

Cellular Cell Bifurcation of Cylindrical Detonations *

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Cellular cell pattern evolution of cylindrically-diverging detonations is numerically simulated successfully by solving two-dimensional Euler equations implemented with an improved two-step chemical kinetic model. From the simulation, three cell bifurcation modes are observed during the evolution and referred to as concave front focusing, kinked and wrinkled wave front instability, and self-merging of cellular cells. Numerical research demonstrates that the wave front expansion resulted from detonation front diverging plays a major role in the cellular cell bifurcation, which can disturb the nonlinearly self-sustained mechanism of detonations and finally lead to cell bifurcations.

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The self-sustained cellular detonation has been observed experimentally in reality, and its three-dimensional front structure has intrigued researchers for decades due to its intrinsic characteristics. The cylindrical detonation can also be self-sustained, but its front appears to be more unstable than general detonations as it propagates. Moreover, cellular cells in cylindrical detonations are successively generated in a continuously enlarging detonation front to keep a roughly constant cell scale. The special process is referred to as cellular cell bifurcation and imposes more difficulty in the understanding of general cellular detonation propagation. Furthermore, all the cellular detonation fronts have a spherically-curved front in each cell, and the wave expansion takes apart more or less in their propagation so that the investigation into the cylindrically-diverging detonation could be invaluable in comprehending fundamental mechanisms of detonation propagation and cellular cell evolution.

Experimental observations on cylindrically-diverging detonations were reported widely^[1,2] in detonation research area, and open-shutter photographs taken during cylindrical detonation divergence were obtained. Those experimental works showed clearly the cellular cell bifurcation and the roughly constant cell patterns, but the essential issues underlying the cellular cell bifurcation are still not clear. A large quantity of numerical investigations on one-dimensional axisymmetric or spherical symmetric detonation has been carried out in the past decades.^[3] Preliminary two-dimensional numerical studies of detonation instabilities have also been conducted for diverging cylindrical detonation waves.^[4] In this Letter, we describe the numerical simulation on cylindrically-diverging detonation, which is carried out by solving

two-dimensional Euler equations implemented with an improved two-step model.^[5] Numerical triple-point contrails and other parameters are recorded during the simulation, from which the cellular cell bifurcation and its primary mechanisms underlying the essential physical issues are figured out.

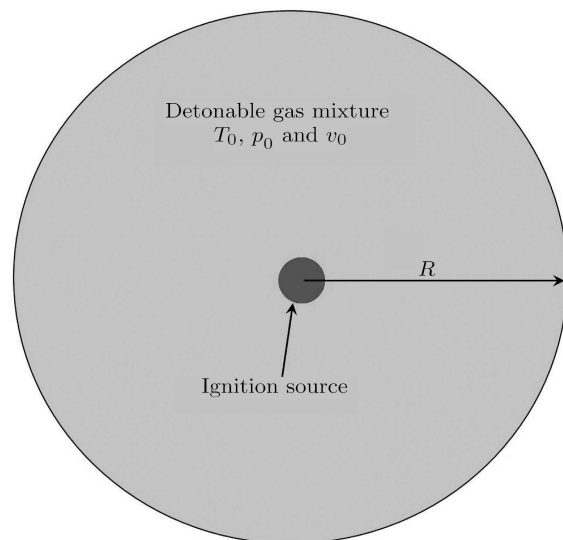


Fig. 1. Computational domain and initial conditions for cylindrically-diverging detonation.

Computational domain and initial conditions for cylindrically-diverging detonation are schematically shown in Fig. 1, where R is the radius of the computational domain filled with a detonable gaseous mixture at a given initial thermo-state. The ignition source is a small column of hot burnt gases from the burst of which a strong cylindrical blast wave will be driven out. The direct initiation is applied here to avoid a long DDT process. Here we take T_0 , p_0 and v_0 standing

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for initial temperature, pressure and velocity, respectively.

In our numerical experiments, the hydrogen and oxygen mixture with the equivalent ratio of 2:1 is filled into the domain, with the initial state of $p_0 = 1.0$ atm, and $T_0 = 293.0$ K. By assuming flow symmetry, the computational domain is simplified as a 30° annular region with an outer radius of 15.5 cm and an inner radius of 0.5 cm to avoid the problem of singularity. Orthogonal grids in the cylindrical coordinate system are applied to this problem, with 3000 grid points uniformly distributed in radial direction and 1000 in circumferential direction.

Figure 2 shows the numerical cellular cell pattern from which the initiation effect of the strong blast wave on the cell pattern is observable in the central area, but decays very quickly in a short time. Beyond the transient region between 20 mm and 40 mm, the cellular cell scale appears to keep a roughly similar size. This indicates that the numerical cellular detonation has been fully developed. By comparing this cell pattern with the experimental open-shutter photographs,^[1,2] the same cellular cell bifurcation process is identified, which indicates a self-organized regeneration of transverse waves. Actually, the cells grow larger as the detonation front expands, and the cell bifurcations resulted from the new transverse wave generation take place when the cells become sufficiently large. From this result, three main modes for the cellular cell evolution are identified, as marked in

Fig. 2, and the detailed descriptions and explanations will be stated as follows.

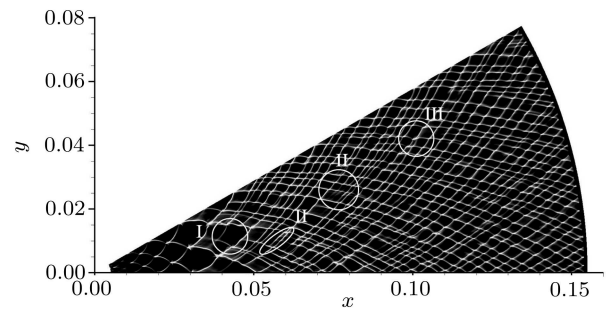


Fig. 2. Cellular detonation cell pattern of cylindrically-diverging detonation.

The first mode of the cellular cell bifurcation is referred to as concave front focusing as shown in Fig. 3. As the detonation front expands cylindrically, the continuously-decaying leading shock results in detonation front decoupling which slows down chemical reactions and makes the front concavely curved. Once the concavely-shaped front develops, the reaction zone and leading shock converging effect becomes dominant, which induces a positive feedback between chemical reactions and the leading shock. More and more energy is concentrated and released in the concave reaction zone, and finally a local explosion takes place. The explosion pushes the leading shock forward and leads to generation of a new pair of triple points shown in Fig. 3(c), where the cell bifurcation takes place.

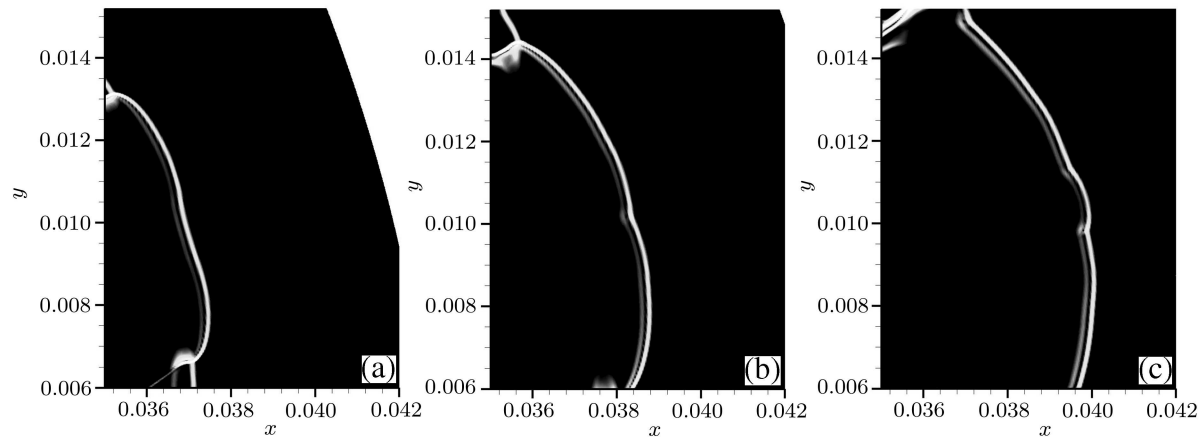


Fig. 3. Wave front configurations at three instants, showing the evolution of concave front focusing.

The second mode is named as kinked and wrinkled wave front evolution, and considered to be the result of front instability. When the wave front curvature becomes sufficiently large, the wave expansion induces decoupling of the leading shock and the chemical reaction zone. Thus, the deformed wave front becomes kinked or wrinkled, as shown in Figs. 4(a) and 4(b), respectively. For the kinked wave front, a

strong perturbation at the joint point of the decoupled and un-decoupled wave front is generated and moving along the detonation front. As the kinked front moves, a triple point is induced from detonation re-ignition. There are two stages observable during the period of mode II: the first stage is development of the deformed detonation front, and the second one is re-ignition of a pocket of explosive gases from which a single triple

point is formed. The wrinkled wave front may contain more transverse perturbations and several single triple-points can be generated, but the fundamental mechanisms appear to be the same with that of kinked wave front.

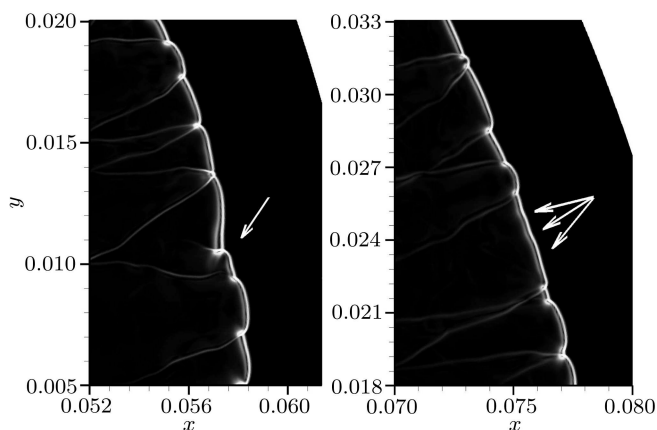


Fig. 4. Wave front configurations of mode II: (a) kinked wave front, (b) wrinkled wave front.

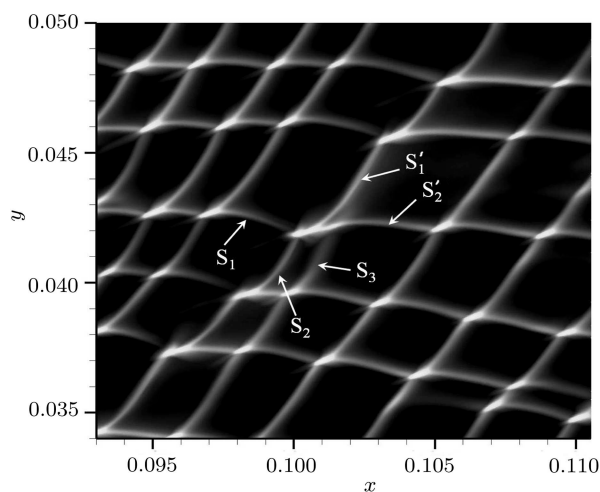


Fig. 5. Detonation cell pattern of mode III, showing self-merging of cellular cells.

The key characteristics of the third mode are shown in Fig. 5, in which three triple-point trajectories are denoted by S_1 , S_2 and S_3 , respectively. With movements of triple points, only two clear trajectories

can be captured, named as S'_1 and S'_2 . This means that two original cells merge into one cell during cell evolution of cylindrically-diverging detonations. Therefore, this mode is named as self-merging of cellular cells. If carefully checking Fig. 5, the two triple points, moving along S_2 and S_3 , propagate in the same direction. Intensive chemical reactions behind the first triple point induces a large amount energy released which increases the thermal state parameters and leaves more exhausted gas in front of the following triple point. Such an environment change weakens the strength of the second triple point and leads to the transformation from a strong triple structure to a weak compression perturbation that diminishes later. Finally, one triple-point disappeared and other two remained to be observable. Cellular cells merging in this mode is caused by triple point interaction because of cell size limitation.

In conclusion, the numerical simulation of cylindrically diverging cellular detonation has been performed successfully, three main modes for the cellular detonation cell evolution have been figured out and referred to as concave front focusing, kinked and wrinkled wave front instability, and self-merging of cellular cells, respectively. The main mechanism results from the detonation self-sustained property that is highly nonlinear and sensitive to flow expansion behind a detonation front. The flow expansion resulting from detonation front diverging is found to be a key factor in cellular cell bifurcation, from which the concave, kinked and wrinkled wave fronts develop. The self-merging of cellular cells is induced by the triple-point interaction in which the two triple points move in the same direction, and acts to remove smaller cellular cells and keep all the cellular cells in a roughly same size.

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