2aPAc4. Numerical simulations of evolution of weak disturbances in vibrationally excited gas

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We consider a model of gas with an exponential law of relaxation of vibrational states of molecules excited by the external energy source (Joule heating in discharges, exothermic chemical reactions, optical pumping, etc). In such a medium, the second (bulk) viscosity coefficient inversion can take place due to the positive feedback between the sound perturbation and the nonequilibrium heat release. Such a medium with the negative viscosity is acoustical active. The existence of stationary nonlinear acoustical structures that are different from the step-wise or saw ?wise shock wave structures are discussed basing on the solutions of general nonlinear acoustical equation [N. Molevich, A. Klimov, V. Makaryan International Journal of Aeroacoustics, 2005, No 3-4]. Using the numerical simulation of full one ?dimensional (1D) system of relaxing gas dynamics, we show that any weak localized acoustical disturbance transforms into the sequence of self-sustained solitary pulses. Collisions of such pulses lead to their full reconstruction after the initial stage of the nonlinear increase of summarized amplitude. Using the 2D - system of relaxing gas dynamics, we consider the evolution of the noise signal into the non - stationary quasi-regular system of colliding self-sustained solitary pulses.
A MODEL OF GAS WITH AN EXPONENTIAL LAW OF RELAXATION OF VIBRATIONAL STATES OF MOLECULES EXCITED BY THE EXTERNAL ENERGY SOURCE

The vibrationally excited gas with the exponential relaxation law

\[ \frac{dE_v}{dt} = \frac{E_e - E_v}{\tau_v(T,p)} + Q \]

is the simplest model of nonequilibrium media with the negative second viscosity [1-3]. Here, \( E_v \) is the energy of the vibrational degrees of freedom of the molecules, \( E_e \) is its equilibrium value, \( \tau_v \) is the vibrational relaxation time, and \( Q \) is the power of an external heat source, that sustaining \( E_e \) (in particular, electric pumping in the discharge or optical pumping).

The initial system of gas dynamics equations for acoustical wave description has the form

\[ P = \frac{\rho T}{M} \text{ } \frac{dp}{dt} + \rho \text{div}\vec{\nu} = 0, \quad \rho \frac{d\vec{\nu}}{dt} = -\nabla P + \frac{\partial}{\partial x_i} \left[ \eta \left( \frac{\partial \vec{\nu}}{\partial x_i} + \frac{\partial \vec{\nu}}{\partial x_j} - \frac{2}{3} \delta_{ij} \frac{\partial \vec{\nu}}{\partial x_k} \right) \right], \]

\[ C_{V\infty} \frac{dT}{dt} + \frac{dE_e}{dt} = \frac{T}{\rho} \frac{dp}{dt} = Q - l + \frac{Z}{\rho} \Delta T. \]

In (2), \( v, T, \rho, P \) are, respectively, the velocity, temperature, density, and pressure; \( l \) is the heat removal; \( d / dt = \partial / \partial t + \vec{\nu} \cdot \nabla \).

Applying the linearization procedure to (1)-(2), we obtain a linear relationship between the perturbations \( E_v, \vec{\nu}, T \sim \exp(ikx - i\omega t) \) in an acoustical wave

\[ E_v = \frac{(C + S_0 \tau_T)(T - S_0 T_0 \vec{\nu} / \rho_0)}{1 - i\omega \tau_v} \]

and a simple dispersion relation

\[ \frac{T_0 k^2}{M \omega^2} = C_V \rho = \frac{1}{\gamma(\omega)}, \]

where

\[ C_V = \left( \frac{\partial h}{\partial \eta} \right)_V = C_{V\infty} + \left( \frac{\partial E_v}{\partial T} \right)_V = \frac{C_{V\infty} - i \omega \tau_v C_{V\infty}}{1 - i \omega \tau_v}, \quad C_p = \left( \frac{\partial h}{\partial \eta} \right)_{p} = C_{p\infty} + \left( \frac{\partial E_v}{\partial T} \right)_p = \frac{C_{p0} - i \omega \tau_v C_{p\infty}}{1 - i \omega \tau_v} \]

are the complex heat capacities of the relaxing medium at constant volume and at constant pressure; \( \gamma(\omega) = \gamma' + i\gamma^* \) is the complex adiabat index; \( k = k' + ik^* \) is the complex wave number; \( u, h = u + P/\rho \) are the internal energy and enthalpy of the medium per one molecule; \( C_{V0} = C_{V\infty} + C_v + S_0 \tau_T, \quad C_{P0} = C_{p\infty} + C_v + S_0 (\tau_T + 1) \) are the low-frequency heat capacities at constant volume and constant pressure in the vibrationally excited gas; \( S_0 = (E_v - E_{e0})/T_0 = Q \tau_v / T_0 \) is the nonequilibrium degree of the medium; \( T_0, \rho_0, E_{e0}, E_v \) are the stationary values; \( \gamma_T = \partial \ln \tau_v / \partial \ln T_0; \quad \tau_v = \tau_v(T_0, \rho_0); \quad C_{V\infty} \) and \( C_{p\infty} \) are the frozen (high-frequency) heat capacities.

Using (3), we get the sound velocity \( c_s = \omega / k' \) and the damping decrement \( \alpha = k^* \). Under the condition \( k^* << k' \), equations (3) yield expression

\[ \alpha = \frac{\omega^2 [\xi(\omega) + \mu]}{2 \rho_0 c_s^2(\omega)}, \]
where $\mu = 4\eta / 3 + \chi (1 / C_V - 1 / C_P) ; \eta$ is the shear viscosity coefficient; $\chi$ is the thermal conductivity; $c_s$ is the sound speed. The general condition of acoustically instability is $\xi(\omega) + \mu < 0$.

The second viscosity and the sound velocity have the usual forms for media with a single relaxation process:

$$\xi = -\frac{P_0}{\omega^2} \gamma(\omega) = -\frac{\xi_0 C_V^2}{C_V^2 + \omega^2 \tau_v^2 C_V^2} , \quad c_s = \sqrt{\frac{C_V^2 + \omega^2 \tau_v^2 C_V^2}{C_V^2 + \omega^2 \tau_v^2 C_V^2}}$$

Here,

$$\xi_0 = \frac{C_v \tau_v (c_{v_0}^2 - c_0^2) \rho_0}{C_V}$$

is the low-frequency second viscosity coefficient; $c_0^2 = \gamma \tau_0 / M$; $c_v^2 = \gamma_0 T_0 / M$; $\gamma_\infty = C_p / C_v$;

$\gamma_0 = C_p / C_v$ are the frozen and equilibrium adiabatic indexes, respectively, $M$ is the molecular mass.

The low-frequency heat capacities $C_{V_0}$ and $C_{p_0}$ depend on the degree of the nonequilibrium $S$. Then, low frequency second viscosity in fact consists of two part $\xi_0 = \xi_{0_1} + \xi_{0_2}$. The “equilibrium” part $\xi_{0_1} = P_0 \tau_v C_v / C_{V_0}$ is positive. The nonequilibrium part $\xi_{0_2} = -P_0 \tau_v (C_{V_\infty} - \tau_T) S_0 / C_{V_0}$ is negative under the condition $\tau_T < C_{V_\infty}$. Hence, the second viscosity is negative under the condition $S_0 > S_{th} = C_v / (C_{V_\infty} - \tau_T)$.

This condition corresponds to the positive feedback between the acoustical perturbation and nonequilibrium heating: nonequilibrium heating increases in compression regions and decreases in rarefaction regions of acoustical perturbation. Such a medium becomes acoustically active (the well-known Rayleigh instability criterion).

For $\mu \neq 0$, the amplification condition $\xi(\omega) + \mu < 0$ is satisfied only at

$$\omega < \omega_{cr} \approx \frac{C_V}{C_{V_\infty} \tau_v} \sqrt{\frac{\xi_0}{\mu_\infty}}$$

where $\mu_\infty = 4\eta / 3 + \chi M (1 / C_{V_\infty} - 1 / C_p)$.

Using relaxation law (1), the propagation of the small – amplitude acoustical perturbations up to the second order of smallness can be described by a generalized nonlinear acoustical equation (GNAE)[1-3]

$$C_{V_\infty} \tau_v (\tilde{\rho}_T - c_{v_0}^2 \tilde{\rho}_{xx} - c_{v_0}^2 \Psi_{\infty} \tilde{\rho}_{xx}^2 - \frac{\mu_\infty}{\rho_0} \tilde{\rho}_{xx}) +$$

$$+ C_v \tau_v \tilde{\rho}_T \left(1 + S_0 \right) \frac{S_0 \left(1 + S_0 \right)}{C_p C_v} + 2 C_{V_\infty} \left(2 S_0 \left(1 + S_0 \right)^2 \tau_T \right)$$

$\Psi_{\infty} = \frac{\gamma_\infty + 1}{2} , \quad \tau_T = \frac{T_0^2 \frac{\partial^2 \tau_v}{\partial T_0^2}}{\tau_v \frac{\partial T_0}{\partial T_0}}$

Here,

$$\Psi_{\infty} = \left[ \frac{S_0 \tau_T \left(1 + S_0 \right)}{C_p C_v} + \frac{1 \frac{S_0 \left(1 + S_0 \right)^2}{C_p C_v} \tau_T}{2 C_{V_\infty}} \right] , \quad \mu_{\infty} = \frac{4\eta}{3} + \chi M \left(1 \frac{1}{C_{V_0}} - 1 \frac{1}{C_p} \right) , \quad \tilde{\rho} = \rho - \rho_0 \frac{\rho_0}{\rho}$$

For $S_0 = 0$, equation (9) leads to $\Psi_{\infty} = (\gamma_\infty + 1) / 2$.

Equation (4) is valid for media with the small dispersion coefficient $m = (c_0^2 - c_v^2) / c_s^2 << 1$. It is the generalized acoustical equation of relaxing media as it describes acoustical perturbations independently of their spectrum.

For waves travelling in one direction ( $\tilde{\rho} = \rho / \rho_0 , \xi = (x - c_s t) / c_s \tau_v , y = \theta / \tau_v \right)$, equation (4) reduces to
\[
(p_y + \frac{\Psi_0}{2} \rho^2 - \mu_o \rho \partial_{\rho} \rho) \partial_{\rho} \rho - \nu(p_y + \frac{m}{2} \rho^2 + \frac{\Psi_0}{2} \rho^2 - \mu_o \rho \partial_{\rho} \rho) = 0,
\]
where \(\mu = \mu / 2 \pi \rho_0\), \(\Psi_0 = \gamma_0 \rho_0 / \gamma_o\), \(\nu = C_{V0} / C_{V0}\).

In the low frequency approximation \( (\partial / \partial \rho \approx \theta \sigma)\), Equation (5) reduces with an accuracy to \( \sim \theta^3 \) to the modified Kuramoto-Sivashinsky equation

\[
\rho_y + \Psi_0 \rho \partial_{\rho} \rho = \mu \rho \rho + \tilde{\mu} \rho \partial_{\rho} \rho + \kappa \tilde{\rho} \partial_{\rho} \rho.
\]

In Equation (6) \( \mu_o = \tilde{\mu}_0 + \tilde{\epsilon}_o \) is the total viscosity, \( \tilde{\epsilon}_o = \tilde{\epsilon}_o / 2 \rho_0 \tau_0 \nu_0^2 \), \( \kappa = C_{V0} \tilde{\beta} / C_{V0} = C_{V0} / C_{V0} \)

(\text{with neglect of } \sim \tilde{\mu}_0^2 \tilde{\rho} \tilde{\rho} \tilde{\rho} \tilde{\rho}). For \( C_{V0} > 0 \), all these coefficients are negative if the second viscosity coefficient is negative.

In the high frequency approximation \( (\partial / \partial \rho \approx \theta^{-1} \partial \rho)\), Equation (5) reduces (with an accuracy to \( \sim \theta^2 \)) to the Burgers equation with a source and integral dispersion

\[
\rho_y + \Psi_0 \rho \partial_{\rho} \rho = \mu \rho \rho - \tilde{\alpha}_o \rho \tilde{\rho} = \tilde{\beta} \tilde{\rho} \partial_{\rho} \rho,
\]

where \( \tilde{\alpha}_o = \tilde{\epsilon}_0 C_{V0}^2 / C_{V0} \rho_0 \tau_0 \epsilon_0^2 \) is the dimensionless gain (at \( \tilde{\epsilon}_0 < 0 \)) of the high frequency sound, \( \tilde{\beta} \approx C_{V0} \alpha_o / C_{V0} \) is the dispersion coefficient. The solutions of Equations (6) and (7) are well known.

A disadvantage of these low-frequency and high-frequency equations is the impossibility of describing the nonstationary evolution of perturbations with arbitrary spectrum. Moreover, if \( \tilde{\epsilon}_0 < 0 \), the Korteweg - de Vries - Burgers equation doesn’t have finite stationary solutions at all, the generalized Kuramoto-Sivashinsky equation has the stationary wave solution in form of the traveling solitary pulse and the Burgers equation with the ‘source’ has solution in form of the traveling quasi-saw-tooth periodical wave. Note, that this periodical wave is evolutionary unstable in relation to perturbations of a longer period. Note also, that the spectrum of stationary wave structures described by these equations is broader than their domain of applicability. Thus, an evolution of acoustical perturbations and stationary wave structures in media with isentropic instability must be investigated basing on Equations (4), (5) without low- or high -frequency approximations.

As an example, we consider the typical laser mixture \( CO_2 : N_2 : He = 1 : 2 : 3 \) (pressure \( P_0 = 1 atm \), temperature \( T_0 = 300K \)), where the acoustical wave generation is observed experimentally. We use the relaxation time dependence

\[
\tau = 10^{10} \frac{M}{\rho} \left[ 0.22 \cdot \exp(-62.75 / T^{1/3}) + 0.99 \cdot \exp(-75.46 / T^{1/3}) + 0.55 \cdot 10^{-2} \sqrt{T} \exp(-58.82 / T^{1/3}) \right]^{-1}
\]

This dependence is valid for \( T=300-2000 K \). For \( T = 300 K \) and \( P = 1 atm \), we obtain \( \tau \approx 10^{-5} \), \( \tau_T \approx -3.4 \); \( \tau_{TT} \approx 15.9 \). In this mixture, the threshold nonequilibrium degree is \( S_{th} \approx 1.5 \cdot 10^{-4} \) (\( \rho P_0 / M = 1.5 W / cm^3 \)).

Dependecies of the sound speed relation \( c_0^2 / c_o^2 \) and the low-frequency nonlinearity coefficient \( \Psi_0 \) on nonequilibrium degree \( S \) are shown in Figure 1.

There are four distinctive fields of the nonequilibrium degree \( S \) in a case of \( \tau_T < 0 \). This corresponds to the relaxation time decrease with the temperature increase.

\textit{Field I:} \( 0 < S < S_{th} \), Here, we have the positive viscosity \( \tilde{\epsilon}_0 > 0 \), the positive dispersion \( c_0 < c_o \), the positive nonlinearity coefficient \( \Psi_0 \approx (\gamma_0 + 1) / 2 \) similar to equilibrium media.
FIGURE 1. Dependencies of the sound speed relation \( c_0^2 / c_\infty^2 \) (a) and the low-frequency nonlinearity coefficient \( \Psi_0 \) (b) on nonequilibrium degree \( S \) in the \( CO_2 \)-containing mixture. Fields of nonequilibrium I-IV are characterized by appreciably different acoustical properties[3].

Field II: \( S_{th} \leq S < S_{\Psi} \); \( S_{\Psi} = \frac{C_{V\infty} + C_v}{-\tau_T} \).

The dispersion and the second viscosity are negative (\( \xi_0 < 0 ; c_0 > c_\infty \)). The nonlinear coefficient \( \Psi_0 \) can be positive or negative. The low-frequency speed can be significantly greater than the high-frequency speed. For \( S = 0.1 \) (\( \zeta P_0 / M = 1kW/cm^3 \)), we estimate \( \xi / \mu < 10^4 \); \( m = 0.095 \); \( \Psi_0 = 1.1 \); \( \Psi_\infty = 1.23 \). The frequency dependencies \( \alpha(\omega) \) and \( c_s(\omega) \) are shown in Figure 2. Here, the band of sound amplification (\( \alpha < 0 \)) is up to \( \omega_{cr} \sim 10^7 s^{-1} \).

Field III: \( S_{\Psi} < S < S_P \); \( S_P = \frac{C_{V\infty} + C_v}{-(\tau_T + 1)} \); \( \tau_T < -1 \) or \( S > S_{\Psi} \); \(-1 < \tau_T < 0 \).

Here, \( \xi_0 < 0 \), \( C_{V\infty} < 0 \), \( C_{p_0} > 0 \); hence, \( c_0^2 < 0 \) and the low-frequency sound can’t propagate.

Field IV: \( S > S_P \); \( \tau_T < -1 \). Here, the second viscosity is negative and such media is acoustically active. The dispersion and \( \Psi_0 \) are positive. The low-frequency sound speed can be significantly smaller than the high-frequency speed. In this field \( C_{p_0} \leq 0 \) and the decrease of temperature takes place in compression zones of the low-frequency perturbation.

In fields II-IV, there exist regions of nonequilibrium \( S \) such that \( \Psi_0 \gg 1 \). Here, acoustical approximation is inapplicable and we should take into account higher orders of acoustical perturbations .

It is interesting to know how these acoustical properties of nonequilibrium media can change the shock wave structure in different fields of nonequilibrium. In the present work, we restrict ourselves to that part of field II where \( \Psi_0 > 0 \). For \( \Psi_0 > 0 \), \( C_{V\infty} > 0 \) and the negative total viscosity , Equation (5) describes three stationary structures that are shown in Figure 2 [1,2].

The most interesting structure is strongly asymmetric solitary pulse (curve3, Fig. 1) with the shock front width \( \sim \mu / \mu_\infty \) and exponential trail \( \bar{\rho}_p \exp v_{\Psi_\infty} / 2 \Psi_\infty \), where \( \bar{\rho}_p = -4v \mu_\infty / (2 \Psi_\infty - \Psi_0) \)[1]. The speed of this pulse

\[
w_p = \frac{\rho \Psi_\infty}{(2 \Psi_\infty - \Psi_0)}.
\]
This pulse is the autowave (self-wave), whose form and amplitude depend on parameters of the nonequilibrium medium only. Note, that obtained forms of shock waves differ from the density jump (step-wise wave) described by the Burgers equation. Moreover, obtained solitary pulse (Figure 2c) is significantly different from the solitary pulse, which is stationary wave solution of tcnononservative Korteweg –de Vries equation. Firstly, the obtained solitary pulse has strongly asymmetric form with the sharp front and the long exponential tail; secondly, as we will show, the obtained solitary pulse is the self-sustained wave because of its amplitude and velocity depend only on parameters of medium and independent of the amplitude and the form of initial nonstationary perturbations.

RESULTS OF THE NUMERICAL SIMULATION

1. The initial step-like disturbance with amplitude $\tilde{\rho} > \tilde{\rho}_{cr} = -2 \Psi_{\infty}/(\Psi_{\infty} - \tilde{\Psi}_{0})$ transforms to the first stationary structure (Figure 2a). The second structure (Figure 2b) are obtained for $\tilde{\rho}_{cr} > \tilde{\rho} > \tilde{\rho}_{cr1} = -2 \Psi_{\infty}/(2 \Psi_{\infty} - \tilde{\Psi}_{0})$. The steps with amplitudes $\tilde{\rho} < \tilde{\rho}_{cr1}$ are unstable and broke down into a periodic sequence of stationary pulses (Figure 3). Each pulse has previous form and amplitude $\tilde{\rho}_p$ (Figure 2c). Thus, such pulse is autowave (self-wave), whose form and amplitude depend on parameters of the nonequilibrium medium only.
The bell-like disturbance transforms into the same pulses and roll waves in trail (Figure 4). These roll waves are autowave too. Their amplitude and period are independent of amplitude and square of the initial bell-like disturbance.

The obtained stationary structures have a wide spectrum and can’t be described by the known equations of the low- or high-frequency approximations.

**FIGURE 4.** Nonstationary disintegration of the initial localized perturbation into sequence of pulses obtained by the numerical solution of GNAE (5) (a) and by the 1D - numerical solution of (1), (2) (b)

2. 2D- weak shock waves destroy into the similar autowave pulse structures (figures 5,6).

**FIGURE 5.** The splitting of the shock wave front for the 2D geometry obtained by the numerical simulation of the system of equations (1), (2).
3. Collision of 1D autowave pulses leads to their full reconstruction after the initial stage of the nonlinear increase of summarized amplitude (Figure 7).
4. Using the 2D - system of relaxing gas dynamics (1),(2), we consider the evolution of the initial noise signal into the non-stationary quasi-regular system of colliding self-sustained acoustical pulses (figure 8).

FIGURE 8. Pattern of colliding self-sustained solitary pulses obtained from initial noise signal in 2D geometry. (a) dependence of density on coordinates x, y; (b) shadow picture of density distribution

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