The usefulness of a 1D hydrodynamic model for the detonation structure for predicting detonation dynamic parameters

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1 Introduction

Numerical prediction of detonation phenomena is currently very difficult. This is primarily due to the highly transient cellular structure, where the scales controlling the chemical evolution and the coupled gas dynamics are too small to be resolved in practical calculations. The smallest scales of the hydrodynamics and of chemical evolutions are a few orders of magnitude smaller than the global reaction thickness of the front, dubbed the "hydrodynamic thickness" [1]. While recent efforts have been devoted to resolve these transient phenomena in direct numerical simulations [2] and large eddy simulations at the meso-scale [3], such simulations are not of practical use, where typical length scales of interest are 10^3 to 10^9 larger than the "hydrodynamic thickness".

A useful formulation of the detonation problem is seeking a macroscopic average description of the detonation structure, such that the transient fast time dynamics associated with the cellular structure are modeled at the subgrid scale, akin to turbulence modeling [4–8]. Such a description for the structure of the detonation front can be more easily incorporated in large scale simulations aimed to study problems in which the detonation dynamics are of prime concern: detonation limits in narrow tubes, detonation initiation, diffraction and the evolution in complex geometries. In such an approach, the description of the reaction zone structure becomes quasi-one dimensional in the direction of propagation of the front. Fig. 1 shows an example of the resulting mean pressure profile for the hydrodynamic mean structure of the front obtained by ensemble averaging the results of large eddy simulations [3]. The figure also shows that the global reaction structure is significantly longer than predicted by the ZND model.

Such a mean profile, along with the other mean hydrodynamic variables of interest (density, speed and energy progress variable) can be obtained to leading order if a mean reaction rate was known. This mean reaction rate would be a function of the complex interaction of the chemical kinetics, unsteady gasdynamics and turbulence driven by the detonation cellular structure, and requires modeling.

Two distinct approaches can be used to obtain appropriate macroscopic rate equations for closure of the hydrodynamic approach. The first, and most difficult, is a bottoms-up approach of beginning with the small

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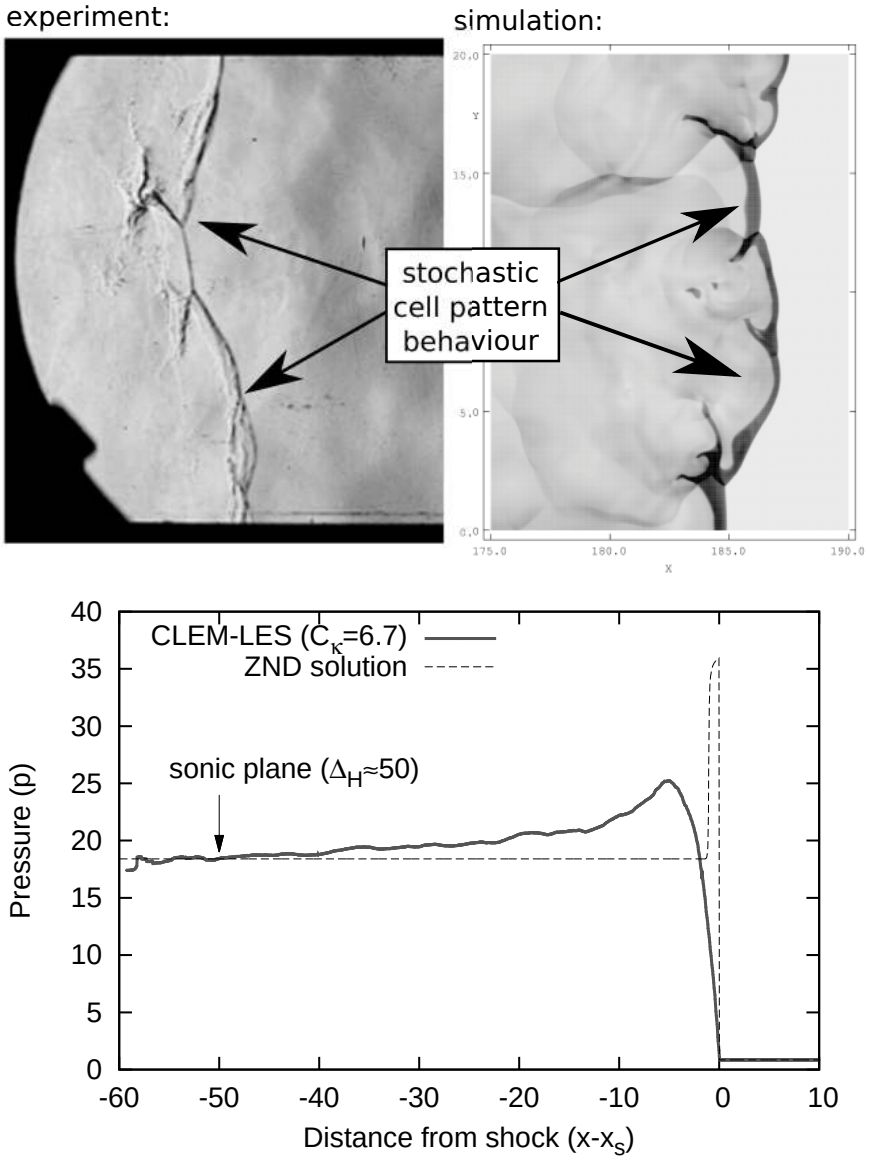

Figure 1: Reaction zone structure of methane-oxygen detonations obtained experimentally and numerically (top) and the average pressure evolution obtained numerically (bottom), compared with the ZND structure [3].

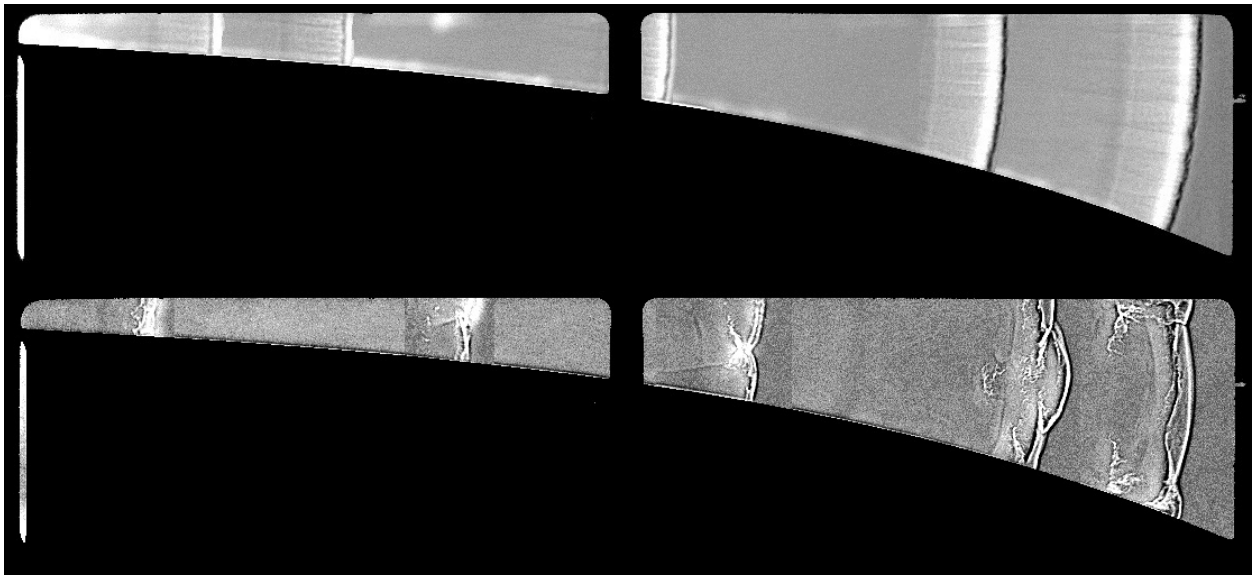

Figure 2: Evolution of a propane-oxygen detonation front in an exponentially diverging 1-m-long channel at 10.3 kPa initial pressure (top) and 3.45 kPa (bottom).

scale phenomena and building to the scale of the cellular structure. The second is less physically satisfying, but much more easily implemented and useful for quantitative predictions. It requires the calibration of the macroscopic rate equations directly from experiments. These can be designed in such a way to unambiguously infer the appropriate rate equation for a given reactive mixture. The present study provides the recent progress made in my research group in both these approaches and suggests directions for future research.

2 Exponential horn experiments for attenuated steady state detonations

A novel technique to achieve detonations propagating at constant mean speeds with an easily modeled loss mechanism has been recently formulated by Radulescu and Borzou [9]. The technique involves propagating a detonation wave in a channel or tube whose cross-sectional area increases exponentially. Fig. 2 shows an example of a cellular propane-oxygen detonation in a laterally diverging channel. For small rates of divergence of the tube, this geometry provides a constant rate of lateral flow divergence. As a result of this constant loss term along any mean stream tube in the direction of motion, the detonation front was found to propagate at a constant mean speed below the Chapman-Jouguet value.

Since the detonation propagates at a mean constant speed, direct observation of the statistically stationary cellular structure is possible, in experiment and simulations. This permits to obtain the average description, and its dependence on the amount of lateral divergence, in a meaningful way. Indeed, the hydrodynamic description not only requires the correct mean profiles to be attained, but also their sensitivity to the velocity deficits, which are controlled by the amount of lateral divergence.

3 Extraction of the mean rate of energy release from the speed measurements

The lateral flow divergence in the exponential horn experiments controls the amount of losses. It was found that a unique dependence between the detonation speed deficit and the lateral flow divergence can be established, as shown, for example, in Fig. 3 for a mixture stoichiometric propane-oxygen. As the divergence increases, the velocity deficit also increases. There is also a well-defined limiting value of divergence beyond which a steady detonation cannot be established.

This unique curve relating the detonation speed and the hydrodynamic streamline divergence differs substantially from the prediction made using the classical ZND model with mass divergence [10] using the full chemical kinetics for the mixture [9], as can be seen in Fig. 3. Cellular detonations are thus generally found to propagate under global divergence rates much larger than permissible for 1D waves. This comes as no surprise and clearly highlights that the global energy release in the cellular detonation differs from that of the steady ZND model by a substantial amount, as is also evident from the structure of the local hydrodynamic description (see Fig. 1).

In spite of the failure of the ZND model to capture correctly the response of the detonation wave to the imposed flow divergence, the experimental data, however, can be used to infer an empirical reaction model for the hydrodynamic average description. Ironically, the hydrodynamic model is the ZND model itself, with the fundamental difference that the global reaction rate represents the mean evolution, as discussed above.

The simplest global rate of energy release is a one-step description, that has two empirical coefficients to be fitted: the pre-exponential rate constant and the activation energy. These two constants can be fitted such that the prediction of the detonation speed deficit matches with experiment. The result of such a fitting exercise is shown in Fig. 3.

The resulting one step model provides an empirical global rate law for energy release in a cellular detonation. It is worth commenting on the magnitude of the two coefficients obtained for the example considered. First the global activation energy for a macro-scopic description is found to be lower than the underlying 0D chemical decomposition along any particle path by more than 50%! This makes a dramatic change in the overall detonation dynamics characteristics, as we will illustrate below. The lower effective activation energies are not surprising, as it was already noted that the enhancement of burning mechanism in turbulent detonations by turbulent mixing suppresses much of the thermal character of the ignition mechanism, yielding effectively lower activation energies [7].

4 Test of the usefulness of the mean description: direct initiation

In order to test the usefulness of the mean hydrodynamic description in predicting general detonation dynamic parameters, we have performed one-dimensional calculations for determining the critical energy for detonation initiation for the sample mixture of propane-oxygen treated above. The calculations were performed in the spherical geometry using a second order exact Riemann solver and adaptive mesh refinement, implemented in the MG code developed by Sam Falle at the University of Leeds. The high energy source was simulated by a high pressure kernel of gas of dimension significantly smaller than the scales relevant to the initiation dynamics. The source energy E denotes the excess of internal energy of the high pressure kernel. Fig. 4 shows, for example the outcome of the shock pressure for a supercritical and sub-critical initiation process, which are controlled by the magnitude of the source energy. The demarcation between

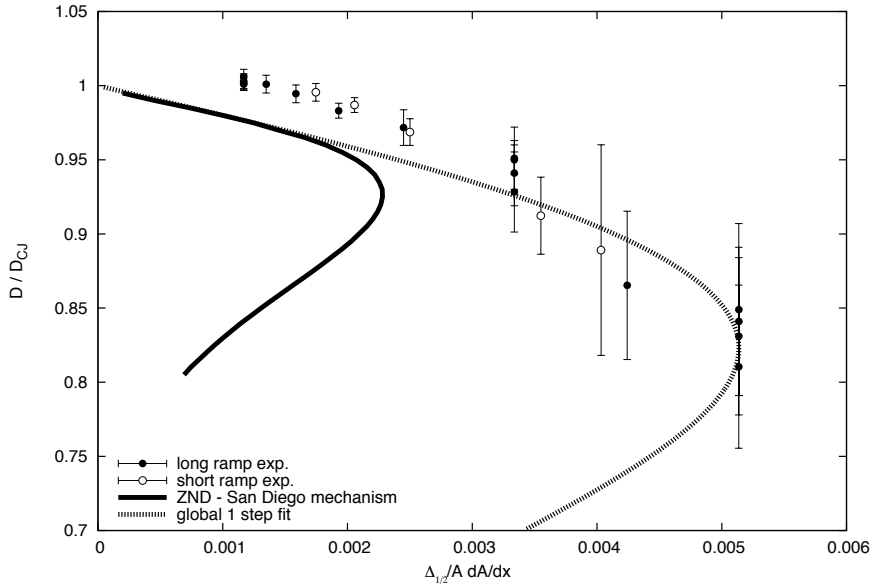

Figure 3: Comparison of the detonation velocity deficit obtained experimentally for different normalized lateral flow divergence with the ZND model prediction using the real chemistry and the fitted global one step reaction rate.

successful initiation and detonation failure can thus be obtained in order to find the critical energy of initiation E. Alternatively, the critical explosion length $R_0 = (E/p_0)^{1/3}$ can also be used as a critical length scale for detonation initiation, where p_0 denotes the initial pressure of the gas.

Fig. 5 shows the performance of this procedure in capturing the experimentally measured critical energy for direct initiation of detonations for propane-oxygen [11]. The agreement with the experimental results for propane-oxygen is excellent. The conclusion of such a comparison is that the hydrodynamic model can be quite successful in reproducing correctly the detonation dynamics, if properly calibrated experimentally to account for the complex cellular detonation structure.

5 The mean reaction rate from first principles

While a meaningful method has been devised above in order to obtain an empirical model of the mean reaction rate from experiment, this approach is not entirely satisfactory, in that it misses the physics of detonation waves and leaves the modeller with little insight into the cause and effect. At present, it is still not clear what aspect of cellular detonations provides the enhancement of the global reaction rates, as compared to a ZND laminar wave. Two schools of thought exist: the first attributes the enhancement to an inviscid mechanism, mainly due to the variability of the lead shock strength and presence of transverse waves, possibly reactive ones. The second attributes the enhancement to the turbulent mixing in the reaction zone. Recent empirical evidence tends to lean towards the second explanation. Indeed, inviscid calculations have shown that the detonability of a given mixture appears to *decrease* as the mixture becomes more unstable [12–14], whereas experiments suggest the opposite trend. Cellular detonations are more easily ignited and

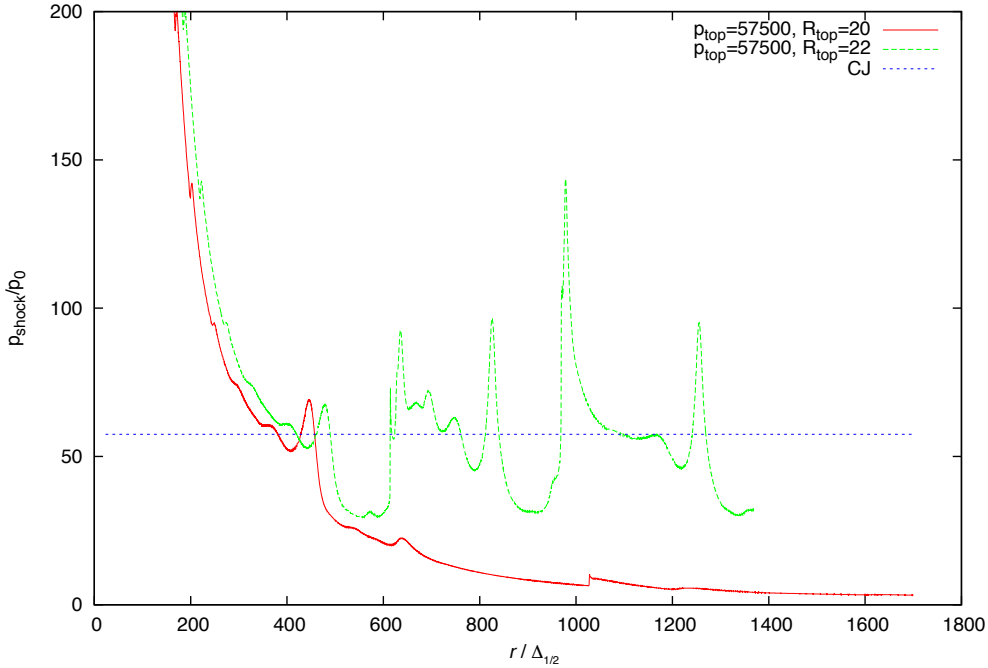

Figure 4: Supercritical and subcritical direct initiation of a propane-oxygen detonation using the the macroscopic reaction model obtained in the exponential horn experiments.

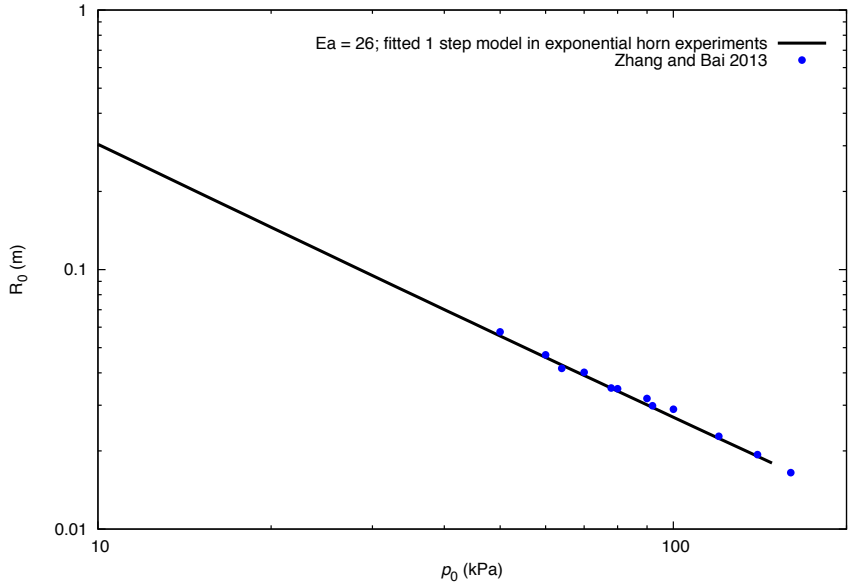

Figure 5: Comparison between the critical detonation initiation explosion radii predicted using the experimentally derived global kinetic law and experiments of Zhang and Bai [11].

harder to quench than predicted by a 1D ZND model, as shown above. It is also only recently that the role of turbulent mixing in detonations has been modelled explicitly, as attempted by Maxwell et al. in large eddy simulations [3]. These simulations suggest that mixing of the reacted and non-reacted gas along shear layers, and enhancement of flame speeds on the surface of non-reacted pockets via turbulence contributes to fundamental modifications of the global rate of energy release in detonations. These calculations confirm the early observations made by Subbotin, that pockets of non-reacted gases burn by diffusive processes [15].

If one accepts that turbulent diffusion plays an important role, deterministic modeling should perhaps be abandoned in favor of a stochastic approach, treating the likelihood of a given particle crossing the detonation front of a given strength to ignite in a finite time t_{ig}, and constructing the histogram of the shock strength in order to reconstruct the global rate of energy release. Progress in our current efforts to characterize the probability density function of shock strengths in experiments and the corresponding distribution of reactivity will be communicated at the conference.

6 Conclusion

The present survey has shown that the mean hydrodynamic description of a detonation wave, provided by the mean rate of energy release is a meaningful concept that permits to predict the various dynamic parameters of detonations. The exponential horn technique, which provides an experimental method to obtain quasi-steady detonations, permits to obtain a statistically stationary reaction zone structure. In turn, it provides a direct way to infer the global reaction zone structure and its dependence on wave speed. This method permits an unambiguous calibration of a global reaction rate to account for the detonation structure of cellular detonations. Use of this global rate law becomes relevant when interested in the dynamics of cellular detonations, such as initiation and failure. Nevertheless, a bottoms-up approach is also required for physical clarity, in order to rationalize and identify the most promising modeling avenue of the global scale mean exothermicity rate law for the hydrodynamic description of the detonation structure.

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