A Remark on Self-sustained Detonations

Liu W.

University of Central Lancashire, School of Engineering, Preston, Lancashire, UK
**Corresponding author's email: wliu1@uclan.ac.uk*

ABSTRACT

The steady self-sustained detonation is theoretically a Chapman-Jouguet detonation. Through solving the basic equations for combustion, the author presents some quasi steady self-sustained detonations that propagate much faster than Chapman-Jouguet detonations. This study shows that the propagations of the quasi steady self-sustained detonations depend upon not only the release energy from their chemical reactions, but also the rates of their chemical reaction.

KEYWORDS: Self-sustained detonation, over-driven detonation, Chapman-Jouguet detonation

NOMENCLATURE

A	dimensionless pre-exponential factor
a_0	refernce velocity
E	total energy
E_a	activation energy
M	Mach number
h_0	heat of combustion
l	length of chemical reaction
p	pressure
p_0	reference pressure
Pr	Prandtl number
q_0	heat of combustion
Re	Reynolds number
Sc	Schmidt number
T	temperature
T_0	reference temperature
t	time
u	mixture velocity
Y	mass fraction

Greek

γ	ratio of specific heats
ρ	density
ρ_0	reference density
$\dot{\omega}$	reaction rate

Subscripts

0	ambient

Superscripts

b	after combustion

INTRODUCTION

Steady and self-sustained detonation is a basic mode of combustion wave propagations. It is maintained by the chemical reactions. only. Having a look at the basic mathematical equations for combustions, we would find two aspects of the reactions: the heat released by the reactions and the rate of the reactions, directly influence the solutions of combustion wave propagations. Therefore, it is envisaged that the speed of the self-sustained detonations should be related to the heat by and the rate of the chemical reactions.

Theoretically a steady self-sustained detonation is Chapman-Jouguet (C-J) detonations. As we have known, C-J detonation is decided by the heat released from the reactions only, and is independent of the rate of the reactions. Furthermore, the speed of C-J detonations is the minimal within all the

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possible detonation modes. In other words, all the self-sustained detonations, when the energy released from their reactions and driving these detonations is the same, will have a same speed of propagation, whatever the differences in their reaction rates are, whether very fast or very slow. This is clearly inconsistent with the observation of the basic equations for combustions.

If a detonation is non-C-J detonation, its speed must be quicker. When a detonation has a propagation speed more than that of a C-J detonation, it is called over-driven detonation in the literature. Now it is generally thought that an over-driven detonation must be driven by not only the chemical reactions but also some external forces, such as an external pressure or input flow velocity, thus it must not be a self-sustained detonation.

In this work, the author numerically solves the Cauchy problem to study whether the quasi steady self-sustained detonations other than C-J detonations exits. Since the author is numerically solving the Cauchy problem and cannot integrate the problem to infinite length, the steady detonations to be found are called quasi steady detonations.

BASIC EQUATIONS

Consider a detonation development in a smooth shock tube. The shock tube has a closed end and an open end. The detonation is initiated in the closed end. After a developing stage, if the detonation becomes steady and is maintained by its reactions only, then this detonation is thought to be steady and self-sustained detonation wave. In this paper, the direct numerical simulation approach is applied to construct all these processes of the detonation development and examine whether a steady and self-sustained detonation wave exists in the set surrounding. The same work can be done by experiments but the advantage of the numerical simulations over the experiments lies in perfect and accurate records of the database.

Complete~~ly~~ understanding of detonations and shock waves certainly needs molecular dynamic theory and chemical reaction dynamics theory. The methodology of the research in this work is however limited to the theoretic framework of continuum. Thus, the minimal spatial scale and temporal scale in this work are respectively about 5 μm and 5 μs, as they are reasonably calculable and sufficiently accurate for the continuum models. It is known that such scales are far beyond the scales in molecular dynamics and molecular reaction courses. Therefore, the detailed processes in molecular dynamics and chemical reactions will be modelled so that the nature of the physicochemical processes is correctly reflected in the continuum framework.

The theoretical models in the numerical simulations are the one-dimensional Navier - Stokes equations for the movement of the gaseous reactant and product and the first-order Arrhenius kinetics for chemical reaction rates. As the purpose of this paper is mainly to deal with the conceptual framework, the simple kinetics is applied but it does not lose the nature of the concerned issue. In fact, this model has been widely used in the other researches and engineering applications as well [1]. The basic equations for the theoretical models are written in the following dimensionless form in with a length of 0.1 m, l, and the sound speed, density, pressure and temperature at the initial states of the reactant mixture, a_0, ρ_0, p_0, and T_0, are used for the reference length, velocity, density, pressure and temperature, respectively.

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

$$\frac{\partial (\rho u)}{\partial t} + \frac{\partial \left(\rho u^2 + p\right)}{\partial x} = \frac{\partial}{\partial x}\left(\frac{4}{3\,\mathrm{Re}}\frac{\partial u}{\partial x}\right), \tag{2}$$

$$\frac{\partial(\rho E)}{\partial t}+\frac{\partial(\rho uE+up)}{\partial x}=-h_0\cdot\rho\dot{\omega}+\frac{\partial}{\partial x}\left(\gamma\frac{4M^2}{3\mathrm{Re}}\cdot u\frac{\partial u}{\partial x}+\frac{\gamma}{(\gamma-1)\mathrm{Re}\,\mathrm{Pr}}\frac{\partial T}{\partial x}\right), \tag{3}$$

$$\frac{\partial(\rho Y)}{\partial t}+\frac{\partial(\rho uY)}{\partial x}-\frac{\partial}{\partial x}\left(\frac{1}{\mathrm{Sc}\,\mathrm{Re}}\rho\frac{\partial Y}{\partial x}\right)=\rho\dot{\omega}, \tag{4}$$

$$\dot{\omega}=AY\exp\left(-\frac{E_a}{T}\right), \tag{5}$$

$$p=\rho T, \tag{6}$$

where u, ρ, p, T, E, Y, h_0 and $\dot{\omega}$ denote the flow velocity, density, pressure, temperature, total energy, mass fraction of reactants, heats of combustion and reaction rate, respectively, while γ, Re, Pr and Sc denote the ratio of specific heats, Reynolds number, Prandtl number and Schmidt number, respectively. In equation (5), A and E_a are the dimensionless pre-exponential factor and activation energy, respectively. The reader is reminded that dimensionless equations are solved in this work.

NUMERICAL METHODS

The finite volume method is used for the spatial discretization in the numerical solutions. The accuracy of this method mainly depends upon flux calculation on the interface between two connected control volumes. The flux calculation involves two routines – reconstruction of the solution within the associated control volume and solution for the Riemann problem corresponding to the Euler equations (1) – (3). In this work a third order WENO scheme is implemented for the reconstruction and the Liou-Steffen (AUSM) flux-vector splitting method [2] is employed for solution of the Riemann problem. After the spatial discretization, a set of ordinary differential equations is generated. A Runge – Kutta scheme of five levels is used to integrate the ordinary differential equations [3]. The numerical methods were verified through solving the shock tube flow and comparing the numerical solution and the exact solution of shock tube flow [4]. The reader can see the detailed implementation and validation of the numerical methods from the paper [5].

Transport terms, i.e., viscous stresses, dissipation of energy, heat conduction and mass diffusion, are included in the basic equations. In order to calculate the fluxes produced by the transport terms, the relevant gradients are computed using finite difference scheme of fourth order. Clarke [6] theoretically found that the influence of the transport terms on combustion wave propagations will significantly decrease with the increase of combustion wave speeds. The numerical simulations in this work find that the transport process plays a minor role in denotation movements, which supports Clarks's conclusion.

Boundary conditions and initial conditions

There are two boundaries. One is imposed by the wall boundary condition. At the second boundary, the non-reflecting open boundary condition is applied [5].

The initial conditions are set with the initial states of real shock tubes. A high temperature and high pressure inertial gas is filled in the closed end, while the reactant gas is separately charged at the other side and its initial states are the same as the reference states in nondimensionalization of the basic equations. The high temperature and high pressure side setting is simply to ensure the reaction can be initialized after the simulation starts.

Mesh-independent solutions

Mesh resolution may be the most critical factor for a numerical simulation. In this work a uniform mesh is applied. Its resolution is assessed by the criterion that the major reaction zone or flame is meshed by more than 100 nodes. The major reaction zone is defined from the reaction starting, to 95% completeness of the reaction.

When initial and unreacted states are at the standard atmospheric conditions, the computational results find that the lengths of the major reaction zones are about 0.5 mm, which is similar to the results in [1]. The major reaction zones are meshed by more than 100 nodes, the corresponding mesh resolutions are therefore about 5 μm.

In the practical computations, the samples of the simulations are regularly checked. If the criterion is broken the mesh will be doubled until the criterion is satisfied. Figure 1 shows the variation of product fraction in a typical reaction zone. One can see that it is quite smooth. In fact, the sensitivity of the solutions to mesh resolutions was studied in this work as well. Figure 2 presents the detonation speeds and Table 1 lists the maximum density, pressure and temperature behind the flame produced on three meshes, double-coarse, criterion-satisfied and double-refined meshes. It can be seen that their differences are small. Therefore, the sensitivity of the mesh, when this criterion is met, is minor. That implies the mesh resolution is sufficiently fine.

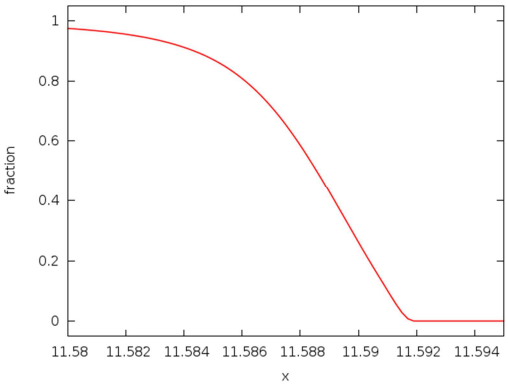


Fig. 1. Mass fraction profile of product within the reaction zone.

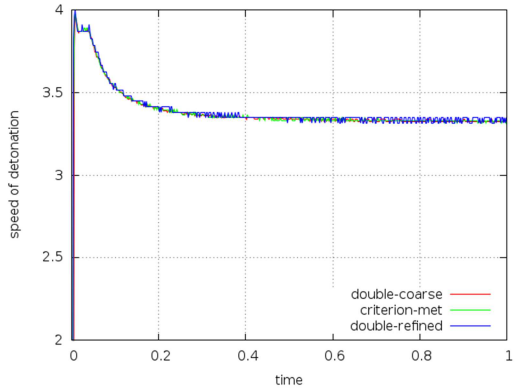


Fig. 2. Detonation speeds produced on three meshes with different resolutions.

Table 1. Results behind the flame produced by different mesh resolutions

	Double-coarse	Criterion-met	Double-refined
Density	4.37	4.45	4.52
Pressure	12.29	12.35	12.41
Temperature	4.143	4.150	4.156

It is necessary to note that the computations in this work are about unsteady flows with high Reynolds numbers. They are therefore inevitably involved in turbulent fluctuations. The amplitude of the fluctuations, compared with the major flows, are however minor and also the fluctuations' frequency is too high to be illustrated in the graphics in this paper. This is the reason why the graphic presentation of the results, like those of others, e.g., [7], looks quite smooth.

COMPUTATIONAL RESULTS AND DISCUSSIONS

After solving the Cauchy problem (1) – (6) built up above, one can obtains the processes of detonation movements and propagation. The solution is comprised of two stages - initiation of detonation and propagation of fully-developed detonation. In what follows, the detailed results about them are presented.

Initiation of detonations

Initiation of detonation is a complex process. In general it can be classified into two different kinds: direct initiation and indirect initiation. In the former, detonation will be directly launched by the ignition. For the latter, however, a fast flame or fast deflagration is initiated firstly. The fast deflagration is then developed. When the fast deflagration is achieved to some certain state, a sudden acceleration of the combustion wave occurs which is called the second explosion in literature. After the acceleration, the detonation is created [5, 8].

Ignition energy in this work is set in the initial condition. It is a key parameter for the successful initiation of detonation and what kind of initiation of detonation takes place. The numerical results show the following regime of initiation.

$$FF \quad < E_0 < \quad II \quad < E_1 < \quad DI\,, \tag{7}$$

where E_0 and E_1 are the two criteria of ignition energy while *FF* represents the fast flame, *II* the indirect initiation of detonation and *DI* the direct initiation of detonation. If the ignition energy is less than E_0 no initiation of detonation happens. When it larger than E_1 direct initiation of detonation will be observed. Between E_0 and E_1 the initiation is indirect and needs a deflagration-to-detonation transition (DDT).

Figure 3 presents four initiations of detonation. The four cases are for the same chemical kinetics. The input parameters for the computations are given in Table 2 in which the ignition energy is measured by the initial temperature of the hot mixture in the ignition zone. From the Fig. 3 we observe that the four cases all experience an induction period that ends at t = 0.02196. After the induction, when ignition temperature is 4 dimensionless units, a direct initiation of detonation is achieved. However, the other three with the lower ignition temperatures, undergo the indirect initiation of detonation. It is important that the final detonation speed of all the four cases, when initiation of detonation is competed, is approaching the same value. Therefore, we can conclude that the final detonation speed and steady detonation state are independent of its initiation course.

Table 2. Parameters of simulated cases

Heat of combustion (q_0)	10.0
Ratio of specific heats (γ)	1.32
Preexponential factor (A)	1.0×10^{6}
Activation energy (E_a)	20.0
Time step width (Δt)	1.0×10^{-5}
Re, Pr, M, Sc	1.0×10^{6}, 0.78, 0.8704, 1.0

Their final detonation speed is 4.49534, while the speed of the corresponding C-J detonation is 3.629403, which therefore indicates that the speed of the self-sustained detonation produced by the

numerical simulations is significantly higher than that of the C-J detonation. As a result, the C-J detonation is not the self-sustained detonation mode for this chemical kinetics.

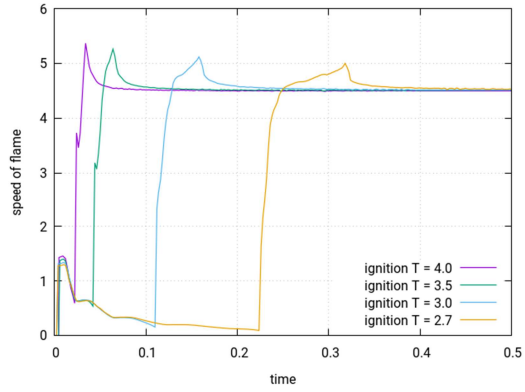
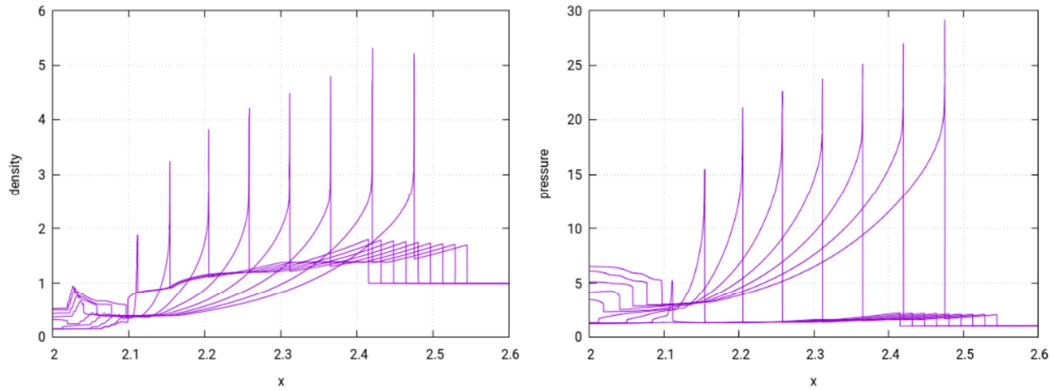
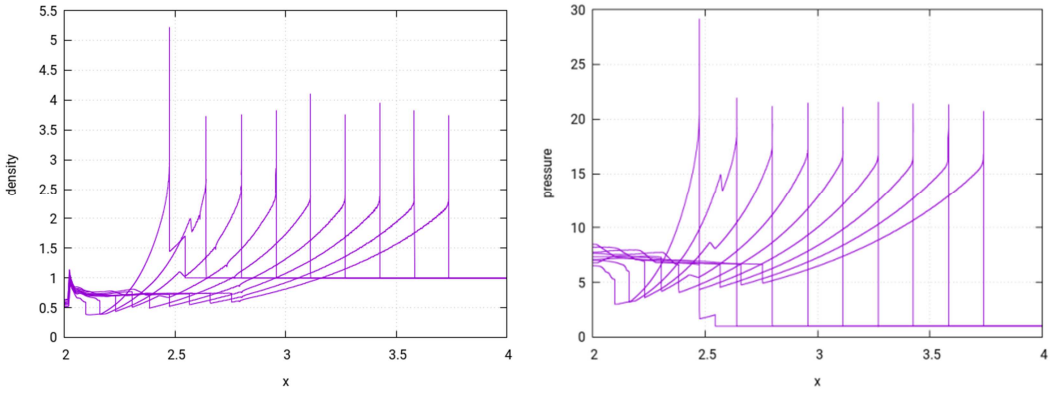


Fig. 3. Flame speeds produced by different ignition temperatures.



(a) Density (b) Pressure

Fig. 4. Density and pressure variations during deflagration-to-detonation transition.



(a) Density (b) Pressure

Fig. 5. Density and pressure variations after transition to detonation.

Figure 4 and 5, respectively, display the profiles of the mixture density and pressure at different time instants for the case with the ignition temperature of 2.7. The time interval for the results is Δt = 0.01. In Fig. 4, there are three jumps of the pressure and density. The leading one with the maximal x coordinate is a neutral shock wave formed in the ignition. The medium jump is growing and speeding up. This jump is just the fast deflagration which is going through a transition to detonation. Because of a higher speed, the fast deflagration will catch up the leading shock wave. The third jump is a reflecting shock wave generated when the two expansion waves after the two flames collide. From Fig. 4 we see that the speed of the third jump is slower than that of its fast deflagration and therefore no interaction occurs.

Figure 5 indicates the fully developed detonation after DDT. The speed of the combustion wave is becoming constant, which shows that a steady self-sustained detonation is obtained.

Influence of chemical reaction kinetics on self-sustained detonation propagation

We now explore the propagation of a self-sustained detonation under different chemical reaction kinetics, but with the same combustion heat, q_0 = 10.0. Because of the same combustion heat, there is only one mode of C-J detonation propagation whose speed is s_{C-J} = 3.629403. Nonetheless, because chemical reaction kinetics are changed in the basic equation (4), the Cauchy problem (1) – (6) produces different detonation propagation.

The chemical reaction kinetics (6) has two parameters, the activation energy and pre-exponential factor. The tests of two groups are therefore done. In the first group, the pre-exponential factor is kept unchanged while the activation energy, E_a, is changed. Figure 8 displays the speeds of the produced detonations. It is observed that the speed of the detonation will increase when the activated energy rises. As a comparison, the speed of the C-J detonation also is plotted in the figure. One can see it is significantly smaller than the speeds of the three numerically simulated detonations.

The profiles of the pressures and temperatures of the two cases are illustrated in Fig. 7. It is seen that the detonation with E_a = 22.5 propagates faster over the detonation with E_a = 17.5. This is consistent with the results in Fig. 6. We also observe that the faster the detonation propagates the larger is the overpressure or temperature produced by the detonation, which is in agreement with the prediction by Rankine-Hugoniot curve.

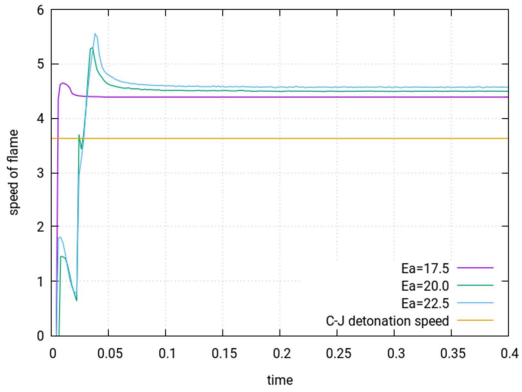
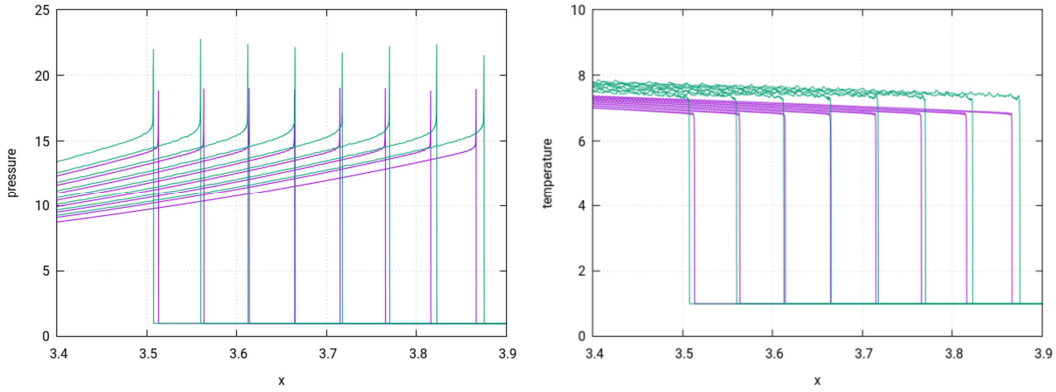


Fig. 6. Variation of detonation speeds for different activation energy E_a .

The second group of tests is of three different pre-exponential factors with the same activated energy E_a = 20.0. The speeds of the detonations for this group are shown in Fig. 8, again different from the speed of the C-J detonation. In particular, the speeds of the detonations generated by the

three tested cases differ from each other. With the increase of the pre-exponential factor the speed of the detonation decreases. This is consistent with the first group of tests.



(a) Pressure (b) Temperature

Fig. 7. Comparison of the profiles of the mixture pressure and temperature at 8 time instants, here the time interval is equal to 0.01; the green is for the detonation with E_a = 22.5 and the purple is for the detonation with E_a = 17.5.

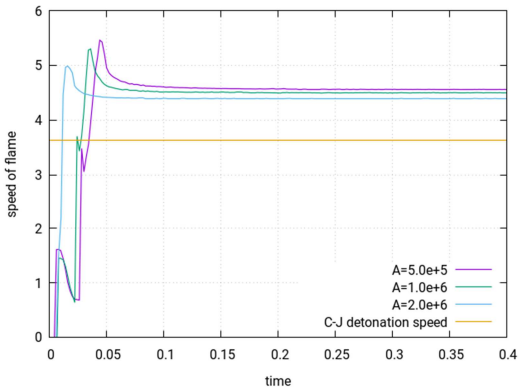


Fig. 8. Variation of detonation speeds against preexponential factor *A*.

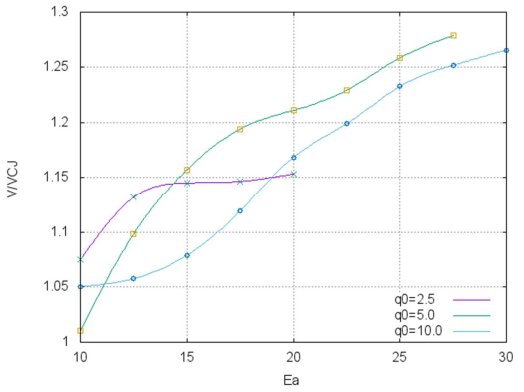


Fig. 9. Detonation speed for different E_a and q_0 ($A = 10^6$).

The results from both groups of tests all proved that the speed and structure of self-sustained detonation depend upon the chemical reaction kinetics.

Relationship between speed of detonation and chemical reaction kinetics

Speed of detonation is actually an eigenvalue of self-sustained combustion system. When the speed of detonation is determined, the structure of detonation will be fixed [9]. The results above have showed that there is a close relationship between the speed of detonation and chemical reaction kinetics. Now we are searching for the relationship. To this end, three groups of simulations were performed. Each group corresponds to a value of combustion heat. In the same group of simulations, the activation energy of (6) is varying from E_a = 10.0 to E_a = 30.0. For all the simulations, the pre-exponential factor is kept the same.

The results of the three groups are summarized on the Fig. 9. In order to generalize the outcomes, all the speeds of detonations are normalized by their own C-J detonation speeds. From the figure we observe as E_a decreases the detonation tends to the a C-J detonation. It is supposed that there is an activated energy which makes the detonation be C-J detonation. If it is true, the C-J detonation is only one of the many possible self-sustained detonations. However, this still needs to be proved theoretically.

On the contrary, however, if E_a becomes larger the detonation will move faster than its C-J detonation. In the other words, the speed of detonation is getting faster with the increase in the activation energy. The quantitative variations of the detonation speeds are displayed on the figure. It is found that the maximal increment of the detonation speed against the C-J detonation speed is about 28% of the cases of the simulations in this work.

Comparison of the solutions of eigenvalue problem

Recently Liu proposed a new theoretical model for generally steady combustion wave propagations [9]. The theoretic model is an eigenvalue problem mathematically. According to this model, the modes of the combustion wave propagations are on discrete distribution. Through solving for this model, we can obtain all the possible self-sustained combustion waves.

Applying the theoretic model to the case of the parameters, $q_0 = 5.0$, $A = 2\times10^5$, $E_a = 15$, and $\gamma = 1.32$, a set of steady self-sustained detonations, corresponding to the parameters are obtained which are all with faster speeds than C-J detonation. The eigenvalue problem gives all the possible solutions of the steady waves, while which one physically occurs, is a problem of the eigen solution realization. In these eigenvalues there is only one which is very close to the speed of detonation produced by the Cauchy problem. Also, the structures of detonations produced by both problems are almost identical. Figure 10, below, shows the speeds of detonations by the eigenvalue approach, the Cauchy problem and C-J detonation.

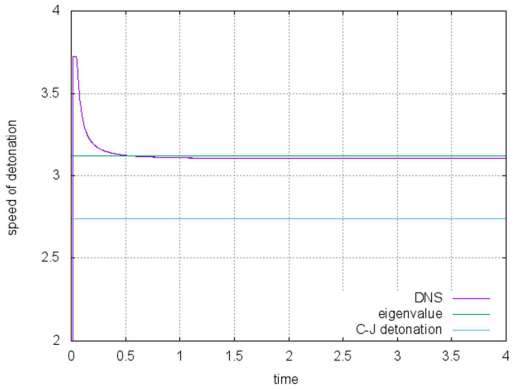


Fig. 10. Comparison of the speeds of detonations produced by DNS, predicted by the eigenvalue problem and its C-J detonation ($q_0 = 5.0$, $A = 2\times10^5$, $E_a = 15$, and $\gamma = 1.32$).

CONCLUSIONS

Two approaches were applied to study the self-sustained detonation. The results produced by both approaches are consistent and identical.

The results of numerical simulations show that there exist the quasi steady self-sustained detonations other than C-J detonations. The speed of quasi steady self-sustained detonations is

dependent on the rate of chemical reactions, that is, the speeds of detonations would be different when their reaction rates are not the same, although the heat released by all the reactions is the same.

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