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A VARIATIONAL PRINCIPLE OF THE HAMILTON TYPE OF NONLINEAR PHENOMENA OF COMBINED TRANSFER

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UDC 536.248:517.972.5

A Lagrange function is given on the basis of which the variational principle of nonlinear combined transfer phenomena is built.

A great applied importance at the present time is possessed by mathematical models found on the use of a system of nonlinear partial differential equations of the form

$$\frac{\partial \vartheta_i}{\partial t}=\sum_{k=1}^{n} a_{ik}(\vartheta)\operatorname{div}(b_{ik}(\vartheta)\operatorname{grad}\vartheta_k)+\omega_i(\vartheta)\quad (i=1,\ 2,\ \ldots,\ n). \tag{1}$$

Here $\vartheta_i=\vartheta_i(x_1,\ x_2,\ x_3,\ t)$ $(i=1,\ 2,\ \ldots,\ n)$ are functions (transfer potentials) which are continuous together with their derivatives; a_{ik}, b_{ik}, ω_i $(i,\ k=1,\ 2,\ldots,\ n)$ are continuous functions of transfer potentials $\vartheta=(\vartheta_1,\ \vartheta_2,\ldots,\ \vartheta_n)$.

By means of this system, e.g., we describe phenomena of combined transfer of an arbitrary number of substances in a continuous medium occupying a volume v, in the presence of sources and sinks of substances and, in particular, phenomena of combined heat and mass transfer [1]. Systems of equations, being particular cases of system (1), lie at the basis of the investigation of biochemical reactions [2-4], nerve conductivity [5], development of malignant tumors [6], etc.

It is known that investigation of system (1) in each concrete case is complicated by difficulties caused by its nonlinearity, and in rare cases is completed in t closed form.

During the recent years in the solution of problems of thermodynamics of irreversible processes, a greater and greater role is played by variational methods. Allowing us partly to eliminate the difficulties connected with nonlinearity of the problems, they in a number of cases allow us to obtain effective approximate solutions of problems of combined transfer [7, 8]. It should be noted that the variational principles forming their basis usually do not use the Lagrange function, i.e., these principles do not possess a Hamiltonian form.

We consider the possibility of using a variational principle of the Hamilton type in the solution of problems leading to a system of equations (1).

Taking as $[t_0,\ t_1]$ an arbitrary segment of time, we write the integral of action in the form

$$I=\int_{t_0}^{t_1}\int_{v}\mathcal{L}\,dv\,dt. \tag{2}$$

We shall assume for a start that some natural boundary conditions are absent. This assumption is equivalent to the assertion that variations of transfer potentials $\delta\vartheta_i$ $(i=1,\ 2,\ \ldots,\ n)$ on the boundary of the volume v are zero at any time instant $t(t_0\leq t\leq t_1)$, and also $\delta\vartheta_i|_{t_0}=\delta\vartheta_i|_{t_1}=0$ within the volume v and on its boundary.

The system of equations (1) can be obtained by means of the variational principle $\delta I=0$, if in (2) we take the Lagrange equation in the form

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Translated from Inzhenerno-Fizicheskii Zhurnal, Vol. 39, No. 3, pp. 475-481, September, 1980. Original article submitted September 28, 1979.

0022-0841/80/3903-0985$07.50

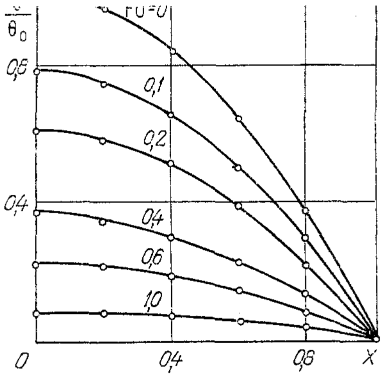

Fig. 1. Comparison of approximate temperature profiles (points) with exact profiles (solid lines) for the case of an infinite plate in dimensionless variables.

$$\mathcal{L}=\frac{\alpha}{2}\sum_{i=1}^{n}\left[\dot{\vartheta}_i-\sum_{k=1}^{n}a_{ik}(\vartheta)\operatorname{div}(b_{ik}(\vartheta)\operatorname{grad}\vartheta_k)-\omega_i(\vartheta)\right]^2\exp\frac{t}{\alpha}, \tag{3}$$

while the parameter α, entering into the Lagrangian (3) is allowed to tend to zero after the process of variation is completed (here by a dot above the symbol we denote a derivative with respect to time).

Indeed, applying with (3) taken into account the system of Euler—Lagrange equations for the generalized coordinates ϑ_i

$$\frac{\partial\mathcal{L}}{\partial\vartheta_i}-\frac{\partial}{\partial t}\frac{\partial\mathcal{L}}{\partial\dot{\vartheta}_i}-\sum_{j=1}^{3}\frac{\partial}{\partial x_j}\frac{\partial\mathcal{L}}{\partial(\partial\vartheta_i/\partial x_j)}+\sum_{j=1}^{3}\frac{\partial^2}{\partial x_j^2}\frac{\partial\mathcal{L}}{\partial(\partial^2\vartheta_i/\partial x_j^2)}=0\quad(i=1,\ 2,\ \ldots,\ n), \tag{4}$$

we obtain after division of both sides by $\exp(t/\alpha)$, expressions of the form

$$\dot{\vartheta}_i-\sum_{k=1}^{n}a_{ik}\operatorname{div}(b_{ik}\operatorname{grad}\vartheta_k)-\omega_i=G_i\left(x_j,\ t,\ \vartheta_i,\ \dot{\vartheta}_i,\ \frac{\partial\vartheta_i}{\partial x_j},\ \ldots,\ \alpha\right)\quad(i=1,\ 2,\ \ldots,\ n).$$

If the Lagrangian is chosen in the form of relation (3), then functions G_i on the right side of the last expression tend to zero under the condition $\alpha\to 0$. With this taken in into account, Lagrangian (3) leads to the system of equations (1).

The approach to the construction of variational principles of the Hamilton type just considered is generalized to the case of nonlinear anisotropic combined transfer of an arbitrary number of substances. This phenomenon takes place when the coefficients of conductivity of the medium for the different substances taking part in the transfer, depend on the directions of transfer. The system of equations (1) is then written as

$$\frac{\partial\vartheta^i}{\partial t}=a^{ik}(\vartheta)\frac{\partial}{\partial x_\alpha}\left(L_{\alpha\beta}^{ik}(\vartheta)\frac{\partial\vartheta^k}{\partial x_\beta}\right)+\omega^i(\vartheta)\quad(i=1,\ 2,\ \ldots,\ n). \tag{5}$$

Here the coefficients $L_{\alpha\beta}^{ik}$ are a tensor of the second rank; over the repeated lower Greek indices summation is carried out from 1 to 3, while over the upper repeated indices i and k summation is carried out from 1 to n. The Lagrange function in this case assumes the form

$$\mathcal{L}=\frac{\alpha}{2}\sum_{i=1}^{n}\left[\dot{\vartheta}^i-a^{ik}(\vartheta)\frac{\partial}{\partial x_\alpha}\left(L_{\alpha\beta}^{ik}(\vartheta)\frac{\partial\vartheta^k}{\partial x_\beta}\right)-\omega^i(\vartheta)\right]^2\exp\frac{t}{\alpha}. \tag{6}$$

Carrying our for (6) the construction of the Euler—Lagrange equations and going to the limit with $\alpha\to 0$, it can be shown that Eq. (5) follows from (6).

We shall demonstrate the possibility of practical application of the formalism under consideration, to investigation of problems of combined transfer with an example of a system of equations of heat and mass transfer ($n=2$, ϑ_1 and ϑ_2 are the transfer potentials of heat and mass of a combined matter):

$$\begin{gathered}c_q\gamma\dot{\vartheta}_1=\operatorname{div}(\lambda_q\operatorname{grad}\vartheta_1)+\varepsilon\rho c_m\gamma\dot{\vartheta}_2+\omega_q(\vartheta_1,\ \vartheta_2),\\ c_m\gamma\dot{\vartheta}_2=\operatorname{div}(\lambda_m\delta\operatorname{grad}\vartheta_1)+\operatorname{div}(\lambda_m\operatorname{grad}\vartheta_2)+\omega_m(\vartheta_1,\ \vartheta_2).\end{gathered} \tag{7}$$

The Lagrange function (3) in this case has the form

$$\mathcal{L} = \frac{\alpha}{2}\left\{\left[\dot{\vartheta}_1 - \frac{1}{c_q\gamma}\operatorname{div}(\lambda_q \operatorname{grad}\vartheta_1) - \frac{\varepsilon\rho}{c_q\gamma}[\operatorname{div}(\lambda_m\delta\operatorname{grad}\vartheta_1 + \right.\right.$$

$$\left.\left. + \lambda_m \operatorname{grad}\vartheta_2) + \omega_m] - \frac{\omega_q}{c_q\gamma}\right]^2 + \left[\dot{\vartheta}_2 - \frac{1}{c_m\gamma}\operatorname{div}(\lambda_m\delta\operatorname{grad}\vartheta_1 + \lambda_m\operatorname{grad}\vartheta_2) - \frac{\omega_m}{c_m\gamma}\right]^2\right\}\exp\frac{t}{\alpha}. \tag{8}$$

We take

$$\lambda_q = \overset{*}{\lambda}_q M_1, \quad c_q\gamma = \overset{*}{c}_q\gamma^* N_1, \quad \varepsilon\rho = \varepsilon^*\rho^* L_1, \quad \lambda_m = \overset{*}{\lambda}_m M_2,$$

$$c_m\gamma = \overset{*}{c}_m\gamma^* N_2, \quad \lambda_m\delta = \overset{*}{\lambda}_m\delta^* L_2, \quad \omega_q = \overset{*}{\omega}_q\Omega_1, \quad \omega_m = \overset{*}{\omega}_m\Omega_2,$$

$$\Delta = \frac{\alpha a_q}{R^2}, \quad K_1 = \frac{1}{N_1}, \quad K_2 = \frac{1}{N_2}, \quad K_3 = \frac{L_1}{N_1 N_2}$$

(here M_i, N_i, L_i, Ω_i ($i = 1, 2$) are continuous functions of the dimensionless transfer potentials θ_1 and θ_2). Then for an infinite plate of thickness R the Lagrange function is written as

$$\mathcal{L} = \frac{\Delta}{2}\left\{\left[\frac{\partial\theta_1}{\partial \mathrm{Fo}} - K_1\frac{\partial}{\partial X}\left(M_1\frac{\partial\theta_1}{\partial X}\right) - \mathrm{Ko}^*\,\mathrm{Pn}\,\mathrm{Lu}\,K_3\left(L_2\frac{\partial\theta_1}{\partial X}\right)\right.\right.$$

$$\left. + \mathrm{Ko}^*\,\mathrm{Lu}\,K_3\frac{\partial}{\partial X}\left(M_1\frac{\partial\theta_2}{\partial X}\right) - \mathrm{Po}_q K_1\Omega_1 + \mathrm{Ko}^*\,\mathrm{Lu}\,\mathrm{Po}_m K_3\Omega_2\right]^2\cdot$$

$$\left. + \left[\frac{\partial\theta_2}{\partial \mathrm{Fo}} + \mathrm{Lu}\,\mathrm{Pn}K_2\frac{\partial}{\partial X}\left(L_2\frac{\partial\theta_1}{\partial X}\right) - \mathrm{Lu}\,K_2\frac{\partial}{\partial X}\left(M_1\frac{\partial\theta_2}{\partial X}\right) - \mathrm{Lu}\,K_2\Omega_2\right]^2\right\}\exp\frac{\mathrm{Fo}}{\Delta}. \tag{9}$$

With $L_n = M_n = N_n \equiv 1$, $\Omega_n \equiv 0$ we consider the sequence of obtaining approximate solutions of concrete problems for the case of an infinite plate. For this we use the method of reduction to ordinary differential equations. Specifying the behavior of the potentials θ_1 and θ_2 with respect to a spatial variable and computing the integral over this variable, the dependence of θ_1 and θ_2 on the criterion Fo will be determined, proceeding from the condition that the Euler—Lagrange equations are satisfied for the variational integral over time.

We denote $A_1 = 1 + \mathrm{Ko}^*\mathrm{Pn}\,\mathrm{Lu}$, $A_2 = \mathrm{Lu}\,\mathrm{Ko}^*$, $A_3 = \mathrm{Lu}$, $A_4 = \mathrm{Lu}\,\mathrm{Pn}$ and will assume in the following that the free index i runs through the values 1 and 2. We take the boundary conditions

$$\theta_i(1, \mathrm{Fo}) = \theta_i(-1, \mathrm{Fo}) = 0, \ \theta_i(X, 0) = \theta_{i0}(1 - X^2), \ \theta_{i0} = \mathrm{const}.$$

We shall assume that the distribution of the transfer potentials satisfies the boundary conditions and has the form

$$\theta_i(X, \mathrm{Fo}) = \theta_{i0}(1 - X^2)\varphi_i(\mathrm{Fo}), \ \varphi_i(0) = 1. \tag{10}$$

For the determination of the unknown functions $\varphi_i(\mathrm{Fo})$ we substitute expressions (10) into relation (9) and in the integral of action

$$I = \int_{\mathrm{Fo}_0}^{\mathrm{Fo}_1}\int_{-1}^{1}\mathcal{L}\,dX\,d\mathrm{Fo} \tag{11}$$

we carry out integration over the spatial coordinate. We obtain

$$I = \int_{\mathrm{Fo}_0}^{\mathrm{Fo}_1}\mathcal{L}(\varphi_1, \varphi_2, \dot{\varphi}_1, \dot{\varphi}_2, \mathrm{Fo})\,d\mathrm{Fo} = \int_{\mathrm{Fo}_0}^{\mathrm{Fo}_1}\frac{\Delta}{2}\left\{\sum_{m=1}^{2}\left[\theta_{m0}^2\dot{\varphi}_m^2 - \right.\right.$$

$$- 5A_{2m}\theta_{10}\theta_{20}\dot{\varphi}_m\varphi_{3-m} + 5A_{2m-1}\theta_{m0}^2\dot{\varphi}_m\varphi_m + \frac{15}{2}(A_m^2\theta_{m0}^2 +$$

$$\left.\left. + A_{m+2}^2\theta_{3-m,0}^2)\varphi_m^2\right] - 15\theta_{10}\theta_{20}(A_1A_2 + A_3A_4)\varphi_1\varphi_2\right\}\exp\frac{\mathrm{Fo}}{\Delta}\,d\mathrm{Fo}. \tag{12}$$

If the integral of action (12) is stationary relative to the functions φ_i, which are independent variables, then the Euler—Lagrange equations

$$\frac{\partial}{\partial \mathrm{Fo}} \frac{\partial \mathscr{L}}{\partial \dot{\varphi}_i} - \frac{\partial \mathscr{L}}{\partial \varphi_i} = 0$$

must be fulfilled; in the given case they have the form

$$\frac{2}{5} \dot{\varphi}_1 + A_1\varphi_1 - A_2 \frac{\theta_{20}}{\theta_{10}} \varphi_2 = \Delta \{\cdots\}_1,$$

$$\frac{2}{5} \dot{\varphi}_2 - A_4 \frac{\theta_{10}}{\theta_{20}} \varphi_1 + A_3\varphi_2 = \Delta \{\cdots\}_2.$$

Carrying out transition to the limit with respect to Δ → 0, we have for determination of the functions φ_i a system of ordinary differential equations of the form

$$\frac{2}{5} \dot{\varphi}_1 = -A_1\varphi_1 + A_2 \frac{\theta_{20}}{\theta_{10}} \varphi_2, \quad \frac{2}{5} \dot{\varphi}_2 = A_4 \frac{\theta_{10}}{\theta_{20}} \varphi_1 - A_3\varphi_2. \tag{13}$$

Its solution with the initial conditions $\varphi_i(0) = 1$ and different real roots of the characteristic equation, e.g., has the form

$$\varphi_1 = \frac{a_2 - 1}{a_2 - a_1} \exp s_1\mathrm{Fo} + \frac{1 - a_1}{a_2 - a_1} \exp s_2\mathrm{Fo},$$

$$\varphi_2 = \frac{a_1(a_2 - 1)}{a_2 - a_1} \exp s_1\mathrm{Fo} + \frac{a_2(1 - a_1)}{a_2 - a_1} \exp s_2\mathrm{Fo}.$$

Here

$$a_i = \frac{A_4\theta_{10}}{\left(A_3 + \frac{3}{5} s_i\right) \theta_{20}};$$

$$s_{1,2} = -\frac{5}{4} \left(A_1 + A_3 \pm \sqrt{(A_1 + A_3)^2 - 4(A_1A_3 - A_2A_4)}\right).$$

The method of reduction to ordinary differential equations, used here to solve the problem with boundary conditions of the first kind, allows us to make, while determining the transfer potentials, the best possible choice in the class of functions having a given a priori dependence on the spatial variable. This, as is seen from the preceding example, leads to simple computations, but does not allow us to construct a converging sequence when computing approximate solutions with a given accuracy, a circumstance which complicates the a priori estimate of the error. At the same time, this method in a number of cases allows us to rapidly obtain a good approximation of the transfer potentials. We shall demonstrate this with the example of the preceding problem, carrying out an a posteriori estimate of the error by comparing the approximate solutions (10) with the exact solutions for the case where $\mathrm{Ko}^* = \mathrm{Pn} = 0$. From (13) we have $\varphi_1 = \exp(-5/2 \times \mathrm{Fo})$. This expression together with expression (10) for the temperature coincides with the analogous problem of heat conduction obtained in [9]. In Fig. 1 we have represented the approximate solutions (10) for the potential θ_1 (points) and the exact solutions of the corresponding problem of heat conduction [10]. The comparison demonstrates their good agreement. We now take the boundary conditions in the form

$$\frac{\partial \theta_i}{\partial X}(1, \mathrm{Fo}) = B_i, \quad \frac{\partial \theta_i}{\partial X}(0, \mathrm{Fo}) = 0, \quad \theta_i(X, 0) = 0, \tag{14}$$

where $B_1 = \mathrm{Ki}_q = \mathrm{const}$; $B_2 = \mathrm{Pn}\,\mathrm{Ki}_q + \mathrm{Ki}_m + \mathrm{const}$.

Following [11], we introduce layers of potentials θ_1 and θ_2 of thickness $\delta_1(\mathrm{Fo})$ and $\delta_2(\mathrm{Fo})$, respectively, developing with time, and divide the process of transfer into two stages. At the first stage ($\delta_i \leq 1$) the profiles of the transfer potentials are represented in the form

$$\theta_i = \frac{B_i}{2\delta_i} [X - (1 - \delta_i)]^2. \tag{15}$$

Substituting (15) into (11), carrying out integration over X within each layer, where nonzero distribution of the transfer potential exists, and solving then the Euler–Lagrange equation obtained in the case Δ → 0, for δ_i with the initial conditions $\delta_i(0) = 0$, we have

$$\delta_1 = \left[5\left(A_1 - A_2\frac{B_2}{B_1\mu}\right)\mathrm{Fo}\right]^{\frac{1}{2}}, \quad \delta_2 = \left[5\left(A_3 - A_4\frac{B_1}{B_2}\mu\right)\mathrm{Fo}\right]^{\frac{1}{2}}. \tag{16}$$

Here the simplex $\mu = \delta_2/\delta_1$ is determined from a quadratic equation obtained with the use of (16).

At the second stage a variation of the potential in the plane $X = 0$ takes place. In this case the boundary conditions (14) are satisfied by the functions

$$\theta_i = q_i + \frac{1}{2}B_iX^2. \tag{17}$$

Here $q_i = q_i(\mathrm{Fo})$. Expressions (17) and (11) lead to the Euler—Lagrange equations relative to the functions q_i, the solution of which in the case of the initial conditions $q_1(\mathrm{Fo}') = 0$, $q_2(\mathrm{Fo}'') = 0$ has the form

$$q_1 = (A_1B_1 - A_2B_2)(\mathrm{Fo} - \mathrm{Fo}'), \quad q_2 = (A_3B_2 - A_4B_1)(\mathrm{Fo} - \mathrm{Fo}''). \tag{18}$$

The instants of ending of the first stages Fo' and Fo" are determined from (16) for $\delta_1(\mathrm{Fo}') = 1$ and $\delta_2(\mathrm{Fo}'') = 1$, respectively.

The results (15)-(18) completely coincide with the solutions of this problem obtained in [8] on the basis of the supplementary form of another variational principle, but the procedure of computations in the given case is somewhat shorter. Also an estimate of the accuracy of approximate solutions is given there and, in particular, it is shown that in form they completely coincide with the quasistationary terms of the corresponding exact solutions [1].

Thus, the variational principle considered allows us to obtain simple approximate solutions of problems of combined heat and mass transfer, and can be used for the solution of also other problems leading to the system of equations (1).

NOTATION

x_1, x_2, x_3, spatial coordinates; t, time; v, region occupied by a body; $\mathscr{L}$, Lagrange function; c_q and c_m, specific heat and mass capacity; γ, density of medium; λ_q and λ_m, coefficients of heat and mass conduction; ε and ρ, criterion and specific heat of phase transformation; δ, Soret coefficient; ω_q and ω_m, rates of heat and substance liberation, respectively, per unit volume; a_q, thermal diffusivity; $(\ )^*$, characteristic quantities with dimensions; X, dimensionless coordinate; Fo, Fourier number; Lu, Pn, Ko*, Lykov, Posnov, and modified Kossovich numbers; Po_q and Po_m, Pomerantsev heat and mass exchange numbers.

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PROBLEM OF A PISTON IN A RELAXING GAS

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UDC 533.6.011.72

The possibility of obtaining an oscillatory inversion of population in $CO_2 + N_2 +$ He mixtures behind nonstationary shock waves is studied.

In [1-5] the possibility of obtaining an inversive population in gases consisting of multiatom molecules by means of thermal methods of pumping. In particular, inversion between the oscillatory levels (04°0-00°1) and (20°0-00°1) of the CO_2 molecule behind stationary shock waves is considered. Below we use the motions of an ideal, non-heat-conducting, perfect gas in the case of the problem of a symmetric piston moving in a $CO_2 + N_2 +$He mixture. For the analysis of oscillatory relaxation, we use the kinetic Anderson model [3, 5].

In a gaseous medium at rest, let the initial instant of motion of a piston obey the law $r_p = \lambda_p t^\delta$, where λ_p, $\delta = \mathrm{const}$. A shock wave is formed in front of the piston [6]; this wave excites oscillatory relaxation leading to an inversive population of the oscillatory levels of CO_2 molecule.

According to the Anderson model [3, 5], the oscillatory levels of CO_2 and N_2 molecules group into two "modes." This is based on the characteristic feature of the CO_2 molecule, which manifests itself in the fact that the strain oscillations ν_2 and the symmetric oscillations ν_1, which very rapidly come into equilibrium with them, have a shorter relaxation time than the asymmetric oscillations ν_3. On the other hand, thanks to the almost equal disposition, the asymmetric oscillations ν_3 rapidly exchange energy with the oscillatory level of the N_2 molecule. Such a feature of the CO_2 and N_2 molecules allows us to unite the oscillations ν_1 and ν_2 into "mode" I, and the oscillations ν_3 and ν into the "mode" II.

Since the lower oscillatory levels are of the major interest, in the case of calculations the model of the harmonic oscillator

$$\frac{dE_I}{dt} = \frac{E_I(T) - E_I(T_I)}{\tau_I} \tag{1}$$

remains valid, analogously for E_{II}, where τ_I, τ_{II} are the characteristic relaxation times; T is the translational temperature. The values τ_I and τ_{II} are certain effective values determined according to the rule of "parallel resistance" [3, 5]. The oscillatory temperatures T_I, T_{II} can be found, using the relations for the quantities E_I, E_{II}:

$$E_I = C_{CO_2} R_{CO_2} \left\{ \frac{\theta_1}{[\exp(\theta_1/T_I) - 1]} + \frac{2\theta_2}{[\exp(\theta_2/T_I) - 1]} \right\}, \tag{2}$$

$$E_{II} = C_{CO_2} R_{CO_2} \frac{\theta_3}{[\exp(\theta_3/T_{II}) - 1]} + C_{N_2} R_{N_2} \frac{\theta}{[\exp(\theta/T_{II}) - 1]}.$$

Here C_{CO_2}, R_{CO_2} are the mass fraction and the gas constant for CO_2; C_{N_2}, R_{N_2} are determined analogously to N_2; $\theta_i = h\nu_i/k$ are the corresponding characteristic temperatures. When computing the level populations in "modes" I and II, we take as valid the Boltzmann distribution over the levels within the "modes" [3-5].

The movement of the gas will be described by Eqs. (1) and (2) in combination with the equations of conservation of mass, momentum, and energy, which can be taken in the form

$$\frac{\partial \rho}{\partial t} + \frac{\partial \rho u}{\partial r} + j \frac{\rho u}{r} = 0,$$

V. A. Steklov Mathematical Institute, Moscow. Translated from Inzhenerno-Fizicheskii Zhurnal, Vol. 39, No. 3, pp. 482-485, September, 1980. Original article submitted August 29, 1979.

0022-0841/80/3903-0990$07.50