Computing Detonations

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Stable Detonations

Detonation modeling begins from the Chapman-Jouguet (CJ) theory [1-4] that appeared more than a hundred years ago and considered an ideal one-dimensional (1D) steady-state detonation wave from the point of view of thermodynamics. The theory does not provide any details about the reaction zone of the detonation wave, but it defines the ideal detonation velocity D_{CJ} as a thermodynamic function which depends on the released energy and the equation of state, and does not depend of the kinetics of energy release.

The next step in detonation modeling was made by Zeldovich [5], von Neuman [6], and Döring [7] who considered a 1D steady-state detonation wave with a reaction zone of a finite thickness. According to the Zeldovich-Neumann-Döering (ZND) model, the energy release begins in a hot, shock-compressed material behind the shock front, and continues until the thermodynamic equilibrium is established. This equilibrium point at the end of the reaction zone corresponds to the CJ point in the Chapman-Jouguet theory. The detonation velocity in ZND model is still equal to D_{CJ} and independent of the kinetics of energy release which affects only the reaction-zone thickness. A nonmonotonic energy release, however, may result in pathological detonation waves [8] propagating with a velocity higher than D_{CJ}.

Both CJ and ZND models are based on exact solutions for 1D steady-state detonation waves, and therefore provide correct asymptotics for multidimensional theories of steady-state detonations. Both models are also used to check the accuracy of stable time-dependent numerical solutions based on Euler equations. Calculated values of D_{CJ} are very close to mean detonation velocities actually measured in experiments for large-diameter systems, providing that the equation of state (EOS) of detonation products and the energy released in a detonation wave are well defined. This is usually not a problem for gaseous systems, but becomes more complicated for condensed explosives that require sophisticated EOS of detonation products calibrated in shock-wave and detonation experiments (see, for example, [9-13]). The computed ZND reaction-zone structure can be compared to the experimental data only for heterogeneous condensed explosives, for which a non-Arrhenius kinetics of energy release ensures the stability of detonation. These computations, however, require the reaction rate law and the EOS of the reactive mixture, both difficult to determine for condensed explosives.

The one-dimensional CJ and ZND models were followed by two-dimensional (2D) theories [14-16] that considered curved detonation fronts in condensed explosives. For example, Wood and Kirkwood [16] expanded the ZND model to describe the axial flow behind a steady-state spherical shock front. They derived integral conservation equations, similar to the Rankine-Hugoniot relations, as well as the relation between the energy release rate and the flow divergence at the sonic point. According to the Wood-Kirkwood model, the steady-state detonation velocity linearly decreases as the front curvature increases.

The next step in development of 2D steady-state detonation models was made independently by Trofimov [17-18] and Bzdil [19-20] who considered the radial structure of the reaction zone behind a convex shock front. They have shown, in particular, that for unconfined or weakly confined detonations, the shock front and the sonic surface intersect at the side surface of the explosive charge. Trofimov's approach was limited to the reactive flow immediately behind the convex shock front and produced a differential equation for the shape of the shock in a cylindrical charge. This equation, however, contains the streamline curvature as an unknown parameter that can be found only by analyzing the whole reaction zone, from the shock to the sonic surface, and from the axis to the edge of the charge. Bzdil performed such an analysis for a weakly curved front and a thin reaction zone, and derived a differential equation for the shock shape that also connects the detonation velocity to the charge diameter. Direct numerical simulations based on reactive Euler equations [21] confirmed the main conclusions of both theories, and also revealed additional details of the 2D reaction-zone structure. In particular, the numerical simulations have shown that the sign of the curvature of the sonic surface can change as the charge diameter decreases. This possibility was not ruled out by Trofimov [18] who qualitatively analyzed the shape of the sonic surface.

Bdzil's approach was generalized by Stewart and Bdzil [22-25] to include time dependence. The resulting detonation shock dynamics (DSD) model includes evolution equations for the detonation front, and is being used as a numerically efficient alternative to direct simulations of detonation propagation in complex geometries. This approach also has an important practical advantage for engineering applications because it does not require the equation of state and the reaction rate law. Instead, $D_n(k)$, the relation between the normal velocity of the detonation front D_n and its curvature k, can be determined experimentally and then used to calculate the detonation propagation for the same explosive in different configurations. A similar approach was proposed by Brun [26-27] who developed his JR model by generalizing the CJ theory to introduce the front curvature and acceleration, and assuming a partial burning in an infinitely thin reaction zone.

Direct time-dependent numerical simulations of condensed-phase detonations based on reactive Euler equations were pioneered by Mader [11] and are still the most precise method for modeling the detailed reaction-zone structure of steady-state detonations [21] and transient detonation phenomena [25]. More detailed simulations become possible as the computational technology develops, but the predictive capabilities of direct numerical simulations for condensed explosives depend on uncertainties in EOS and energy release rates.

Unstable Detonations

Most of the steady-state detonation models do not apply to gas-phase detonations that are intrinsically unstable [28] and form complex multidimensional dynamic structures involving transverse shocks and triple-shock configurations propagating along and behind the leading shock front. These structures has been widely investigated experimentally and theoretically since the middle of the last century. Tony Oppenheim actively participated in these studies [29-39] by developing experimental techniques, measuring detonation parameters, and analyzing the detonation structures. He also wrote reviews [29-31,34-35,37,39] which traced the history and current progress in this fast-developing field, and strongly advocated the importance of gas detonation studies for future propulsion systems. His reviews contain a comprehensive list of references on the pioneering experimental and theoretical works on detonation structures in gases than we will omit here for brevity.

Numerical studies of multidimensional gas-phase detonations begin in late seventies and early eighties in the work of Taki and Fujiwara [40], Oran et al. [41], and Markov [42], who showed that the problem of evolution of initially perturbed shock in a reactive medium can be solved using numerical integration methods with low numerical diffusion. These 2D numerical models were based on the reactive Euler equations and correctly reproduced the complicated dynamic structure of unstable detonation waves and the characteristic cellular pattern formed by the trajectories of triple points. Further 2D simulations [43-51] showed how detonation structures form and how they depend on the thermodynamic properties of the system, the kinetics of energy release, and the channel width. The detailed structure of triple-shock configurations was investigated in [48]. Unreacted gas pockets reported in numerical simulations [41,43-45] and experiments [43,52] were further studied in [53-54] and shown to be a common feature of cellular detonations. The unreacted pockets become more pronounced when the scaled activation energy E_a/RT_S (where T_S is the post-shock temperature of unreacted material in the ZND model) increases, and degenerate into "keystone" features (also observed in experiments [55]) when E_a/RT_S decreases. The difference between the theoretical ZND reaction-zone structure and the averaged 1D reaction-zone structure resulting from 2D numerical simulations of cellular detonations also increases for higher E_a/RT_S. Larger values of E_a/RT_S result in more irregular cellular structures [54] that are characterized by higher pressures at triple points, the higher frequency of appearance and disappearance of these points, and larger variations of the local shock velocity. The average detonation velocity, however, remains equal to D_{CJ}.

Both experiments [56-57] and simulations with a one-step chemical kinetics [58-59] show that when E_a/RT_S increases above 6.5, the cellular patterns produced by an unstable detonation front become complicated by small secondary cells embedded inside the main structure. This happens when the overdriven parts of the detonation front become unstable enough to develop secondary triple points during the time between two collisions of the primary triple-shock configurations [60]. High-resolution numerical simulations performed for $E_a/RT_S = 12.4$ [61] were able to reproduce the complex behavior of marginal detonations in a flat channel. The modeled structures involved primary and secondary triple-shock configurations, trans-

verse detonations, and triple points resulting from instability of transverse detonations. These simulations performed for a one-step Arrhenius kinetics showed that formation of multi-level cellular structures in detonation waves does not necessarily require the complex chemistry, though two stages of energy release with disparate timescales can also cause secondary detonation cells [62].

Three-dimensional (3D) numerical simulations of unstable detonations [63-70] are usually performed with lower numerical resolution compared to 2D simulations, and do not show significant qualitative differences with 2D results. The detonation cell size seems to be about the same in 2D and 3D simulations [66], but still differs from experimental values when calculated for a specific system. Intrinsically 3D phenomena, such as rectangular and diagonal cellular structures in rectangular tubes [69-70] and single-spin detonations [64] in round tubes are qualitatively reproduced by simulations.

In spite of extensive experimental and numerical studies of gas-phase detonations, theoretical descriptions of highly nonlinear multidimensional structures produced by unstable detonations are still mostly phenomenological and do not provide enough information for computing parameters of detonation structures, unless empirical correlations are used (see, for example, [71]). Although Borissov and Sharypov [72-73] and Stewart and Yao [74-75,24] derived evolution equations that describe propagation of cellular detonation fronts, direct numerical simulations are still the main method of modeling gas-phase detonations. As the computational technology develops, computing cellular detonations becomes a routine test for numerical methods designed to solve reactive fluid dynamics problems. These computations may involve a detailed chemistry, multiphase reactive systems, molecular transport properties, an adaptive mesh refinement, and sophisticated boundary conditions. The progress in computational technology also facilitates modeling of large-scale phenomena involving multiple detonation cells, such as the detonation diffraction [76].

Astrophysical Detonations

Detonation as a general mechanism for propagation of supersonic reaction waves appears in several astrophysical theories, including Type Ia supernovae [77-80], the transition of neutron matter into strange matter in neutron stars [81], phase transitions in early universe [82], and star formation [83].

Thermonuclear detonations are believed to play a key role in Type Ia supernova explosions [77-79]. These detonations appear as a result of deflagration-to-detonation transition inside white dwarf stars, and propagate through the carbon-oxygen degenerate matter with the velocity about 10,000 km/s. The energy is produced by a network of thermonuclear reactions that begins with the original ^{12}C and ^{16}O nuclei and ends in the formation of ^{56}Ni, or lighter elements, depending on the density. Thermonuclear detonations are unstable and able to form several levels of detonation cell structures [78] that correspond to different stages of energy release with different characteristic times.

Detonation is considered as a propagation mechanism for self-supported waves of star formation in intergalactic medium that may be responsible for formation of large-scale structure in the universe [83]. These very large waves involve an intergalactic shock which compresses large amounts of gas and triggers star formation in this gas. Massive stars that form behind the shock release energy into the interstellar medium through several mechanisms, including supernova explosions. This energy supports the shock propagation and continuing star formation. Stability of these detonations was not yet considered, and the kinetics of energy release in these waves is still not well defined.

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