Multi-processor simulation of forming a detonation wave in shock tube on the molecular process level.

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The Monte Carlo nonstationary method of statistical simulation (MCNMSS) (another name DSMC) with weight factors [1] was used in calculations. It takes into account all processes of heat-mass transfer automatically. Development of computers permits now to simulate by MCNMSS gas processes in which a local mean free path of molecules (l) is much less than a character size of this process in some points of space. One of them is detonation in a tube. Numerical study of a process of forming a detonation wave in the gas on the molecular process level gives a lot of useful information.

Simulation was carried out in the one-dimensional coordinate space and in the three-dimensional velocity space. At an initial moment, the low-pressure channel (LPC) was filled up by gas *A*. And the high-pressure chamber (HPC) of a shock tube was filled up by gas *C*. The simulation started after removing a diaphragm between HPC and LPC. It was supposed that chemical reaction $A+M\rightarrow B+M$ (M=*A*,*B* and *C*) took place. The ratio of molecular masses (m_i) of gases *A*, *B* and *C* was:20:20:1. This is analogous to the case of internal molecular energy release. The threshold of the reaction Q_{AB} was equal to $25kT_1$ (k is the Boltzmann constant, T_1 is the temperature in LPC and HPC at the initial moment of time). The energy release in reaction Q was equal to $402.6\ kT_1$. It was supposed that during the collision of two particals ,the reaction occurs if the total energy of their relative motion is higher than Q_{AB}. All considered molecules were treated as hard spheres with equal diameters without internal structure. Particles reflected elastically from walls at boundaries of the simulation region. In the beginning of the simulation the ratio of pressures in HPC and LPC was equal to 100. In order to the size of spatial cell (Dx)did not exceed l in the gas, the size of spatial cell in HPC was 20 once smaller than that in LPC at the beginning. During the simulation, that part of LPC where the molecules from HPC have enter, got new cells with the size in 20 once smaller. The initial average number of model particles per cell N was equal to 360 both in LPC and in HPC.

In considered case m_A is equal to m_B. And there is the Hugoniot analytical relation [2]:

$$p_2/p_1=(4+2Q/kT_1- n_1/n_2)/(4\ n_1/n_2-1).$$

Here, indices 1 and 2 refer to parameters ahead of and behind a wave, p_i is a pressure and n_i is a numerical density of a gas.

It is easy to obtain from this analytical expression of the Chapman-Jouguet condition. If to denote $z=2Q/kT_1$ then

$$n_1/n_2=\{[2(z+5)-(4z^2+15z)^{1/2}]/10\}.$$

This expression gives the following parameters of the Chapman-Jouguet condition for our case: n_1/n_2=0.6254, p_2/p_1=538.4, T_2/T_1=338, velocity of detonation D=6.11u (u is the most probable thermal velocity of molecules of component *C* at the beginning).

Parallel calculations were carried out by means of a multi-processor computer. Domain decompositions of a simulation region was performed. Standard Message Passage Interface (MPI) [3] was used to communicate data between processors and 176 processors were used. The modeled region spread from 0 to $6264\,l_н$ ($l_н$ is l in LPC at the initial moment). Boundary between LPC and HPC was placed at $x=5889\,l_н$.

Ignition of gas *A* started at the moment of time $t\approx 200\,l_н/u$ in vicinity of $x=5625\,l_н$. A period of reaction induction was shot because of low value of Q_{AB}. And the shock front didn't form at this time. Figures 1-3 shows the results of simulation at the moment $758.3\,l_н/u$. As one can see, parameters of the flow in the region $1750<x/l_н<2500$ remained constant: $n_2/n_1\approx 1.25$, $p_2/p_1\approx 380$ $T_2/T_1\approx 290$. These values are in 20%, 30% and 15% respectively less then for the Chapman-Jouguet condition. Range of variation of D is $(6.05\div 6.3)u$. The region of constant parameters of the product *B* increased with time of simulation. This is the case of weak (low-pressure) detonation. The behavior of velocity of the product *B* wasn't simple.

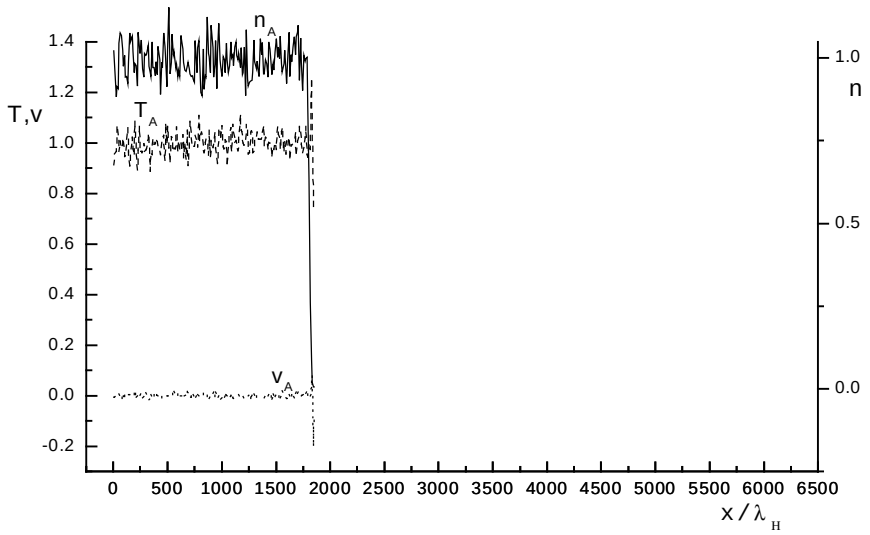

Fig. 1. Profiles of numerical concentration n_A (—), total kinetic temperature T_A (---) and velocity v_A (···) of reagent *A*. Concentration is normalized to initial concentration of reagent *A*, temperature – to T_1, v - u.

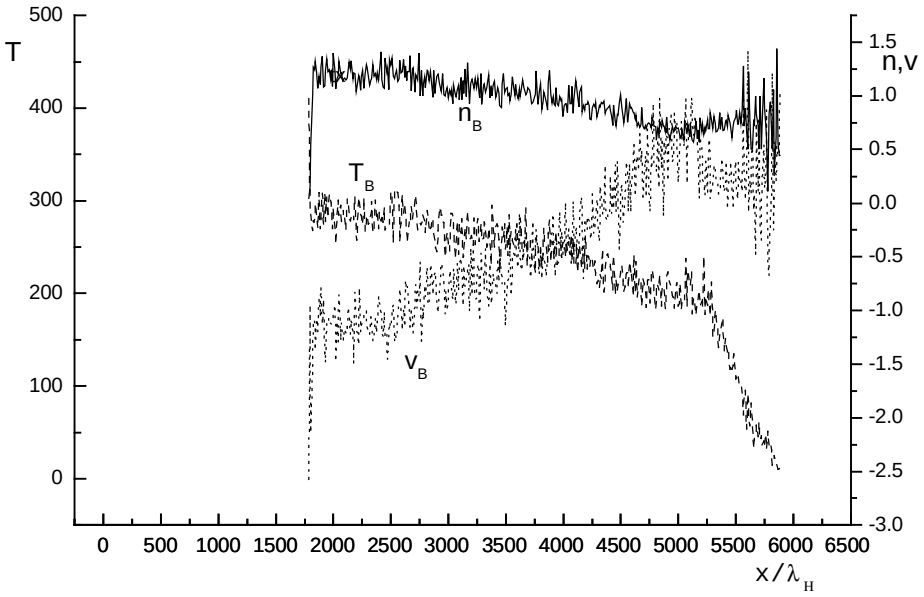

Fig. 2. Profiles of numerical concentration n_B (—), total kinetic temperature T_B (---) and velocity v_B (···) of product *B*.

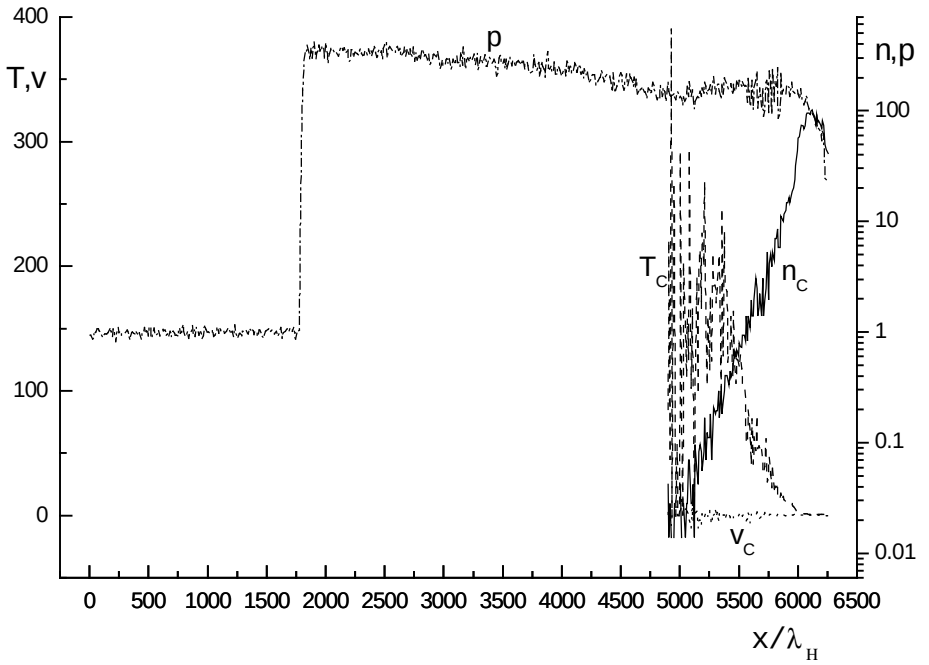

Fig. 3. Profiles of numerical concentration n_C (—), total kinetic temperature T_C (---), velocity v_C (···) of gas C and total pressure p (-·-·-). Pressure is normalized to initial pressure of reagent A .

The presented results show possibilities of using MCNMSS for simulation of detonation wave. This is only a beginning of the work. Possibly increase of modeled region and N heighten a precise the results. There is no serious problem to consider more complex cases with several components and reactions in LPC.

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