SIMPLE MODEL OF A DETONATING GAS FOR USE WITH THE DIRECT MONTE – CARLO SIMULATION TECHNIQUE

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Summary: The research on gaseous detonation has recently become a very important issue because of increasing importance of gaseous fuels. We propose to use the Direct Monte – Carlo Simulation technique, which is a very powerful tool for solving complex flow problems. We propose a very simple model of a molecular collision, which makes it possible to increase the thermal energy of a gas, which is similar to the processes in the flame. We show then, that this model can produce the wave, which has all the features, characteristic for a detonation wave.

INTRODUCTION

The research on gaseous detonation has recently become a very important issue, in connection with increasing importance of gaseous fuels.
The Direct Monte – Carlo Simulation (DMCS) technique [1] has proven to be a very powerful tool for solving complex flow problems. It offers also a possibility of taking into account the relaxation phenomena and chemical reactions [1, 2], as well as influence of solid walls (friction and heat exchange). However the relaxation phenomena and chemical reactions increase substantially complexity of the computer programs and the necessary computing times. Fortunately, in the case of simulating gaseous detonation, considerable simplifications can be made thanks to the fact, that in a detonation wave the state of the medium is far from equilibrium, therefore combustion proceeds very fast and 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 with walls, and move along straight lines with constant speed between collisions. We assume for simplicity, that all molecules are identical hard spheres. We assume, finally, that some of the molecules, uniformly distributed in space, carry certain amount of "internal" energy (of unspecified character), 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 velocity (Fig.1a). If this is the case, the relative velocity of the molecules after collision is increased suitably (Fig.1b).

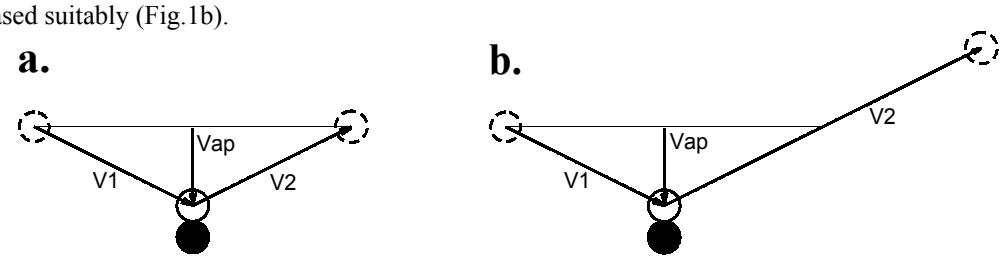

Fig. 1. Collision of two molecules in reference frame connected with one of them:
a. – elastic, b. – with energy release.
V1– relative velocity of the molecules before collision, V2 – after collision,
Vap – "velocity of approach" of the molecules.

RESULTS

To prove, that the proposed model can actually simulate the detonation wave, calculations for various geometries were performed.
Fig. 2 presents the simplest case – a plane, perpendicular wave, moving along x – axis in a positive half-space. The wave was initiated by removal of a diaphragm, placed at x = 100 units of length (mean free paths) from the origin of coordinates. The gas in front of the diaphragm contained 10 per cent of the molecules carrying the "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 was 10 times higher than that of the driven gas. The pressure was such, that after the diaphragm removal the shock wave with Mach number Ms = 2 was produced.
The presented figure shows the diagrams of the gas temperature in terms of distance along the x – axis for the initial situation and for 15 subsequent instants, equally spaced in time. Formation of the primary shock wave after the diaphragm removal is clearly visible. Later, the shock gradually speeds up, transforming into a detonation wave, which then moves with constant speed and constant intensity, as expected.

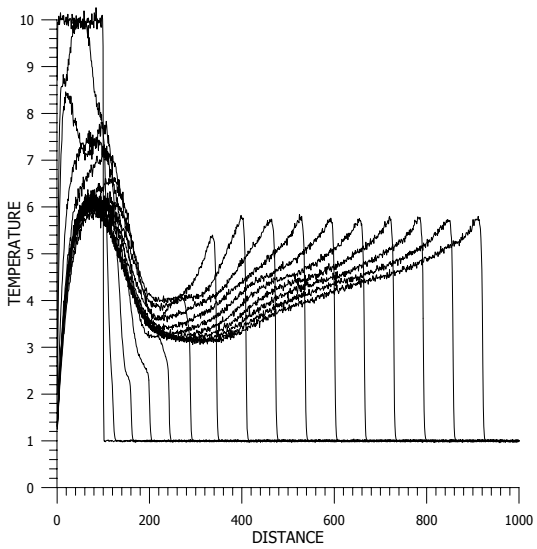

Fig. 2. Formation of a plane detonation wave without influence of walls.

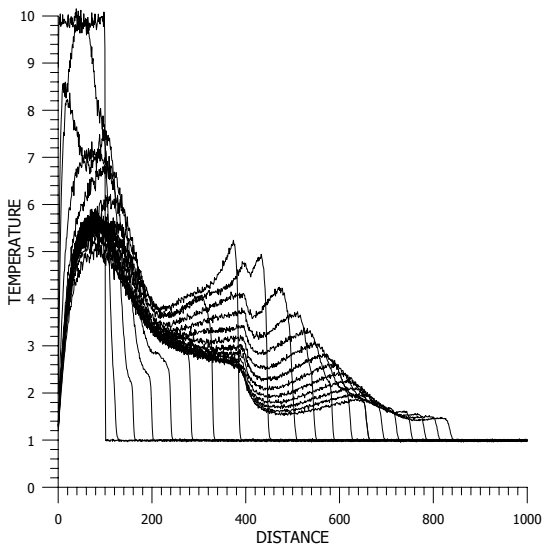

Fig. 3. Formation and decay of a detonation wave in a narrow pipe.

Fig. 3 shows similar picture for the wave, moving in a cylindrical pipe, in the same gas. The diameter of the pipe was equal to 100 mean free paths of the gas molecules. For x < 400 the molecules reflected from the pipe walls specularly, i.e. without exchange of tangential momentum and energy. For x > 400 the molecules reflected diffusely, i.e. their average kinetic energy after reflection corresponded to the temperature of the wall and the average tangential momentum was equal to zero.
The left part of the picture, up to x = 400, looks similarly to that in Fig. 2 – formation of shock and detonation waves 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.

Acknowledgements

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References

[1] G.A. Bird: Molecular gas dynamics and the direct simulation of gas flows, Clarendon Press, Oxford, 1994.

[2] P.S. Larsen, C. Borgnakke, in *Rarefied Gas Dynamics* (ed. M. Becker and M. Fiebig), **1,** Paper A7, DFVLR Press, Porz-Wahn, Germany, 1974.