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Half-Cell Law of Regular Cellular Detonations *

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Numerical simulations illustrate the half-cell law of regular cellular detonations propagating in confined space, i.e., the number of cells always maintains an integral multiple of half cell. The cells adapt themselves larger or smaller to the size of the unconfined space by maintaining the cell scale larger or smaller than the original cells of detonation.

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During the propagation of cellular detonations, multi-wave detonation fronts will leave a special cellular pattern on the smoked foil placed in the test section, which is regarded as the tracks of high-speed shear forces originated from triple-point in the multi-wave detonation front.[1,2] Commonly, the cell size is one of the characteristic gas dynamic parameters for regular cellular detonations and depends mainly on the properties and initial thermo-states of gaseous mixture.[3] Numerical studies on the regular cellular detonation have shown that the size of cell finally reaches to a roughly constant value which does not depend on the initially artificial perturbations.

Neither in experiments nor in numerical simulations, it is seldom considered to choose the width of test sections or computational domains to be an integral multiple of the cell scale. However, both the numerical and experimental cellular patterns take a quite regular form in the whole region where the cellular detonation propagates. This implies that the cellular detonation has an inherent ability to adapt to the width of domain. It is believed that the self-organized generation of the transverse waves plays an important role in the cellular pattern variations, but no further studies were reported to clarify such a fundamental issue in detonation physics.

The numerical simulations were carried out by solving the two-dimensional Euler equations with one-step chemical reaction model. The key parameters in the chemical reaction model are the reaction rate, the active energy, the equilibrium constant and the molar weight ratio of the reactant to the product. Two-dimensional Euler equations in Cartesian coordinates can be expressed as

$$\frac{\partial}{\partial t}\begin{bmatrix}\rho\\ \rho u\\ \rho v\\ \rho E\\ \rho\lambda\end{bmatrix}+\frac{\partial}{\partial x}\begin{bmatrix}\rho u\\ \rho u^2+p\\ \rho uv\\ (\rho E+p)u\\ \rho\lambda u\end{bmatrix}+\frac{\partial}{\partial y}\begin{bmatrix}\rho v\\ \rho uv\\ \rho v^2+p\\ (\rho E+p)v\\ \rho\lambda v\end{bmatrix}=\begin{bmatrix}0\\0\\0\\0\\S\end{bmatrix}, \tag{1}$$

where ρ, p, u, v are the density, gas pressure, velocities in x and y directions, respectively; λ represents the progressive variable measuring chemical reaction and S is the chemical reaction source term. E denotes the total energy of the gas mixture and is defined as

$$E=\frac{p}{(\gamma-1)\rho}+\frac{1}{2}(u^2+v^2)+(1-\lambda)Q, \tag{2}$$

where γ is the specific heat ratio and Q is the chemical reaction heat released per unit mass of reactants. For one-step reversible chemical reactions, source term S can be expressed as

$$S=(1-\lambda)\cdot k_f\cdot e^{E_a/R_oT}-\lambda\cdot k_b\cdot e^{E_a/R_oT}, \tag{3}$$

where k_f and k_r represent the forward and the reverse reaction rate, respectively. E_a, R_o, and T in Eq. (3) are the active energy, the general gas constant, and the gas temperature T is calculated by

$$p/\rho=[(1-\lambda)R_A+\lambda\cdot R_B]T, \tag{4}$$

where R_A and R_B are the gas constant for the reactant and the product, respectively. For a reversible chemical reaction, $k_r=k_f/\pi_e$, where π_e is the equilibrium constant. In this reaction model, the reactive gas mixture is described by the constant parameters k_f, π_e, E_a, Q, γ, R_A, and R_B, as well as the initial state parameters p_0, ρ_0, and T_0.

The convective terms of the governing equations are discretized with the DCD finite difference scheme of a 2th order precision both in space and time:

$$\begin{aligned}\frac{\Delta \boldsymbol{U}}{\Delta t}=&-\frac{1}{\Delta\xi}\big(\boldsymbol{F}^+_{i+1/2,L}-\boldsymbol{F}^+_{i-1/2,L}+\boldsymbol{F}^-_{i+1/2,R}\\&-\boldsymbol{F}^-_{i-1/2,R}\big)-\frac{1}{\Delta\eta}\big(\boldsymbol{G}^+_{j+1/2,L}-\boldsymbol{G}^+_{j-1/2,L}\\&+\boldsymbol{G}^-_{j+1/2,R}-\boldsymbol{G}^-_{j-1/2,R}\big)+\hat{\boldsymbol{S}},\end{aligned} \tag{5}$$

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where

$$\boldsymbol{F}^{+}_{i+\frac{1}{2},L} = \boldsymbol{F}^{+}_{i} + \frac{1}{2}\boldsymbol{\Phi}_A \min\mathrm{mod}\{\Delta\boldsymbol{F}^{+}_{i-\frac{1}{2}}, \Delta\boldsymbol{F}^{+}_{i+\frac{1}{2}}\},$$
$$\boldsymbol{F}^{-}_{i+\frac{1}{2},R} = \boldsymbol{F}^{-}_{i+1} + \frac{1}{2}\boldsymbol{\Phi}_A \min\mathrm{mod}\{\Delta\boldsymbol{F}^{-}_{i+\frac{1}{2}}, \Delta\boldsymbol{F}^{-}_{i+\frac{3}{2}}\},$$
$$\boldsymbol{G}^{+}_{j+\frac{1}{2},L} = \boldsymbol{G}^{+}_{j} + \frac{1}{2}\boldsymbol{\Phi}_B \min\mathrm{mod}\{\Delta\boldsymbol{G}^{+}_{j-\frac{1}{2}}, \Delta\boldsymbol{G}^{+}_{j+\frac{1}{2}}\},$$
$$\boldsymbol{G}^{-}_{j+\frac{1}{2},R} = \boldsymbol{G}^{-}_{j+1} + \frac{1}{2}\boldsymbol{\Phi}_B \min\mathrm{mod}\{\Delta\boldsymbol{G}^{-}_{j+\frac{1}{2}}, \Delta\boldsymbol{G}^{-}_{j+\frac{3}{2}}\}.$$

In the above equations, ΔF^+ and ΔG^+ represent the forward differencing of F and G, $\Delta F^-, \Delta G^-$ represent the backward one, and

$$\boldsymbol{\Phi}_A = \boldsymbol{I} \mp \frac{\Delta t}{\Delta\xi}\boldsymbol{\Lambda}^{\pm}_A, \quad \boldsymbol{\Phi}_B = \boldsymbol{I} \mp \frac{\Delta t}{\Delta\eta}\boldsymbol{\Lambda}^{\pm}_B. \tag{6}$$

The "min mod" function is defined as

$$\min\mathrm{mod}(x, y) = \mathrm{sgn}(x) \cdot \max\big\{0, \min[|x|, y\mathrm{sgn}(x)]\big\}. \tag{7}$$

Initial conditions of the gas mixture are taken to be the pressure $p_0 = 1\,\mathrm{atm}$, the temperature $T_0 = 300\,\mathrm{K}$, the polytropic exponent $\gamma = 1.4$ The parameters of chemical reactions are specified as $E_a = 24\,\mathrm{kJ}$, $\pi_e = 20$, $k_f = 8.5 \times 10^8$, $Q = 1.58 \times 10^6\,\mathrm{J}$, and $R_A = R_B = 287.096\,\mathrm{J/(mol\,K)}$.

Figure 1 shows the present physically-simplified test case and its computational domain. It is a two-dimensional channel with a thin splitting plate. The channel width is H, and the distance h, between the splitting plate and the upper channel wall is adjustable to produce two separated channels with the required width. The initially cellular detonation with a certain number of regular cells propagates from left to right and it is pre-computed with a long time so that the quasi-steady propagating state could be reached. Once the detonation enters into the two separated channels whose width is not exactly an integral multiple of half cell, the self-organized generation of the transverse waves will take place, and result in different cellular patterns related with h variations.

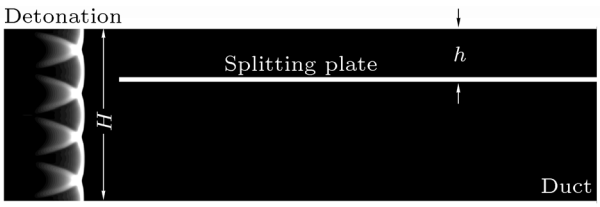

Fig. 1. Problem specification and computational domain.

In the present test case, the total channel width $H = 2.5\,\mathrm{mm}$ and the distance h is taken to be a variable parameter for different numerical experiments. The whole channel is initially charged with a combustible gas mixture and the chemical reaction progress variable is set to be $\lambda = 0$. At the inflow boundary, a two-dimensional cellular detonation is specified in the upstream position of the splitting plate based on the pre-computation, and its cell size is $l = H/4 = 0.625\,\mathrm{mm}$. Slip boundary conditions are applied on the channel walls and the non-reflection condition is applied at the outflow boundary.

The different cellular patterns are obtained by varying the distance h between the splitting plate and the upper channel wall. Three physical issues which may interact with each other in different ways are examined and discussed in detail. The first one is the total number of the cells along cross-section with the variation of the channel width. Whether or not the cell number variation meets the integral multiple of half-cell will be demonstrated by checking the total number in each experiment. The second one is the critical cell size: the maximum size and the minimum size between which the cellular detonation could be sustained without cell bifurcation or merging. The last one is the variation of thermo-dynamic parameters while the cell becomes larger or smaller. The effort will be made to explore the mechanism of the self-reorganized generation of transverse waves. It is believed that the self-reorganized generation of the transverse waves induces cell bifurcation or mergence and makes the cells adapt to the channel passage in which the cellular detonation propagates.

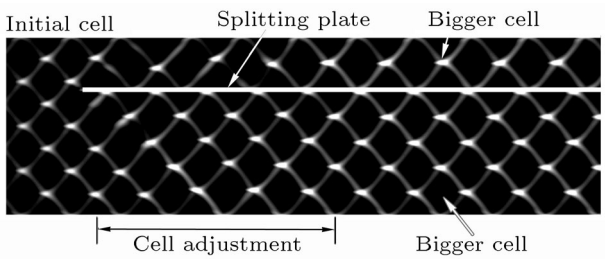

Fig. 2. Cellular structures recorded by shock pressure for $h/l = 1.2$.

The first numerical experiment was carried out by setting $h/l = 1.2$, and the cellular pattern of the numerical results is plotted in Fig. 2. The cellular pattern is computed by recording the historical pressure peaks. There are obvious three parts in this figure: the left part is the initially cellular pattern before the detonation front reaches the splitting plate, the middle part shows irregular cells which indicate a transition region, and the right one shows a quasi-steady propagation of the transmitted detonation. It is observable that the total number of the cells is 4 in the left parts, but 3.5 in the right part. There is only one cell in the upper channel, and two and half cells are in the lower channel. This means that after the self-organization of transverse waves, the total number of cells in the whole channel is reduced from 4 to 3.5. The cell in the

upper channel becomes larger, about 1.2 times larger than the initial cell size. The cells in the lower channel also become larger, but its size is about 1.12 times than the initial cell size. The region where the irregular cells occur is referred to as the transition region because the self-organization of transverse waves takes place there. The total number of the cells is 3.5 after the detonation reaches a steady state in the two separated channels, and it is seven times of the half cell. This role is referred to as the half-cell law that states the cell number that possibly exits must be integral multiple of the half-cell for a regular cellular detonation.

Figure 3 shows the distributions of dimensionless local maximum pressure $p_{\max}$ along the upper and lower walls of the channel. It is observed that from the left boundary to the front edge of the splitting plane, two curves are overlaid together. After the cellular detonation front enters the separated channel, the shock pressure distributions demonstrate obvious difference, which indicates the detonation transition. Once the detonation regains its quasi-steady state, the shock pressures take the regularly periodic distribution. The local maximum pressure distribution along the upper wall is higher than that along the lower wall, and both of them are higher than that in the initial detonation. The corresponding physical issue observed from Fig. 2 is that the cell size in the upper channel is larger than that in the lower channel, and the both are larger than the initial cell size.

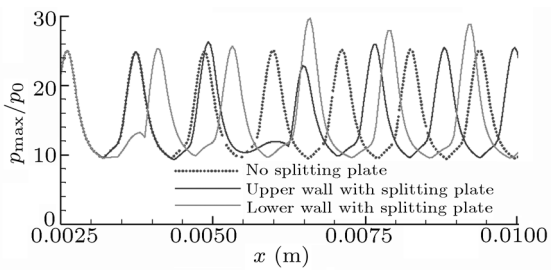

Fig. 3. Local maximum pressure distributions on the walls with $h/l = 1.2$.

The above-mentioned phenomenon is an interesting physical issue that is closely related with the nature of cellular detonations and is reported by Deng *et al.*[4] Generally speaking, for a cellular detonation with a certain cell size, the higher the shock pressure is, the wider the reaction zone is. If the shock pressure is lower, the reaction zone is narrower.

Figure 4 shows the numerical result of the case with $h/l = 1.16$. In this case, the width of upper channel is slightly larger than the size of initial cells. After the self-organization of detonation transverse waves, the number of cell in the upper channel is 1 and the size of the cell increases to 1.16 multiple of the size of initial cells. In the low channel, the number of cells is 3, but the size of the cell diminishes to 0.95 multiple of initial cells. In this case, the total number of detonation cells maintains 4, although the sizes of cells in upper and lower channel have changed. The self-organization of transverse waves inclines to match the 'half-cell' criteria.

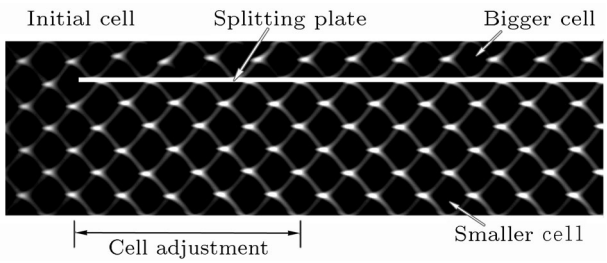

Fig. 4. Cellular structures recorded by the shock pressure ($h/l = 1.16$).

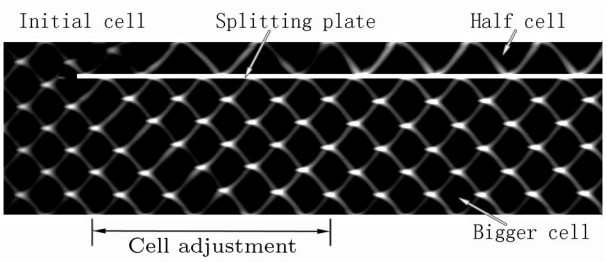

Fig. 5. Cellular structures recorded by the shock pressure ($h/l = 0.82$).

Figure 5 shows the numerical result of the case with $h/l = 0.82$. In this case, the width of upper channel is smaller than the size of initial cells. After the self-organization of transverse waves of detonation, the number of cell in the upper channel is 0.5 and the size of the half cell increases to 1.64 multiple of the size of initial half cell. In the low channel, the number of cells is 3, the size of the cell increases to 1.06 multiple of initial cells. The self-organization of transverse waves inclines to match the half-cell criteria.

In all the above cases with different h/l, the self-organizations of transverse waves of detonation meet the half-cell criteria. New cells may be smaller or larger than the initial cellular structures. For the detonation with regular cells propagating in confined space, the evolution of cellular structures is influenced by the transverse scale of the space, besides the properties of gas mixture and its initial parameters.

Obviously, there are several different modes of the self-organization of the transverse waves, which correspond to the different behaviour of the cellular structure evolution. Some limits may exist between the different modes. In the above cases, with the change of the splitting plate position in the range of 2.5–3.5 multiple of the initial cells, the number of cells in the lower channel may be 2.5 or 3. There is a limit be-

tween the two cellular structure modes. From the numerical results, the limit lies in $h/l = 1.18$. The maximum size of the cell in the lower channel is about 1.128 multiple of the size of the initial cells, which corresponds to 2.5 cells in the lower channel. If the size of the cells increases further, the number of cells in the lower channel jumps to 3 discontinuously.

In conclusion, the self-organizations of transverse waves of a detonation with regular cells take place in confined space, which result in the change of sizes of the cells behind the detonation. The self-organization of transverse waves comes from the collision of the triple-point in the detonation front and inclines to match with the half-cell criteria, that is, the total number of cells always maintains an integral multiple of half cellular cell. According to the half-cell criteria, the size of cellular structures of a detonation in confined space may be larger or smaller than that of the detonation in unconfined space.

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