Journal of Loss Prevention in the Process Industries 36 (2015) 394–403

Contents lists available at ScienceDirect

Journal of Loss Prevention in the Process Industries

journal homepage: www.elsevier.com/locate/jlp

Numerical study of cellular detonation structures of methane mixtures

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ARTICLE INFO

Article history:
Received 15 September 2014
Received in revised form
10 March 2015
Accepted 11 March 2015
Available online 12 March 2015

Keywords:
Gaseous detonation
Transverse wave
Detonation cell
Critical tube diameter
Critical initiation energy
Detonation velocity
Methane
Chemical kinetics
Irregular multifront structure

ABSTRACT

A two-step model of the kinetics of detonation combustion of methane in mixtures with an oxygen and air has been developed. The proposed model of the kinetics of detonation combustion of methane appears to be reasonably accurate within the confines of the assumptions and is consistent with the second law of thermodynamics. Constants of the model have a clear physical meaning. The model is useful for multi-dimensional numerical simulations of detonation processes. A numerical simulation of a two-dimensional (2D) structure of the detonation wave (DW) in a stoichiometric methane–air mixture in a wide range of channel height has been performed. The changes in the 2D structure of the self-sustaining DW on variations of the height of the channel have been studied. From the analysis of the flow structure, the dominant size of the detonation cell for stoichiometric methane–air mixture determines to be 34 ± 1 cm, and 0.3÷0.35 cm for methane–oxygen mixture. These values are in good agreement with all known experimental data. The transverse size of the detonation cell is a characteristic size of the DW front structure. Based on this value, it is possible to determine such parameters of detonation as critical conditions of detonation combustion, the critical energy of direct initiation, detonation propagation limits, etc., i.e. to estimate the detonation hazard of gaseous mixture and its use in various schemes of detonation propulsion systems. The 2D simulations were reproduced the DW irregular cellular structure with all its main features observed in the experiment: a chaotic uncoordinated movement of the main transverse waves; the presence of a fine (secondary) cell structure at the transverse waves themselves; the existence of numerous secondary transverse waves at the leading shock front, forming a hierarchy of the decreasing the size DW front perturbations; and a significant number of pockets of the unburned mixture at a considerable distance behind the DW front, etc. Numerical simulation of irregular structure of the multi-front DW has been conducted for a real hydrocarbon–air mixture with an adequate description of all its thermal and chemical properties.

1. Introduction

Extensive experimental and theoretical studies of gas detonations (Voitsekhovskii et al., 1966; Fickett and Davis, 1979) have shown that the actual structure of the detonation front is very different from that predicted by the one-dimensional Zeldovich theory (Zeldovich et al., 1955). The flow behind a plane detonation wave front is unstable. Due to the growth of the initial disturbances, the leading shock front is no longer smooth and exhibits a complex time-periodic structure. The main element of this structure is a triple configuration consisting of a Mach stem (overdriven DW), an incident wave (decaying DW), and a reflected (transverse) wave adjacent to the first two waves at the triple point (Voitsekhovskii et al., 1966; Fickett et al., 1979).

Collisions of transverse waves moving over the DW front in opposing directions lead to the reproduction of the front structure in time. The trajectories of triple points are two intersecting families of lines that form a network of diamond cells. These detonation structures are fixed in the experiment on the soot imprints (Voitsekhovskii et al., 1966; Fickett et al., 1979; Nettleton, 1987). The transverse size of the cell, a_0, determined as the average distance between the trajectories of one family measured in the direction normal to DW propagation, is a characteristic size of the DW front

Abbreviations: DW, Detonation wave; TW, Transverse wave; CJ, Chapman–Jouguet; TVD, Total variation diminishing; MUSCL, Monotonic Upstream-Centered Scheme for Conservation Laws; ASIRK, Additive semi-implicit Runge-Kutta; HLLC, Harten, Lax, van Leer, Contact (surface); CPU, Central Processing Unit.

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http://dx.doi.org/10.1016/j.jlp.2015.03.012
0950-4230/

structure.

One of the most important problems in the theory of dynamic systems is the formation and destruction of ordered gas-dynamic structures in a reactive medium. An example of such a self-organizing system is a multifront (cellular) DW steadily propagating in a reacting gas mixture. The complex three-dimensional and time-dependent structure of the front of these waves propagating in constant cross-section channels shows some order, whose geometrical parameter is the size of the elementary cell of the DW a_0. Based on this value, it is possible to determine such parameters of detonation as critical conditions of detonation combustion, the critical energy of initiation (Vasil'ev and Grigor'ev, 1980), detonation propagation limits, etc., i.e. to estimate the detonation hazard of gaseous mixture.

Based on the currently available experimental data, gas mixtures can be divided into several groups (Voitsekhovskii et al., 1966; Fickett et al., 1979; Nettleton, 1987) according to the degree of regularity of cells: 1) mixtures with a very regular detonation-cell structure (all cells at soot imprints are strikingly similar in size and shape); 2) mixtures with a slightly irregular structure (cells are slightly different in size and shape); 3) slightly regular mixtures with an appreciable variation in cell size; 4) mixtures with a highly irregular structure (cells vary greatly in both shape and size, and the characteristic size of the structure can be determined quite subjectively).

The first group includes, for example, hydrogen–oxygen mixtures highly diluted with argon. The last group includes hydrocarbon–air mixtures. A particularly high degree of irregularity is observed fir methane–air mixtures, for which it is very difficult to identify a characteristic ordered spatial structure and the size of the detonation cell a_0 can only be interpreted as a quantity averaged over the soot imprints in different parts of the detonation tube and over many experiments.

In our previous numerical simulation (Trotsyuk, 1999) of the two-dimensional cellular DW structure in hydrogen–oxygen mixtures, good agreement was obtained between the numerical results and experimental data on the size a_0 over a wide range of initial pressures and degrees of dilution with argon. A two-scale (bifurcation) cellular detonation structure was first found in numerical studies of the DW structure in hydrogen–oxygen mixtures with the addition of hydrogen peroxide (Fomin et al., 2006; Vasil'ev et al., 2010). Note that in the vast majority of studies, regular cellular structures in model gas mixtures have been simulateded; see the literature review in papers by Fomin et al. (2006) and Vasil'ev et al. (2010). Real mixtures are studied using detailed kinetic mechanisms of gas reactions. The use of this method in multi-dimensional numerical simulations is hampered by its cumbersomeness, programming difficulties, and high demands on computing power. Therefore, such studies are relatively few, and they also model DWs with regular or slightly irregular cell structures. As regards studies of irregular detonation structures, an irregular cellular structure was obtained in calculations of Gamezo et al. (1999, 2000) for a model mixture with thermochemical parameters very different from those of a real gas mixture resulted. Use was made of a simple chemical kinetics in the form of a single Arrhenius-type equation which described an irreversible exothermic reaction with high activation energy. Two-dimensional irregular structure of detonation in methane–air mixture is numerically obtained firstly by Kessler et al. (2010, 2011), using a one-step irreversible Arrhenius equation also.

The objectives of this work are to develop an approximate model for the kinetics of chemical reactions to describe the detonation combustion of methane based gaseous mixtures and to perform a numerical simulation of the irregular multifront (cellular) structure of a two-dimensional detonation wave in a stoichiometric methane–air mixture under the standard initial conditions.

1.1. Governing equations and model of chemical kinetics

The dynamics of the compressible chemically reactive medium is described by the two-dimensional Euler equations.

The chemical reaction in the DW is described according to our model for the combustion of methane using the two-step model of the detonation kinetics (induction period and main heat release stage step) first proposed by Korobeinikov et al., 1972). The induction period for methane mixtures is calculated by the empirical formula of Soloukhin (1970) suggested in paper (Vasil'ev, 1998). As shown by Vasil'ev (1998), the induction kinetics of Soloukhin (1970) provides the best fit to the available experimental data on the size of the detonation cell a_0 in methane based mixtures when using an analytical model of the detonation cell (Vasil'ev and Nikolaev, 1976).

A two-step model for the kinetics of chemical reactions in hydrogen–air mixtures (NFZT model) was developed in Nikolaev (1978); Nikolaev and Fomin (1982); Nikolaev and Zak (1988); Fomin and Trotsyuk (1995) As in (Korobeinikov et al., 1972), the reaction is divided into two steps: the induction period and the heat-release step. The model includes one ordinary differential equation for the molar mass of the mixture after the induction period and explicit algebraic formulas for the internal energy and the adiabatic index as functions of the pressure p and temperature T. The model adequately describes chemical equilibrium in hydrogen–air and hydrocarbon–air mixtures, allowing calculations of the molar mass, internal energy, and isentropic index of the mixture as functions of T and p using explicit algebraic formulas. The model is highly accurate and consistent with the second law of thermodynamics, and the constants of the model have a clear physical meaning.

In this paper, the two-step kinetic model NFZT is modified to describe the chemical reaction in detonation waves in methane–air mixtures:

$$CH_4 + a_1H_2 + a_2O_2 + a_3N_2 + a_4Ar + a_5H_2O,\ a_2 > 0.5.$$

We replace the real multistep processes occurring during the induction period by some *brutto*–reaction chosen from the following considerations.

At the end of the induction period, the temperature increase (and, hence, the total heat release of the chemical reactions) is small. Therefore, we choose the *brutto*–reaction so that its heat Q_τ is much lower than the maximum possible heat release Q_{max} from the total recombination of the reaction products with the formation of CO_2 and H_2O molecules.

Considering that the induction period involves chemical reactions associated with the formation and increase in number of active centers and the disintegration of methane molecules, we assume that during the induction period, all methane molecules decomposed to form CO molecules.

In accordance with the foregoing, during the induction period, all methane molecules will sooner or later undergo the following chemical reactions:

$$CH_4 + O_2 \rightarrow CO + OH + 1.5H_2,\ \text{if } a_2 \geq 1, \quad (1)$$

$$CH_4 + a_2O_2 \rightarrow CO + (2a_2 - 1)OH + (2.5 - a_2)H_2,\ \text{if } 1 > a_2 \geq 0.5. \quad (2)$$

If the initial mixture contains molecules of H_2O, H_2, N_2, and Ar, we assume that they are not involved in chemical reactions during the induction period.