Turbulent Combustion in Cellular Detonations

A. A. Efimenko and S. B. Dorofeev
Russian Research Center "Kurchatov Institute"

Moscow, 123182, Russia
E-mail: efimenko@iacph.kiae.ru

Introduction

It is generally accepted that main reaction mechanism in detonations is autoignition via adiabatic compression of reactive media by leading shock waves, and one in deflagrations is connected with turbulent transport. Real detonations are unstable and have a complex transient three-dimensional structure, commonly known as cellular detonation structure. The cellular structure is believed to be very essential feature of real detonations. It was shown experimentally by Dupre, et al. (1988) that if acoustic absorbing dumps transverse shocks out, the detonation fails. This is why the existence of the cellular structure is often considered to be an indication of the detonative regime of combustion.

Although a detailed theory of three-dimensional transient structure of detonations has not been developed, multidimensional numerical simulations were able to reproduce main features of the structure (see, e.g., Oran (1987), Bourlioux and Majda (1991), Quirk (1994), Gamezo, et al. (1999) and other publications). All this simulations were made using Arrhenius type of reaction kinetics, ranging from a single one-step global reaction to detailed chemical reaction mechanisms. Autoignition mechanism via adiabatic compression was assumed to be responsible for chemical energy release.

Transient three-dimensional structure of real detonations involves mutual interactions of numerous transverse shocks, and their interactions with shear layers and density gradients resulting from chemical reactions. These interactions are powerful vorticity production mechanisms and can be responsible for intensive turbulent transport of energy and species, thus, providing an additional energy release mechanism in detonations. The first attempt to introduce turbulence in description of energy release mechanism in detonations was made by White (1961). More recently, Lee (1991), Shepherd (1994) and Efimenko, et al. (1994) were trying to attract attention to this subject. However, turbulence combustion in the reaction zone was not usually considered to play an important role in detonations.

The problem of turbulent combustion as an additional mechanism of energy release in detonations got a new impulse in connection with ideas of Lee (2000) and Dionne, et al. (2000) to generalise description of fast turbulent deflagrations and non-ideal detonations. According to Lee, if various mechanisms of shock-shock, shock-vortex, shock-density gradients, are included, cellular detonations and fast deflagrations in rough tubes can be described by the same propagation mechanism. The autoignition mechanism of classical detonation theory may also play a role in propagation of detonations. It is possible to assume that relative contribution of adiabatic compression and turbulent combustion (in general sense, including shock-wave interactions) may have variable contributions depending on wave speed, and other factors.

If turbulent combustion is introduced as important mechanism for energy release in real detonations, what does it mean for description of detonation cellular structure? The models,

which were used to study intrinsic features of detonation cellular structure, all involve the Arrhenius function for chemical reaction rates. The main features of the cellular structure were reproduced in simulations, at least qualitatively. Correlations were observed between the size of the cells and characteristic reaction length, determined from Arrhenius reactions. The development of instabilities, which result in cellular structure, were connected with strong temperature dependence of reaction rate on local temperature. In the case of turbulent energy release mechanism one should not expect such a strong temperature dependence of reaction rate, as it given by reaction mechanisms in real system. The question arises: is it possible to observe formation of the cellular structure itself, if strong temperature dependence of reaction rate is eliminated? Generally, the turbulent flow with multiple shock-wave interactions can provide the dependence of reaction rate on local flow conditions. What type of instability can be formed in this case? Is it similar to cellular detonation instability typical for real detonations? In the present paper we try to address these questions. The model is proposed that mimic some features of the energy release in turbulent reactive flows. The instability is introduced in the model by a function of reaction rate on local flow conditions. No temperature dependence of combustion rate is assumed in the model. The structure of combustion waves in reactive gas is studied numerically in a series of time-dependent 2D simulations.

Model

Eulerian gasdynamic model (B05 code) with special energy release function were used in series of 2D time-dependent simulations of reactive flow. The gasdynamic solver used is based on first order 3D Eulerian explicit upwind flux method with central difference approximation for pressure gradient. All the calculation parameters are assigned at the vertices of uniform grid. The calculation scheme is based on the equations of motion of the gas in the form of energy, momentum, and mass conservation.

Simplified thermodynamic model was used, in which equation of state of ideal gas is applied to the mixture of gases with constant heat capacities. The efficient values of heat capacities of the reactants and products were chosen to describe typical gaseous fuel-air mixture.

The combustion model implemented in B05 code is similar to effective turbulent burning velocity function. The burning rate was a function of vorticity in each particular calculation cell:

$$\frac{\partial C}{\partial t} = \rho \cdot \frac{K}{\Delta z} \cdot f(|rot\,\vec{V}|), \qquad (1)$$

where C is mass fraction of reactants, ρ - density, K – rate constant, V – flow speed. Function f was given by the following expression: $f(x) = (1+.02 \cdot x) \cdot exp(.49-(.7+.0004 \cdot x)^2)$. The shape of the function is presented in Fig. 1. The reaction was allowed in a mesh point, if one of neighbors has reactant concentration C less than 0.5. Thus a thin reaction front was formed, having width of about 2 to 3 mesh points. The propagation velocity of such a front relative to unburned mixture was approximately equal to the value of $2 \cdot K$ at $f(x) = 1$.

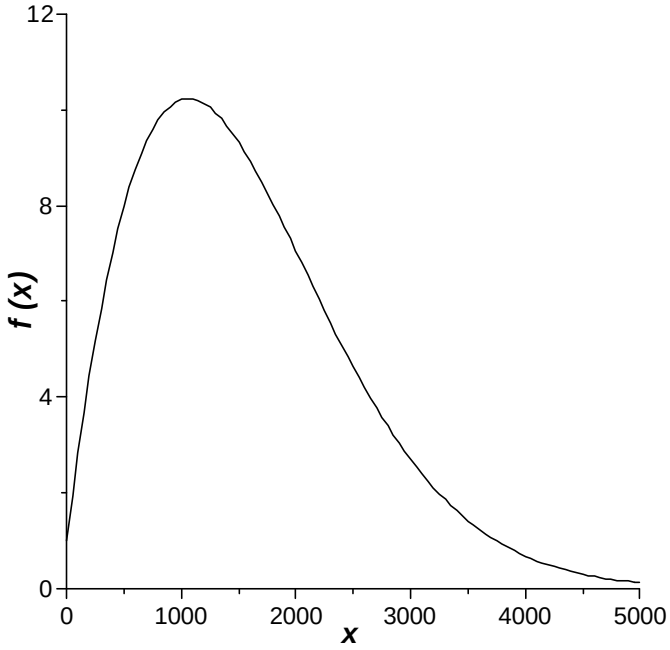

Figure 1. Burning rate function *f* versus vorticity.

The combustion model used in calculations was not aimed to describe real combustion rate in turbulent flow. With these model we tried to mimic one important feature of turbulent combustion rate: its dependence on the vorticity. As typical for turbulent combustion, the reaction rate increases with vorticity, then comes to saturation, and then decreases with further increase of vorticity. It is important to notice, that the burning rate does not depend on temperature at al. It depends, however, on local flow conditions, and can introduce instability in the solution.

Results and discussion

Propagation of a combustion wave in 2D channel was studied in the series of calculations. A small volume (2x2 mesh points) of combustion products at initial pressure was used to start the combustion process. The constant *K* in the burning rate was varied in the calculations. After initial acceleration, for a certain values of reaction rate constant a quasi-steady propagation of detonation wave was observed. The speed of propagation was very close to the Chapman – Jouguet detonation speed. The instability of the wave front was developed very fast, within propagation distances of about the channel width. The instability resulted in formation of cellular structure typical for real detonations. Examples of soot tracks are shown in Figs. 2 and 3. To model soot tracks, a map of maximum local overpressures achieved during all the process was recorded in calculations. Examples are shown for the mixture with thermodynamic parameters corresponded to 11.5% vol. of hydrogen in air at initial temperature and pressure of 300K and 1 atm. Variation of reaction rate constant resulted in corresponding changes of detonation cell sizes. As it is typical for simulations with Arrhenius kinetic models, the characteristic size of the cells is inversely proportional to reaction rate constant.

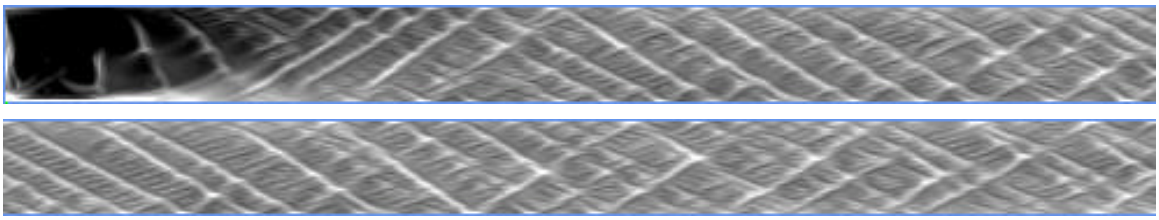

Figure 2. Computer model of soot tracks with constant K = 60 m/s. Wave direction is from left to right. Upper plot shows initial development of the cellular structure, the lower one – following on structure. Pressure range is 2.0 ÷ 0.8 MPa.

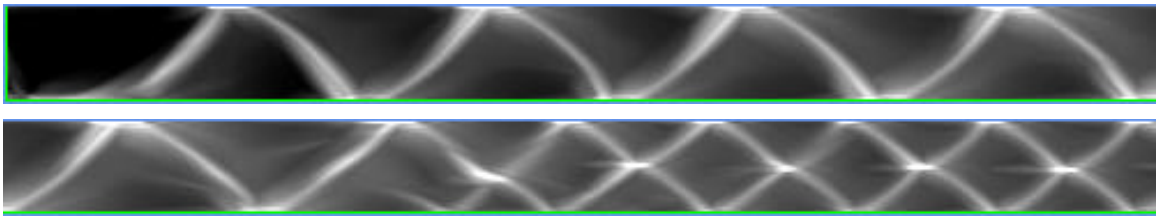

Figure 3. Computer model of soot tracks with constant K = 30 m/s. Wave direction is from left to right. Upper plot shows initial development of the cellular structure, the lower one – following on structure. Pressure range is 3.0 ÷ 0.7 MPa.

Results of calculations show that the energy release model, which does not include any temperature dependence of the reaction rate is able to produce cellular detonation instability similar to that observed with Arrhenius reaction rate models. The key element of the model, which was responsible for the development of cellular instability is that reaction rate depended on vorticity. No instability was observed in calculations, if reaction rate was given by Eq. (1) with $f(x) = 1$.

In the model presented here, the reaction was not initiated through mixture compression behind the lead shock. The mixture was just burning with an effective rate dependent on local flow conditions. Thus, cellular detonation instability cannot be considered as an indication that autoignition via adiabatic compression is the main mechanism of energy release in detonations. The mechanism similar to reaction via transport of energy and species is able to be responsible for development of cellular detonation instability. This observation permits to assume that turbulent combustion may be an additional important mechanism of energy release in multidimensional detonations.

Summary

We have presented results of two-dimensional time dependent simulations of detonation processes in reactive gas with artificial energy release model. The model was used that mimics some features of the energy release in turbulent reactive flows. An effective turbulent burning velocity was assumed with the burning rate dependent on vorticity. No temperature dependence of combustion rate was assumed in the model.

It was found that for a certain range of burning rate constants detonations were formed, and instability was developed with cellular structure typical for real detonations. No cellular instability was observed in calculations, if reaction rate did not depend on vorticity. Variations

of reaction rate constant resulted in corresponding changes of detonation cell sizes. As it is typical for simulations with Arrhenius kinetic models, the characteristic size of the cells was inversely proportional to reaction rate constant.

The results showed that cellular detonation instability cannot be considered itself as an indication that autoignition via adiabatic compression is the main mechanism of energy release in detonations. The mechanism similar to reaction via transport of energy and species is able to be responsible for development of cellular detonation instability.

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