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On the mechanism of flow evolution in shock-tube experiments

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ABSTRACT

The paper studies numerically the flow development behind the shock wave propagating inside the tube. The detailed analysis of the flow patterns behind the shock wave allows determination of the gas-dynamical origins of the temperature non-uniformities responsible for the subsequent localized start of chemical reactions in the test mixture. In particular, it is shown that the temperature field structure is determined mainly by the mechanisms of boundary layer instability development. The kinetic energy dissipation related to the flow deceleration inside boundary layer results in local heating of the test gas. At the same time, the heat losses to the tube wall lead to the cooling of the gas. Therefore the temperature stratification takes place on the scales of the boundary layer. As soon as the shock wave reflected from the end-wall of the tube interacts with the developed boundary layer the localized hot regions arise at a certain distance from the end wall. The position of these hot regions is associated with the zones of shock wave interaction with roller vortices at the margin between the boundary layer and the bulk flow. Formulated mechanism of the temperature field evolution can be used to explain the peculiarities of non-steady shock-induced ignition of combustible mixtures with moderate ignition delay times, where the ignition starts inside localized kernels at distance from the end wall.

1. Introduction

One of the main problems related to the experimental study of chemical reactions kinetics in gases is the accurate interpretation of gas dynamics affecting the chemical processes inside a reactor. The problem of the detailed account of gas-dynamical processes becomes of paramount interest, especially when studying the exothermal reactions such as combustion of fuel-oxygen mixtures [1,2] or pyrolysis of hydrocarbons, which in some cases could also yield to the heat release [3,4]. The pattern of the gas-dynamical field determines the structure of ignition kernel and subsequent evolution of the exothermal wave. Thus, it is a known fact that in case of so-called mild ignition [1] the reaction initiation takes place inside localized hot spots forming at a certain distance from the closed end of the shock tube behind the reflected shock wave. Non-steady reaction wave evolution takes place in the gaseous mixture with non-uniform temperature distribution and finally different combustion regimes including detonation could be realized. In view of this, it is of paramount importance to understand clearly how the flow develops and what patterns of temperature field are formed.

Unfortunately, the experimental data on the flow characteristics are limited by utilized experimental technique, which usually includes pressure gauges or schlieren visualization, and, at best, provides only one- or two-dimensional representation of the process. Pure theoretical analysis also cannot provide the overall pattern of the process since the nature of its development is three-dimensional and absolutely non-linear. Therefore, the most informative method to understand the peculiarities of flow evolution inside the reactor is the numerical analysis. As soon as it became possible to carry out high-precision numerical simulations utilizing powerful supercomputer systems a certain number of studies were devoted to the peculiarities of flow evolution inside reactors [5–8]. Most of them were carried out assuming some approximations such two-dimensional flow, adiabatic walls or inflow modeled by the inlet boundary condition. Moreover, generally, researchers were using conventional numerical techniques not devoid of numerical dissipation and dispersion errors. Due to this fact it was not possible to resolve with high enough accuracy all the peculiarities of the flow evolution including gas-dynamical instabilities and behavior of the vortical structures. It should be also noted that commonly one studies numerically the shock waves in diatomic gases that determines relatively fast growth of boundary layer behind the incident shock wave [9]. Independently of the boundary layer structure, the interaction of reflected shock wave with a relatively thick boundary layer, in that case, causes rather fast breaking of the vortices into the bulk flow. In turn, this leads

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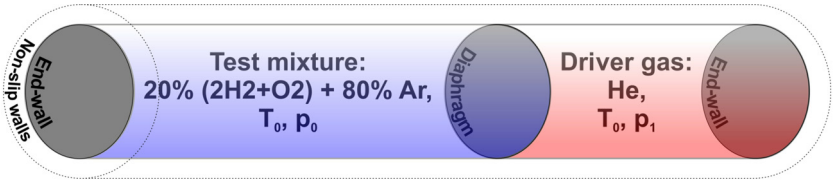

Fig. 1. Schematic problem setup.

to the additional gas heating due to vortices kinetic energy dissipation into heat (herein, numerical dissipation could determine a highly overestimated intensity of this process compared with the reality, moreover the spatial structure of the temperature field could be significantly distorted). In case of adiabatic walls, the gas inside boundary layer occurs to be heated via the same mechanism of kinetic energy dissipation in the shear flow. Therefore the vortices breakaway also transfer this heat from the boundary layer to the bulk flow. Due to this, the most probable position of ignition kernel formation is somewhere inside the bulk flow. Despite this mechanism seems to be quite physically reasonable, there are experimentally observed regimes with ignition taking place in the region adjacent to walls [10,11] that can be related to the peculiarities of boundary layer evolution in mixtures strongly diluted with a monatomic inert gas such as argon. According to this, it is quite questionable to generalize the results of obtained numerical data on the wide range of regimes observed experimentally.

The main goal of this work is to visualize and analyze numerically the flow evolution behind shock wave propagating in the shock tube. The interpretation of the formed flow structures is provided in terms of boundary layer instability. We also provide the detailed analysis of the temperature field development and define the origins of temperature non-uniformities formation and their localization. Taking all of these results into account the gasdynamical mechanism responsible for ignition kernels formation is formulated.

2. Problem setup

Taking into account the critical overview of numerical studies presented above we have formulated the following problem setup. We considered the tubes of different geometries, including 2D channel, 3D channel with rectangular cross section and 3D tube of round cross section. The tube was divided into two chambers by infinitely thin diaphragm. One of the chambers was filled with test mixture (20% ($2H_2 + O_2$) / 80% Ar) at given temperature and pressure (T_0, p_0), and the second chamber – with pressurized driver gas (He at T_0 and p_1). Calculations were carried out for $T_0 = 300$ K, $p_0 = 0.355$ atm, p_1 was varied in the range from 1.1 atm to 14.0 atm that corresponded to the variation in the shock wave speed D from 500 m/s to 1000 m/s. The side walls of the tube were modeled as no-slip isothermal solid surfaces. Isothermal boundaries were considered as an approximation of thermal conducting wall. In addition the series of calculations with adiabatic boundaries were implemented to understand the rate of gas heating due to the viscous dissipation. Tube was closed from both ends. Schematically the problem setup is shown in Fig. 1.

To reproduce the flow patterns evolution a conventional non-reactive Navier–Stokes system of gasdynamical equations was used. The model included compressibility, viscosity, thermal conductivity and multicomponent diffusion. The governing equations are as follows:

$$\frac{\partial \rho}{\partial t} + \frac{\partial \rho u_j}{\partial x_j} = 0 \tag{1}$$

$$\frac{\partial \rho u_i}{\partial t} + \frac{\partial \rho u_i u_j}{\partial x_j} = \frac{\partial \sigma_{ij}}{\partial x_j} - \frac{\partial p}{\partial x_i} \tag{2}$$

$$\frac{\partial \rho Y_k}{\partial t} + \frac{\partial \rho Y_k u_j}{\partial x_j} = -\frac{\partial \rho Y_k V_{k,j}}{\partial x_j} \tag{3}$$

$$\frac{\partial \rho E}{\partial t} + \frac{\partial \rho E u_j}{\partial x_j} = \frac{\partial \sigma_{ij} u_j}{\partial x_i} - \frac{\partial p u_i}{\partial x_i} + \frac{\partial}{\partial x_i}\left(\lambda(T)\frac{\partial T}{\partial x_i}\right) - \frac{\partial}{\partial x_j}\left(\rho \sum_k h_k(T) Y_k V_{k,j}\right) \tag{4}$$

$$\sigma_{ij} = \mu(T)\left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} - \frac{2}{3}\delta_{ij}\frac{\partial u_l}{\partial x_l}\right) \tag{5}$$

where x_i – spatial coordinates, t – time, ρ – density, p – pressure, T – temperature, u_i – the components of velocity vector, Y_k – the mass fraction of kth species, E – the specific total energy, σ_{ij} – the viscous stress tensor, $V_{k,j}$ – the components of diffusion velocity vector of kth species, $\lambda(T)$ – the mixture-averaged thermal conductivity, $\mu(T)$ – the mixture-averaged dynamic viscosity, h_k – the enthalpy of kth species. Diffusion velocities are calculated in zeroth-order Hirschfelder–Curtiss approximation [12], taking into account correction velocity [13] to ensure mass conservation. Pure species transport coefficients are evaluated utilizing the first principles of gas kinetic theory [14]. Mixture averaged properties are calculated from the pure species parameters with conventional averaging methods [14].

Thermodynamic characteristics of the mixture are related with use of equations of state:

$$\varepsilon = \frac{p}{\rho(\gamma - 1)} \tag{6}$$

$$\frac{p}{\rho} = \frac{RT}{\overline{M}} \tag{7}$$

where ε – the specific internal energy, $\gamma(T, Y_k) = \frac{C_p}{C_V}$ – the adiabatic index of the mixture, $\overline{M} = (\sum_k (Y_k/M_k))^{-1}$ – the averaged molar mass, M_k – the molar mass of kth species, R – the universal gas constant. Here heat capacities and enthalpies are calculated using the interpolation of tabulated data [15].

To obtain an accurate solution of the formulated problem we utilized a low dispersive and low dissipative numerical method based on the Compact Accurately Boundary-Adjusting high-Resolution Technique (CABARET) [16]. CABARET is an explicit finite-difference second-order in space and time scheme with divided calculation of the fluxes and conservative variables that provides unique low-dissipative properties. For solving non-linear flow problems CABARET uses flux correction method directly based on the maximum principle on flux variables and does not require any parameter tuning or flux limiters. Non-linear correction ensures accurate balance between dispersion and dissipation errors [16]. This contemporary numerical algorithm was recently successfully implemented to solve a wide range of multiscale unsteady gasdynamical problems, among which aero acoustic problems of jet noise generation and subsonic flow over airflow at zero attack angle [17,18], ocean gyres modeling [19], direct numerical simulation of the vortex pair interaction and jittering vortex systems [20], solving Landau–Lifshitz fluctuating hydrodynamics equations [21]. Results, obtained with CABARET, have shown a good agreement with experimental data and have been validated by conventional

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