NUMERICAL MODELING OF SHOCK WAVE TO DETONATION TRANSITION IN METHANE–AIR MIXTURE IN TUBE WITH CENTRAL BODY

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For the purpose of obtaining fast deflagration-to-detonation transition (DDT) in pulse detonation engines (PDE), detonation initiation in methane–air mixture in tube with a profiled central body was studied by numerical modeling. The shape of central body was optimized to minimize the distance of detonation onset. As a result of numerical calculations, the optimal geometrical parameters of the central body were suggested for further experiments.

1 Introduction

The detonation is the most effective way to use the chemical energy of substance and it allows the efficiency of technological burners and jet engines to be improved [1]. The basic advantage of pulse detonation is a combination of high fuel efficiency to high values of temperature and velocity of detonation products. Due to thermal convection, a heat transfer from detonation products to the heat target is essentially higher in PDE than in traditional burners. At present, the possibility of practical use of pulse detonation of natural gas for increasing the efficiency of power plants is actively investigated [2].

The main problem on the way of implementation of pulse detonation of natural gas in practice is associated with its low detonability.

Therefore, DDT is considered as a main technique of detonation initiation. For fast DDT, it was suggested to use a number of special devices [3] with the aim to intensify the process of combustion from laminar to turbulent flames, which speed is high enough to generate weak shocks that then passed through focusing obstacles to initiate a detonation. The main attention previously has been concentrated around focusing of shock waves in nozzles [4–6]; in the present work, for the same purposes, it is offered to use the shaped central body. The effectiveness of the approach is investigated by numerical modeling of shock wave propagation (with Mach number M = 3.0–3.8) in a tube with central body.

2 Problem Description

The central body with diameter d is located in the symmetry axis of the tube with inner diameter $D = 94$ mm (Fig. 1). The central body consists of frontal part which has a conic or parabolic section described by angle α, cylindrical insert with length L, and tail part which has conic, or parabolic, or elliptic section described by angle β. The blockage ratio of tube cross section is defined as $\mathrm{BR} = (d/D)^2$. At the initial time, the tube is filled with stoichiometric methane-air mixture (with weight composition $N_2 = 0.725$, $O_2 = 0.220$, and $CH_4 = 0.055$) at normal conditions (pressure $p_0 = 0.10$ MPa and density $\rho_0 = 1.13$ kg/m^3). Inflow type of boundary condition is set on the left side of computational domain. The parameters (pressure, density, and velocity) are the same as behind a shock wave of Mach number M_0. It leads to propagation of the shock wave from left to right. Under certain conditions, the interaction

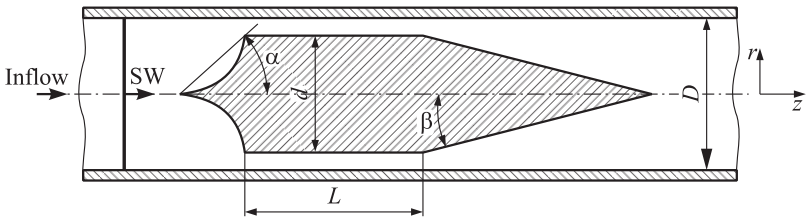

Figure 1 Scheme of computation domain: tube and central body

of the shock wave with central body can lead to self-ignition of some volume of mixture due to local temperature growth; as a result, it can lead to detonation onset in the tube.

The goal is to find out the optimal shape of central body (blockage ratio BR, length of insertion L, and values of angles α and β) for detonation onset.

3 Mathematical Model

The governing equations of the mathematical model include the equations of conservation of mass, momentum, and energy for nonviscous and nonheat-conducting ideal gas in the cylindrical coordinate system:

$$
\begin{aligned}
[\rho r]_t + [\rho u r]_z + [\rho v r]_r &= 0\,; \\
[\rho u r]_t + \left[\left(\rho u^2 + p\right) r\right]_z + [\rho u v r]_r &= 0\,; \\
[\rho v r]_t + [\rho u v r]_z + \left[\left(\rho v^2 + p\right) r\right]_r &= p\,; \\
[E r]_t + [(E+p)\, u r]_z + [(E+p)\, v r]_r &= r\dot{Q}\,; \qquad (1) \\
[\rho Y_i r]_t + [\rho Y_i u r]_z + [\rho Y_i v r]_r &= r J_i\,. \qquad (2)
\end{aligned}
$$

Here, ρ is the gas density; Y_i is the mass fraction of the ith substance of multicomponent gas mixture; u and v are the axial and radial components of the velocity vector; p is the pressure; and $E = \rho(e + (u^2 + v^2)/2)$ is the total energy where $e = \int\limits_0^T C_v(T)\, dT$ is the internal specific energy of the gas. The specific heat of the gas was calculated using the known temperature dependences of the specific heats [7]:

$$C_v(T) = \sum_{i=1}^{N_g} Y_i C_{vi}(T)\,.$$

To close the system, the equation of state of an ideal gas was used:

$$p = \rho R T \sum_{i=1}^{N_g} \frac{Y_i}{\mu_i}\,,$$

where R is the universal gas constant; T is the temperature; and μ_i is the molecular weight of the ith species. Based on the known reaction

rates w_k and the standard enthalpies of formation of the species ΔH_i^0, the source of mass J_i and heat $\dot{Q}$ in the right side of Eqs. (2) and (1) were calculated as

$$J_i = \mu_i \sum_{k=1}^{N_r} (\nu''_{ik} - \nu'_{ik})\, w_k\,; \quad \dot{Q} = \sum_{k=1}^{N_r} w_k Q_k\,;$$

$$Q_k = \sum_{i=1}^{N_g} (\nu'_{ik} - \nu''_{ik})\, \Delta H_i^0\,.$$

4 Kinetic Scheme of Methane Oxidation

The chemical transformations were described by a set of N_r irreversible chemical reactions:

$$\sum_{i=1}^{N_g} \nu'_{ik} A_{ik} \xrightarrow{k} \sum_{j=1}^{N_g} \nu''_{jk} B_{jk}$$

where A_{ik} are the initial reactants; B_{jk} are the products of the kth reaction; and ν'_{ik} and ν''_{jk} are the stoichiometric coefficients. The reaction rate was presented as

$$w_k = A_k \left(\frac{P}{P_0}\right)^{m_k} \exp\left(-\frac{(E_a)_k}{RT}\right) \prod_{i=1}^{N_g} \left(\frac{\rho Y_i}{\mu_i}\right)^{v'_{ik}}$$

where A_k is the preexponential factor; $(E_a)_k$ is the activation energy; m_k is the parameter that describes the pressure dependence of the

Table 1 Kinetic mechanism of methane oxidation

No.	Reaction	Q_k, kJ/mol	E_a, kJ/mol	A_k, l, mole, s	m_k
1*	$CH_4 + (3/2)O_2 = CO + 2H_2O$	519	209	$4 \cdot 10^{11}$	0.0
2	$2H_2 + O_2 = 2H_2O$	484	88	$7 \cdot 10^{13}$	−0.5
3	$2CO + O_2 = 2CO_2$	566	88	$8.5 \cdot 10^{12}$	−1.5
4	$CO + H_2O = CO_2 + H_2$	41	174	$1 \cdot 10^{12}$	−1.0
5	$CO_2 + H_2 = CO + H_2O$	−41	208	$3.1 \cdot 10^{13}$	−1.0

*Reaction rate $w_1 = A_1\,(P/P_0)^{m_1} \exp(-(E_a)_1/(RT))[CH_4][O_2]$.

reaction rate; and P_0 is the atmospheric pressure (101 325 Pa). In calculations, the oxidation of methane was modeled using a five-step overall kinetic mechanism (Table 1). Based on this scheme, the calculations of self-ignition delays are in good agreements with experimental data.

5 Numerical Method

The principle of splitting of physical processes [8] underlying the numerical implementation was used to solve the model equations step-by-step: first, the subsystem of convective transfer and pressure work is solved by Godunov–Kolgan method [9], thereafter, the subsystem of chemical transformation which is a set of ordinary differential equations is solved using Runge–Kutta method based on Dorman and Prince formulae with self-operated time step control [10]. The domain decomposition is used in computer code to speed up calculations. The implementation uses MPICH-MPI library to organize boundary data interchange between subdomains.

6 Results

The calculations were performed on a cylindrical uniform rectangular grid with a computational cell size of 0.2 mm. The parameters of central body are summarized in Table 2. The last column in the table shows whether detonation onset has been fixed in the computational domain. Figure 2 shows the dependence of the lead shock wave speed in the vicinity of tube wall vs. distance.

In preliminary calculations, it was established that parabolic shape with $\alpha = 40^\circ$–45° is optimal for the frontal part to obtain a detonation. Numerical modeling and experiments with shaped nozzles [6, 11, 12] show that for reliable detonation initiation, blockage ratio BR should be about 0.7. Therefore, the calculations with central body have been carried out with BR = 0.6–0.7. It was found that it is easy to initiate detonation in a tube with central body which has conical section and BR = 0.6 or parabolic section and BR = 0.7 with all other conditions being equal. In both cases, the detonation arose in an overdriven mode, and it had essential nonplanar front structure.

Table 2 Parameters of central body

No.	Shape	M_0	α	β	L, mm	BR	Detonation
1	Parabolic/conic*	3.75	45	7	120	0.6	+
2		3.5	40	3	80	0.7	−
3		3.5	40	6	120	0.6	+
4		3.5	45	6	120	0.7	−
5	Parabolic/elliptic†	3.5	45	7	120	0.7	+
6		3.5	45	7	120	0.6	+
7		3.3	45	7	120	0.6	−
8		3.3	45	7	120	0.7	−
9		3.3	45	3	120	0.7	−
10	Parabolic/parabolic‡	3.5	40	3.5	60	0.6	+

*Frontal part has parabolic section, curve equation is $r^2 = az + b$, tail part has conical section, curve is $r = az + b$.

†Tail part of central body has elliptic section, curve is $a(z-b)^2 + (r-c)^2 = d^2$.

‡Both frontal and tail parts have parabolic section, curve is $\pm r^2 = az + b$.

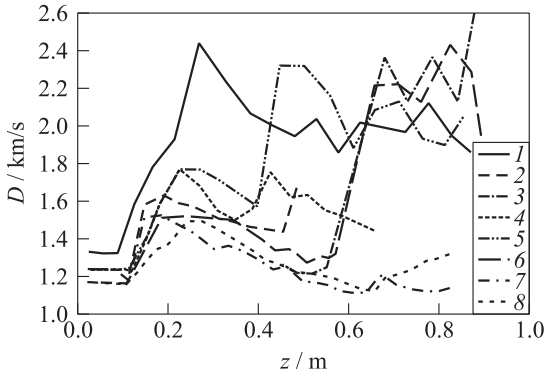

Figure 2 Shock wave velocity vs. distance

For runs 1 and 6, shadow graphs are shown in Fig. 3. In run 1, the velocity of shock wave increases from 1310 m/s ($M_0 = 3.75$) at inlet to 2440 m/s at the gap exit, then it begins to go down and gradually approximates to the velocity of Chapman–Jouguet detonation (according to thermodynamics calculations, it is equal to 1800 m/s). However, the

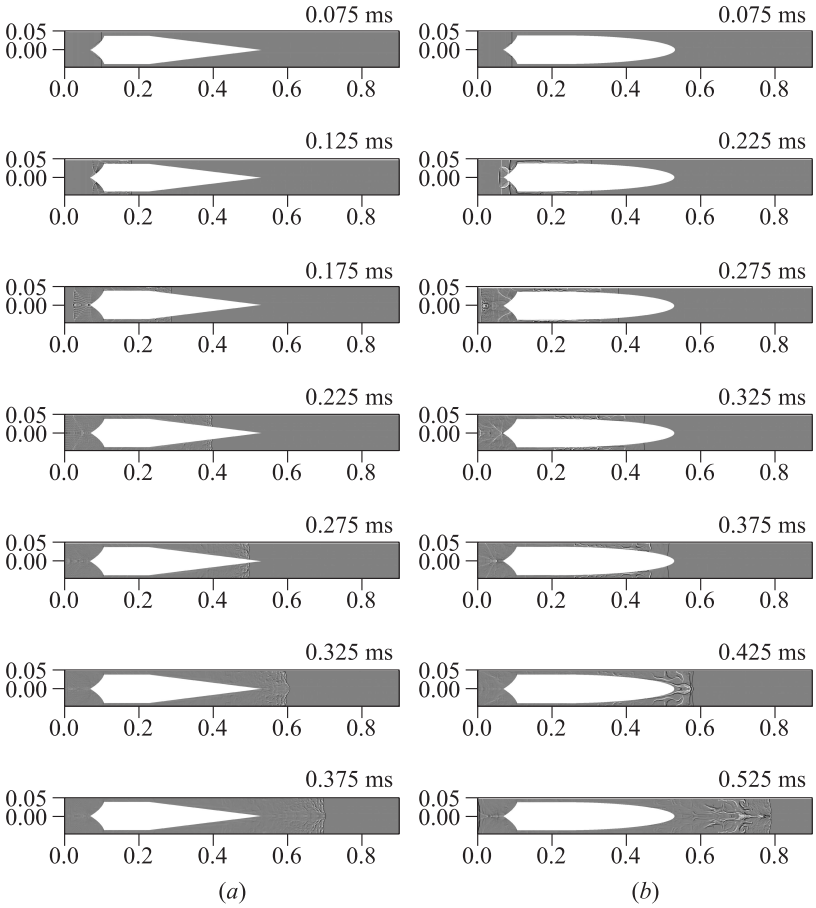

Figure 3 Shadow graphs: (*a*) run No. 1; and (*b*) run No. 6

pulses are remained and the velocity of the detonation wave oscillates in the range of 1840–1950 m/s.

In run 6, the velocity of shock wave at inlet is equal to 1230 m/s ($M_0 = 3.5$), then it increases to 1520 m/s in the gap and continues to grow until the detonation is set at a distance of 0.65 m with the velocity of 2240 m/s which quickly drops down to 1940 m/s.

7 Concluding Remarks

The possibility of using a central body in tubes to shorten the distance required for detonation initiation was shown by means of numerical modeling. At suitable assumptions on chemical kinetics, the onset of detonation was observed in calculations for the initial shock wave Mach number above $M_0 = 3.5$.

It was revealed that according to expectations, the shape of central body and blockage ratio have an effect on critical parameters for the onset of detonation. The optimal blockage ratio is 0.6-0.7 depending on the body shape. The optimal shape of the frontal part of the body is paraboloid with $\alpha = 40°$. As for the shape of the tail part of the body, it was found that for high angles corresponding to abrupt drop in cross section, the critical Mach number was close to the normal velocity of Chapman–Jouguet detonation. It appeared that conical or elliptical configuration of the tail with angle $\beta = 6°$–$7°$ is optimal for detonation initiation with a shock wave of lowest intensity.

Acknowledgments

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References

1. Frolov, S. M., A. E. Barykin, and A. A. Borisov. 2004. Thermodynamic cycle with detonating combustion of fuel. *Khim. Fiz.* 23(3):17–25. [In Russian.]
2. Frolov, S. M., V. S. Aksenov, K. A. Avdeev, A. A. Borisov, P. A. Gusev, V. S. Ivanov, A. S. Koval', S. N. Medvedev, V. A. Smetanyuk, F. S. Frolov, and I. O. Shamshin. 2014. A prototype of the pulsed detonation burner operating on natural gas. *Transient combustion and detonation phenomena*. Eds. G. D. Roy and S. M. Frolov. Moscow: TORUS PRESS. 401–412.
3. Frolov, S. M. 2009. Detonation initiation techniques for pulse detonation propulsion. In: *Progress in propulsion physics*. Eds. L. T. DeLuca, C. Bonnal, O. Haidn, and S. Frolov. Advances in aerospace sciences EUCASS book ser. Moscow–Paris: TORUS PRESS – EDP Sci. 1:321–340.
4. Frolov, S. M., and V. S. Aksenov. 2009. Initiation of gas detonation in a tube with a shaped obstacle. *Dokl. Phys. Chem.* 427(1):129–132.

5. Semenov, I. V., P. S. Utkin, V. V. Markov, S. M. Frolov, and V. S. Aksenov. 2009. Numerical and experimental investigation of detonation initiation in profiled tubes *22nd Colloquium (International) on the Dynamics of Explosion and Reactive Systems*. Minsk, Republic of Belarus. Paper No. 168.
6. Frolov, S. M., V. S. Aksenov, and A. A. Skripnik. 2014. Detonation initiation in natural gas–air mixture in a tube with focusing nozzle. *Transient combustion and detonation phenomena*. Eds. G. D. Roy and S. M. Frolov. Moscow: TORUS PRESS. 196–203.
7. U.S. Dept. of Commerce, National Bureau of Standards. 1970. JANAF: Thermochemical tables. 2nd ed. Washington, D.C.
8. Kovenja, V. M., and N. N. Janenko. 1981. *The method of splitting in problems of gas dynamics*. Novosibirsk: Nauka. 304 p. [In Russian.]
9. Kolgan, V. P. 1972. Application of the minimum-derivative principle in the construction of finite-difference schemes for numerical analysis of discontinuous solutions in gas dynamics. *Uch. Zap. TsAGI* 3(i6):68–77.
10. Hairer, E., S. P. Norsett, and G. Wanner. 1987. *Solving ordinary differential equations I. Nonstiff problems*. Springer-Verlag. 528 p.
11. Frolov, S. M. 2008. Fast deflagration-to-detonation transition. *Russ. J. Phys. Chem. B* 2(3):442–455.
12. Frolov, S. M., and V. S. Aksenov. 2009. Initiation of gas detonation in the tube with shaped narrowing of the tube cross-section. In: *Combustion and explosion*. Ed. S. M. Frolov. Moscow: TORUS PRESS. 2:26–30. [In Russian.]