Numerical Simulation of Spin Detonation in Square Tube

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Introduction

Spin detonation has been known since 1927 when Campbell and Woodhead [1] published their experimental study of CO/O2/H2 detonation. Several years later Bone et al. [2] found spin detonations in CO/O2 mixtures in various shapes of tube such as triangle, square and rectangular. They could see that (1) detonation spins well; (2) detonation head rotates and quiescent mixture does not; and (3) there is a pitch angle of spin. More recently, Schott [3] showed the structure of spinning detonation with smoked foil records and Lee et al. [4] reviewed gaseous detonation where the detail of such smoked foil records of spinning detonations in circular and square cross-sections.

Many studies have been done for the structure of spinning detonation experimentally and theoretically up to now. Meanwhile numerical study of spinning detonation has not appeared very recently until a fast computer is developed when the interest on such spin detonation work is gone. A very fast numerical work on spin detonation was performed by Washizu and Fujiwara [5] to show a spinning mode of detonation in double circular tube with a H_2/O_2 two-step reaction mechanism.

The present paper presents a numerical study of spinning detonation in a square cross-section tube in the first time. The structure and propagation mechanism of spin detonation in the square tube are discussed in detail, especially a difference between spin detonations in circular and square cross-sections.

Numerical Methods

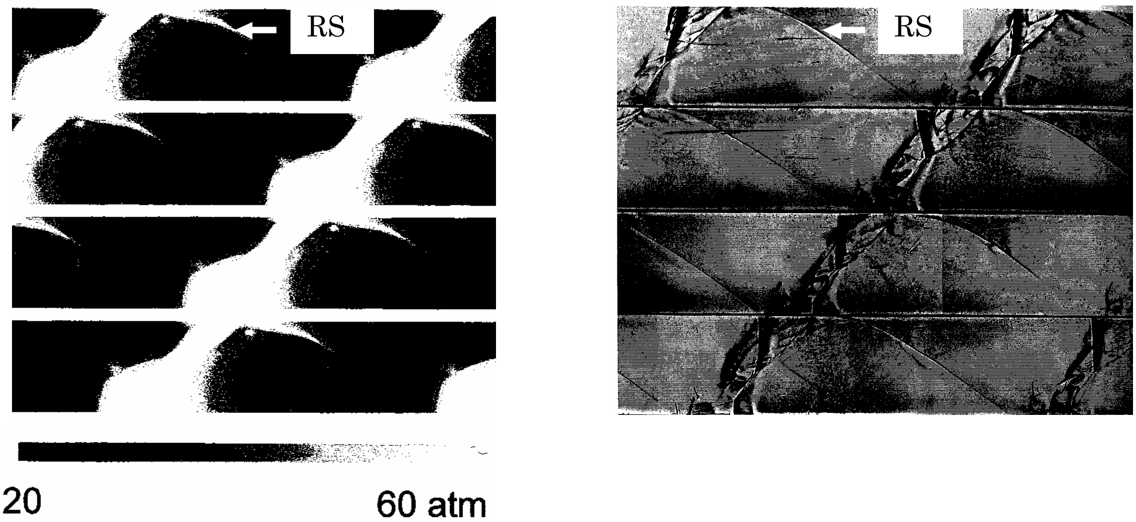
Compressible 3D Euler equations are applied together with mass conservation equations of 9 chemical species; H_2, O_2, O, H, OH, HO_2, H_2O_2, H_2O, and N_2. A semi-implicit technique is used to treat production terms in the governing equations implicitly and other terms explicitly. A non-MUSCL modified-flux type TVD scheme developed by Harten and Yee [6] is applied in convection terms and a point implicit method to production terms. A 2nd-order Strang type fractional step method is used for time integration. A Petersen and Hanson H_2-air reaction model [7] for 9 species and 18 elementary reactions is treated for the present calculation.

Computational grid sizes for 3D calculation are 5μm x 5μm x 5μm and the grid number is 200 x 200 x 600. The grid size of 5μm corresponds to one thirty third of the half reaction distance of H_2/air of 167.3μm. The boundary conditions are treated as adiabatic, non-slip, and non-catalytic at walls and a H_2/air mixture at stoichiometric condition, 1 atomospheric pressure, and 298 K of temperature with CJ velocity upstream, and flowing-out with CJ pressure downstream. As for initial conditions, 1D results are pasted three-dimensionally with an initial perturbation of asymmetric profiles of un-reacted gases behind detonation.

The present calculation is performed using NEC SX-6 1 node (8CPU) of ISAS/JAXA. The program is paralleled by Open MP system.

Results and Discussion

Figure 1 shows the numerical smoked foil records in 1 x 1 mm tube obtained by maximum pressure record in H_2/air mixture (Fig.1-(a)) and the experimental smoked foil records in 3/4 x 3/4 in tube obtained by Lundstrom [4] in C_2H_2/O_2/Ar mixture (Fig.1-(b)). A distinct feature, which is different from spin detonation in circular tube, is seen in the figure: that there is a wall effect which provides complicated wave interactions such as a reflected shock indicated in the figure as RS. Since the numerical results are obtained from the maximum pressure history, the detailed numerical smoked foil profiles are not seen in the figure, but if the described pressure limit is lowered, the further detailed structure will appear.



(a) Numerical results presently obtained

(b) Experimental results obtained by E.A. Lundstrom, Berkeley [4]

Fig.1 (a) Maximum pressure history on the wall and (b) smoked foil records of spin detonation in square tube; detonation propagates from left to right.

The series of pressure and temperature profiles behind the detonation front are shown in Figs.2 and 3, respectively. In both figures the detonation front rotates in clockwise which may depend on the initial conditions. When the triple point hits the wall, high pressure and high temperature regions come out, which phenomena is quite different from the spin detonation in a circular cross-section. The interesting results are observed in the hydrogen molecule profiles (not shown in this abstract) that the fuel is consumed completely one or two tube widths, although un-reacted pockets are seen behind the detonation front. Furthermore the tailing phenomena seems not to appear in the spin detonation in square tube, while there is one for that in circular tube. It is found that this spin detonation has CJ detonation velocity.

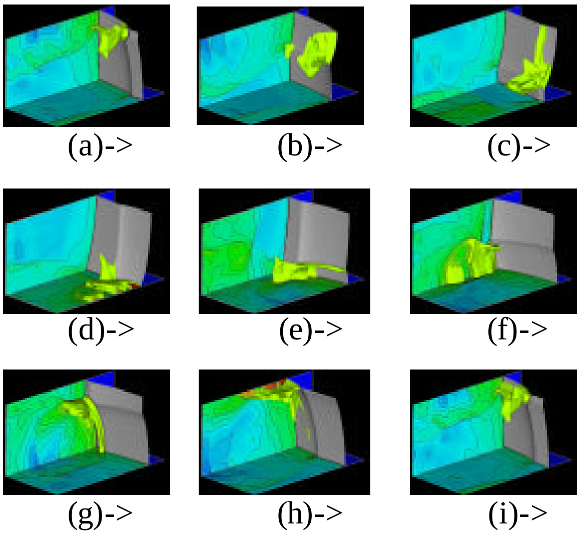


Fig.2 Series of pressure profiles behind spin detonation wave where blue color is 1 atm and red color is 60 atm. The gray is the spin detonation front. Detonation front spins clock wise; (a)->(b)->(c)->(d)->(e)->(f)->(g)->(h)->(i)->(a)->…

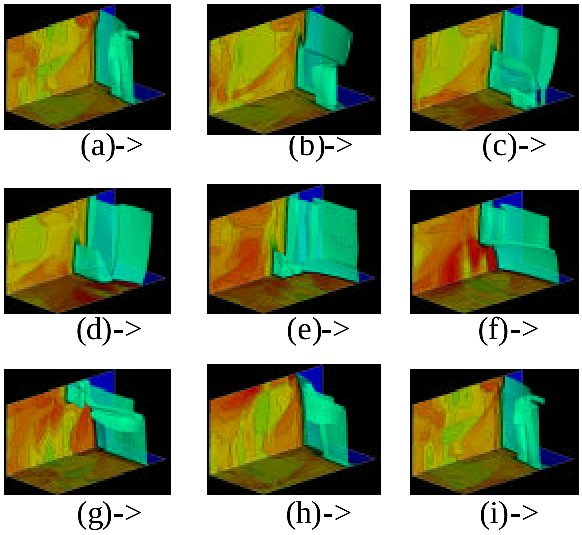


Fig.3 Series of temperature profiles behind spin detonation wave where blue is 300 K and red is 3700 K. The blue-green is the spin detonation front. Detonation front spins clockwise; (a)->(b)->(c)->(d)->(e)->(f)->(g)->(h)->(i)->(a)->…

Conclusion

Spin detonation in square tube is studied numerically using compressible 3D Euler equations. From the results the following are found:

(1) The detonation spins clockwise with a CJ speed of 1970 m/s.
(2) The feature of the numerical smoked foil records agree with that of experimental one.
(3) There is no tailing so far.
(4) The spin pitch angle is about 51 degrees which coincidently agree with experimental one.

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