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Optimization of Detonation Dampers for Ducts Transporting Gaseous Fuels.

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Abstract One of the important contemporary technological problems is connected with necessity of extinguishing detonations, which may occur in pipelines transporting gaseous fuels. To achieve this goal usually a matrix of narrow channels is placed across the flow inside the pipeline. In our recent papers [1], [2] we have shown, that channels with sharp changes of cross-section should be more efficient in this respect than traditionally used straight channels with constant cross-section area. In the present paper we demonstrate how detonation behaves in channels with changes of cross-section under realistic conditions – if the channel cross-section is of dimensions acceptable technologically. At the same time we take into account the fact, that if friction and heat exchange at the walls are present, gas flowing through the channels accelerates and its density decreases considerably. The result of our considerations is a selection of, possibly, optimum shape of the channels of a detonation damper.

1   Introduction

The necessity of extinguishing detonation, which may occur in pipelines transporting gaseous fuels, creates nowadays a very important technological problem. The standard devices used for this purpose consist of matrices of very narrow channels. Cooling the gas by cold walls of such channels may extinguish the flame and stop detonation. Detonation may also be extinguished if the cross-section of the channel transporting gas increases abruptly at some place. The desired effect is achieved if the generated rarefaction waves decrease sufficiently the temperature of the flame ([3], [4], [5], [6]). It has been shown, that simultaneous use of both methods – using narrow channels with variable cross-section – may give even better results ([1], [2]). Additional profit would come here from the fact, that the flow in narrow channels is usually laminar; the abrupt change of the cross-section introduces some turbulence and this way enhances cooling by the walls.

There are, however, some doubts connected with results presented in the papers [1] and [2]. The most important is connected with the fact, that these results were obtained for very narrow channels – about 5 micrometers wide only. It is not clear how detonation waves would behave in channels of larger cross-section, sufficiently large to be technologically acceptable. In particular, it is not clear how detonation waves would behave in such channels, when flow parameters, density and velocity, vary along the channel. Apart from that, although it has been shown, that in very narrow channels with abrupt changes of cross-section the flow resistance is not bigger than in straight channels [2], this might not be true for wider channels. To overcome the possible increase of resistance it might be necessary to increase the cross-sections of the channels, which would affect the efficiency of the device, so that the net result might not be worthwhile.

The present paper is devoted to clarification of these problems. The method used for this purpose is the numerical simulation with the DSMC technique.

There is one point, which should be noted here. The device for extinguishing detonation, as mentioned above, has, as a rule, a form of a thick steel plate (of the order of 50 mm thickness), with large number of holes of diameter equal to a fraction of a millimeter. It is impossible to drill large number of such holes in a solid steel plate. Instead, such device is usually manufactured from thin steel sheets, with narrow and shallow grooves, pressed firmly together. Such method of manufacturing makes it possible to produce the channels of the device of nearly arbitrary size and shape.

2   Method of Simulation

The simulations presented in this paper were performed with the standard Direct Simulation Monte – Carlo (DSMC) technique [7]. The DSMC technique makes it possible to simulate the fluid flows in various geometrical configurations and it also offers a possibility of taking into account the relaxation phenomena and chemical reactions ([8], [7]). This, unfortunately, increases complexity of the computer programs and the necessary computing times. However, in the considered case considerable simplifications can be made because in a detonation wave the medium is far from thermodynamic equilibrium, combustion proceeds very fast and the relaxation processes at the molecular level may be disregarded. The factor of prime importance is the produced thermal energy.

3   Model of a Detonating Medium

In the present work we investigate only the influence of shape and size of the channel upon the flow inside it, and upon the process of extinguishing detonation. A very simple model of the detonating medium ([6], [9]) may therefore be used. It has been assumed, that all molecules of this medium are identical, hard spheres. Part of them, uniformly distributed in space, carry certain amount of "internal" energy (of unspecified character). The remaining molecules are "inert" – they can carry no "internal" energy and cannot accept it in any way. The "internal" energy of a molecule may be transformed into kinetic energy during collision with an "inert" molecule, provided that the colliding molecules approach each other with sufficiently high "velocity of approach" (Fig. 1). As the result, the relative velocity of the molecules is increased suitably.
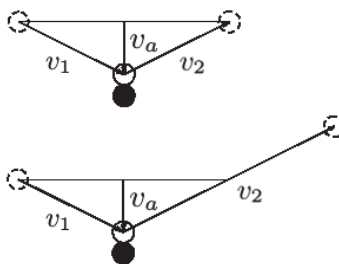

Fig.1. Collisions of two molecules in reference frame connected with one of them. Top – elastic, bottom – with energy release; v_1 – relative velocity before collision, v_2 – relative velocity after collision, v_a – "velocity of approach".

A molecule which had lost its "internal" energy may regain it in a collision with an "inert" molecule if their "velocity of approach" is higher than velocity corresponding to

this "internal" energy. The relative velocity of the molecules is then decreased suitably.

The assumed "internal" energy of a single molecule was such, that the relative velocity of the colliding molecules was increased by the value equal to 10 times the most probable molecular speed. The "threshold velocity of approach" of the colliding molecules, necessary to release the "internal" energy, was equal to about 5.48 (exactly $\sqrt{30}$) times the most probable molecular speed.

4 Interactions with Solid Walls

To simulate the interactions of the molecules with walls the very simple model introduced by J.C. Maxwell [10] has been employed: molecules reflect from the walls either specularly (without exchange of tangential momentum and energy) or diffusely (molecules are adsorbed by the wall and re-emitted in directions selected at random, with energies corresponding to temperature of the reflecting wall). The ratio of the number of molecules reflected diffusely to the total number of the reflected molecules (called "accommodation coefficient", α) may vary from 0 to 1. The value $\alpha = 0$ (purely specular reflections) corresponds to no exchange of tangential momentum and energy, the value $\alpha = 1$ corresponds to maximum possible exchange (maximum friction and cooling). For majority of the so-called "technological surfaces" the accommodation coefficient is close to unity, i.e. practically all molecules reflect from the walls diffusely.

5 Simulation of Flow in Channels of Larger Cross-Section

The described model of interactions of the molecules with walls makes it possible to extend the results of flow simulations in very narrow channels to channels of larger cross-section. According to the model, the walls influence the flow through diffuse reflections of the molecules only. The specular reflections cause neither momentum, nor energy exchange. The influence of walls upon the flow depends therefore only on the ratio of the number of molecules reflecting diffusely to total number of molecules in the flow.

Since, for "technological surfaces" the reflection of molecules is usually diffuse and in wide channels the ratio of the number of molecules reflecting from walls to total number of molecules is smaller than in narrow, it may be expected that artificial decrease of the assumed accommodation coefficient will produce, in the narrow channel, the flow picture similar to that in the channel of larger cross-section.

It is easy to show, that the value of accommodation coefficient necessary to simulate the channel of given dimensions is inversely proportional to its hydraulic radius.

It should be pointed out, that the described method cannot be used in the case of the narrowest channels, if the flow is close to free-molecular. The criterion is the value of the Knudsen number, which should not be larger than 0.01 – 0.02.

6 Details of Simulations

We simulate the behaviour of stationary flow and detonation waves in five channels of different geometries, as shown in Fig.2.

Channel 1 (standard shape) was straight, of rectangular cross-section of size 70 x 70 units and length 1300 units (the unit of length was equal to 1 mean free path of the molecular motion at initial conditions). Channel 2 was similar to channel 1, only its length was equal to 1900 units.

Channel 3 was designed for investigation of influence of cross-section changes. In channel 4 there was additional influence of sharp turns. In channel 5 the sharp decreases of cross-section were removed.

The widths of channels 3, 4 and 5 were equal to 70 units; other dimensions are given in Fig. 2.
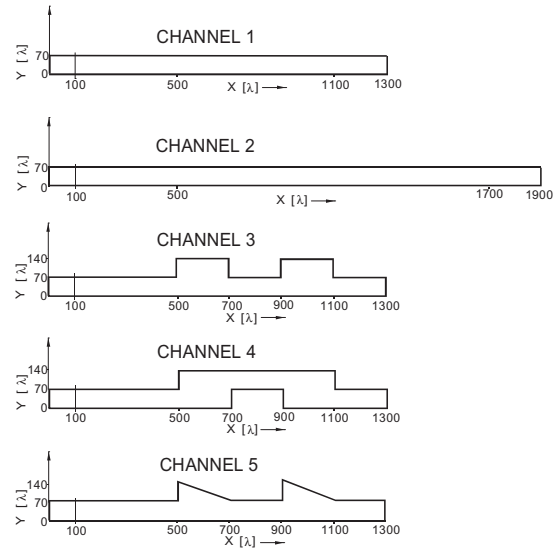

Fig.2. Shapes of the considered channels. λ – mean free path at initial conditions.

The interior of the channels was divided into cubic cells of dimension equal to 1 unit. Each cell contained initially about 5 simulated molecules.

In each channel, 100 units from its left end, there was a "diaphragm" separating the hot driving gas from the rest of the channel. The temperature of the driving gas was at least 10 times higher than temperature of the gas behind the "diaphragm" and the number density was equal to about 0.9 of the number density in that region. Removal of the "diaphragm" produced a shock, strong enough to be transformed into a detonation wave.

At both ends of each channel, 500 units from its left end and 200 units from the right end the molecules were reflected from the walls specularly, i.e. without exchange of tangential momentum and energy. Such region of flow without losses behind the "diaphragm" was necessary for the detonation to develop. The flow without losses at the other end of the channel was assumed to enable checking whether the extinguished detonation would not reappear.

In the central part of each channel the molecules were reflected from the walls with accommodation coefficient $\alpha = 0.05$, or $\alpha = 0.145$. At the dimension of the channel cross-section equal to 70 units, i.e. $\sim 5\mu$m, this corresponds to simulated channels acceptable technologically (dimension of the cross-section ~ 0.1mm, or ~ 0.035mm).

The simulation consisted of two stages. During the first stage – generation of the stationary flow – the molecules were allowed to escape freely from the right (low-pressure) end of the channel. The escaping molecules were then transferred to the place at low-pressure side of the "diaphragm", which created certain pressure difference between the ends of the channel and, after sufficiently long time (not less than 100000 steps – usually

about 90 hours of computing time of the desktop computer DELL PowerEdge T30) it led
to establishing stationary flow.

The second stage was initiated by the "diaphragm" removal. It produced the shock
wave, which subsequently was transformed into a detonation wave.

7   Results

7.1   Stationary Flow

Fig. 3 shows distributions of flow parameters along the channels in simulated stationary
flow: in channel 1, at accommodation coefficients $\alpha = 0.05$ and $\alpha = 0.145$, in channel 3
at accommodation coefficient $\alpha = 0.05$. Fig. 3, upper, left, shows the distributions of
density, Fig. 3, upper, right – velocity, Fig. 3, lower, left – pressure, and Fig. 3, lower,
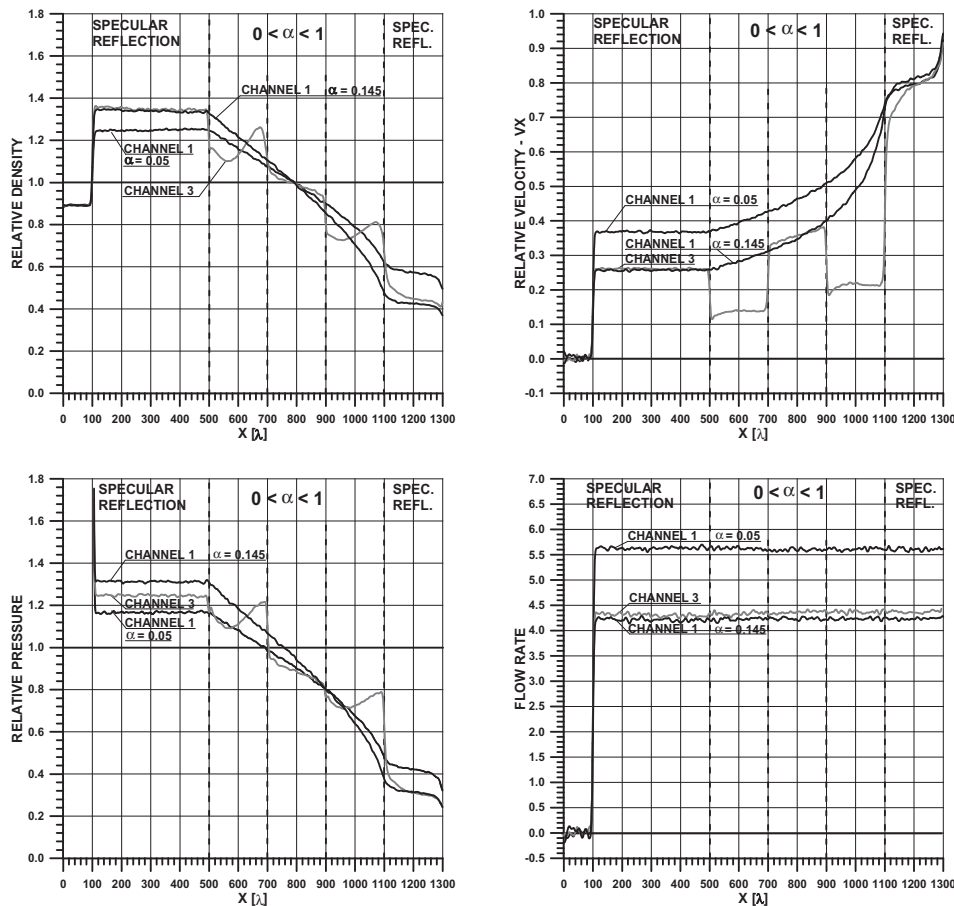right – flow rate (product of local density and velocity).

Fig.3. Distributions of parameters along the channels in stationary flow: in channel 1,
for $\alpha = 0.05$ and $\alpha = 0.145$, and in channel 3, for $\alpha = 0.05$. Upper, left – density, upper,
right – velocity, lower, left – pressure, lower, right – flow rate. The vertical dotted lines
separate different parts of channels – see Fig. 2.

Fig.   4 shows similar distributions for channel 2, at accommodation coefficient

$\alpha = 0.145$. Distributions of stationary flow parameters for channels 4 and 5 (which are similar to those for channel 3) are not presented.

In the above figures density and pressure are related to their initial values (before beginning of the flow) and velocity – to the initial value of the most probable velocity of the molecular motion. All parameters are averaged over the local cross-section of the channel.

The variations of density, velocity and pressure along the channel in stationary flow are appreciable. The pressure drop along the straight channel 1, at accommodation coefficient $\alpha = 0.05$ is smaller than that along channel 3 (Fig. 3, lower, left) and the flow rate is larger (Fig. 3, lower, right). This means, that resistance to the flow in the straight channel is smaller than in the channel 3 (with abrupt changes of cross-section).
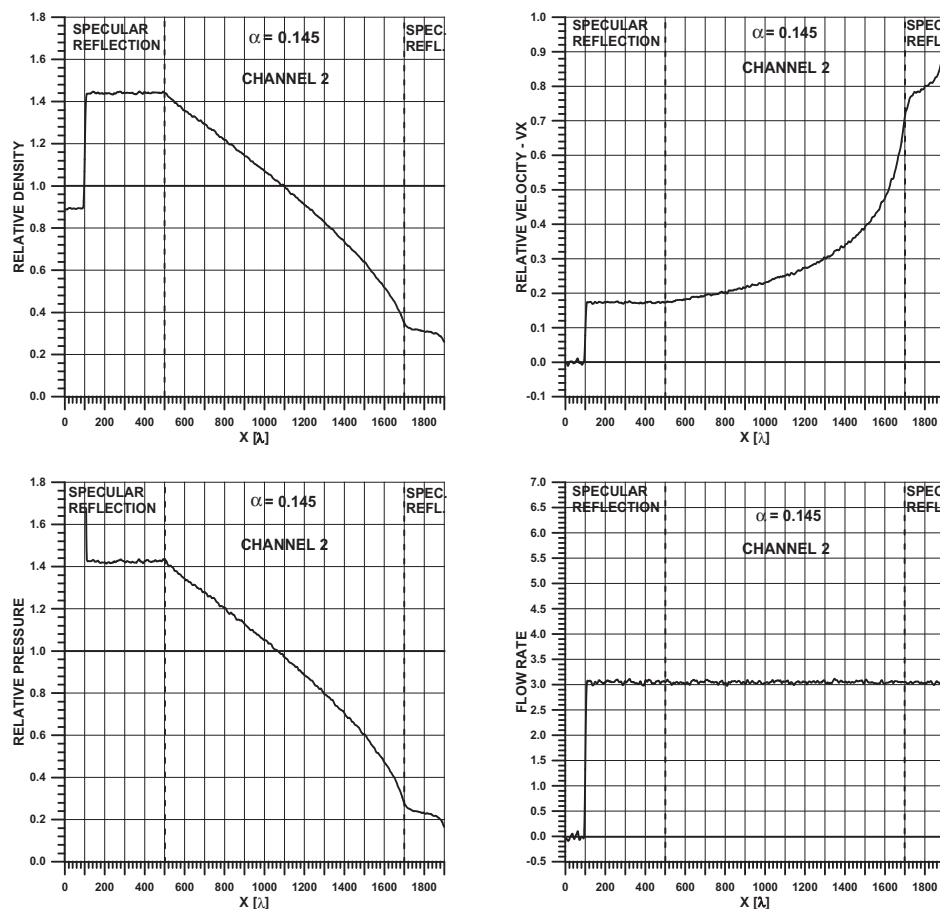

Fig.4. Distributions of parameters along channel 2 in stationary flow, for $\alpha = 0.145$. Upper, left – density, right – velocity, lower, left – pressure, right – flow rate.

To make it more precise, the coefficients of hydraulic resistance were calculated from the standard formula:

$$\zeta = 2\Delta p/(\rho u^2)$$

where Δp – pressure drop along the channel, ρ – density and u – velocity in region $100 < x < 500$. The coefficient of hydraulic resistance of channel 3 is 2.27 times larger than that of the straight channel 1 at $\alpha = 0.05$.

In the straight channel 1, at accommodation coefficient $\alpha = 0.145$, (equivalent to channel 0.035mm wide at $\alpha = 1.0$) the flow rate is lower than that in channel 3, but it is very close to it (Fig. 3, lower, right). The pressure drop is only slightly higher. The calculated coefficient of hydraulic resistance is only 11% higher than that for channel 3. From the point of view of the flow resistance this channel may be considered nearly equivalent to channel 3.

In the long, straight channel 2, at accommodation coefficient $\alpha = 0.145$, the calculated coefficient of hydraulic resistance is 2.76 times higher than that for channel 3.
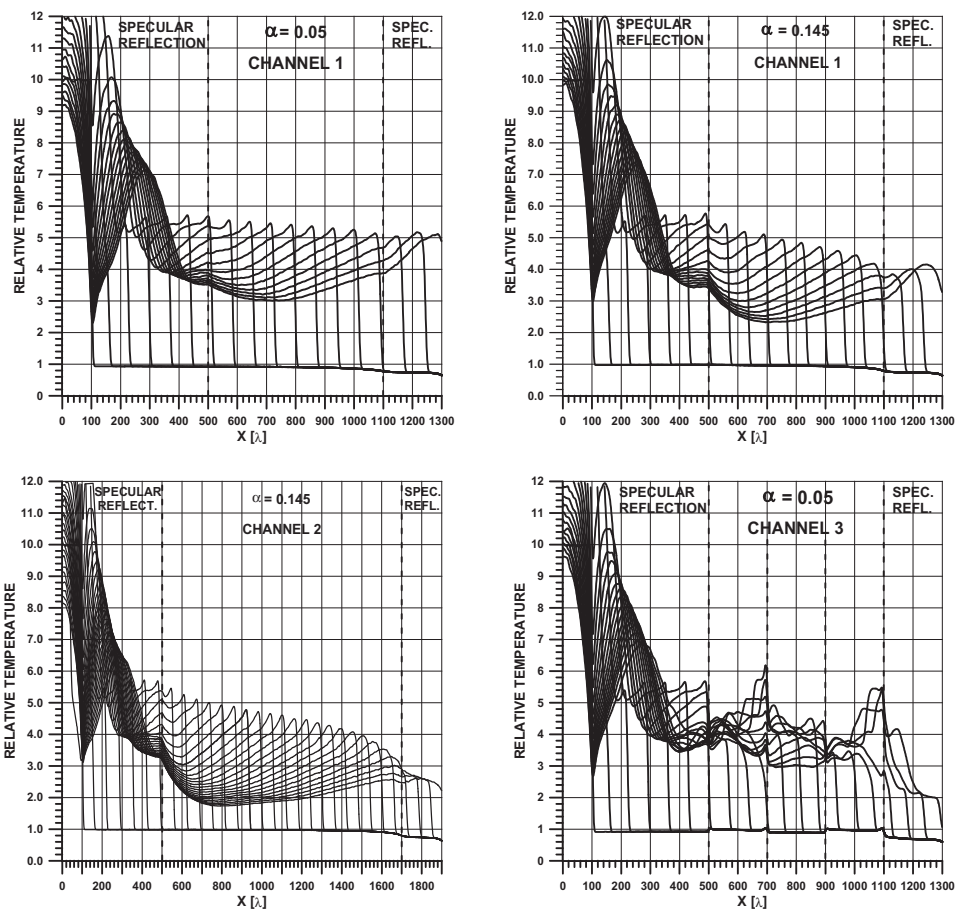
7.2   Detonation

Fig.5. Temperature distributions in a number of time instants in channels 1, 2 and 3, with detonation waves progressing into stationary flow. 10% of "energetic" molecules in all channels. Upper, left – channel 1, $\alpha = 0.05$, upper, right – channel 1, $\alpha = 0.145$, bottom, left – channel 2, $\alpha = 0.145$, bottom, right – channel 3, $\alpha = 0.05$.

In this section we present the diagrams of temperature along the channels, uniformly distributed in time, resulting from simulation of the behaviour of a detonation wave in the stationary flow inside the considered channels. The amount of "energetic" molecules in all channels is equal to 10%.

In Fig. 5 – upper, left, the diagrams of temperature inside channel 1, at $\alpha = 0.05$ are shown. The detonation wave, fully formed after "diaphragm" removal in the initial part of the channel, in its central part is affected very weakly – its amplitude decreases by about 9% only. In the end part of channel, where no friction and heat exchange are present, it evidently regains its intensity.

In Fig. 5 – upper, right, the diagrams of temperature inside the channel 1, at $\alpha = 0.145$ are shown. As before, the detonation wave is fully formed after "diaphragm" removal. In the central part of the channel its amplitude decreases by about 30%. Still, after entering the part of channel with no friction and heat exchange it regains its intensity.

In Fig. 5 – lower, left, the diagrams of temperature inside the channel 2, at $\alpha = 0.145$ are shown. The detonation wave is fully formed after "diaphragm" removal and in the central part of the channel its amplitude gradually decreases. This decrease becomes much faster close to the end of this part of the channel, so that only relatively weak shock wave, separated from the hot gas, enters the part of channel with no friction and heat exchange. It may be expected, that after leaving the damper, this shock wave will gradually decay.

In Fig. 5 – lower, right, the diagrams for channel 3 at $\alpha = 0.05$ are presented. Formation of the detonation is here similar to that in the previous cases. The passage to the first area of increased cross-section causes appreciable decrease of intensity of the wave. However, at the end of this area, before the decrease of cross-section, the gas temperature locally increases.

In the next, narrow part of the channel the intensity of the wave remains approximately the same as before, however temperature behind the wave decreases. The picture in the second area of increased cross-section is similar to the first one, only the temperatures are lower. Finally, the wave, which appears in the last, narrow part of the channel, with no friction and heat exchange, is no longer a detonation wave. It is a relatively weak shock wave, separated from the hot gas, which probably is no longer burning. It may be expected, that after leaving the damper, this shock wave will gradually decay.
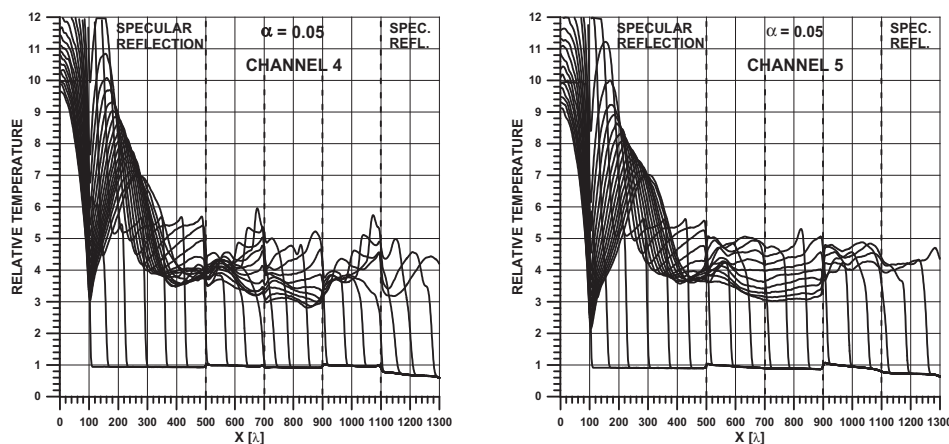

Fig.6. Temperature distributions in channel 4 (left) and channel 5 (right), at $\alpha = 0.05$ and 10% of "energetic molecules". Detonation waves progressing into stationary flow.

In Fig. 6 the diagrams for channels 4 and 5 at $\alpha = 0.05$ are presented. In both cases the wave entering the end part of the channel is strong; it may be expected, that it will

subsequently regain its original intensity and structure. It has been found in separate simulations, that these two channels extinguish detonation if percentage of "energetic" molecules is not larger than about 6%.

It may be concluded, that among all considered channels only channel 2 and channel 3 can extinguish detonation of the assumed intensity. However, as found in the previous chapter, the coefficient of hydraulic resistance of channel 2 is 2.76 times higher than that of channel 3. Channel 3 is therefore the most favourable for use in detonation dampers.

8   Conclusions

- A successful method of DSMC simulation of flow in channels of a detonation damper of technologically acceptable dimensions has been proposed.

- It has been found, that presence of abrupt changes of cross-section of narrow channels, used in detonation dampers, generally increases efficiency of damping. As shown in our earlier paper [2], if the channels are very narrow it does not necessarily increase the flow resistance.

- In channels of technologically acceptable dimensions ($\sim$ 0.1mm width, or more), presence of the abrupt changes of cross-section increases both, efficiency of detonation damping and flow resistance. Increase of efficiency generally seems to be more pronounced than increase of resistance.

- Out of all considered shapes channel 3 seems to be the best: it is about as efficient as the longer and narrower channel 2 and its flow resistance is much lower.

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