DIFFUSION PROBLEMS IN THE LINEAR THEORY OF GASDYNAMIC AND CHEMICAL LASERS

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The system of linear equations of multicomponent convective diffusion is reduced consistently with allowance for the features of the relevant laser devices. A criterion for the realization of a purely diffusion regime is established. A method of diagonalization of the diffusion coefficient matrix is given; it reduces the multicomponent problem to a series of one-component problems. The superposition of relaxation modes is discussed. A diffusion type hydrofluoric laser illustrates the influence of angular asymmetry of the particles on the output power of the radiation.

1. If the kinetic processes that determine the parameters of gasdynamic and chemical lasers (see the reviews [1-3]) are to be established precisely, it is frequently necessary to take into account the diffusion characteristics of a nonequilibrium flux. A considerable number of laser systems have been developed in which the diffusion transport of atoms and molecules is the dominant kinetic process [4, 5].

By using simplified estimates of the "diffusion contributions" to the relaxation times and also other parameters that directly determine the gain, power, and efficiency of lasers, one can seriously distort the results of calculations [6] or even arrive at a qualitative contradiction to experimental data [7]. In this paper, I consider linear boundary-value diffusion problems whose solutions must be taken into account. These problems admit either a direct analytic or simple numerical solution, so that the results can be used to improve the model theories of lasers like those in [8-10].

2. In the framework of the phenomonological description of vibrational relaxation of the levels, combined in "blocks", of the basic laser components (for example, in the Landau–Teller approximation [8] and the Courant–Friedrichs–Levi stability conditions [11]) one can proceed from the following system of linear equations of convective diffusion:

$$\frac{\partial n_i}{\partial t} + \mathbf{v}\nabla n_i - \sum_{k=1}^{p} D_{ik}\nabla^2 n_k + \alpha_i n_i = 0, \qquad \mathbf{v} = \sum_{i=1}^{p} n_i \mathbf{v}_i. \tag{2.1}$$

Here $\mathbf{v}$ is the vector of the mean velocity of the flux; α_i are dissipative coefficients; and D_{ik} are diffusion coefficients which, to a good approximation, can be regarded as scalar quantities related to one another by the Onsager relations.

We find a criterion that enables one to distinguish a purely diffusion regime of operation of the laser. If $l_{\parallel}$ and $l_{\perp}$ are the characteristic longitudinal and transverse dimensions of the laser channel (or rather that part of it in which the diffusion process is important), the criterion can be formulated as

$$t_c \gtrsim 10 t_d, \quad t_c = l_{\parallel}/v, \quad t_d = l_{\perp}^2/\langle D_{ik}\rangle \tag{2.2}$$

where t_c and t_d are the times of convective and diffusion passage of a particle. Introducing the Schmidt and Reynolds numbers for the flux, Sc and Re respectively, we can rewrite (2.2) as

$$\mathrm{Sc}\ \mathrm{Re} \lesssim 0.1\ l_{\parallel}/l_{\perp} \tag{2.3}$$

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The opposite inequality corresponds to the fast-flow regime [12]. Neither this nor the intermediate case [13] will be considered.

Apart from the neglect of the second term, on the basis of (2.3), a further formal simplification of (2.1) can be achieved by the change of variables

$$m_i = n_i e^{\alpha_i t} \tag{2.4}$$

Then (2.1) is replaced by

$$\frac{\partial m_i}{\partial t} = \sum_{k=1}^{p} D_{ik}^* \nabla^2 m_k \tag{2.5}$$

$$D_{ik}^* = D_{ik} e^{(\alpha_i - \alpha_k) t} \tag{2.6}$$

The literature data (see, for example, [3, 6, 10]) enable one to make a comparative estimate of the quantities t_d and the differences $\alpha_i - \alpha_k$ in the exponential in (2.6). It is found that a large number of practically interesting cases are characterized by

$$|\alpha_i - \alpha_k| < t_d^{-1} \tag{2.7}$$

i.e., to a fair degree of accuracy one can ignore the difference between the dissipative coefficients in the multicomponent problem and proceed from the system of equations

$$\frac{\partial n_i}{\partial t} = \sum_{k=1}^{p} D_{ik} \nabla^2 n_k - \alpha n_i \tag{2.8}$$

3. In the thermodynamics of irreversible processes in the solution of problems described by equations of the type (2.8), one attempts, using different approximations, to "decouple" the system or ignore the nondiagonal terms of the matrix D_{ik} of diffusion coefficients. As a rule, such procedures are hard to justify and their use introduces uncontrollable errors into the calculations [14, 15].

Note that (2.8) is transformed into a system of p independent equations by the diagonalization of D. We consider an auxilliary nonsingular square matrix g with elements g_{ik} whose rank is the same as that of D. Multiplying the equations of the system (2.8) by the corresponding elements of g_{ij}, summing over i, and also replacing the subscripts i by k in terms with single summation, we find

$$\frac{\partial}{\partial t} \sum_{k=1}^{p} g_{kj} n_k = \operatorname{div} \operatorname{grad} \sum_{k=1}^{p} n_k \sum_{i=1}^{p} g_{ij} D_{ik} - \alpha \sum_{k=1}^{p} g_{kj} n_k, \quad j = 1, 2, \ldots, p \tag{3.1}$$

We introduce the notation

$$G_j = \sum_{k=1}^{p} g_{kj} n_k, \quad H_j = \frac{1}{g_{kj}} \sum_{i=1}^{p} g_{ij} D_{ik} \tag{3.2}$$

after which the system (3.1) can be written in the form

$$\partial G_j / \partial t = H_j \nabla^2 G_j - \alpha G_j, \; j = 1, 2, \ldots, p \tag{3.3}$$

where the coupled terms are absent. The elements of the diagonalized matrix, H_j, can be found from the condition

$$\det (D_{ik} - H \delta_{ik}) = 0 \tag{3.4}$$

The solution of the system of equations (2.8) is

$$n_i = \sum_{j=1}^{p} g_{ij}^{-1} G_j \tag{3.5}$$

where g^{-1} is the inverse matrix.

Returning to the more complicated case, when (2.7) does not hold, we note that an investigation was made of the convergence of the iterative scheme in accordance with which coefficients α_j of the form

$$\alpha_j = \frac{1}{G_j} \sum_{k=1}^{p} \alpha_k g_{kj} n_k \tag{3.6}$$

are introduced in (3.3) and in the first approximation the n_k are found using (3.5). As a rule, more than two iterations are not required.

4. After reduction of the multicomponent diffusion problem, we arrive at an equation of the form

$$\partial n/\partial t = D\nabla^2 n - \alpha n \tag{4.1}$$

where the subscript i has been omitted. Specifying a definite geometry of the system and solving (4.1), one can obtain the complete relaxation matrix

$$Y_{mnq} = \gamma_{mnq} \exp(-t/\tau_{mnq}), \quad \sum_{m,n,q} \gamma_{mnq} = 1 \tag{4.2}$$

Suppose, for example, that the diffusion occurs in a cylindrical cavity, L and R being the length and radius of the cylinder. Separating the four arguments (r, φ, z, t) of the function n in (4.1) by the Fourier method, and making some calculations [16], we find

$$n(r, \varphi, z, t) = \sum_m \sum_{n=1}^{\infty} \sum_{q=0}^{\infty} C_{mn}' [K_q' \cos(q\varphi) + M_q' \sin(q\varphi)] \, J_q(\mu_{mq} r) \cos(\nu_n z) \exp\{-[D(\mu_{mq}^2 + \nu_n^2) + \alpha] t\} \tag{4.3}$$

Here K_q', M_q', C_{mn}' are constants to be determined from the initial and boundary conditions; $\nu_n = (2n-1)\pi L^{-1}$ and μ_{mq} are the roots of the transcendental equation

$$J_q(\mu_{mq} R) = 0 \tag{4.4}$$

J_q is the symbol of a Bessel function, and in the summation over m one need take into account only the positive roots of Eq. (4.4). As can be seen from (4.3), the matrix elements in the expression (4.2) are determined by

$$\tau_{mnq} = [D(\mu_{mq}^2 + \nu_n^2) + \alpha]^{-1} \tag{4.5}$$

In the case of spherical geometry, the solution can be written in the form

$$n(r, \theta, \varphi, t) = \sum_m \sum_{n=0}^{\infty} \sum_{q=0}^{\infty} C_{mn}'' P_n^{(q)}(\cos\theta) [K_q'' \cos(q\varphi) + M_q'' \sin(q\varphi)] (\mu_{mn} r)^{-1/2} J_{n+1/2}(\mu_{mn} r) \exp\{-[D\mu_{mn}^2 + \alpha] t\} \tag{4.6}$$

where $P_n^{(q)}(\cos\theta)$ are associated Legendre functions, and the exponential dependence of the elements of the relaxation matrix Y is determined by the term

$$\tau_{mn} = [D\mu_{mn}^2 + \alpha]^{-1} \tag{4.7}$$

which contain only two indices instead of three (degeneracy).

We mention here a formal similarity with the problem of longitudinal relaxation of optically oriented atoms in a cell with inert or organic inhibitor [16-18]. As in the problem, in this case one can expect appreciable changes of τ_{mnq} and γ_{mnq} in (4.2) because of the absence of symmetry in the distribution of the diffusing particles with respect to the angle φ. This must have an appreciable effect on the output characteristics of the laser – the integral gain, the laser power, mode structure, etc. Such an effect has been observed: in [19] the choice of a particular asymmetric position of a hydrogen injector in a subsonic HF electric-discharge mixing laser made it possible to improve the output parameters of the laser appreciably. Similar cases can also be found in the investigations of laser systems with chemical pumping (see [3]).

From the point of view of the solution of (4.3), asymmetry in the angular distribution of the diffusing particles amounts to retention of the summation over q and the need to find the roots μ_{mq} in (4.4) for different values of q. To make the calculations less cumbersome, it is convenient to use the generalized coordinates x_φ introduced in the study of multidimensional problems of the theory of neutron transfer [20]. The transition to a symmetric distribution of the particles with respect to φ then corresponds to degeneracy of x_φ in the Cartesian coordinate x.

5. We illustrate the use of the general expressions in a definite example. Let us calculate the power W of the radiation leaving an HF flow diffusion system operating under laser conditions. Let I_0 be the intensity of the radiation entering the laser. In the z direction we assume that the beam has dimensions unity, and along the x (along the flux velocity) and y (along the segment bounded by the flow axis and the "flame front" [4]) axes we integrate in accordance with the formula

$$W = I_0 \int_0^x \left[\exp\left(\int_0^{y_0} \varkappa \, dy\right) - 1\right] dx \tag{5.1}$$

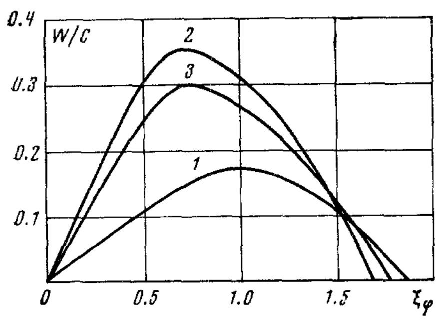

Fig. 1

In the approximation of a laminar front [21]

$$y_0 = A\sqrt{Dx/v} \tag{5.2}$$

where A is a constant of order unity, v is the flux velocity,

$$\varkappa = \chi\hbar\omega\, N_0\,([HF^*] - [HF^\circ]) \tag{5.3}$$

$\varkappa$ is the local gain (the notation is standard [22] and therefore not explained) for which, following the model of [10], one can readily write down an ordinary differential equation. The important parameters in this equation are χI_0, and also Q_H and Q_M, which are the products of the concentration of H_2 molecules and the concentration M of the particles and the reaction rates $\bar{Q}_H$ and $\bar{Q}_M$ respectively:

$$H_2 + F \xrightarrow{\bar{Q}_H} HF^* + H \tag{5.4}$$

$$HF^* + M \xrightarrow{\bar{Q}_M} HF^\circ + M \tag{5.5}$$

These three quantities determine two dimensionaless ratios:

$$\lambda_1 = Q_H/Q_M, \quad \lambda_2 = 2\chi I_0/Q_M \tag{5.6}$$

which are convenient in the interpretation of different particular solutions of the problem.

As a result of solution of the equation for $\varkappa$, substitution of this solution into (5.1), and integration with allowance for $\varkappa \leqslant 0.5$ we obtain

$$W = Cb_1\sqrt{1-b_1}\left\{a_1\left[\sqrt{\xi_\varphi} - \mathrm{Daw}\left(\sqrt{\xi_\varphi}\right)\right] - \frac{a_2}{b_2}\left[\sqrt{\xi_\varphi} - \frac{\mathrm{Daw}\left(\sqrt{b_1\xi_\varphi}\right)}{\sqrt{b_1}}\right] + \frac{2}{3}a_3\xi_\varphi^{3/2}\right\} \tag{5.7}$$

The symbol Daw denotes the Dawson integral, which is tabulated and can be expressed in terms of the error function of imaginary argument:

$$\mathrm{Daw}(x) \equiv \left(\sqrt{\pi}/2i\right)\exp(-x^2)\,\Phi(ix)$$

The variable ξ_φ is related to the generalized coordinate x_φ, which takes into account the azimuthal asymmetry of the flux of diffusing H_2 molecules as follows:

$$\xi_\varphi = (1+\lambda_2)\,\zeta_\varphi = Q_m v^{-1}(1+\lambda_2)\,x_\varphi \tag{5.8}$$

The remaining quantities in (5.7) are

$$b_1 = \frac{\lambda_2}{1+\lambda_2}, \quad b_2 = \frac{\lambda_1}{1+\lambda_1}, \quad a_1 = \frac{b_2(2-b_1)}{b_2-1}, \quad a_2 = \frac{1+b_2-b_1}{b_2-1}, \quad a_3 = b_1 - 1 \tag{5.9}$$

The characteristic result of calculation in accordance with (5.7) is shown in Fig. 1. Along the axes we have plotted ξ_φ and W/C (C is constant) and for simplicity we have taken the limiting case $\lambda_1 \to \infty$; physically it means that the reaction of formation of active molecules (5.4) is completed within the "flame front." Here, λ_2 is a variable parameter and, for curves 1 and 2, takes the values 1 and 4. These two curves correspond to the case when there is no angular asymmetry in the distribution of the diffusing particles, i.e., $x_\varphi = x$ for them. For curve 3, as for curve 1, $\lambda_2 = 1$, but the assumption of a symmetric distribution of the particles with respect to φ has been lifted and it has been assumed that the injector of H_2 molecules is shifted with respect to the axis of the system in the radial direction through a radial distance R/4. Accordingly, the scale along the abscissa has been deformed, i.e., here $x_\varphi \neq x$.

It is evident from a comparison of the curves that the output power of the laser can be appreciably improved by the superposition of the relaxation modes when the reacting molecules are injected asymmetrically. This method of optimizing diffusion-type lasers, which is formally equivalent to increasing the gain for transitions of the P-branch of induced electrodipole radiation, evidently warrants further study.

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