NONLINEAR DYNAMICS OF ACOUSTIC INSTABILITY IN A NONEQUILIBRIUM CHEMICALLY ACTIVE GAS: NUMERICAL MODELING AND SHOCK-WAVE STRUCTURE

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Abstract: The dynamics of unstable sound waves in a chemically active, vibrationally excited gas is considered. Based on the MUSCL (Monotone Upwind Scheme for Conservation Laws) gasdynamic method, a one-dimensional numerical model is constructed and a computational tool is developed for studying various stages of acoustic instability evolution in nonequilibrium vibrationally excited gas flows, taking into account irreversible first-order chemical reactions, viscosity, thermal conductivity, heating, and cooling. The numerical model features high spatial resolution and second-order accuracy, allowing for the consideration of various models of chemical reactions and vibrational relaxation times. To improve computational performance, the numerical algorithm is parallelized using OpenMP technology. Conditions imposed on the parameters of a chemically active, nonequilibrium medium are determined to construct an initial quasi-steady state with a slow and monotonic change in gasdynamic quantities. This initial state can be technically implemented in a real experimental setup, allowing for the study and comparison of the nonlinear dynamics of acoustic instability using both numerical and physical modeling. It is shown that accounting for chemical energy release increases the intensity and spatial scale of shock wave pulses formed at the final nonlinear stage of acoustic instability development. It has been found that, under certain conditions, shock-wave pulses can excite high-intensity detonation waves even when the contribution of chemical energy release to the total equilibrium gas heating power is insignificant ($\sim$ 10%). In the detonation excitation region, two strong shock waves are formed, with the pressure at their front increasing by a factor of 40–70. These detonation waves propagate in opposite directions from the excitation region at velocities of approximately Mach 6–8, completely burning out the chemically active reactant in their path. It is shown that the numerical model accurately describes the flow structure in the detonation combustion region behind the shock-wave front. With an optimal choice of spatial resolution, the detonation wave width accounts for more than 100 computational cells and its structure agrees well with theoretical models — the Rankine–Hugoniot shock adiabat and the Chapman–Jouguet condition.

Keywords: nonequilibrium gas; vibrational relaxation; chemical reactions; acoustic instability; shock-wave pulses; detonation waves; numerical modeling; MUSCL method; parallel computing; OpenMP

DOI: 10.30826/CE26190102 **EDN:** AMUKIX

Figure Captions

Figure 1 General scheme of the calculation model of a plane-parallel channel filled with a nonequilibrium chemically active gas

Figure 2 Distribution of levels of the heating and cooling balance function $\Phi(\bar{T},\bar{T}_a)$ for different values of β_0: (*a*) 0.1; and (*b*) 0.2. The solid blue line corresponds to the zeros of function Φ for $\hat{Y} = 1$, in the shaded area $\Phi < 0$, and in other zones $\Phi > 0$. The dash-dashed line shows the value of the critical activation temperature $\bar{T}_a^*$. The dash-dotted line shows the offset of the boundaries of $\Phi = 0$ at $\hat{Y} = 0.7$

Figure 3 Solutions of the system of equations (11)–(13) for models A1–A4 and B1–B4 from the table. Shown are the time dependences $\bar{t}$ of: temperature $\bar{T}$ for monotonic (*a*) and oscillating (*b*) solutions; and degree of nonequilibrium of the medium S (*c*). Diagram (*d*) shows the boundary of thermal instability on the plane of parameters $(S, \beta\bar{T}_a)$: circles depict the positions of the models at the initial time, and triangles — on the time interval $50 \le \bar{t} \le 70$

Figure 4 Distribution of the dimensionless acoustic increment $\bar{\alpha}$ on the parameter plane $(\lg\bar{\omega}, \bar{T}_a)$ for different values of β_0: (*a*) 0.1; and (*b*) 0.2

Figure 5 Spatial distributions of the dimensionless density $\bar{\varrho}(\bar{x})/\gamma$ at different stages of the evolution of acoustic instability in a nonequilibrium chemically active gas in models A0, A5, and A6: (*a*) $\bar{t} = 80$; and (*b*) $\bar{t} = 400$

Figure 6 Evolution of shock wave pulses and excitation of detonation waves in model A1. The occurrence of detonation waves at three successive instants of time $\bar{t} = 169$ (*1*), 170 (*2*), and 171 (*3*) is shown for density (*a*), pressure (*b*), and temperature (*c*). The flow structure in the region of propagation of two diverging detonation waves is shown in (*d*) at time $\bar{t} = 194$ for the gasdynamic quantities $\bar{p}$, $\bar{\varrho}$, $\bar{T}$, $\bar{T}_v$, and $\bar{Y}$

Figure 7 Dependence of the propagation velocity of the wavefront $\bar{u}_s$ (*a*) and the maximum amplitude of the relative density disturbance $\widetilde{\varrho}_{\max} = (\bar{\varrho}_{\max} - \bar{\varrho}_0)/\bar{\varrho}_0$ in wave (*b*) from the distance $\bar{x}$ to the source. The values for the first maximum of the wave packet in models A0–A6 are shown. Box (*b*) compares the growth rates of the disturbance amplitude for the second maxima in numerical calculations (A0–A6) and a linear model (see Fig. 4) in which the disturbance growth function $\propto \exp\{0.145\,\bar{x}\}$ is shown as a dotted line

Figure 8 Dynamics of the detonation wave propagating to the right for the numerical model A1 (see the table and Fig. 6*d*): (*a*) distributions of density, pressure, and temperature in the vicinity of the detonation wave front at different moments of time; (*b*) relative changes in the intensity and velocity of the detonation wave over time ($\delta_f(\bar{t}) = f(\bar{t})/f(\bar{t} = 186)$ where $f = \{\bar{\varrho}_{\max}, \bar{p}_{\max}, \bar{T}_{\max}, \bar{u}_{\mathrm{sh}}\}$)

Figure 9 The structure of the shock wave propagating to the right for the numerical model A1 (see the table) at time $\bar{t} = 194$ (see Fig. 6*d*): (*a*) spatial distributions of the flow parameters in the vicinity of the shock wave front ($1 - \bar{p}$; $2 - \bar{\varrho}$; $3 - \bar{T}$; $4 - \bar{T}_v$; $5 - \bar{c}_s$; $6 - \bar{u}' = |\bar{u} - \bar{u}_s|$; $7 - \mathrm{M} = \bar{u}'/\bar{c}_s$; and $8 - Y$); and (*b*) thermodynamic state diagram $(\hat{P}, \hat{V})$ where **A** is the initial state ahead of the shock wave front at $\bar{x} \approx 340.66$; **B** is the state behind the shock wave front at the point of maximum pressure jump at $\bar{x} \approx 340.6$; **C** is the state behind the shock wave front in the vicinity of the maximum temperature and $\mathrm{M} \approx 1$ at $\bar{x} \approx 339.47$. The vertical dotted lines in (*a*) delimit the subsonic and supersonic flow regions. The dotted line in (*b*) shows the Rankine–Hugoniot shock adiabat for an equilibrium gas (curve **D**), the dashed line shows the shock adiabat for a nonequilibrium medium taking into account chemical heat release (17) with $q \approx 11.3$ (curve **E**), and the solid line shows the numerical solution (red broken curve **AB**)

Table Caption

Parameters of numerical models

Acknowledgments

The work was supported by the Russian Science Foundation (grant No. 23-71-00016, https://rscf.ru/project/23-71-00016/. The research is carried out using the equipment of the shared research facilities of HPC computing resources at Lomonosov Moscow State University.

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Received July 30, 2024
After revision January 26, 2026
Accepted February 2, 2026

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