Application of Direct Monte-Carlo Method for Simulation of Gaseous Detonation

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Introduction

The research on detonation in gases has recently become a very important issue because of increasing importance of gaseous fuels. The urgent technological problem is connected with detonation in pipelines and the necessity of extinguishing it. The devices used for this purpose usually consist of matrices of very narrow channels. Cooling the gas by cold walls of such channels may extinguish the flame and stop detonation.
The Direct Monte-Carlo Simulation (DMCS) technique [1] has proven to be an excellent tool for simulating flows in various geometrical configurations – particularly in narrow channels. It offers also a possibility of taking into account the relaxation phenomena and chemical reactions [1, 2], these unfortunately increase complexity of the computer programs and the necessary computing times. However, in the case of detonation, considerable simplifications can be made thanks to the fact, that in a detonation wave combustion proceeds at high temperature and at very high speed, therefore all relaxation processes at the molecular level may be disregarded. The only important factor, that remains, is the produced thermal energy.

Model of a Combustible Gas

As always in the Monte-Carlo simulations we treat the gas as an ensemble of molecules, which collide with each other and move along straight lines with constant speed between collisions. We assume for simplicity, that all molecules are identical, hard, elastic spheres. We assume, finally, that some of the molecules, uniformly distributed in space, carry certain amount of “internal” energy, the same for each of them. This may be transformed into kinetic energy during collision with another molecule (carrying no energy), provided that the two colliding molecules approach each other with sufficient (“threshold”) speed. If this is the case, the relative speed of the molecules after collision is increased suitably.

Details of Calculations

To check whether the proposed model can actually simulate the detonation wave, several calculation runs for various geometries were performed. We employed the

standard DMCS procedure, according to Bird [1], and the selection of molecules for collisions was performed with the ballot-box scheme, as proposed by Yanitskiy [3].
The calculations were performed in one- and three-dimensional geometry. In 1-D geometry (plane wave, no walls) the number of molecules was about 5000, in 3-D geometry it ranged from about 3 to 8 million. The calculation area was divided into 1100 cells in 1-D geometry and 1.5 to 4 million cells in 3-D geometry.
The wave was initiated by instant removal of a "diaphragm", placed at x = 100 units of length. The gas in front of the diaphragm contained either 10 or 30 per cent of the molecules carrying "internal " energy. The energy released in a single collision was such, that the relative velocity of the colliding molecules was increased by the value equal to 10 times the most probable molecular velocity. The temperature of the driver gas (behind the diaphragm) was 10 times higher than that of the driven gas. The pressure was such, that, after the diaphragm removal, the shock wave of Mach number Ms = 2 was produced.

Results

Figures 1–4 show some selected results of the performed simulations.

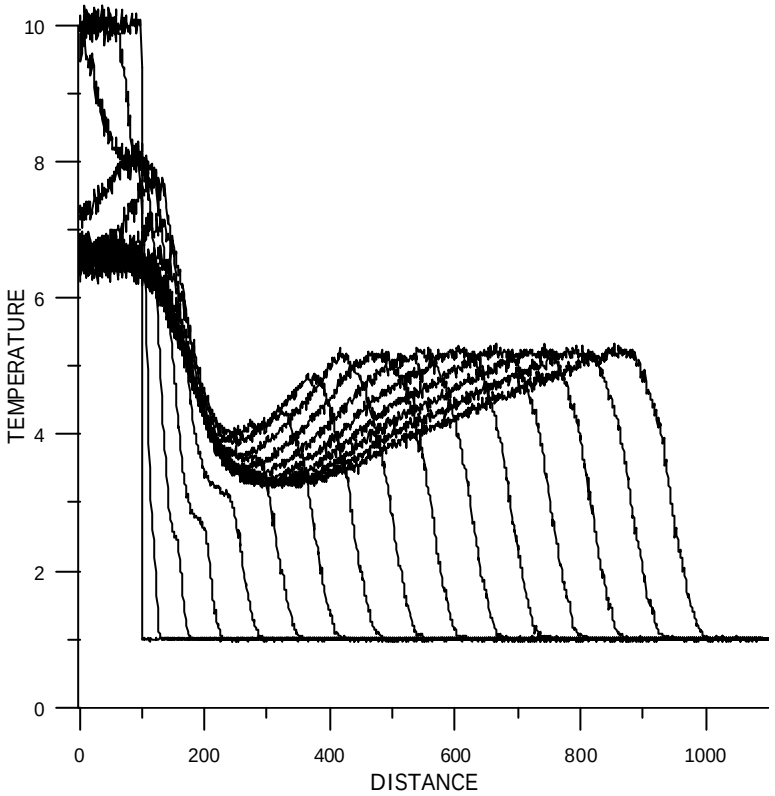

Fig. 1. Formation of the plane detonation wave without influence of walls.

Figure 1 shows the simplest case – a plane, perpendicular wave, moving along x – axis in a positive half-space, in a gas containing 10 per cent of the "energetic" molecules. The figure contains diagrams of the gas temperature in terms of distance along the x – axis (measured in mean free paths of the gas molecules) for the initial situation and for 15 subsequent instants, evenly spaced in time. Formation of the primary shock wave after the

diaphragm removal is clearly visible. The shock then gradually speeds up, transforming into a detonation wave, which afterwards moves with constant speed and constant intensity, as expected.

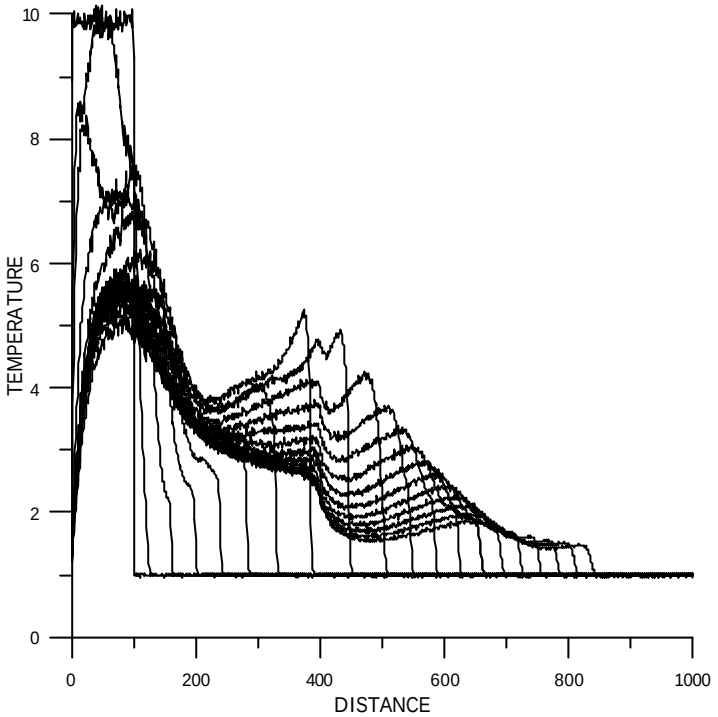

Fig. 2. Formation and decay of the detonation wave in a pipe under friction and heat exchange at the walls.

Figure 2 shows similar picture for the wave, moving in a cylindrical pipe in the same gas. The diameter of the pipe is equal to 100 mean free paths. For $x < 400$ the molecules reflect from the walls specularly, i.e. without exchange of tangential momentum, and energy. For $x > 400$ the molecules are reflected diffusely, i.e. after reflection their average energy corresponds to the temperature of the wall, and the average tangential velocity equals zero.

The left part of the picture, up to $x = 400$, looks similarly to that in Fig. 1 – formation of shock and detonation wave is evident. For $x > 400$ however, the walls cool the gas down, below the ignition point, and the shock moves ahead, unsupported by the flame front, getting weaker and weaker.

In Fig. 3 the configuration is the same as in Fig. 2, only the gas contains 30 per cent of the "energetic" molecules. Here, the amount of released energy is so large, that the walls are not able to absorb it. After entering the pipe with rough and heat conducting walls the detonation wave slows down a little bit and decreasas its intensity, still it moves steadily forwards. For this kind of gas, to stop detonation it is necesary to have larger ratio of the wall surface to the volume of the pipe – i.e. the pipe of smaller diameter.

Figure 4, which corresponds to the sixth line of Fig. 3, shows the shape of the detonation wave, slightly curved under the influence of the boundary layer. This curvature is evidently rather weak.

Conclusions

A method of simulation of the detonation phenomenon, based on the Direct Monte-Carlo Simulation technique has been proposed. This method makes it possible to study detonation in narrow channels and its decay under the influence of wall friction and heat exchange. This method may possibly be used for optimizing the devices stopping detonation in pipes.

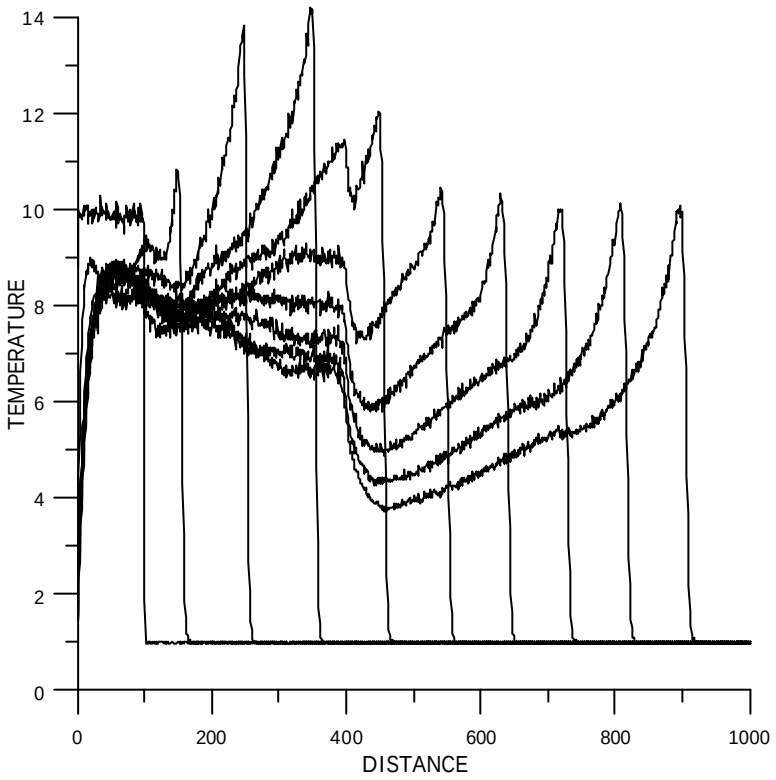

Fig. 3. Detonation wave in a highly energetic gas, in a pipe with friction and heat exchange.

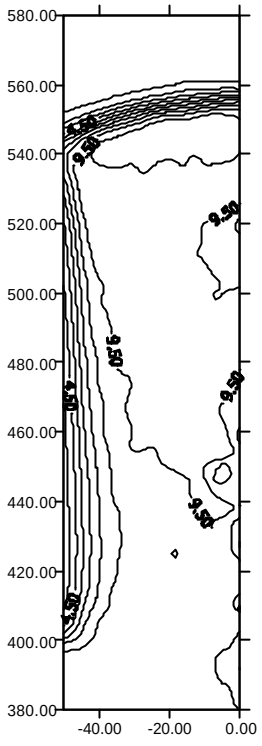

Fig. 4. Shape of the detonation wave in a narrow pipe, under the influence of the boundary layer.

References

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