NUMERICAL MODELING OF UNSTABLE DETONATION IN HEPTANE VAPOR-AIR MIXTURES

Hong Tao and Qin Chengsen
Institute of Applied Physics and Computational Mathematics,
P. O. Box 8009, Beijing 100088, China
e-mail: hong_tao@mail.iapcm.ac.cn

ABSTRACT: The stability problem of one-dimensional gaseous detonation in heptane-air mixtures is numerically analyzed. Three step reaction mechanism is used to describe chemical reaction. The ignition condition is the gas with high velocity and high temperature. Three kinds of solution are obtained. First, as the velocity of ignition gas is slow the detonation fails to develop. Second, the pressure history becomes double oscillation after several single oscillations. The last is much more complex solution that pressure history is very irregular.

INTRODUCTION

The classical theory of ZND[1] assumes that detonation waves are one dimensional steady traveling wave with a structure that is composed of a leading shock followed by a reaction zone. But in fact stable one-dimensional detonation waves are seldom observed. The experiments demonstrate that in many cases detonations are complicated unstable wave patterns. One of the instability is pulsating detonation. In most of previous work on unstable detonation chemical reaction is one-step Arrhenius mechanism such as the work by Ficket & Jackbson(1972)[2], Abouseif & Toony(1982)[3], Bourlioux & Majda(1991)[4], He & Lee(1995)[5], except the work by Short & Quirk(1997)[6], in which they used three step chain-branching reaction.

In this paper a three step reaction mechanism, based on the two-step mechanism by Westbrook & Dryer is employed to study the pulsating detonation wave. The model includes the reaction of hydrocarbon with oxygen producing monoxide and water vapor. The model also contains two reversible reactions that include the dissociation of carbon dioxide and water. One-dimensional simulations are used to determine the development of the pulsating detonation in heptane vapor with air mixture of same equivalence ratio which equals 1.

ANALYSIS MODEL

Numerical simulation of gas phase detonation are based on the compressible, time-dependent conservation equations for mass, momentum and energy.

Mass conservation

$$\frac{\partial \rho}{\partial t}+\frac{\partial(\rho u)}{\partial x}=0 \tag{1}$$

Momentum conservation

$$\frac{\partial \rho u}{\partial t}+\frac{\partial(\rho u^2+p)}{\partial x}=0 \tag{2}$$

Energy conservation

$$\frac{\partial}{\partial t}\left[\rho(e+0.5u^2)\right]+\frac{\partial}{\partial x}\left[\rho u(e+0.5u^2)+pu\right]=Q_c \tag{3}$$

Where ρ,u, p, e are density, velocity, pressure and specific internal energy respectively. Q_c is the chemical heat release term. The chemical reaction occuring in the system are symbolized by $\sum_j a_{jr} x_j \leftrightarrow \sum_j b_{jr} x_j$. The stoichiometric coefficients must satisfy $\sum_j \left(a_{jr} - b_{jr}\right) W_j = 0$. W_j is the molecular weight. In this paper the detonatible mixtures are heptane vapor with air. The model of chemical reaction mechanisms is a three-step described by the following[7,8]:

$C_7H_{16}+7.5O_2=7CO+8H_2O$ (r1) $2CO+ O_2 \leftrightarrow 2CO_2$ (r2) $2H_2+O_2 \leftrightarrow 2H_2O$ (r3)

The gaseous phase is a mixture of chemical gases with seven components. The concentration of each component is Y_j□j=1,…,N,N=7□,where j=1 corresponds to heptane vapor, j=2 oxygen, j=3 nitrogen, j=4 carbon dioxide, j=5 water vapor, j=6 monoxide, j=7 hydrogen. In a multispecies fluid in which chemical reaction occur, the mass equation for individual species is the following:

$$\frac{\partial(\rho Y_j)}{\partial t} + \frac{\partial}{\partial x}(\rho Y_j u) = \dot{\rho}_j^c \tag{4}$$

$$\dot{\rho}_j^c = W_j \sum_r \left(b_{jr} - a_{jr}\right)\omega_r \tag{5}$$

the chemical heat release term in the energy equation is

$$Q_c = \sum_r Q_r \omega_r \tag{6}$$

$$Q_r = \sum_j (a_{jr} - b_{jr})(\Delta h_f^0)_j \tag{7}$$

ω_r is chemical reaction rate. $(\Delta h_f^0)_j$ is the heat of formation of species j at absolute zero. The equation of state of gaseous phase is

$$p = \rho RT \sum_{j=1}^{N} Y_j / m_j \tag{8}$$

The second order accurate MacCormack finite difference equation is used along with FCT-technique[9,10] for above equations.

RESULTS AND DISCUSSIONS

The initial conditions are pressure and temperature with velocity discontinuity separating two regions in the computational domain.

$0 \le x \le L_{ign}$, $p=p_{ign}$,$\rho=\rho_{ign}$, $u=u_{ign}$, $T=T_{ign}$; $x>L_{ign}$,$p=p_0$, $\rho=\rho_0$, $u=0$

L_{ign} is the length of ignition area. In ignition area, the gas is in high velocity and high temperature with the same in initial. Here the ignition condition in all calculations is the same as the following:

The calculation is carried on in the range of 2m and time limit is 1000μs. The mixture is heptane vapor-air with equivalence ratio Φ=1. Table 1 lists the initial condition of calculation. There are three kinds of ignition condition. First kind of case 1,2 and 3 is the different gas velocity with same pressure and temperature. Second kind of case 1 and 4 is with different ignition length L_{ign}. Last kind of case 1,5 and 6 is with different temperature and pressure of same velocity.

Table 1. Initial condition for computation

	Case 1	Case 2	Case 3	Case 4	Case 5	Case 6
L_{ign}/cm	16	16	16	8	16	16
p_{ign}/Mpa	2.58	2.58	2.58	2.58	2.95	2.21
u_{ign}/m/s	1000	800	600	1000	1000	1000
T_{ign}/K	2800	2800	2800	2800	3200	2400

Figure 1-6 shows the pressure history of leading shock wave of detonation of case 1-6. Three kinds of solution are obtained. First, as the velocity of ignition gas is slow the detonation fails to develop such as in figure 3. Second, the pressure history becomes double oscillation after several single oscillations as in figure 1,2,5. The last is much more complex solution that pressure history is very irregular as in figure 4 and 6. It seems that there are no regular single oscillation solution in this problem.

REFERENCES

1.Fickett,W. and Davis W.C., Detonation, University of California Press, 1979, p. 230-288

2.Fickett,W., Jacobson J.D. & Schott, G.L. Calculated pulsating one-dimensional detonation with induction-zone kinetics, AIAA, 10, 514-516,1972

3.Abouseif, G.E., and Toony,T.Y., Theory of Unstable One-Dimensional Detonations, Combustion and Flame,45:68-94,1982

4.Bourlioux, A., Majda, A.J. & Roytburd, V. Theretical and numerical structure for unstable one-dimensional detonations. SIAM J. Appl. Maths 51,303-343,1991

5.He,L. And Lee,J.H.S., Dynamical Limit of one-dimensional detonations, Phys. Fluids 7(5):1151-1158, 1995

6.Short,M. And Quirk,J.J., On the nonlinear stability and detonability limit of a detonation wave for a model three-step chain-branching reaction, J. Fluid Mech., vol. 339,pp.89-119,1997

7.Westbrook,C.K., Dryer,F.L, Simplified Reaction Mechanisms for the Oxidation of Hydrocarbon, Combustion Science and Technology, 27:pp.31-43(1981)

8.Kiehne,T.M., Matthews, R.D ., Wilson, D.E., An Eight Step Kinetics Mechanism for High Temperature Propane Flames, Combustion Science and Technology, 54: pp. 1-23 (1987)

9.Book, D.L., Boris, J.P.,Hain,K., Flux-Corrected Transport □:Generalization of the Method, J. Computational Physic*s*, 18:pp. 248-283(1975)

10.Taki S., Fujiwara T., Numerical Simulation of Triple Shock Behavior of Gaseous Detonation, Eighteenth International Symposium on Combustion, The Combustion Institute, Pittsburgh, PA, 1981,pp.1671-1681

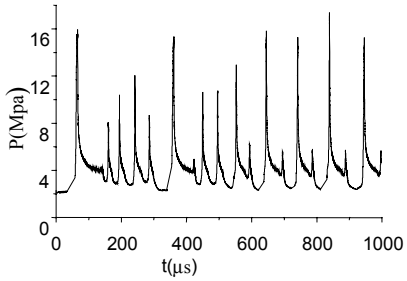

Fig.1 pressure history of case 1

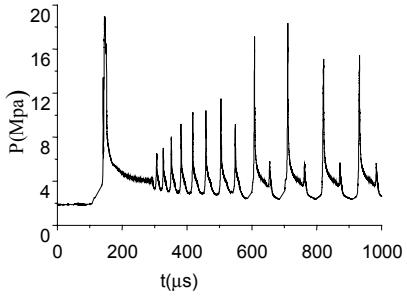

Fig.2 pressure history of case 2

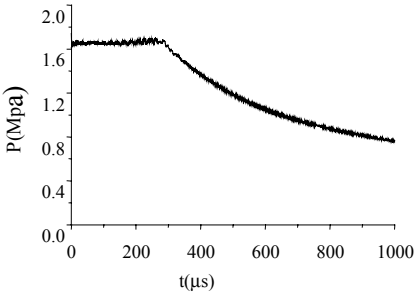

Fig.3 pressure history of case 3

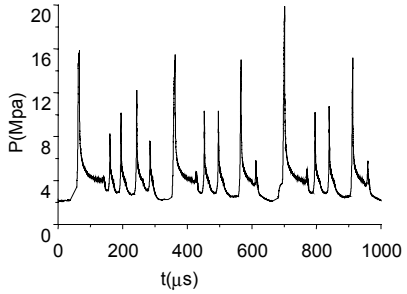

Fig.4 pressure history of case 4

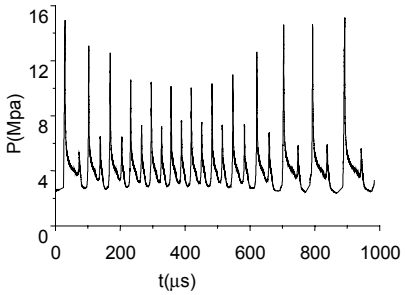

Fig.5 pressure history of case 5

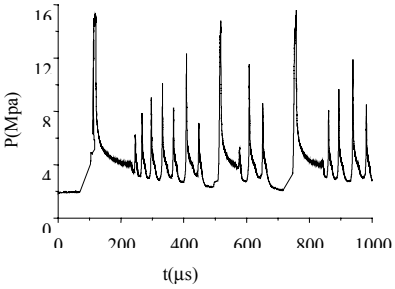

Fig.6 pressure history of case 6