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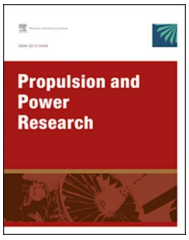

ORIGINAL ARTICLE

Numerical simulations of cellular detonation diffraction in a stable gaseous mixture

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Abstract In this paper, the diffraction phenomenon of gaseous cellular detonations emerging from a confined tube into a sudden open space is simulated using the reactive Euler equations with a two-step Arrhenius chemistry model. Both two-dimensional and axisymmetric configurations are used for modeling cylindrical and spherical expansions, respectively. The chemical parameters are chosen for a stable gaseous explosive mixture in which the cellular detonation structure is highly regular. Adaptive mesh refinement (AMR) is used to resolve the detonation wave structure and its evolution during the transmission. The numerical results show that the critical channel width and critical diameter over the detonation cell size are about 13 ± 1 and 25 ± 1, respectively. These numerical findings are comparable with the experimental observation and confirm again that the critical channel width and critical diameter differ essentially by a factor close to 2, equal to the geometrical scaling based on front curvature theory. Unlike unstable mixtures where instabilities manifested in the detonation front structure play a significant role during the transmission, the present numerical results and the observed geometrical scaling provide again evidence that the failure of detonation diffraction in stable mixtures with a regular detonation cellular pattern is dominantly caused by the global curvature due to the wave divergence resulting in the global decoupling of the reaction zone with the expanding shock front.

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1. Introduction

When a gaseous detonation wave emerges from a confined geometry, either a channel or a circular tube, into an open area filled with the same reactive mixture, the detonation will fail if the channel width or tube diameter is less than some critical value [1,2]. This phenomenon has long been a well-defined fundamental problem in understanding both initiation and failure of detonation waves. Knowledge of the critical geometrical dimension also has practical applications such as in the design of initiators for pulse detonation engines (PDE), e.g., when the detonation transmits from the small pre-detonator to the main thrust tube of the pulse detonation engine [3–7]. At specific initial conditions, these critical parameters have rather unique values for a given detonable mixture and can thus be considered as an alternative length scale that provides an assessment of the relative detonation sensitivity of a combustible mixture.

For common fuel-air mixtures which are typically unstable with an irregular detonation front structure embedded with small scale instabilities, the universal relationship for the critical tube diameter d_c has been well established to be $d_c = 13\lambda$ where λ is the characteristic detonation cell size [8–10]. Critical widths, w_c, for the successful transformation of a planar to a cylindrical detonation are also measured in a number of experiments using a thin annular or rectangular channel and show that w_c/λ is roughly about 3 [11,12]. However, in very special mixtures such as those with high argon dilution (e.g., acetylene-oxygen mixtures with argon dilution above 70% well within the detonation limit), the aforementioned empirical correlations become invalid and experiments have shown that the scaling can be up to $d_c \sim 25\lambda$ and w_c/λ as much as 12 [11,13–15]. In highly argon diluted mixtures, the cellular detonation structure is very regular or appears to be piece-wise laminar and, hence, it has long been suggested that the detonation stability or cell structure regularity plays an important role in the detonation undergoing a sudden expansion into open space and leads to the breakdown in the scaling between stable and unstable mixtures. Lee [16] proposed two mechanisms, one local and one global for the diffracted wave to explain the phenomenon and the difference in the λ scaling between stable and unstable mixtures. For common fuel-air, unstable mixtures, the phenomenon is characterized by the re-initiation of local explosion centers, that is linked to the effect of instabilities. For stable mixtures where the cellular structure is very regular and instability plays a less important role (e.g., explosive mixtures such as acetylene-oxygen with high percentage of argon dilution), Lee argues that the failure occurs due to the global mechanism, like an ideal Zel'dovich-von Neumann-Döring (ZND) detonation, where the curvature of the attenuated detonation exceeds some critical value required for self-sustained propagation [17].

Although a number of numerical studies on the detonation diffraction can be found in the literature, e.g., [18–22] for gaseous mixtures as well as [23–25] for multiphase explosives, very few focus on Lee's conjecture, to discriminate between the two failure mechanisms in unstable and stable mixtures. The λ scaling observed from experiments has not yet been recovered numerically due to several limitations. A number of studies have been restricted only to two-dimensional (channel) configuration, low grid resolution, simplified one-step Arrhenius chemical kinetics, and the diffraction of an initial planar ZND detonation. In this study, a series of high resolution, numerical simulations using the two-dimensional (channel) and axisymmetric (tube), reactive Euler equations with a two-step reaction model are performed to investigate the evolution of the cellular detonation wave expanded from a small channel or tube to a larger open space in a stable mixture with highly regular cellular pattern. While it is difficult to simulate with confidence detonation waves in unstable mixtures due to the necessity to resolve various sources of instability inside the structure, for stable mixtures a sufficient level of numerical resolution can be achieved presently using adaptive mesh refinement to correctly capture the regular detonation structure and its evolution. The objectives of this work are two-folds. The numerical simulations provide the flow field during the diffraction phenomenon and confirm the critical thickness and tube diameter correlations with cell size for stable mixtures. The numerical values of w_c/λ and d_c/λ obtained from both two-dimensional and axisymmetric computations are compared to the predictions of failure mechanisms proposed by Lee [16]. If the mechanism of failure for stable detonations is based on curvature, as suggested by Lee, this should result in a 2:1 relationship between d_c and w_c. The curvature of a cylindrical surface is half that of a spherical one, as curvature in one direction does not exist, therefore the theory expects $w_c \approx d_c/2$, a geometrical factor of two. It is worth mentioning that this geometrical relation was also suggested previously through the analysis of a series of experimental data by Vasil'ev [26].

2. Problem formulation and numerical details

The present simulation of gaseous cellular detonation diffraction is based on the inviscid, reactive Euler equations for either a two-dimensional ($\boldsymbol{Z}=0$) or axisymmetric flow in channel or circular tube, respectively. Written in conserved form, these equations are represented by:

$$\frac{\partial \boldsymbol{U}}{\partial t}+\frac{\partial \boldsymbol{F}}{\partial x}+\frac{\partial \boldsymbol{G}}{\partial r}+\frac{\boldsymbol{Z}}{r}=\boldsymbol{S}$$

where the conservative state vector $\boldsymbol{U}$ and the flux vectors $\boldsymbol{F}$, $\boldsymbol{G}$, $\boldsymbol{Z}$ and the source term $\boldsymbol{S}$ are given by:

$$\boldsymbol{U}=\begin{pmatrix}\rho\\ \rho u\\ \rho v\\ E\\ \rho y_1\\ \rho y_2\end{pmatrix},\quad \boldsymbol{F}=\begin{pmatrix}\rho u\\ \rho u^2+p\\ \rho uv\\ u(E+p)\\ \rho uy_1\\ \rho uy_2\end{pmatrix},\quad \boldsymbol{G}=\begin{pmatrix}\rho v\\ \rho uv\\ \rho v^2+p\\ v(E+p)\\ \rho vy_1\\ \rho vy_2\end{pmatrix}$$

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