研究論文

A Simplified Analysis on The Magic Numbers in Detonation

by Hiroyuki MATSUI and Mitsuo KOSHI

Analytical calculations with simplified models of detonation have shown the good agreement with the experimentally observed critical conditions for initiating directly an unconfined spherical detonation. The relation between the cell size of detonation propagating in straight tubes and the critical tube diameters, i.e., experimentally observed magic number 13 is well reproduced theoretically in a stoichiometric mixture of hydrogen and oxygen over the initial pressures of 0.1 to 5 atmospheres. The nature of the magic number seems to be explained by the relation of local and bulk detonability limits caused by the physical loss terms due to the boundary conditions.

1. Introduction

Physical or chemical constants (or quasi−constants) which are universally valid for a variety of experimental conditions have sometimes appeared too difficult to explain by the existent theories, thus they are often called "magic numbers". Examples can be found in the field of detonation studies ; it has been long discussed why the circular tubes must have a diameter d_c large enough to accomodate at least 13 transverse waves for directly initiating an unconfined spherical detonation if the tube is connected to a large volume vessel[1)-3)], i.e.,

$$d_c = M_1 \lambda \quad (M_1 \cong 13) \tag{1}$$

where, λ is the maximun width of the transverse waves. Usually the trace of the interacting transverse waves appers regular cellular feature, so λ is often called "cell size". Unfortunately, no clear explanation of the physical and/or chemical reason for this magic number has come out so far.

Also for many fuel−oxygen mixtures, Westbrook and coworkers have shown that chemical induction length for onedimensional ZND model, Δ can be well correlated with the cell size λ by multiplying 29[4)], i.e.,

$$\lambda = M_2 \Delta \quad (M_2 \cong 29) \tag{2}$$

Received on October 11, 1989

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where, Δ has been estimated by use of calculated induction delay time τ in an adiabatic, constant volume system then multiplied by the flow speed behind a plane shock wave with C−J velocity. This finding is very useful because one can easily evaluate the critical tube diameter for inducing the direct detonation only by performing rather simple computations of elementary chemical processes. Recent development of the large−scale computers has enabled ones to perform detailed calculations of 2−or 3−dimensional reacting flows and some demonstrations of the local shock wave interactions leading to the cellular structures in detonation waves have been reported[5)-7)].

Although these experimental and computational works have suggested that there exists a close correlation between the chemical reaction rates and the cellular structure of the detonation, trials of the physically or chemically based explanations for these magic numbers seem not yet successful. The present study has been undertaken in order to investigate the nature of these magic numbers, i.e., the critical conditions of the propagation of detonation by using simplified fluid dynamic models. Such simplifications may introduce some uncertainties in the calculated results and the discussions may be limited to a qualitative level, however, it will be advantageous for exploring the relations between the chemical reactivity and the local and global propagation limits more clearly rather than performing time consuming com-

putation of the fluid dynamic conservation equations. As for the chemical reactions, on the other hand, it is desirable to employ the exact expressions for the rates of heat release behind strong shock waves of fuel−oxygen mixture, because the test have to be performed over a wide range of experimental conditions, if otherwise, the chemical term can introduce too much uncertainties (because of its nonlinear nature) for making discussions of the critical condition. Thus, a stoichiometric mixture of hydrogen and oxygen has been employed as a test of the investigation, since the reaction mechauism of it is considered as almost established. Detailed elementary reactions for the mixture haves been numerically solved simultaneously with the simplified fluid dynamic conservation equations.

2. The model and the analyses for direct transition of a planar to a spherical detonation

A conceputual model for expressing the transition of a planar to a spherical detonations is illustrated in Fig.1. If the incident detonation propagating in a circular tube is well above the critical condition for the transition, the detonation front starts to expands semispherically at the exit to free volume, as is shown in Fig.1−a. In contrast, the detonation front starts to shrink at the exit as is shown is Fig.1−b, if it is below the critical condition because the loss term caused by the Prandtle−Meyer expansion overwhelms its ability of recovering to the selfsustained propagation of detonation. From these considerations, the critical condition for the direct transition of a planar to spherical detonation should be just in the intermediate of these two cases and may be illustrated as shown in Fig.1−c. The planar detonation propagating in a circular tube with a critical tube diameter d_c is assumed not to change its cross section even after it starts to propagate in a unconfined situation at its critical condition. This situation is, of course, unrealistic since the free detonation surrounded by explosive gas mixture is rather unstable and so, cannot keep its cross section constant very long. According to this simplified critical condition, a planar detonation wave propagating in a tube with a constant cross section will suffice a loss of mass when the surrounding wall is suddenly removed, and the averaged loss term behind a planar detonation front can be easily evaluated by formulating the following conservation equations

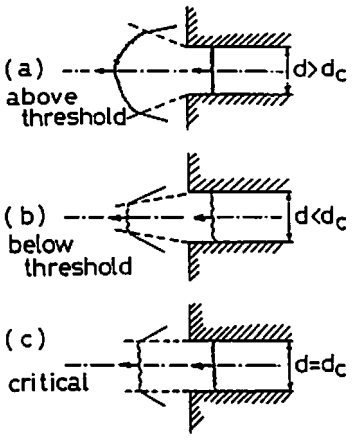

Fig. 1 Conceptual illustrations of the transition of a plane to a spherical detonation.

for a steady free detonation[8].

mass conservation : $d(\rho uA)/dz=0$ (3)

momentum conservation :

$$d[(\rho u^2+p)A]=pdA/dz \quad (4)$$

energy conservation :

$$udu/dz+C_p dT/dz-\Sigma_j(\Delta h_j)dY_j/dz=0 \quad (5)$$

where, ρ is the total density of gas mixture, u the flow velocity for the coordinate fixed to the shock front, A the coss section area of the reactive flow, p the pressure, z the distance from the shock front, C_p the averaged specific heat under constant pressure, T the temperature, Δh_j the heat of formation of jth species per unit mass, and Y_j the mass fraction of the jth species, respectively. The equation governing chemical reactions is given by,

$$dY_j/dz=(m_j/\rho)dC_j/dz \quad (6)$$

where, m_j and C_j denote the molecular weight and molar concentration of jth species, respectively. Equations (3) − (6) can be rewritten in the following forms ;

$$dp/dz=[(\gamma-1)\rho M^2/(M^2-1)]\,[dQ/dz-\xi_1] \quad (7)$$

and

$$\xi_1=[a^2/(\gamma-1)]\,d(\log A)/dz \quad (8)$$

where, γ is the ratio of specific heats, a the frozen sound speed, and M the local Mach number defined as, M=u/a, respectively. ξ_1 (the averaged loss term caused by the free expansion) has been simultaneously evaluated by use of Newton approximation,

$$p=p_0+\rho_0 D^2(dA/dz)^2/[1+(dA/dz)^2] \quad (9)$$

where, p_0, ρ_0, and D denote the initial pressure, initial density, and the steady detonation velocity, respective

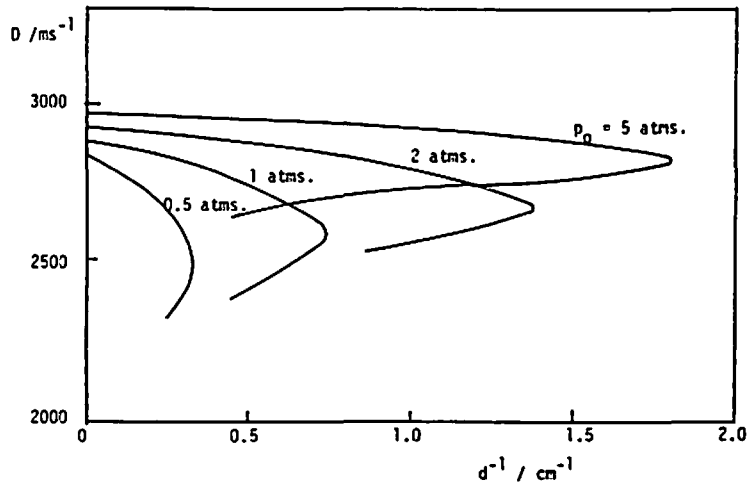

Fig. 2 Calculated results on the detonation velocity with free boundary for a stoichiometric mixture of H_2 and O_2

ly. The rate of heat production by the chemical reactions per unit mass,

$$dQ/dz=\Sigma_j(\Delta h_j)dY_j/dz \qquad (10)$$

has been also solved simultaneously. The elementary reactions used in this study are the same as those of Westbrook[9]. As the dissociation and recombination of HO_2 are expected to be in the fall−off region at high pressures[10], the present calculations are limited only for the low pressure range ($p_0=0.1-5$ atmospheres) where the rate constants at low pressue limit can be used. Equations (7)−(10) have been integrated by using Gear's method with an assumed value of D by which an initial condition is given by Rankine−Hugoniot relations for nonreactive flow. Search for the eigenvalue D has been continued until the generalized C−J condition,

$$dQ^*/dt=\xi_1^* \qquad (11)$$

has been satisfied, where the asterisk denotes quantities at the C−J condition : M=1. During the integration, γ has been reevaluated in each integral step, although it is assumed as a constant in the derivation of Equation (7). As the variation of γ is very small, such approximation has not brought significant errors. The results of the present calculations on the detonation velocity is shown is Fig.2 against the inverse of the tube diameter, d^{-1}. The solutions give dual−eigenvalues for D for a fixed tube diameter. The higher values of the solution on D agrees very well with that calculated by using ideal C−J theory at sufficiently large tube diameters. Also it is shown that no solution exist for $d<d_c$, thus d_c is decided theoretically for free detonation. As shown in Fig.3, the calculated results on d_c agrees very well with the experiment by Matsui and Lee[11]; the present model for expressing the critical condition of the direct initiation of a spherical detonation seems reasonable. Also the calculated magic number M_1 ($=d_c/\lambda_e$) is shown in the same figure, where, λ_e is the cell size decided in the experimental work by Manzhaley et al[12]. In this work, the mean value of λ_e has been given by the following form,

$$\log \lambda_e=-0.969 \log p_0-0.878$$

where, λ_e and p_0 are expressed in cm and atms. units, respectively. It is found that the limit of the propagation of free detonation agrees very well with a condition of $d_c/\lambda_e=13$ for the wide range of initial pressures. So, as far as empirical cell size is admitted, it may be reasonable to conclude that the magic number M_1 can be roughly explained by the present simplified analysis, at least for the detonation of the stoichiometric mixture of hydrogen and oxygen.

3. Discussion of the local cellular structure of detonation in a straight tube

Evaluation of the size of the cellular structure in detonation wave traversing in a straight tube is essentially difficult since one should solve nonsteady three dimensional conservation equations coupled with many elementary reactions. According to the detailed examination of the detonation structure propagating in a tube, both experiment[13] and computation[7] suggest that the interactions of traversing waves normal to the tube axis periodically produce local explosions,

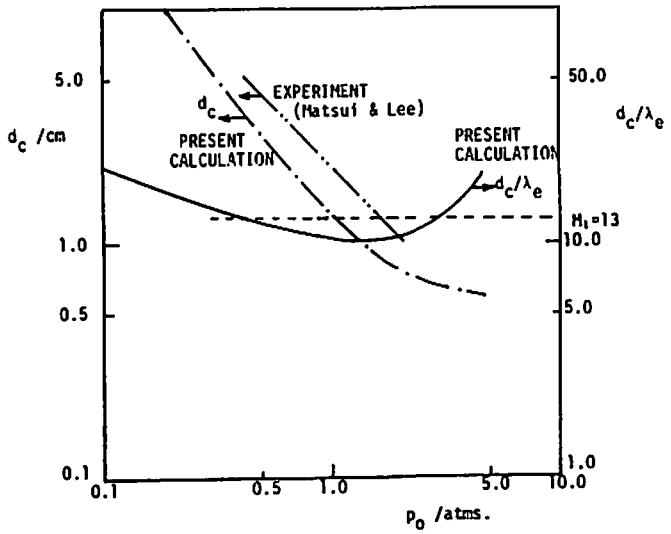

Fig. 3 Comparisons of the calculated critical tube diameter and the magic number, $M_1=d_c/\lambda_e$ with experiment in a stoichiometric mixture of H_2 and O_2.
(d_c by present calculation ;—·—, d_c by experiment by Matsui and Lee ;—··—,d_c/λ_e by present calculation ;——)

and so the detonation front is composed of such many local explosions associated with curved shock fronts (see Fig.4). Thus, it may be interesting to investigate the nature of this microscopic explosion associated with a curved shock front.

By using an assumption of axial symmetric flow behind a spherical leading shock front, the conservation equation of mass along the symmetric axis for steady flow is approximately expressed by[14] ;

$$d(\rho u)/dz=-2\rho(D-u)/(R_s-z) \quad (12)$$

where, R_s is the radius of the leading shock front. Together with the conservation equations for momentum and energy, the following ordinary differential equation is derived.

$$dp/dz=[(\gamma-1)\rho M^2]/(M^2-1)[dQ/dz-\xi_2] \quad (13)$$

and,

$$\xi_2=2a^2(D-u)/[(\gamma-1)(R_s-z)u] \quad (14)$$

where, ξ_2 denotes the loss term caused by the flow deflection behind nonplanar leading shock front. The solutions of Equations (13) and (14) can be obtained by the same procedure as discussed in the previous section. A generalized C−J condition,

$$dQ^*/dz=\xi_2^* \quad (15)$$

is satisfied at M=1 when an exact eigenvalue of the detonation velocity is given as an initial condition.

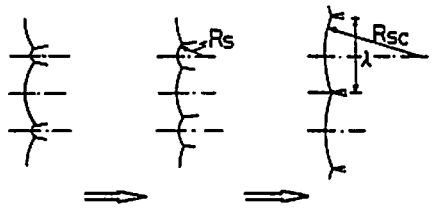

Fig. 4 The model for describing the propagation of the local explosion of detonation.

The calculated detonation velocity is shown in Fig.5 against nondimensional shock radius, R_s/λ_0. The critical condition for sustaining steady propagation of detonation is found to lie in the range,

$$R_{sc}/\lambda_0=2.5-5 \quad (16)$$

for the stoichiometric mixture of hydrogen and oxygen with initial pressures, $p_0=0.1-5$ atmospheres, where R_{sc} denotes the critical shock wave radius for realizing selfsustainance of a steady detonation.

The physical meaning of solving Equation (13) is to evaluate the approximate magnitude of loss term caused by the curved shock front which characterize the microscopic structure of the detonation wave propagating in a straight tube, so, it is assumed in this study that R_{sc} represents the shock wave radius when the microscopic cellular structure is at its maximum

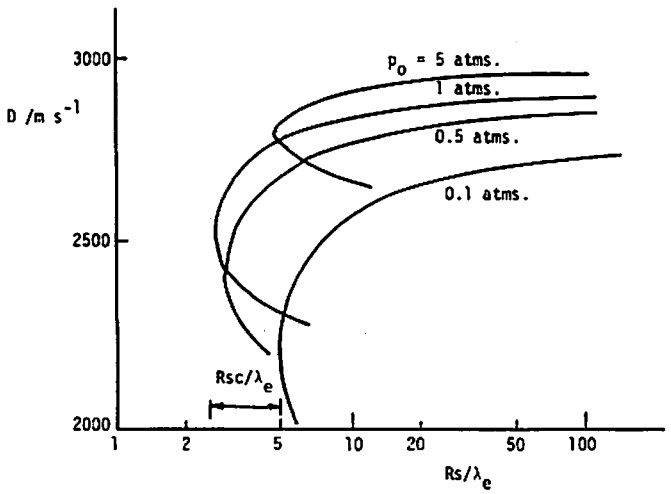

Fig. 5 The calculated detonation velocity with a spherical leading shock front in a stoichiometric mixture of H_2 and O_2.

size. One should then decide a coefficient k which is defined as,

$$k=R_{sc}/\lambda \quad (17)$$

from the theoretical consideration. As λ represents the maximum width of the periodically produced transverse waves, the inclination of the shock front must not be too large in order to initiate the successive local explosion at the intersection of the adjuscent shock waves. There is a critical condition for the shock wave angle to sustain a subsonic flow behind an oblique shock wave. As this condition corresponds to a strong interaction (so can lead to a local explosion very quickly), it is used to evaluate k in this study, i. e.,

$$k=2\cos\alpha_c \quad (18)$$

where, α_c is the critical angle of the shock wave slope against z axis, and it is easily evaluated by the following equation,

$$\tan[\alpha_c-\sin^{-1}[(\gamma-1)/2\gamma)]^{1/2} = 2\cot\alpha_c \sin 2\alpha_c/(\gamma+\cos 2\alpha_c) \quad (19)$$

The calculation shows that k is approximately equal to 2 when γ is assumed to be equal to that at C−J condition. Calculations on the maximum cell size λ has been performed by using Equation (17) and the results are compared with those of experiment in Fig.6.

The calculated cell size agrees pretty well with the experimental one, λ_e ; this indicates the validity of the assumptions introduced in this study. Thus, it is very likely that the maximum cellular width corresponds,

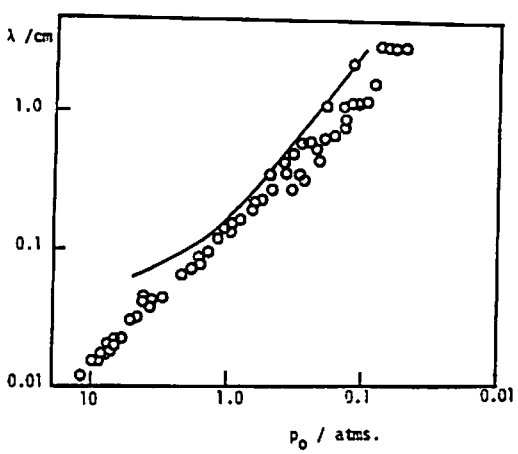

Fig. 6 A comparison of the calculated cell width, λ with experiment (present calculation;——,experimental cell width, λ by Manzhaley et al; ○)

roughly speaking, to the critical condition of the selfsustainance of the microscopic detonation with a spherical leading shock front.

This finding may be explained phenomenologically as follows. The microscopic explosion initiated at the interaction of transverse waves rapidly expands with decaying propagation velocity until $R_s=R_{sc}$, where the propagating shock waves have an ability of producing new explosions if it is still sufficiently strong enough to sustain detonation by itself. So, in a so called steady detonation, there seems to occur a

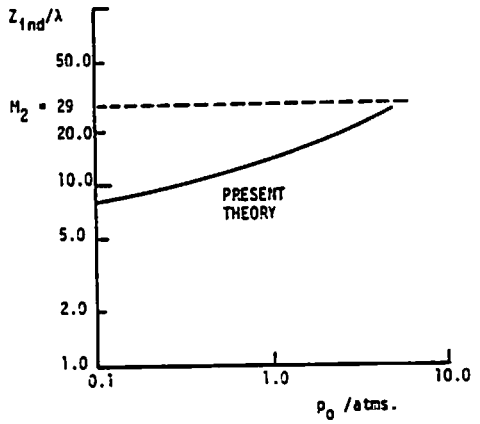

Fig. 7 Pressure dependence of the calculated magic number, $M_2 = z_{ind}/\lambda$ and comparison with empilical value, 29.

resonance condition for wave production among the microscopic explosions, and this resonance condition seems to be associated with the critical condition of each local explosion.

The velocity of the propagation of the local explosion along z axis, D_m varies in the range, $D_i > D_m > D_c$, where, D_i and D_c denote the initial and the critical detonation velocity, respectively. Of course, the time and space averaged value of D_m should correspond to the macroscopic detonation velocity, D, but no theoretical evidence can be supplied in this point.

In Fig.7, the calculated result on the second magic number, $M_2 = \lambda/z_{ind}$ is shown against initial pressure p_0. Here, z_{ind} is the computed induction length which is defined as the reaction length required for the achievement of 5% increment of temperature. The present result indicates that λ/z_{ind} is about 8 at $p_0 = 0.1$ atms. (28% of $M_2 = 29$ given by Westbrook[4]), but the agreement becomes better as p_0 increases. The difference of the magnitudes on M_2 however, seems not serious because both the temperature and pressure histories along which chemical kinetic equations are integrated are different each other.

4. Conclusion

From the above discussions, it is suggested that the local cellular structure of detonation propagating in a straight tube is caused by the quasiresonant behaviour of the interacting transverse waves which is represented by a spherical leading shock front in this study. The resonant nature is likely to be strongly related to the critical condition for the selfsustainance of microscopic explosions.

The bulk nature of the propagation of quasisteady detonation, on the other hand, can be expressed pretty well by the onedimensional ZND model even in describing the critical condition for the direct initiation of a spherical detonation.

Thus, it is likely that the magic number $M_1 = 13$ is the representation of the relation between the microscopic and the macroscopic limits of selfsustainance of detonation.

However, the validity of the models and the assumptions have been tested only for a stoichiometric mixture of H_2 and O_2 at present. If the same conclusion is obtained for the different fuel−oxygen mixtures as well, the conclusion of this study will become more evident.

Also the elementary reactions associated with HO_2 used in this study seems insufficient for describing the rate of chemical energy release at higher pressure range. The successive studies including some hydrocarbons−oxygen mixtures with modified elementary reactions are now being continued.

References

1) Mitrofanov, V. V., and Soloukhin, R. I., Sov. Phys. Dokl. 9, 1055 (1964)
2) Edwards, D.H., Thomas, G. O., and Nettleton, M.A., J.Fluid Mech. 95, 79 (1979)
3) Lee, J.H., Knystautas, R., and Guirao, C.M., Proceedings of The International Specialist Meeting on Fuel−Air Explosion, Montreal, Canada, p.157, University of Waterloo Press, (1982)
4) C.K.Westbrook, The Chemistry of Combustion Processes ed.by T.M.Sloane, ACS Symposium Series 249, p.175, (1983)
5) Taki, S.and Fujiwara, T., AIAA J., 16, 73 (1978)
6) Taki, S. and Fjiwara, T., Proceedings of 18th Symp. (international) on Comb., p.1671, The Combustion Inst. (1981)
7) Reddy, K.V., Fujiwara, T., and Lee, J.H., Memories of Faculty of Engineering, Nagoya Univ., 40, No.1 (1988)
8) Tsuge, S., Furukawa, H., Matsukawa, M., and Nakagawa, T., Astronautica Acta, 15, 377 (1970)
9) Cobos, C.J., Hippler, H., and Troe, J., J.Phys.Chem., 89, 342 (1985)

10) Westbrook, C.K., Fuel－Air Explosions, ed. by Lee, J.H.S. and Guirao, C.M., Univ.of Waterloo Press (1982), p.189
11) Matsui, H. and Lee, J.H., 17th Symp. (International) on Comb., p.1269 The Combustion Inst.(1979)
12) Manzhaley, V.I., Mitrofanov, V.V., and Subottin, V.A., Fiz.Goren.Vzr., 10, 102 (1974)
13) Takai,M., Studies on The Gaseous Detonation, Ph.D.Thesis (in Japanese) (1974)
14) Matsui, H., Moritani, A., Yoneda, K. and Asaba,T., Proceedings of 8th Symp. (International) on Detonation, p.168 NSWC MP 86－184 (1985)

爆轟におけるマジックナンバーの評価について

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簡単なモデルにより酸水素系の爆轟限界を計算した結果，直接起爆条件は自由壁の爆爽に対応する限界爆轟直径と良く一致することが見出された。更に微細な爆爽のセル構造は球面衝撃波を伴う爆轟限界と良い対応を示している。これらのことから爆轟限界におけるセル構造の数が約13である理由は微視的な球面衝撃波を伴う局所的爆発が準定常的にくり返し発生可能な限界と巨視的な平面波で近似される爆轟波の定常な伝播限界における両者のスケール効果を反影していると解釈できる。

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