XXI ICTAM, 15–21 August 2004, Warsaw, Poland

THE CELLULAR STRUCTURE AND ITS TRACKS OF A $\mathrm{H_2/O_2/AR}$ DETONATION WAVES

X. Y. Hu*, J. Czerwinska* N. Adams*, B. C. Khoo**
*Technical University of Dresden, Dresden 01062, Germany
**National University of Singapore, Singapore 119260, Singapore

Summary In this paper, the cellular structure and its tracks of a two-dimensional ordinary detonation wave in low pressure $\mathrm{H_2/O_2/Ar}$ mixture simulated with detailed chemical reaction model, high order scheme and high resolution grids are investigated. The regular cellular structure is produced by introducing perturbations in the reaction zone of a steady one-dimensional detonation wave. The calculated structure shows a double-Mach like strong type configuration, in which strong ignition is observed behind the transverse wave. It is also observed that there are three different structure tracks associated with different triple points or the kink on the transverse wave. The comparisons with previous experiments indicates the presence of strong structure for an ordinary detonation.

INTRODUCTION

It is well known that gaseous detonation wave has cellular structure. The tracks of structure recorded on smoke foils have been observed in experiments, and the regions enclosed by these tracks are called detonation cells. The structure usually involves triple-wave/Mach configuration with the combination of incident shock wave (I), Mach stem (M) and transverse wave (T). Two types of structure, i.e the weak structure and the strong structure, are observed in experiments. The weak structure is characterized by single-Mach configuration with the associated transverse wave being merely shock wave, while the strong structure is characterized by multi-Mach configuration with much stronger transverse wave leading to strong ignition. It is widely accepted that, in a marginal detonation, the cellular structure is of the strong type. As much smaller detonation cell size and the associated structure can not be resolved easily and directly by experiments, it is still quite an open issue whether an ordinary detonation possesses a strong structure (Fickett and Davis 1979). From the late 1970's, numerical simulation has been employed and increasingly so to study the cellular structure to reveal details that can not be determined easily in experiments. Recently, the multi-step, detailed reaction model has been employed with some success. With this model Oran et al (1998) calculated the cellular structure tracks for the low pressure $\mathrm{H_2/O_2/Ar}$ mixture. However, the coarser resolution employed may have led to unclear structure and tracks which are difficult to verify the actual structure type. In this paper, the cellular structure and its tracks are investigated by two dimensional numerical simulations with both detailed reaction model and high resolution.

MODELING AND COMPUTATIONAL INITIALIZATION

This simulation models an ordinary detonation propagating in a two-dimensional channel with stoichiometric $\mathrm{H_2/O_2}$ diluted by 70% argon at initial pressure and temperature given as 6.67kPa and 298K, respectively. A 9 species, 19 elementary reactions model is used for hydrogen-oxygen combustion. The 5th order WENO-LF scheme, which is able to resolve the different discontinuities accurately and has small numerical dissipation, is employed. The time discretization for the fluid dynamic terms is the 3rd order TVD Runge-Kutta method which is combined with an stiff ODE solver. The initial condition, which is an one-dimensional steady detonation wave, is perturbed by introducing random disturbances for the first time-step of chemical kinetic integrations.

HIGH RESOLUTION REGULAR CELLULAR STRUCTURE

Figure 1 shows the detailed structure with $0.025mm$ grid size, which is about $1/200$ of the reaction zone length. One can find that the wave configuration resembles to some extent that of a double-Mach reflection of a shock wave. The main difference between them is the second triple wave configuration in the cellular structure is transitional-Mach like. Hence, the whole structure shows stronger strength than a merely double-Mach configuration. The ignition front, which is approximately defined by the concentration discontinuity, suggested that all the ignitions after the Mach stem, the incident wave, and transverse wave are associated with strong shock induced ignition processes. The structure shows clearly multi-Mach configuration with more than one triple points and the presence of strong transverse wave ignition. Therefore, one can conclude that the cellular structure is of the strong type.

CELLULAR STRUCTURE TRACKS

In the present work, the structure tracks are obtained by recording the maximum flow velocities on all grid nodes in the time history. Figures 2 and 3 show the numerical detonation cells as an analogue of smoke foil tracks and how the tracks are left after the sweeping of the structure, respectively. Generally, it can be observed that there are three tracks left by the structure (see Fig. 2). The first track is left by tangential velocity discontinuity on the first slip line S. The second track is left by the tangential velocity discontinuity on the second slip line S'. The third track is left by the region near the kink point c to the extending transverse wave. Table 1 shows the details of comparisons between the numerics and experiments

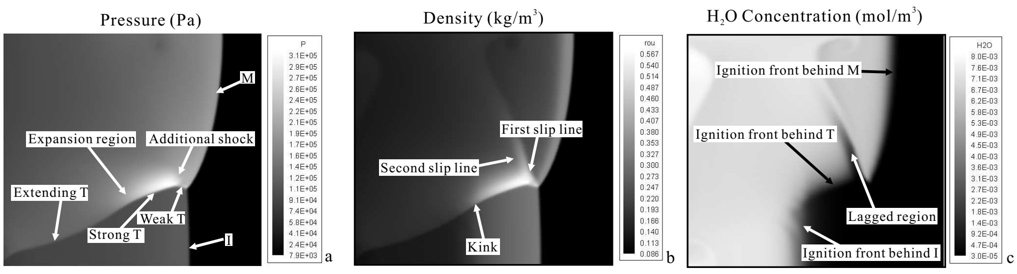

Fig. 1 Cellular tructure with one transverse wave with 0.025mm grid size
a)pressure, b)density, c)d)H_2Oconcentration

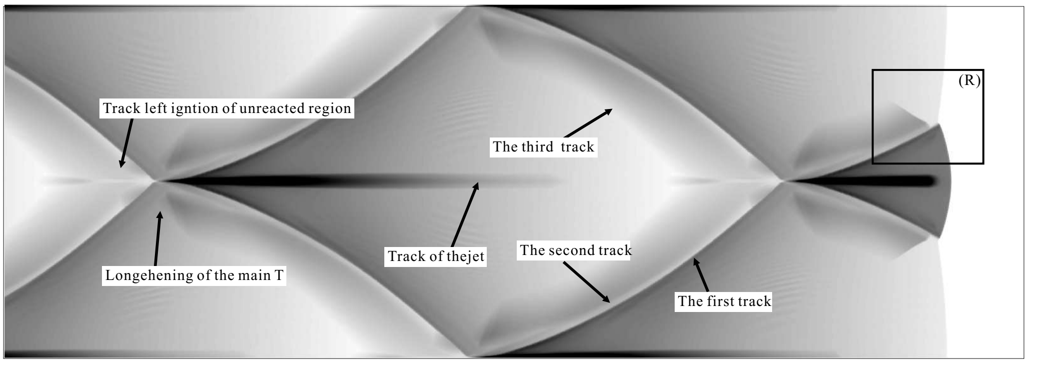

Fig. 2 Numerical detonation cells in a 8mm channel (region (R) is produced schematically in Fig. 3

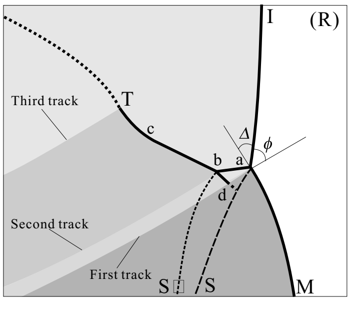

Fig. 3 The making of structural tracks
in a numerical detonation cell

Table 1 Comparison of cell geometries
between simulation and experiments

Cell geometries	Current results	Experiments [a]
Width/length (d/l)	0.55	$0.5 \sim 0.6$
Exit angle (β)	$< 10^o$	$5^o \sim 10^o$
Entrance angle (α)	40^o	$32^o \sim 40^o$
Track angle (ω)	30^o	$\sim 30^o$

[a] From Strehlow (1968)

(Strehlow 1968). Strehlow's (1969) argument for the presence of weak structures in ordinary detonations is based on the ground that the observed structure tracks are "single lines". However, if the experimental smoke foil tracks in Strehlow (1968) are analyzed further, the "single line" is actually a narrow band. In this band, less soot is removed compared to the neighboring regions. This narrow band is very similar to the narrow band reflected in Figs. 2 and 3 and recorded by by region lying between the first and the second tracks. This concurrence of the simulation and experiment suggests the presence of a strong structure for the ordinary detonation in $H_2/O_2/Ar$ mixture. As many experimental smoke foil data (Fickett and Davis, 1979) for *different* ordinary detonations show that the structure tracks are actually narrow bands too, it may be surmised that strong structures exist for other reactive systems.

CONCLUDING REMARKS

In this paper, the cellular structure and its tracks of an ordinary detonation in $H_2/O_2/Ar$ mixture are investigated by a two-dimensional simulation. The calculated high resolution results suggested a strong structure which left three different tracks associated with different triple points or the kink on the transverse wave. The comparisons with previous experiments indicates the presence of strong structure for an ordinary detonation.

References

[1] W. Fickett, W.C. Davis: *Detonation* (University of California, Berkeley, 1979)
[2] .S. Oran, J.E. Weber, E.I. Stefaniw, M.H. Lefebvre, J.D. Anderson: *Combust. Flame* **113** 147-163, 1998
[3] R.A. Strehlow: *Combust. Flame* **12** 81-101, 1968
[4] R.A. Strehlow RA: *Astronaut Acta* **14** 539-548, 1969