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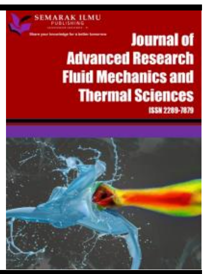

Numerical Study of Detonation Waves in Gas Suspensions with Spatially Inhomogeneous Particle Concentration Distribution in Sharply Expanding Pipes

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ABSTRACT

The article presents some results of a numerical study of detonation waves in gas suspensions with a spatially inhomogeneous distribution of particle concentration in sharply expanding pipes obtained by the large particle method. The purpose of the research is to study the influence of pipeline geometry and longitudinally spatially inhomogeneous distribution of particle concentration on the propagation of detonation waves in gas suspensions. It is shown that the size of the narrow and wide parts of the pipeline, as well as, the spatially inhomogeneous distribution of particle concentrations, qualitatively and quantitatively affect this process. Three detonation modes have been identified: continuous wave propagation, complete cessation, and partial disruption with subsequent recovery. It has been established that, at a fixed total mass of suspension, a layer with a linearly decreasing law of change in the concentration of unitary fuel particles better attenuates detonation waves than with a linearly increasing and homogeneous one.

1. Introduction

Research works are currently being actively carried out around the world aimed at studying the characteristics of the propagation of shock and detonation waves in various media, both experimentally and theoretically. In this direction, the most relevant research is modeling the processes of propagation of explosive and detonation waves in gas suspensions in pipes of various configurations.

The propagation of detonation waves in pipes with sudden expansion is a complex process. When the propagation of detonation waves passes from the narrow part of the pipe to the wide part, their propagation, depending on the influence of the defining parameters, can continue or stop. Modes of

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propagation of detonation waves (subcritical, critical and supercritical) discovered first in experiments by Zel'dovich *et al.,* [1]. In the subcritical mode there is a complete cessation, in the critical mode there is a partial breakdown with subsequent recovery, in the supercritical mode there is continuous propagation of the wave. Kindracki [2] conducted experimental studies of the initiation of detonation in a kerosene-oxidizer mixture in a short pipe. The minimum tube diameter and the minimum energy level that ensures direct initiation of detonation are determined by Gui *et al.,* [3]. They numerically studied detonation diffraction in a T-tube filled with a stoichiometric mixture of hydrogen/oxygen/argon using the Euler equations with detailed finite velocity chemistry. The details of the transient behavior of diffracting detonation in high-speed flows are discussed. Warimani *et al.,* [4] studied the influence of thermodynamic detonation factors on the operation of a pulse detonation engine. Dou and Khoo [5] used three-dimensional numerical modeling to study the influence of the initial disturbance on the structure of the detonation front in a narrow channel. For the initial disturbance, two types of disturbances are used. One of them is a random disturbance, and the other is a symmetric disturbance superimposed inside the strip along the diagonal direction on the leading detonation front. The results show that the two types of disturbances lead to different processes. Continuous detonation combustion of hydrogen-air mixtures in annular combustion chambers of different sizes and designs was studied experimentally by Wang *et al.,* [6] and Lin *et al.,* [7]. Arienti and Shepherd [8] studied the influence of reaction parameters on flows during diffraction of a plane detonation wave behind a step. The existence of three propagation modes has been confirmed, which are designated as subcritical (detonation failure), critical (partial failure with recovery) and supercritical (continuous propagation). The possibility of the emergence of a system of transverse waves at the detonation front in one of the regimes has been indicated. Pantow *et al.,* [9] present the results of a numerical analysis of the flow structure in comparison with experimental schlieren photographs of the propagation of cellular detonation in a channel with a section discontinuity. The possibility of partial disruption of detonation with subsequent reinitiation when a diffracted wave is reflected from the wall of a wide part of the channel with further integration of the shock wave of the combustion front is shown. Kapila *et al.,* [10] studied the processes of diffraction of a detonation wave in a two-phase medium on a reverse step. A powdered explosive characterized by a high detonation speed (7600 m/s) was considered. The average parameters of the mixture were determined without phase separation, and the flow structure turned out to be qualitatively similar to gas mixtures. Roy *et al.,* [11] provide a review of fundamental and applied research aimed at creating pulsating detonation engines. Much attention in these works was paid to the analysis of the propagation of detonation waves in limited volumes and channels of complex shape. By Sorin *et al.,* [12], in order to characterize the transfer processes and quantify the criteria for transfer to the receiving chamber, a study of the diffraction of self-sustaining detonation from a cylindrical pipe on various geometric configurations was carried out. By Bivol *et al.,* [13], the formation of an overcompressed detonation wave in methane-oxygen mixtures in an axisymmetric channel of variable cross-section was experimentally studied. The velocities and pressures at the front of the detonation wave were determined depending on the composition of the mixture. Kratova *et al.,* [14] numerically studied the processes of diffraction of a plane detonation wave in a gas suspension in a flat channel with a discontinuity in the cross-section. The influence of the geometric parameters of the channel and particle size on the propagation of detonation in a wide part of the channel was studied. It has been established that for a flow with a reverse step at the exit from the channel, three modes of detonation propagation are possible: subcritical, critical and supercritical. In the work, using specific examples, it is shown that the occurrence of these modes depends on different values of the channel and particle. Fedorov *et al.,* [15,16] considered the exit of detonation waves from a flat channel into a region with a linear expansion of the cross section of the channel. The process of transition of a detonation wave into an expanding section and further propagation is analyzed. Numerical results of the flow at various expansion angles are presented. Three modes of detonation propagation have been established: supercritical, critical and subcritical. Kutushev *et al.,* [17] present the results of a numerical study of the propagation of detonation waves in monodisperse gas suspensions in sharply expanding pipes. The influence of the diameter and mass content of unitary fuel particles and the geometry (size of the narrow and wide parts) of the pipeline on this process was studied. The dependences of the critical ratio of pipe diameters of a composite pipeline on the relative mass content of unitary fuel particles of different sizes are presented. By Burnashev *et al.,* [18], the results of a numerical study of the patterns of propagation of detonation waves in polydisperse (two-fraction) gas suspensions in sharply expanding pipes are presented. The influence of mono- and polydispersity of unitary fuel particles and their relative mass content, as well as pipeline geometry on the patterns of propagation of detonation waves, has been studied. Nazarov [19] studied the processes of propagation of detonation waves in cases when suddenly expanding pipes are completely or partially filled with gas suspensions across the cross section. The influence of the height of the transverse heterogeneity of the particle concentration distribution on the process under consideration has been studied. It has been established that the critical value of the height of transverse spatial heterogeneity decreases monotonically with increasing relative mass content of gas suspension.

Thus, an analysis of the current state of research on the problem on this topic has shown that the influence of the spatially inhomogeneous distribution of the concentration of unitary fuel particles has not been sufficiently studied.

The main goal of this work is to study the pattern of propagation of detonation waves in gas suspensions with a spatially inhomogeneous distribution of particle concentration in a wide part of sharply expanding pipes.

2. Methodology

2.1 Formulation of the Problem

Let a pipeline be given, consisting of pipes of length $L\,(L = L_0 + L_1 + L_2)$ and diameters D_1 and D_2 (Figure 1), the narrow part of which is filled with a homogeneous, and the wide part of the pipe is filled with an inhomogeneous gas suspension of unitary fuel in the longitudinal section. The distribution of the initial concentration of particles in the wide part of the pipeline in the longitudinal section obeys a linearly increasing or linearly decreasing law $\rho_2(z,0) = Az - B;\ A,\ B = const$. For comparison, it is also considered the case of a uniform distribution of the initial particle concentration. At the initial time, a perturbation of the gas in the form of a triangular shock wave is produced at the left end of the pipe in region 0 $\left(0 \le L_0 \le z_f\right)$, which ignites the monofuel–air mixture in region 1 $\left(z_f < L_1 \le z_*\right)$ of the narrow part of the pipeline. Given sufficient energy of the initiating shock wave, it is required to model the explosion of the air-fuel mixture in such a way that of a stationary heterogeneous detonation wave forms in the narrow pipeline region and then passes to the wide region 2 $\left(z_* < L_2 < z_{**}\right)$ of the pipeline. It is required to study the influence of the longitudinal spatial heterogeneity of the distribution of the concentration of unitary fuel particles in a wide part of the pipeline on the process of propagation of detonation waves.

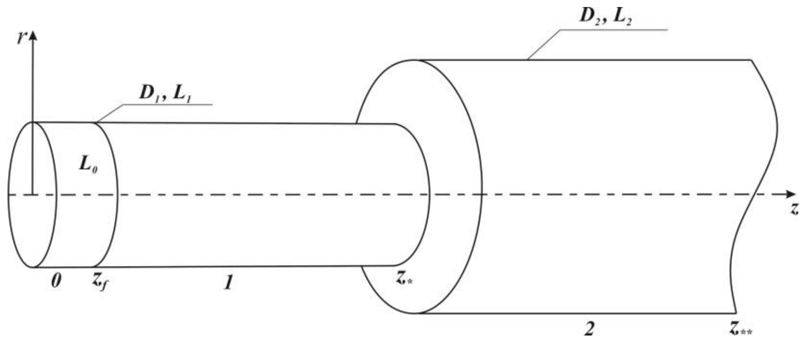


Fig. 1. Schematic representation of the pipeline

2.2 Mathematical Model

The system of equations for two-dimensional plane unsteady motion of gas and particles of unitary fuel has the form the previous studies [20-22]

Mass conservation equations

$$\frac{\partial \rho_1}{\partial t}+\frac{1}{r}\frac{\partial(\rho_1 v_{1,r} r)}{\partial r}+\frac{\partial(\rho_1 v_{1,z})}{\partial z}=J_{21},$$

$$\frac{\partial \rho_2}{\partial t}+\frac{1}{r}\frac{\partial(\rho_2 v_{2,r} r)}{\partial r}+\frac{\partial(\rho_2 v_{2,z})}{\partial z}=-J_{21}, \tag{1}$$

Equations of conservation of mass for an inert gas and gaseous products of combustion of a gas mixture

$$\frac{\partial \rho_{11}}{\partial t}+\frac{1}{r}\frac{\partial(\rho_{11} v_{1,r} r)}{\partial r}+\frac{\partial(\rho_{11} v_{1,z})}{\partial z}=0, \qquad \frac{\partial \rho_{12}}{\partial t}+\frac{1}{r}\frac{\partial(\rho_{12} v_{1,r} r)}{\partial r}+\frac{\partial(\rho_{12} v_{1,z})}{\partial z}=J_{21}, \tag{2}$$

Equations conservation for the number of dispersed particles

$$\frac{\partial n_2}{\partial t}+\frac{1}{r}\frac{\partial(n_2 v_{2,r} r)}{\partial r}+\frac{\partial(n_2 v_{2,z})}{\partial z}=0, \quad \alpha_2=\frac{1}{6}\pi d_2^3 n_2, \tag{3}$$

Phase momentum conservation equations

$$\frac{\partial(\rho_1 v_{1,r})}{\partial t}+\frac{1}{r}\frac{\partial(\rho_1 v_{1,r} v_{1,r} r)}{\partial r}+\frac{\partial(\rho_1 v_{1,r}\, v_{1,z})}{\partial z}+\frac{\partial p}{\partial r}=-F_{2,r}+J_{21} v_{2,r},$$

$$\frac{\partial(\rho_1 v_{1,z})}{\partial t}+\frac{1}{r}\frac{\partial(\rho_1 v_{1,r} v_{1,z} r)}{\partial r}+\frac{\partial(\rho_r v_{1,z}\, v_{1,z})}{\partial z}+\frac{\partial p}{\partial z}=-F_{2,z}+J_{21} v_{2,z},$$

$$\frac{\partial(\rho_2 v_{2,r})}{\partial t}+\frac{1}{r}\frac{\partial(\rho_2 v_{2,r} v_{2,r} r)}{\partial r}+\frac{\partial(\rho_2 v_{2,r} v_{2,z})}{\partial z}=F_{2,r}-J_{21}v_{2,r}, \tag{4}$$

$$\frac{\partial(\rho_2 v_{2,z})}{\partial t}+\frac{1}{r}\frac{\partial(\rho_2 v_{2,r} v_{2,z} r)}{\partial r}+\frac{\partial(\rho_2 v_{2,z} v_{2,z})}{\partial z}=F_{2,z}-J_{21}v_{2,z},$$

Equations of heat flux to particle phases

$$\frac{\partial(\rho_2 e_2)}{\partial t}+\frac{1}{r}\frac{\partial(\rho_2 e_2 v_{2,r} r)}{\partial r}+\frac{\partial(\rho_2 e_2 v_{2,z})}{\partial z}=Q_{12}\eta(-J_{21})-J_{21}e_2, \tag{5}$$

Equations conservation for the total energy of the mixture

$$\sum_{i=1}^{3}\left[\frac{\partial(\rho_i E_i)}{\partial t}+\frac{1}{r}\frac{\partial(\rho_i E_i+\alpha_i p)v_{i,r} r}{\partial r}+\frac{\partial(\rho_i E_i+\alpha_i p)v_{i,z}}{\partial z}\right]=0,$$

$$\rho_1=\sum_{k=1}^{2}\rho_{1,k}, \qquad \rho_{1,k}=\rho_{1,k}^0\alpha_1, \qquad \rho_i=\rho_i^0\alpha_i, \quad \rho_1^0=\sum_{k=1}^{2}\rho_{1,k}^0, \qquad v_i^2=v_{i,r}^2+v_{i,z}^2,$$

$$\alpha_1+\alpha_2=1, \qquad E_i=e_i+0.5v_i^2, \quad \eta(z)=\begin{cases}0, & z<0\\ 1, & z\geq 0\end{cases} \qquad (i=1;\ 2).$$

The mean and actual densities, the volume content, the mass velocity, and the specific and total energies of phase i are denoted as $\rho_i, \rho_i^0, \alpha_i, v_i, e_i$ and E_i respectively (*i*=1 – gas, *i*=2 – particles); ρ_{11}, ρ_{12} and ρ_{11}^0, ρ_{12}^0 are average and true densities of the gas phase components; v_{1r} and v_{1z} are the components of the velocity v_i; n_2 and d_2 number density and particle diametr; p is the pressure of the gas mixture; $F_{2,r}$ and $F_{2,z}$ - components of the interfacial friction force; Q − heat exchange in gas suspension; J_{21} − intensity of interfacial mass transfer; η − Heaviside function.

Closing relations, initial and boundary conditions of the problem are specified similarly to Kutushev [23].

The problem was solved using the large particle method [24,25].

3. Results

Figure 2 shows the calculated profiles of pressure (a) and mass velocity (b) of the gas mixture during the formation of a heterogeneous detonation wave in the narrow and wide part of the pipeline, propagating through initially at rest homogeneous gas suspensions (in the narrow part), and then inhomogeneous, i.e. with a linearly increasing change in the concentration of unitary fuel particles (in a wide part) on the symmetry axis at different times. The diameter of the particles of unitary fuel was $d_2=30$μm, the initial relative mass content of particles in the mixture in the narrow part of the pipeline was $m_{20}=2$. The distribution of the initial concentration of particles in the wide part of the pipeline was determined by formula $\rho_2(z,0)=Az-B,$ corresponding to a linearly increasing change in the concentration of particles of unitary fuel, where $A=0.16;\ B=4;$

$25 < z \leq 50$. The radius of the narrow part of the pipeline is $R_1 = 0.1$ m, and the radius of its wide part is $R_2 = 0.3$ m. It can be seen that as the shock wave penetrates into the region of the gas suspension, convective heating of the powder particles occurs to the ignition temperature and their subsequent combustion. The combustion wave, formed behind the front of the passing shock wave, gradually intensifies (curves 1-3 in Figure 2(a)) and, in the limit, reaches the regime of a Chapman–Jouguet heterogeneous detonation wave (curves 4-5 in Figure 2(a)). The movement of gas and particles of unitary fuel behind a wave of heterogeneous detonation is one-dimensional. The above means that by the time gas-dynamic disturbances arrive at the place of sharp expansion of the pipeline, the wave of heterogeneous detonation becomes stationary. In the following, the stage of wave motion is shown, corresponding to the exit of the detonation wave from the narrow part of the pipeline into its wide part. In the wide part of the pipe, the pressure decreases due to the expansion of the pipeline diameter (curves 6-7 in Figure 2(a)). Subsequently, a gradual increase in pressure is observed (curves 8-9 in Figure 2(a)). The conducted research indicates the possibility of interrupting or continuing the process of propagation of a heterogeneous detonation wave in a pipeline through a sudden expansion of the flow in a wide part of the pipe. In this case, it should be noted that the process of combustion propagation in the detonation mode does not stop.

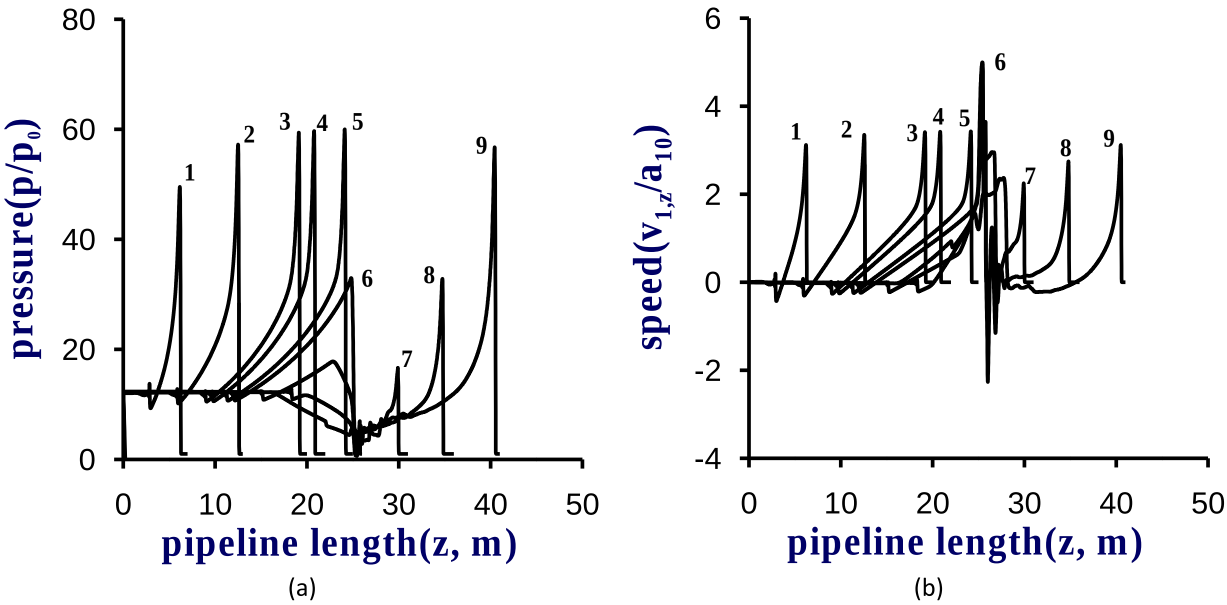
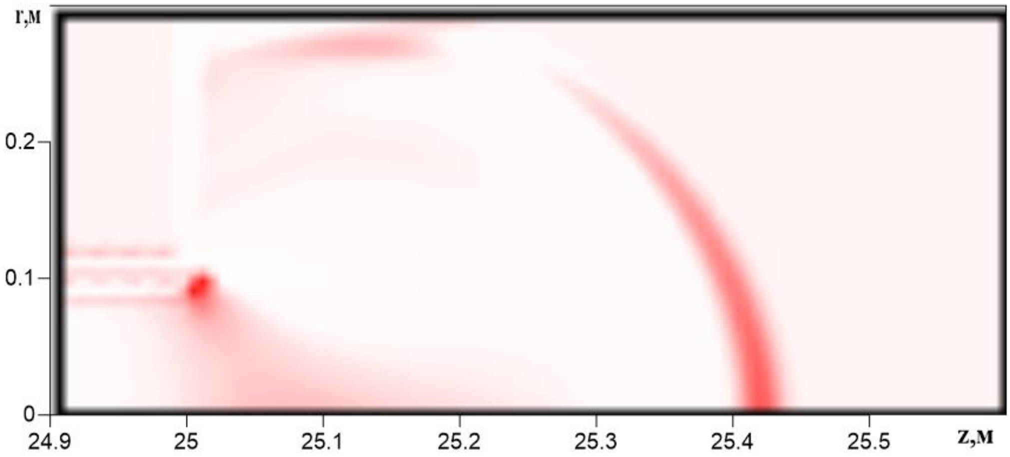
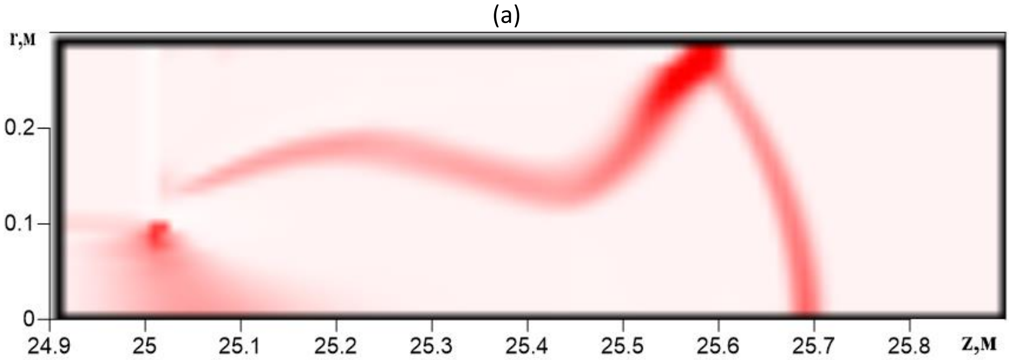


Fig. 2. Profiles of pressure (a) and mass velocity (b) of the gas mixture on the axis of symmetry in the narrow and wide part of the pipeline

Figure 3 demonstrates the initial stage of two-dimensional wave motion, corresponding to the interaction of the diffracted part of the detonation wave with the lateral surface of a wide part of the pipeline at moments in time. All parameters are similar to those in Figure 2. From Figure 3(a) it can be seen that the wave emerging from the narrow part of the pipeline does not immediately reach the pipeline wall. Figure 3(b) illustrates the reflection of a wave from the side wall of the pipeline.



(a)



(b)

Fig. 3. Distribution of pressure (p/p_0) of gas in a wide part of the pipeline at different values of time

Figure 4 shows the calculated profiles of pressure (a) and mass velocity (b) of the gas mixture during the formation of a heterogeneous detonation wave in the narrow and wide part of the pipeline, propagating through initially at rest homogeneous gas suspensions (in the narrow part), and then inhomogeneous, i.e. with a linearly decreasing change in the concentration of unitary fuel particles (in the wide part) on the symmetry axis at moments of time. The particle diameter of the unitary fuel was $d_2 = 30$ μm, the initial relative mass content of particles in the mixture in the narrow part of the pipeline was $m_{20} = 2$. The distribution of the initial concentration of particles in a wide part of the pipeline is determined by formula $\rho_2(z,0) = Az + B$ corresponding to a linearly decreasing change in the concentration of particles of unitary fuel, where $A = -0.16;\ B = 8;\ 25 < z \leq 50$. The radius of the narrow part of the pipeline is $R_1 = 0.1$ m, and the radius of its wide part is $R_2 = 0.3$ m. In the wide part of the pipeline, the pressure initially decreases due to the expansion of the pipeline diameter (curves 4). When detonation waves propagate through a heterogeneous gas suspension with a linearly decreasing mass content of suspended particles, an increase in detonation waves (in pressure) is observed (curves 5-6), and subsequently an acceleration of detonation waves with a gradual decrease in pressure (curves 7-8). An increase in pressure observed in the interaction of detonation waves with a dusty space is due to a sharp deceleration of the flow by dense layers of suspension. When detonation waves propagate through a gas suspension, the gas flow first involves particles from the denser layers of the gas suspension, then particles from the less dense layers of the gas suspension. Calculations show that when detonation waves propagate through a heterogeneous gas suspension with a linearly decreasing mass content of unitary fuel particles, it leads to a gradual cessation of detonation.

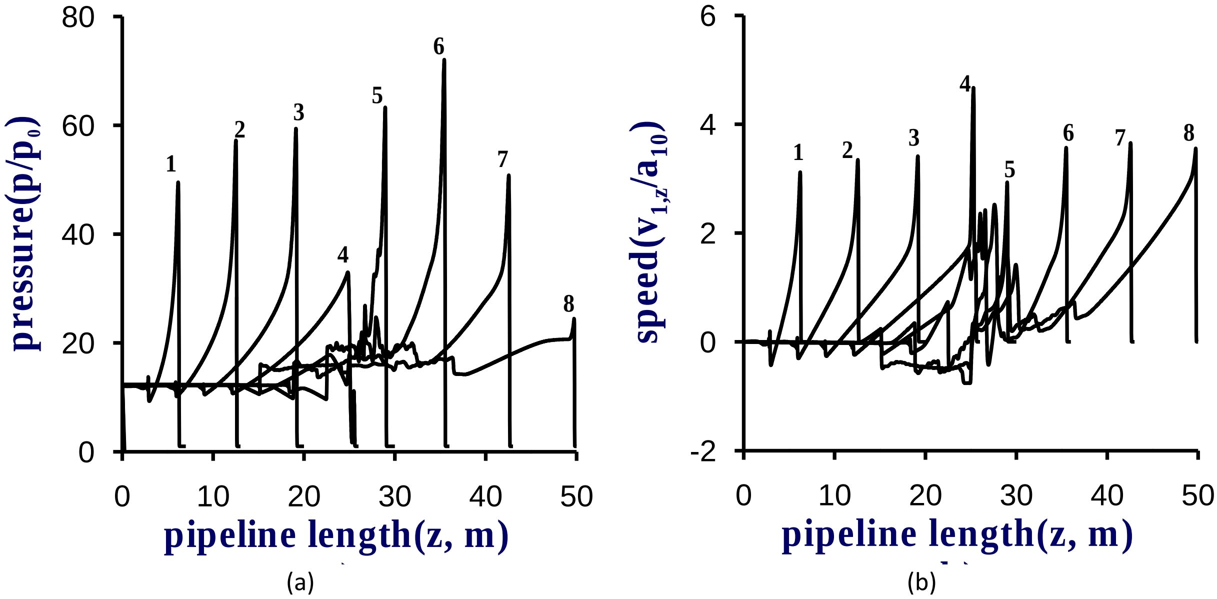


Fig. 4. Profiles of pressure (a) and mass velocity (b) of the gas mixture on the axis of symmetry in the narrow and wide part of the pipeline

Below, the influence of the heterogeneity of unitary fuel particles on the propagation of detonation waves in a wide part of the pipeline is studied numerically. Figure 5 shows the envelopes of the maximum pressures behind the combustion waves on the axis of symmetry in the wide part of the pipeline. The particle diameter of the unitary fuel was $d_2 = 30$ μm, the initial relative mass content of particles in the mixture in the narrow part of the pipeline was $m_{20} = 2$. The radius of the narrow part of the pipeline is $R_1 = 0.1$ m, the radius of its wide part is $R_2 = 0.3$ m. With fixed parameters of the pipeline and gas suspension, for uniform and linearly increasing laws of change in the initial concentration of particles, a continuation of detonation is observed, and with a linearly decreasing one, detonation is gradually disrupted in the wide part of the pipeline.

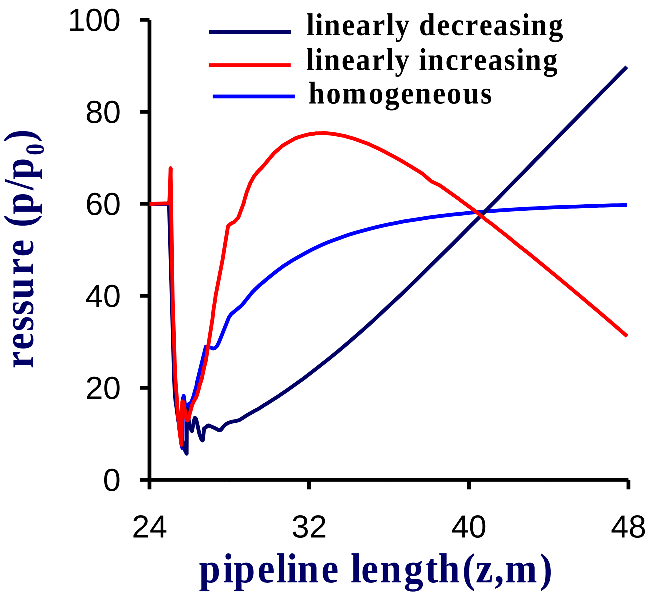
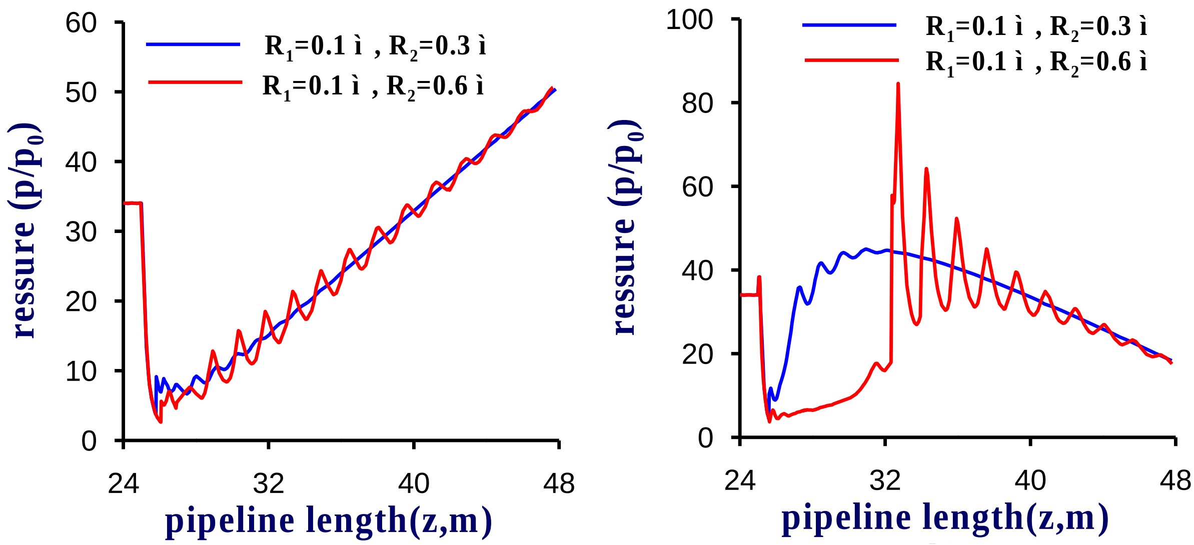


Fig. 5. Envelopes of maximum pressures behind combustion waves on the axis of symmetry in wide parts of the pipeline

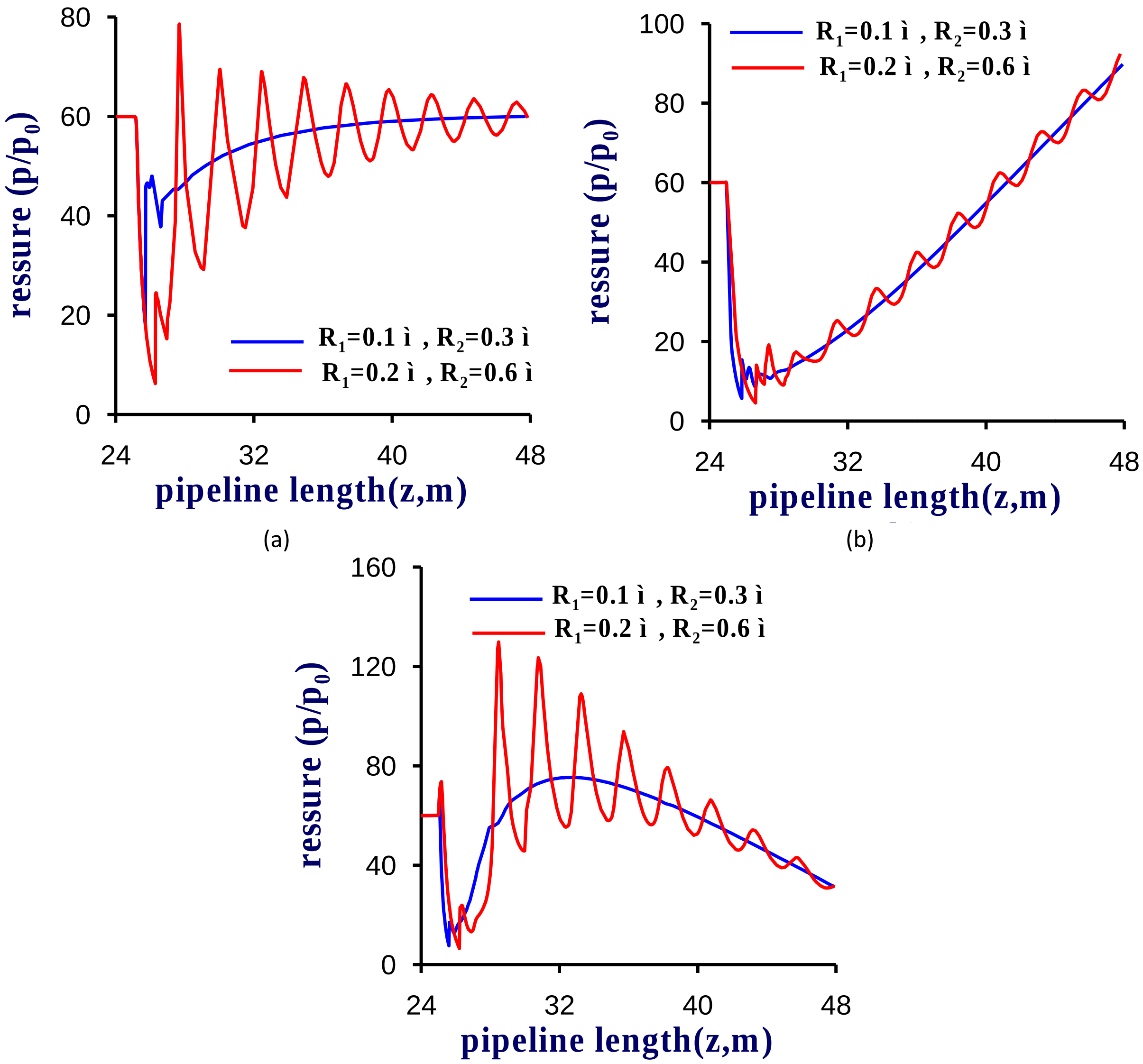
The work numerically studied the effect of changing the size of a wide part of the pipeline on the propagation of detonation waves in gas suspensions of unitary fuel. Figure 6 shows the envelope of maximum pressures behind combustion waves on the axis of symmetry in wide parts of the pipeline. The particle size is $d_2 = 15$ µm, the initial relative mass content is $m_{20} = 1$. Figure 6(b) shows that when $R_1 = 0.1$ m and $R_2 = 0.6$ m, the detonation wave decays in part $25 \le z \le 31$, and the detonation wave recovers in part $z > 31$. In wide parts of the pipeline at $R_1 = 0.1$ m, $R_2 = 0.6$ m, an oscillatory nature is observed throughout the entire region of the wide part of the pipeline. It can be seen that an increase in the diameter of the wide part of the pipeline leads to a qualitative change in the propagation of detonation waves in its wide parts.



(a) (b)

Fig. 6. Envelopes of maximum pressures behind combustion waves on the axis of symmetry in wide parts of the pipeline

Below are some results of a numerical study of the effect of changing the size of the narrow and wide parts of the pipeline on the propagation of detonation waves in spatially homogeneous and inhomogeneous gas suspensions of unitary fuel. Figure 7 shows the envelope of maximum pressures behind combustion waves on the axis of symmetry in wide parts of the pipeline. The particle size is $d_2 = 30$ µm, the initial relative mass content is $m_{20} = 2$. As the pipe width increases, the recovery of the detonation process lags. In wide parts of the pipeline at $R_1 = 0.1$ m, $R_2 = 0.3$ m, an oscillatory character is observed in the area adjacent to the beginning of the wide part of the pipeline, and at $R_1 = 0.2$ m, $R_2 = 0.6$ m throughout the entire area of the wide part of the pipeline. It can be seen that increasing the diameters of the narrow and wide parts of the pipeline leads to a qualitative change in the propagation of detonation waves in its wide parts.



(a) (b)

(c)

Fig. 7. Envelopes of maximum pressures behind combustion waves on the axis of symmetry in wide parts of the pipeline

4. Conclusions

This study examined the influence of the initial distribution of unitary fuel particle concentration on the propagation structure of transient detonation waves in rapidly expanding tubes. It is shown that when detonation waves pass through layers of a gas suspension with increasing or decreasing laws of change in particle concentration, an increase or decrease in the waves is observed, respectively. An increase in the diameter ratio $\left(D_2 / D_1\right)$ of pipelines leads to pressure oscillation in a wide part of the pipeline due to the reflection of the shock wave from the pipeline wall. The conditions for the occurrence of three detonation modes have been identified: continuous wave propagation, complete cessation, and partial disruption with subsequent recovery. Using computational experiments, it was established that at a fixed total mass of suspension, a layer with a linearly decreasing law of change in the concentration of unitary fuel particles is better at attenuating detonation waves than with a linearly increasing and homogeneous one.

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