Simulation of gas detonation in a constant-cross-section channel initiated by instantaneous heating at its closed end for an $O+O_3+He$ mixture

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The one-dimensional problem was studied. A constant-cross-section tube was filled with gases A and B at a fixed initial temperature. The reactants were diluted with the lightest inert gas E (He). After the ignition of the reacting gas, the rapid heating at one closed end of the tube to a certain temperature results in the initiation of a reversible reaction involving molecules with substantially different weights, $A + B \rightleftarrows 2\ C$ (an analog of the only important reaction $O + O_3 \rightleftarrows 2\ O_2$ under the simulation conditions), with the energy thresholds for the forward and reverse reactions. The latter resulted in realistic values of the rate constant and the heat release for this reaction. All calculations were performed by the direct simulation Monte Carlo method with variable weight factors on a multiprocessor computer. It was found that the reaction rate ahead of the detonation front is much higher than the equilibrium rate behind the front.

Key words: detonation wave, direct simulation Monte Carlo method, chemical reaction, one-dimensional approximation.

The results of extensive calculations for detonation waves are available.[1] However, correct calculations of the formation of a detonation wave in a constant-cross-section channel initiated by instantaneous heating at one closed end of the channel is an important and very complex problem even in the one-dimensional approximation. This is due to the appearance of high gradients of the gas flow parameters, resulting in the formation of very narrow nonequilibrium zones that strongly influence wide flow regions. Processes in these zones should be considered at the molecular level. Generally speaking, the consideration of other flow regions can be restricted to the hydrodynamic level. However, this raises the problem of correct joining the results obtained by different methods. Obviously, it is more correct to always use the method that allows one to consider the entire system at the molecular level. Modern computer facilities make it possible to employ the direct simulation Monte Carlo (DSMC) method that was first proposed by Bird.[2,3] This method allows one to obtain results without actually solving the Boltzmann equation. It should be noted that DSMC automatically takes into account all details of the heat and mass transfer.

Such a simulation is feasible.[4] In addition, though in another statement of the problem, the results of DSMC simulation of the detonation have been reported earlier. The pioneering investigations[5,6] were followed by an ideologically interesting attempt[7] to simulate the non-steady detonation for one- and two-dimensional cases. A large linear size of the spatial cell, which was equal to the mean free path in unperturbed gas ahead of the front (λ), was used. For this reason, the size of the spatial cell in the wave front is ~2 times larger than the local, mean, free path, which should lead to at least low-accuracy results of the simulation. Simulations of the detonation in a shock tube for different thresholds of a chemical reaction, which is analogous to that used in Refs 5 and 6, were also carried out.[8—11]

The simulations of the detonation performed earlier at the molecular level used fast model reactions between the model components (see, for example, Refs 4—11). In the present study, we made an attempt to find and simulate a much more realistic chemical interaction between naturally occurring compounds by the DSMC method using real, although very fast, reactions. The influence of the translational nonequilibrium conditions on these reactions at the detonation wave front was investigated.

Calculation Procedure

A constant-cross-section tube filled with gases A and B at the initial temperature T_1 was considered. The reactant gases were diluted with an inert gas E. After the ignition of the reactant gas, a rapid heating of one closed end of the tube to the temperature T_c results in the initiation of a reversible reaction involving molecules with substantially different weights, $A + B \rightleftarrows 2\ C$ (an analog of the only important reaction $O + O_3 \rightleftarrows 2\ O_2$ under the simulation conditions) with the energy thresholds for the forward and reverse reactions $E_{AB} = 9.6kT_n$ and $E_{CC} = 190.6kT_n$, respectively (k is the Boltzmann constant). At $T_1 = 262$ K, these

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thresholds (as well as the rate constants) correspond to the realistic case for this reaction (for details of the rate constant calculations, see Ref. 2, Chapter 12.1). It was assumed that the reaction proceeds if at the instant of the collision the energy of the relative motion of the molecules along the line connecting the centers of the molecules is higher than or equal to the threshold value (for details see Ref. 2, Chapter 4.3). The weight ratio of the components A, B, C, and E was 4 : 12 : 8 : 1 (like for O, O_3, O_2, and He), and the ratio of the initial molar concentrations of the components A, B, and E was 1 : 1 : 5.

An analysis[12] of the scheme of the O_3 decomposition showed that, under the simulation conditions, it is sufficient to take into account only the reaction $O + O_3 \rightleftarrows 2\,O_2$.

The energy threshold E_{AB} = 5 kcal mol^{-1} was taken from Ref. 12. The threshold E_{CC} was re-calculated from thermodynamic relations. In the calculations, it was assumed that the difference between the thresholds of the reverse and forward reactions is equal to the heat effect.

All molecules were treated as solid spheres with the same diameter. Upon colliding with the closed end at temperature T_c, a molecule was reflected at a velocity randomly specified in accordance with the half-Maxwellian distribution with T_c ($T_c/T_1 = 6$). In this case, the molecules are elastically reflected from the opposite end of the tube.

The version of the DSMC technique with variable weight factors used in the present study has been described earlier.[13,14]

The simulation was performed in the one-dimensional coordinate space and in the three-dimensional velocity space. Initially, 360 model particles of each sort were, on the average, placed in a spatial cell. The calculations were performed using 48 processors of the MVS1000M supercomputer at the Joint Supercomputer Center of the Russian Academy of Sciences (JSCC RAS). The block decomposition of the simulation region was used.[4]

Results and Discussion

We succeeded for the first time in observing the appearance of the detonation wave by the simulation of gas detonation in a constant-cross-section channel initiated by instantaneous heating of one its closed end. The results obtained at the instant 370.08 are shown in Figs 1—3. Hereinafter, the time is normalized to λ/u, where u is the most probable thermal velocity of the particles with the mass m_E ($u = (2kT_1/m_E)^{0.5}$) at the initial moment. The distance along the flow was normalized to λ. The concentrations n were normalized to the initial concentration of the component A, the temperature was normalized to T_1, and the longitudinal velocities along the flow v were normalized to u. Since the behavior of the profiles of the gas B is analogous to that observed for the gas A, these profiles are not given as a rule. Figure 3 additionally shows the profile of the total pressure p normalized to the initial pressure p_1. Upon the formation of a small amount of the gas C near the hot wall, peaks of the total pressure, concentrations, and the temperatures of the gases A and B appear at the same places. A very rapid evolution of these excitations leads to the formation of a detonation wave.

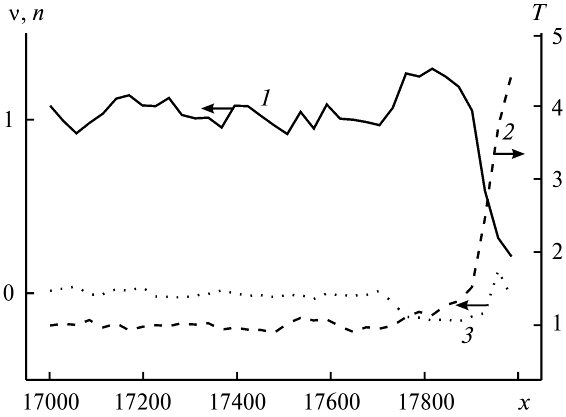

Fig. 1. Profiles for the reactant n_A (*1*), T_A (*2*), and v_A (*3*) at the time instant t = 370.08.

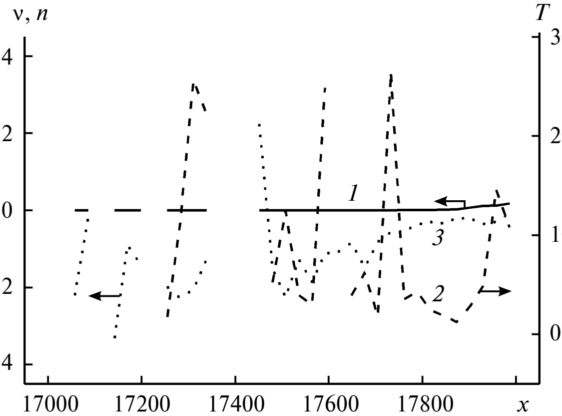

Fig. 2. Profiles for the product n_C (*1*), T_C (*2*), and v_C (*3*) at the time instant t = 370.08.

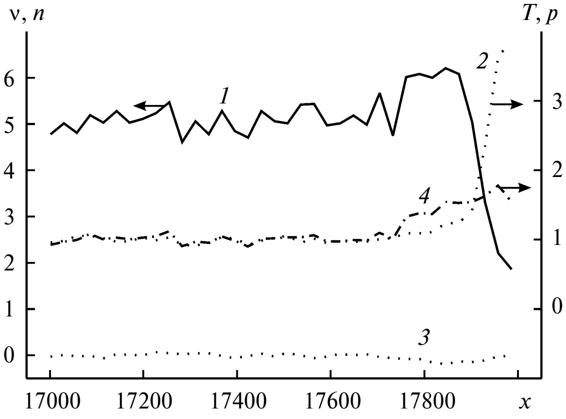

Fig. 3. Profiles for the inert gas n_E (*1*), T_E (*2*), and v_E (*3*), and the total pressure p (*4*) at the time instant t = 370.08.

The results obtained at the instant 4320.25, when the detonation wave already formed, are presented in Figs 4—6. As mentioned above, the behavior of the profiles of the gas

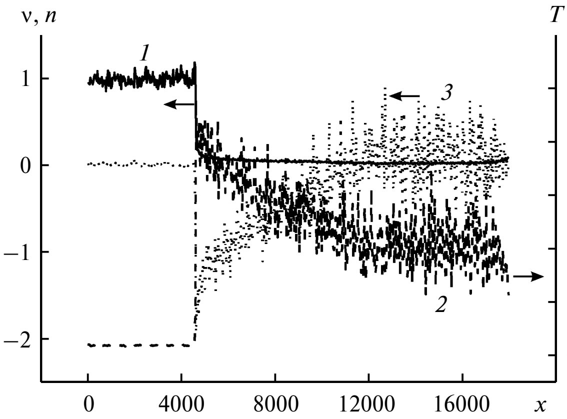

Fig. 4. Profiles for the reactant n_A (*1*), T_A (*2*), and v_A (*3*) at the time instant $t = 4320.25$ with a space step of 28.126.

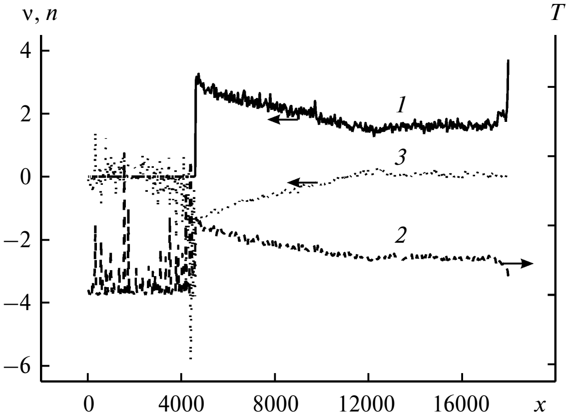

Fig. 5. Profiles for the product n_C (*1*), T_C (*2*), and v_C (*3*) at the time instant $t = 4320.25$ with a space step of 28.126.

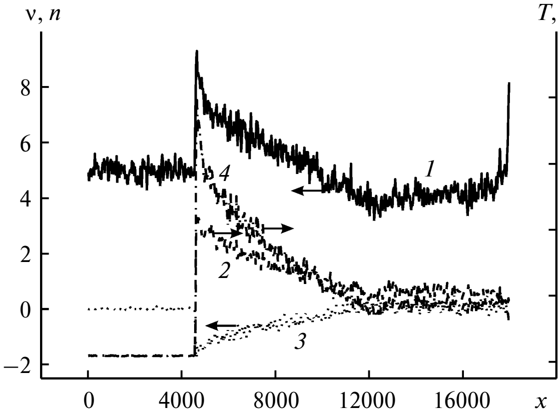

Fig. 6. Profiles for the inert gas n_E (*1*), T_E (*2*), and v_E (*3*), and the total pressure p (*4*) at the time instant $t = 4320.25$ with a space step of 28.126.

B is analogous to those of the gas A. Hence, these profiles are not considered. It can be seen that the flow immediately behind the front behaves like a expansion wave.

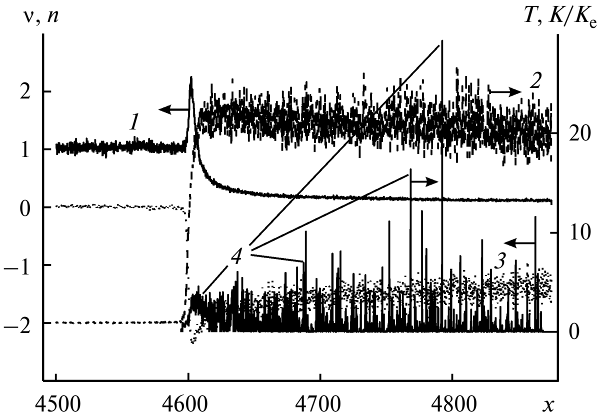

Fig. 7. Profiles for the reactant n_A (*1*), T_A (*2*), and v_A (*3*), and the reaction rate coefficient k/k_e (*4*) at the time instant $t = 4320.25$ with a space step of 0.15.

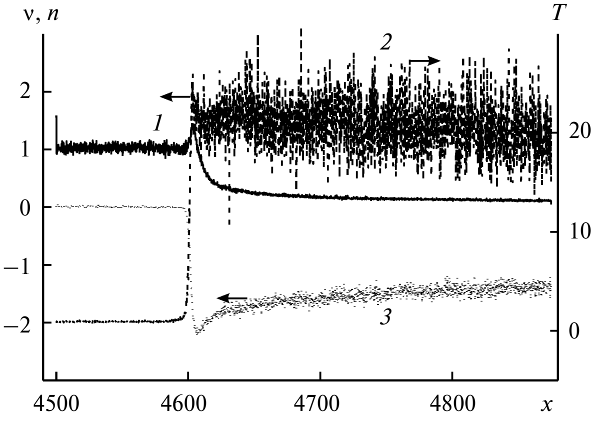

Fig. 8. Profiles for the reactant n_B (*1*), T_B (*2*), and v_B (*3*) at the time instant $t = 4320.25$ with a space step of 0.15.

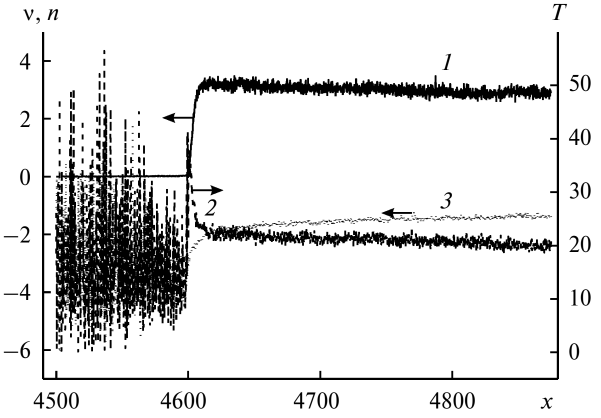

Fig. 9. Profiles for the product n_C (*1*), T_C (*2*), and v_C (*3*) at the time instant $t = 4320.25$ with a space step of 0.15.

The previous plots were constructed using the flow parameters taken with a space step of 28.126 in the spatial cell of a linear size 0.15.

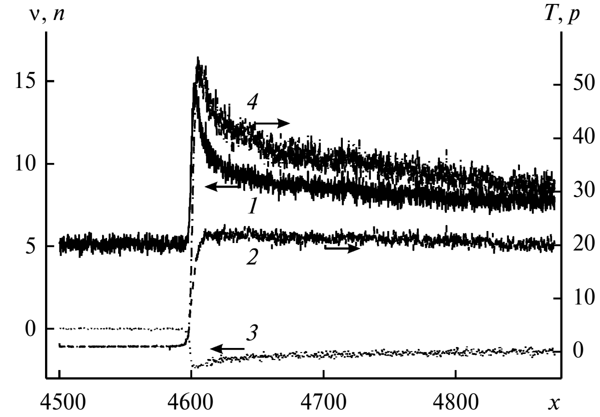

Fig. 10. Profiles for the inert gas n_E (*1*), T_E (*2*), and ν_E (*3*), and the total pressure *p* (*4*) at the time instant t = 4320.25 with a space step of 0.15.

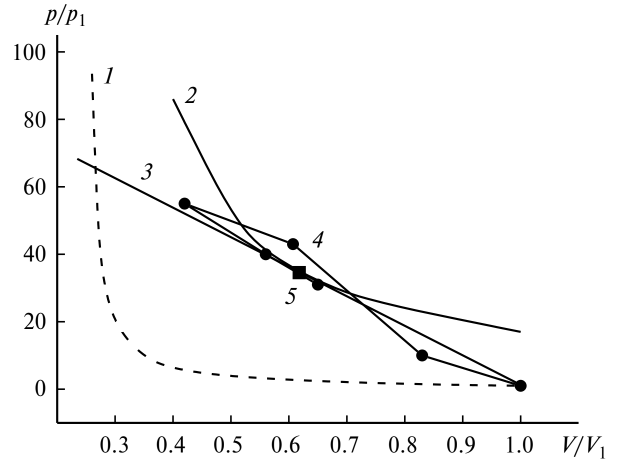

Fig. 11. Hugoniot curves and the evolution of a gas mixture as it goes through the detonation front depending on the volume per unit mass *V*: the shock adiabat (*1*), the detonation adiabat (*2*), the Rayleigh line (*3*), the evolution path of the model mixture through the front determined for a number of points (*4*), and the Chapman—Jouguet point (*5*).

Therefore, for the instant 4320.25, we also present the detailed structure of the propagating detonation wave front, that is, the flow parameters in each spatial cell (Figs 7—10). In the system of coordinates related to the wave front, the flow pattern shows a steady-state behavior. Thus, matching the coordinates x = 12431 and x = 4594 at the time instants 2245.13 and 4320.25, respectively, gives identical flow parameter profiles within statistical error. As the flow parameters evolve into the quasi-steady state, p/p_1 = 31. The Hugoniot shock and detonation adiabats for the case under consideration are shown in Fig. 11. This figure also presents the evolution of the model mixture as it goes through the detonation front. It can be seen that at the Chapman—Jouguet point, one has p/p_1 = 34.5, which is similar to the value mentioned above. The detonation wave velocity determined from the simulation is 3.8, being very similar to the Chapman—Jouguet velocity (3.84) calculated according to the formula (129.9) from Ref. 15. It should be noted that the evolution path of the model system (curve *4*) passes near the Rayleigh line (*3*) but does not intersect curve *1*. Consequently, the processes is evolved qualitatively, and nothing more, in terms of the Zeldovich—von Neumann—Doering theory.

Figure 7 additionally shows the profile of the forward reaction rate coefficient *K* normalized to the rate constant behind the front K_e obtained by the simulation. As can be seen from Fig. 7, the reaction rate ahead of the detonation front is much higher than the equilibrium rate. It should be noted that certain increased values (up to 30 times) are observed far behind the front. An increase in the reaction rate compared to its equilibrium value behind the front is a very important result. This is due to the steady nonequilibrium flow in the vicinity of the detonation front, which can be obtained only by solving the problem at the molecular level. This result cannot be obtained in the treatment of the problem at the macrolevel, because the hydrodynamic equations already imply the translational equilibrium for each component at each point of the flow.

It should be noted that the concentration peak for the component A ahead of the detonation wave is higher (~2.4 times (see Fig. 7) compared to the unperturbed gas) than that for the heavier component B (~1.5 times higher (see Fig. 8) compared to the unperturbed gas).

Therefore, we found a real chemically interacting gas mixture, in which the detonation was simulated at the molecular level. For the title method of detonation initiation, we succeeded for the first time in observing the appearance of the detonation wave. It was shown that the reaction rate ahead of the detonation front is several times higher than the equilibrium rate behind the front. This is a very important result. Although some of the flow parameter profiles determined in the front are nonmonotonic, they do not quantitatively correspond to the classical profiles of the Zeldovich—von Neumann—Doering theory because the induction period of the reaction in the flow is virtually absent. This takes place in spite of the fact that the model is quite realistic.

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