

# The equation of state of a mixture of dense gases, taking into account the detailed chemical composition

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Developing numerical methods for calculating gas-dynamic flows and wide-range universal equations of state allow one to solve a wide range of scientific and technological problems. The construction of quantitative models of dense reacting gases is an urgent task, which at the present level of scientific understanding and technical capabilities can be solved at a high level.

In this paper, the statistical Monte-Carlo method was used to construct the equation of state for dense reacting gases. The substance was considered as a set of point objects (molecules) interacting with the central pair potential. Additionally, molecules have internal degrees of freedom, whose energy depends only on temperature. To determine the equilibrium chemical composition, pressure, and total energy of the system, the mechanics of motion of a small ensemble of particles (100 pieces) was modeled. For homogeneous systems, it is quite enough to determine the equilibrium chemical composition. The paper pays attention to the selection of parameters of pair interaction potentials for describing the behavior of dense gases under conditions of shock waves and detonation of condensed explosives. To calculate the parameters of compositions based on compounds from C, N, O, H, a thermodynamic parameters calculator with access via the Internet (<http://ancient.hydro.nsc.ru/chem>) was developed.