a singularity appears at the end of the initiation zone in the rate equation perturbation, Thus they replaced the radiation condition by a condition avoiding that singularity. However the resulting spectrum still suffers from the same pathology.

2 Inert shocks and Rankine-Hugoniot detonations

A shock wave described as a discontinuity is unconditionally linearly stable to non-planar perturbations in ideal gases [14]. However in the absence of length- or time scales linear analysis is unable to identify planar modes for nonreactive shocks, no matter for what fluid. In contrast, for arbitrary fluids, in certain ranges of values of $\delta = -\dot{m}^2 \big/ \left(\partial p/\partial v|_H\right)$, the ratio slope of the Rayleigh over the slope of the Hugoniot line, either unstable nonplanar modes growing exponentially in time appear, or marginally stable ones, with the shock emitting constant amplitude acoustics [15, 16, 17]. Here $\dot{m}$ is the mass flow rate, p is pressure and v is specific volume, both along the Hugoniot line; index H refers to the partial derivative computed along the Hugoniot line. Using M for the Mach number on the downstream side of the shock and σ for the ratio post- and pre-shock density, the three cutoff values are

$$\delta_1 = -1 - 2M, \quad \delta_K = \frac{M^2\sigma - (1-M^2)}{M^2\sigma + (1-M^2)}, \quad \delta_2 = 1 \tag{1}$$

They found that for δ outside the interval (δ_1, δ_2) the shock is unstable, that it is stable between the Kontorovich value δ_K and δ_2, and marginally unstable, emitting acoustics between δ_1 and δ_K. They do not mention however that δ_2 being the tangency point between the Rayleigh and Hugoniot line, shocks for $\delta > 1$ might violate the second law, in which case it is an existence limit.

Landau & Lifschitz [18] argued that in fluids in which shocks satisfying the second law are compression shocks, these are linearly stable to planar deformations, as confirmed by more recent work [19]. They mentioned however (p. 329) the possibility whereby shocks might be nonlinearly unstable, i.e. susceptible to non-linear break up, as "not having been adequately investigated." As an extension of his work on detonations (see below), Erpenbeck [12] revisited linear stability of shocks to non-planar perturbations, largely confirming previous Soviet results, but because, in contrast with D'yakov, Zaidel, Iordanskii and Kontorovich, who used to ratio of the slopes of the Hugoniot and Rayleigh lines as the independent parameter, he used the Grüneisen parameter $\Gamma = \left. \partial p/\partial s\right|_\rho \big/ (\rho T)$, he missed the limit corresponding to tangency between the two lines, when the conversion becomes singular, since the relationship between δ and Γ is:

$$\Gamma = \frac{2(\delta - M^2)}{(\sigma-1)(\delta-1)M^2} \tag{2}$$

so that since for $\delta \to 1$, $M \to 1$, the value of Γ corresponding to $\delta_2 = 1$ depends upon the limit of $(M-1)/(\delta-1)$.

Gardner [20] showed that under the conditions for transverse linear instability, shock waves are indeed also susceptible to planar nonlinear break up, as anticipated by Landau and Lifschitz [18]. Zaidel [21] revisited and confirmed previous linear stability results, also using the Laplace transform. Kuznetsov [22, 23] expanded upon Gardner's work, concluding that since the mechanism considered in linear stability studies is not how planar shocks break up, linear analysis is not as reliable as the nonlinear breakup model.

Rankine-Hugoniot detonations, i.e. planar reactive shocks, are susceptible to non-linear break up for mixtures obeying the ideal gas law [11], and it is possible to extend the proof to a broad range of fluid models featuring a Hugoniot line with vertical asymptote. Because, following Erpenbeck [12] hence using the Grüneisen parameter as the independent variable, the linear analysis of Majda and Rosales [10] only identified two of the three limits, corresponding to δ_1 and δ_K for inert shocks, but as Erpenbeck for inert shocks [12], they missed the stability limit that occurs at the Chapman-Jouguet point where the relationship between δ and the Grüneisen parameter is singular. The results of Majda and Rosales [10] are easily recovered from those of Zaidel and Kontorovich, leading to limits still expressed by Eq. (1) using M and σ evaluated across the reactive shock. Thus, in contrast with inert shocks, no close relationship is found between nonlinear breakup and linear stability limits.

3 Square wave detonations

Following Gardner [20] and Kuznetsov [22, 23] for nonreactive shocks, and Bauwens et al. [11] for single jump detonations, the potential non-linear breakup of the two singular zones in the square wave model is now investigated. The steady square wave structure is made up of a nonreactive shock, an induction zone in which at leading order the solution is spatially uniform, a thin reaction zone also consisting of a discontinuity and either an equilibrium zone with infinite length, or, for chain-branching kinetics with initiation much slower than chain-branching, an infinite zone of quasi-equilibrium, in which chain-branching no longer occurs [8]. As seen above, for realistic mixtures, the leading shock is usually stable. However, it is now shown that the reaction zone is susceptible to non-linear breakup, in which it is replaced by a non-reactive planar solution. To that effect, it is shown, as done by Gardner for inert shocks [20], that the Riemann problem associated with the jump across the reaction zone with zero thickness admits, in addition to the reactive solution, a second, non-reactive one, in which the initiation zone is effectively destroyed.

One might expect that this second solution would, like in the case above, consist of an expansion wave moving into the initiation zone and a shock moving downstream. However the solution found consists of two expansion waves, and of course a contact surface in the intermediate region, separating unburnt and burnt fluid, at which in the absence of diffusion reaction no longer takes place. In the initiation region, the solution is uniformly equal to that at the von Neumann state, point N, with velocity u_N, speed of sound a_N and pressure p_N. Past the reaction zone, at point B, these are u_B, a_B and p_B, with $p_N > p_B$ but $u_B > u_N$. An expansion wave moving into fluid at the von Neumann state ending at both pressure and velocity matching pressure and velocity in the downstream region would correspond to a situation in which neither a shock or an expansion wave is required on the downstream side. Since $p_N > p_B$ but $u_B > u_N$, one notes that there exist expansion waves moving toward point N, ending either at $u = u_B$ or at $p = p_B$. Considering a wave ending at $p = p_B$, and calling velocity at its end $\hat{u}$, then, while both u_B and $\hat{u} > u_N$, $\hat{u}$ could be larger or smaller than u_B and $\hat{u} = u_B$ provides the cutoff between shock or expansion wave moving downstream. Indeed, if $\hat{u} > u_B$, then a somewhat weaker expansion wave will end up at a pressure above p_B, with velocity still above p_B, which is consistent with a shock moving downstream. However a wave now ending at $u = u_B$ with end pressure $\hat{p} > p_B$ would be too strong for a shock downstream. Thus a solution is obtained made up of expansion wave, contact surface and shock, with for the intermediate pressure $\bar{p}$, $p_B < \bar{p} < \hat{p}$, while for the intermediate velocity $\bar{u}$, $u_B < \bar{u} < \hat{u}$.

If however if $\hat{u} < u_B$, the expansion wave moving toward point N must be stronger than the wave for which pressure at the end matches p_B. As shown in Fig. 1 for an ideal gas, a solution can still be constructed, now made up of two expansion waves moving in opposite directions, and still with a contact surface in the intermediate region, now with $\hat{p} < \bar{p} < p_B$, and $\hat{u} < \bar{u} < u_B$.

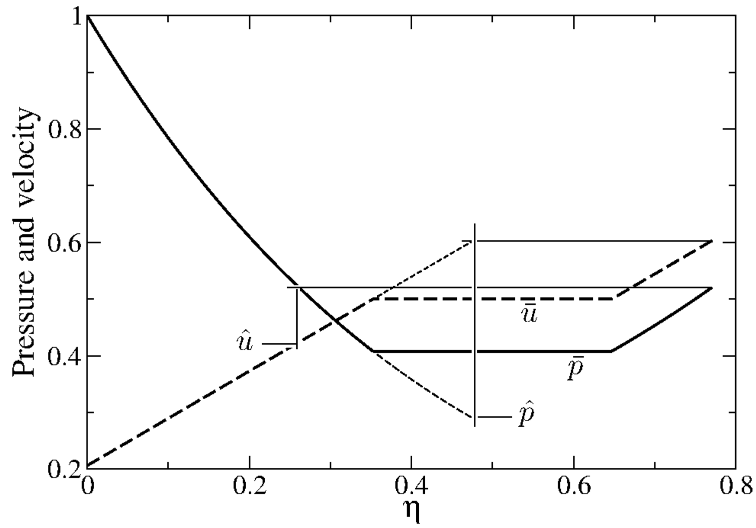

Figure 1: Breakup of the reaction zone: existence of a non-reactive solution (ideal gas). Thick continuous line: pressure p/p_N; thick dashed line: velocity scaled by pre-shock value u_0. $\eta = x/u_0 t$ with zero at point N. Contact surface at $\eta = \bar{u}/u_0$.

To determine which of two possible solutions will occur, one needs to compare either $\hat{u}$ and u_B or $\hat{p}$ and p_B. If $\hat{p} < p_B$ then the solution is made up of two expansion waves. For a mixture obeying the ideal gas law, in an expansion wave moving into fluid at the von Neumann state, velocity u, speed of sound a and pressure p are related by

$$u + \frac{2a}{\gamma - 1} = u_N + \frac{2a_N}{\gamma - 1}, \quad \frac{a}{a_N} = \left(\frac{p}{p_N}\right)^{(\gamma-1)/2\gamma} \tag{3}$$

Eliminating a and solving for p, for $u = u_B$ thus $p = \hat{p}$,

$$\hat{p} = p_N \left[1 - \frac{(\gamma - 1)(u_B - u_N)}{2a_N}\right]^{2\gamma/(\gamma-1)} < p_B \tag{4}$$

For a detonation wave with Mach number M_0 and state B corresponding to a discriminant

$$\Delta = (M_0^2 - 1)^2 - 2M_0^2(\gamma^2 - 1)Q \tag{5}$$

with maximum Δ for the heat release $Q = 0$, the inert shock, and $\Delta = 0$ for a Chapman-Jouguet wave, after some algebra that condition becomes

$$\left\{1 - \frac{(\gamma - 1)(M_0^2 - 1 - \sqrt{\Delta})}{2\sqrt{[2\gamma M_0^2 - (\gamma - 1)][(\gamma - 1)M_0^2 + 2]}}\right\}^{2\gamma/(\gamma-1)} < \frac{1 + \gamma M_0^2 + \gamma\sqrt{\Delta}}{2\gamma M_0^2 - (\gamma - 1)} \tag{6}$$

Which can be shown to be satisfied for the entire range of M_0 and Δ, except in the nonreactive case $\Delta = (M_0^2 - 1)^2$ when both sides equal 1 and equality is obtained. Thus at least for ideal gas, the thin reaction zone is susceptible to nonlinear break up into two expansion waves. The expansion wave moving toward the von Neumann point leads to a drop at leading order in the temperature in an increasingly longer part of the initiation zone. In contrast, with the square wave model, initiation only leads to temperature increasing at the perturbation level. The initiation process is thus effectively destroyed, which is consistent with the thin reactive zone being replaced by a non-reactive interface located at the control surface.

Previous results for slow initiation (hence actually a square wave structure) analyzing stability in which the main reaction zone was resolved [24] are consistent with the current observation: they exhibited a purely real unstable mode on a time scale resolving the reaction zone. Thus on the longer time scale associated with the initiation zone, the growth will reach a magnitude increased by a factor like the ratio of these time scales, i.e. leading order. These results are consistent with [2] in that the Zaidel paradox simply points toward the most unstable modes being of a faster magnitude, since determined by stability of the main reaction zone. They are also consistent with the Zaidel stability initial value problem being ill-posed since the inverse transform does not exist so that the solution in physical space of an initial value problem cannot be reconstructed from the Fourier modes. Physically, the instability is initiated by an expansion wave moving into the initiation zone, immediately affecting the structure at leading order. Such a solution cannot be represented as a set of Fourier modes at a perturbation level.

4 Conclusion

In a square wave structure, the main reaction zone represented as a discontinuity is found to be susceptible to non-linear break up into a non-reactive structure. Such a break up immediately affects the initiation zone at leading order, as a front travels which progressively becomes shallower, a situation that cannot be reduced to a set of Fourier modes at the perturbation level. This explains why the Zaidel model is ill-posed as an initial value problem and why its spectrum is pathological. These results are also consistent with the presence of a singularity in the perturbation accounting for incipient kinetics in the initiation zone, for single step Arrhenius kinetics in the high activation energy limit [13].

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