Mach Reflection in Detonations Propagating through a Gas with a Concentration Gradient

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1 Introduction

The instabilities occurring in a gaseous detonation front produce the well-known cellular structures which can be reproduced numerically by recording the maximum pressure history in a computational domain. Up to date, nearly all studies concerning detonation cells, no matter if experimental or numerical, were focused on perfectly homogeneous mixtures. Although there is a need to consider inhomogeneous mixtures in safety assessment studies [1], hardly any fundamental research has been done in this field, so far.

Due to its low molecular weight, especially hydrogen is prone to forming horizontal layers with oxidizers in accident scenarios. In a previous study [2] the authors experimentally investigated deflagrations in horizontal tubes using different vertical concentration gradients as initial conditions. Possibly the first study to investigate detonation propagation perpendicularly to a concentration gradient was done by Ishii and Kojima [3]. It was observed that the occurring detonation cells were distorted from the usual diamond shape to a more parallelogram shape. In the present study the investigation of detonations propagating perpendicularly to a concentration gradient is continued analytically and numerically. Questions concerning the differences to detonations in homogeneous media regarding detonation front shape, instabilities (soot print), propagation velocity and pressure loads on the enclosing geometry are addressed.

2 Fundamental considerations

We study a detonation propagating in an infinitely long, two-dimensional channel. The fuel concentration varies in the direction perpendicular to the channel axis. In particular, we consider a hydrogen-oxygen mixture which is stoichiometric at the top of the channel (hydrogen mole fraction $x_{H2} = 66.7\%$) and has a linearly decreasing hydrogen content towards the bottom. First, we neglect the role of detonation instabilities and consider steadily propagating reaction fronts only. Assuming that the detonation propagates at any point with the local Chapman-Jouguet (CJ) velocity into the axial direction would lead to a continually increasing time lag between the arrival of the detonation front at the top and at the bottom of the channel. However, it can be shown that after an initial acceleration the curvature of the detonation front remains unchanged: assuming that any point in the reaction front is a source

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from which the detonation propagates into all directions at the local CJ velocity (Huygens' principle), the curvature of the leading detonation front can be determined iteratively: constructing the detonation front as the envelope of all circular waves emanating from the detonation front formed in the previous iteration (with the radius of each circle being proportional to the local CJ velocity), a converged solution is quickly achieved. An example is displayed in Fig. 1, showing a case where the hydrogen content decreases linearly by 10% from the top to the bottom of the channel (corresponding to an almost linear decrease in CJ velocity). The resulting propagation velocity of the entire detonation front is determined completely by the maximum CJ velocity within the inhomogeneous mixture.

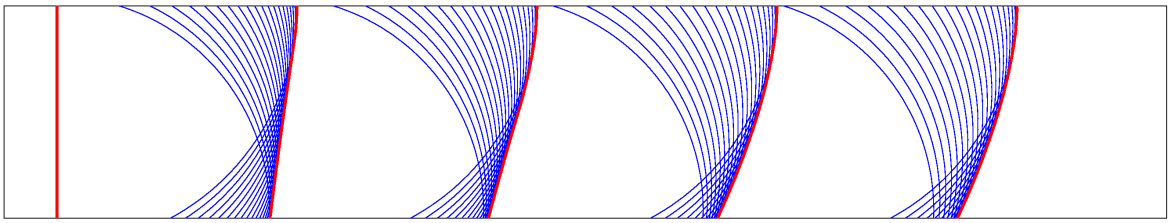

Figure 1: Reconstruction of a detonation front in a medium with vertically varying CJ velocity using Huygens' principle. Blue: circles emanating from the shock front with radius being proportional to the local CJ velocity. Red: envelope of all circles. Due to self-similarity of the problem, no length scale is given.

This is a very simple method for getting a first impression of the detonation front. However, it violates the boundary condition that the flow on the lower wall must always be parallel to the wall. The adjustment that will occur in the actual flow can be explained using a second, very simple model: By splitting the detonation front into an inert leading shock and an infinitely thin heat release zone, three different ways of adjustment to the wall can be distinguished (see Fig. 2):

- Case A: if the deviation from a normal shock is small, the flow immediately behind the shock remains subsonic ($M_2 < 1$). In this case, the leading shock is bended in the vicinity of the wall in order to allow wall-parallel flow.
- Case B: if $M_2 > 1$ and the deflection angle θ_1 caused by the incident shock is small, it can be compensated by a reflected shock (deflection angle $\theta_2 = -\theta_1$).
- Case C: if $M_2 > 1$ and the deflection angle θ_1 is too large to be compensated by the reflected shock, the flow adjusts to the wall by developing a Mach stem.

An overview of some calculations for the hydrogen-oxygen case with increasing concentration gradient is given in Table 1. It contains the Mach number M_1 and the incident angle β_1 of the shock close to the lower wall (where the hydrogen content is minimal), gained with the method shown in Fig. 1. From these quantities, the deflection angle θ_1 and the post-shock Mach number M_2 are computed using the oblique shock relations (see e.g. [4]). If $M_2 > 1$, the maximum deflection angle $\theta_{2,max}$ that can be achieved with a reflected shock is computed as well. It can be observed that in the case with a 10% concentration gradient, the Mach number behind the leading shock just exceeds unity, so that $\theta_{2,max}$ is very small and the transition from case A to case C occurs. Also for higher concentration gradients it can be seen that $|\theta_{2,max}| \ll |\theta_1|$ so that regular reflection (case B) never occurs in this configuration. Further calculations showed that regular reflection can only be expected in gases with low heat release (leading to low Mach numbers M_1) and extreme concentration gradients (leading to high incident angles $\beta_1 \ll 90°$).

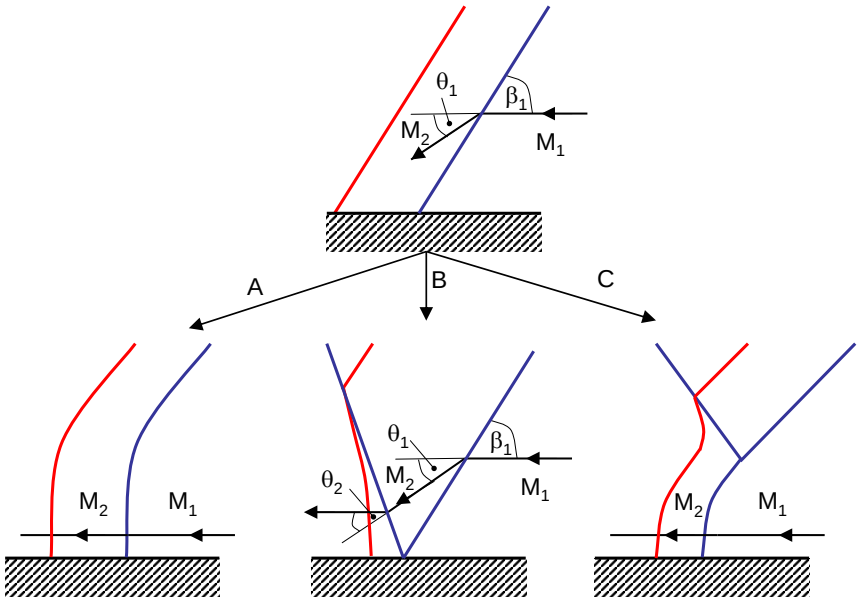

Figure 2: Sketch of the problem (top) of non wall-parallel flow behind an oblique shock and the three possible solutions (bottom). Blue: shocks. Red: heat release zone.

linear gradient	0%	5%	10%	20%
$x_{H2,max}$	66.7%	66.7%	66.7%	66.7%
$x_{H2,min}$	66.7%	61.7%	56.7%	46.7%
M_1	5.32	5.65	5.96	6.52
β_1	90°	72°	66°	47°
M_2	0.41	0.81	1.04	1.40
θ_1	0°	41°	42°	40°
$\theta_{2,max}$	-	-	-0.4°	-10°
case	A	A	C	C

Table 1: Shock angles and Mach numbers gained with Huygens' method.

3 Simulation results

The real structure of a detonation front is more complicated than in the theoretical investigations shown so far, as instabilities perturb the leading shock. In order to study the effect of instabilities, we numerically solve the reactive Euler equations in a 2D simulation. The domain has a height of $2\,\mathrm{mm}$ and a uniform grid spacing of $\Delta x = \Delta y = 0.01\,\mathrm{mm}$. The conservation equations are discretized with a high resolution, Godunov-type central scheme [5]. The gas is at an initial temperature of $293\,\mathrm{K}$ and a pressure of $0.1\,\mathrm{MPa}$. It is ignited by patching a region close to the left end of the domain with the CJ values of a stoichiometric hydrogen-oxygen mixture. Different fuel concentration gradients within the unburned gas are being examined.

For a first impression of the detonation instabilities, a very simple model was used. In this model, all gas properties are assumed to be constant (notably the molecular weight W and the ratio of specific heats γ) and only the heat release q is a function of the fuel mass fraction y_{fuel}. The reaction is modelled as a one-step irreversible Arrhenius reaction. In this model, it can be shown that the CJ velocity D_{CJ} varies

according to

$$D_{CJ} \sim \sqrt{q} \sim \sqrt{y_{\text{fuel}}}$$

The problem is that the Mach number of a CJ detonation also varies with $\sqrt{y_{\text{fuel}}}$, as the sound speed in the unburned mixture is constant, while in reality the sound speed depends heavily on gas composition. Consequently, this model which has successfully been applied to many problems in homogeneous mixtures does not reproduce the real effects and therefore never showed Mach reflection in any of the cases studied.

In a second model, it was tried to capture the full physics by defining the gas as a multi-component mixture consisting of the species H_2, O_2, H_2O, O, H, OH, HO_2 and H_2O_2. The temperature-dependent mixture properties are taken form the Chemkin thermodynamic database [6]. The chemical reaction is modelled using the mechanism by O'Conaire et al. [7].

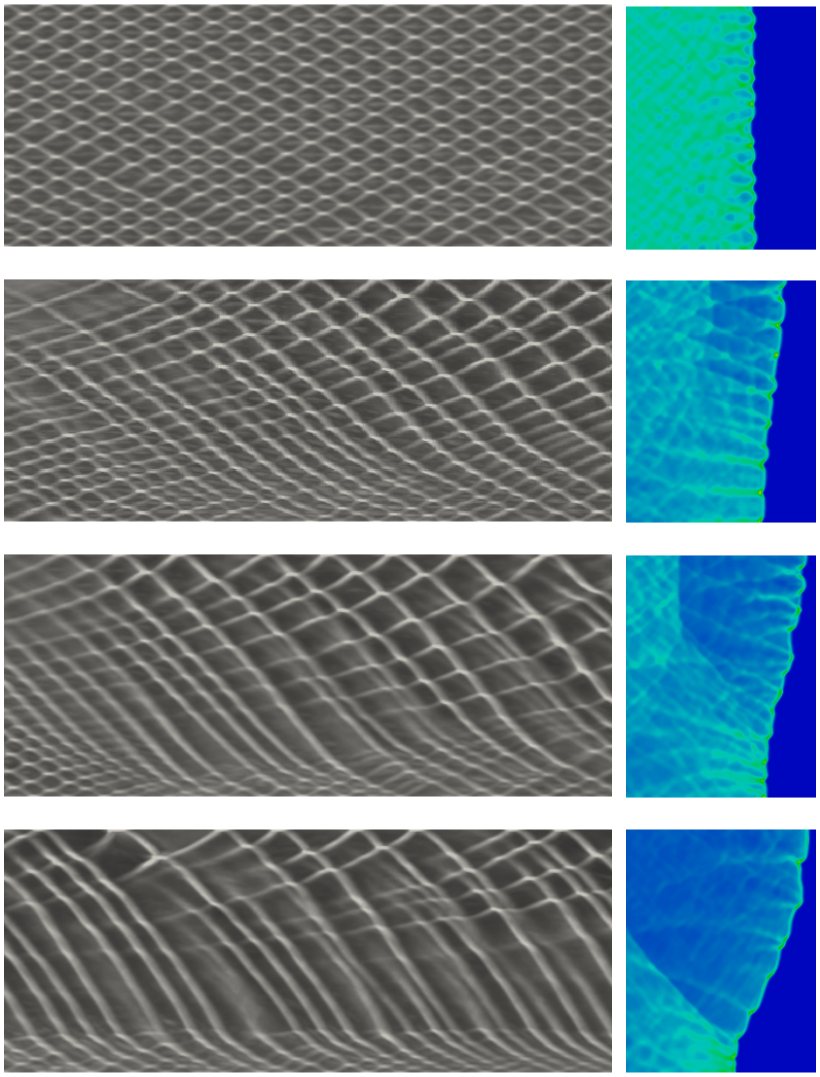

Figure 3: Maximum pressure history (left) and instantaneous pressure field (right) in the multi-component simulation. The homogeneous case is shown on top, followed by increasing concentration gradient (5%, 10%, 20%).

With this model the four cases from Table 1 have been studied. In the homogeneous case, the instabilites evolve as expected. Upwards and downwards running triple points intersect and leave a symmetric cellular pattern in the numerical soot print (=maximum pressure history, Fig. 3). In the case with a 5% concentration gradient, the distortion of the detonation cells observed in the experiments by Ishii and Kojima [3] is reproduced. It can be explained by the locally varying velocity of the triple points caused by the locally varying hydrogen content. Instantaneous visualizations of the pressure show a detonation front which is inclined in the middle of the channel, but remains perpendicular in the vicinity of the channel walls. As expected from the theoretical investigations in Table 1, no reflections of the leading shock can be seen. In the case with a 10% concentration gradient, reflection occurs via a Mach stem. It is relatively weak, as the theoretical Mach number behind the incident shock is just a little above unity, but causes a series of secondary reflections in the trailing flow behind the detonation. The distortion and the irregularity of the detonation cells in the numerical soot print in Fig. 3 increases compared to the 5% case. In the case with a 20% concentration gradient, the Mach stem can clearly be seen. It causes high pressure loads on the lower wall although the hydrogen content there is much lower than in the upper part of the channel. The numerical soot print shows an interesting pattern: the downwards-running triple points produced by the detonation instabilities in the upper part of the channel are not reflected when they run into the Mach stem. Therefore, hardly any upwards-running triple points can be seen and the cellular pattern is replaced by unidirectional lines in some part of the channel. In the region behind the Mach stem, there are triple points running in both directions, but the cellular pattern is very small due to the increased compression compared to a planar CJ detonation. The soot print can clearly be divided in a part caused by the instabilities behind the oblique shock and a part caused by the instabilities behind the Mach stem.

Concerning the propagation velocity of a detonation, an increasing velocity deficit with increasing concentration gradient is observed (up to 7% velocity deficit for a 20% concentration gradient compared to the homogeneous, stoichiometric case). However, it is important to note that the propagation velocity is still higher than the CJ velocity of a homogeneous mixture with the same hydrogen content.

4 Conclusions

The simplified analysis in section 2 leads to a first approximation for the detonation front curvature and reflection in a medium with a concentration gradient. It is shown that for a hydrogen-oxygen mixture, the front will adapt to the wall either by (subsonic) front bending or by Mach reflection. Regular reflection is very unlikely to occur. These effects have been confirmed by Euler simulations. Additional effects have been revealed by the simulations, such as a very unusual soot print caused by Mach reflection in the case of a strong concentration gradient. In this case, the pressure loads on the enclosing structure are very asymmetric. The propagation velocities are between the CJ velocity of the stoichiometric gas (the maximum hydrogen content in the tube) and the CJ velocity of a homogeneous mixture with the same (average) hydrogen content. The authors are looking forward to experimental confirmation of these observations.

This project is funded by the German Federal Ministry of Economics and Technology (Project No. 1501338) which is gratefully acknowledged.

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