

# Light Induced Drift and Heat Transfer of One-Component Gas in a Capillary

V.G. Chernyak · A.P. Polikarpov

Received: 27 November 2009 / Accepted: 25 May 2010 / Published online: 8 June 2010  
© Springer Science+Business Media, LLC 2010

**Abstract** The processes of heat transfer and drift of rarefied gas in a capillary due to velocity-selective excitation of atoms by monochromatic light have been investigated. On the basis of kinetic equation the kinetic coefficients defining surface and bulk mechanisms of light induced transfer phenomena in dependence on the Knudsen number, the ratio of the rate of radiative decay of the excited level to the frequency of intermolecular collisions and the accommodation coefficient were calculated.

**Keywords** Gas · Molecule · Light · Drift · Heat flux · Accommodation

## 1 Introduction

The phenomenon of the light-induced drift (LID) predicted in the works [1, 2] consists in the appearing of the gas flow due to the velocity-selective absorption of the radiation by the gas particles and presence of the buffer gas. Later the full accumulated information on the LID was summarized in the monograph [3]. It's well known that electromagnetic wave propagating in one-component gas along the boundary surface stimulates the macroscopic gas flow along this surface—surface light induced drift (SLID) [4]. There must exist two conditions. Firstly, the radiation should be a traveling light wave whose frequency is close to that of an electronic transition of atoms or vibrational-rotational transition of molecules. The Doppler effect leads to the velocity-selective absorption of the radiation by the gas particles. The effective resonant velocity interval  $\Delta v$  is determined by the following conditions:  $\mathbf{k}\Delta v \sim \Gamma$  ( $\mathbf{k}$ —wave vector,  $\Gamma$ —homogeneous width of absorption line of the molecular transition).

---

V.G. Chernyak · A.P. Polikarpov (✉)  
Department of Physics, Ural State University, Ekaterinburg 620083, Russia  
e-mail: alexey.polikarpov@usu.ru

V.G. Chernyak  
e-mail: vladimir.chernyak@usu.ru

A.P. Polikarpov  
IUSTI, Université de Provence, Technopôle de Château-Gombert, 13453 Marseille Cedex 13, France

The second condition is that excited and unexcited particles must interact with the wall in different ways.

LID is unavailable in an unbounded gas owing to the momentum conservation law. But light induced heat transfer (LIHT) can occur in an unbounded one-component gas.

In the work [5] the so-called bulk mechanism of light induced drift of one-component gas near the boundary surface has been predicted. The nature of this phenomenon consists in the fact that collision cross sections for excited and unexcited particles are different. As a rule for excited atoms the collision cross section is larger, so that the mean free path is smaller than that for unexcited particles. As a consequence the thickness of the Knudsen layer for macroscopic flux of excited particles is smaller than that for the oppositely directed flux of unexcited particles. So these fluxes are not compensated. This effect is absent in an unbounded gas due to the momentum conservation law. But in the case of the bounded gas it leads to the overall gas flux along the surface in the direction of motion of unexcited particles.

Light induced heat transfer in some sense is analogous to the mechano-caloric effect. In other words, it's the difference of the energy flux of gas flow (Umov's vector) and enthalpy.

Surface LID was investigated in a slip flow [6] and a free molecular regimes [7]. Surface and bulk LID of one-component gas in a capillary has been studied in works [8, 9] in the whole range of Knudsen number ( $Kn$ ). In the work [8] the integro-momentum method with collision integral of second-order [10] was applied to solution of kinetic equation. In the work [9] the results of the LID velocity calculations on the basis of the same kinetic equation were obtained by the discrete velocity method. In the work [11] the light-induced heat transfer (LIHT) of the gas in a capillary has been investigated in addition to LID. As distinct from the models used in [8, 9], it is based on the third-order approximation [10] for the linearized collision integral providing an accurate description of the joint heat and mass transfer processes. The evident limitation of the results [11] connects with the proposition that the rate of radiative decay of the excited level  $\Gamma_m$  is considerably smaller than intermolecular collision frequency  $\gamma_i$ , i.e. frequency parameter  $\Gamma_{mi} = \Gamma_m/\gamma_i \ll 1$ . Obviously, it imposes certain restrictions on the theory in the case of low gas pressure when the intermolecular collision frequency is too small. Moreover, in [11] the coupled set of integral equations for the velocity of gas drift, shear stresses and heat flux has been solved by the Bubnov-Galerkin method which gives the opportunity to obtain explicit results in a whole range of Knudsen number for the average values of physical quantities over the capillary cross section, but it can not describe their profiles.

In this work the light induced transfer processes at different values of Knudsen number and frequency parameter  $\Gamma_{mi}$  are investigated. On the basis of numerical solution of the model kinetic equations by the discrete velocity method the average values over the capillary cross section and profiles of LID and LIHT were calculated. The numerical results obtained with certain accuracy can be applied to the estimation of approximate theories describing light induced transfer processes.

## 2 Statement of the Problem

Let us consider the steady-state flow of one-component gas in a circular-cylindrical tube of radius  $r_0$ . A traveling light wave is propagating along the axis  $z$  coinciding with the axis of the capillary. The gas particles are assumed to be in two quantum states—ground  $n$  and excited  $m$ . The radiation frequency  $\omega$  is slightly detuned from the center of the absorption line at  $\omega_{mn}$ , i.e.,  $\Omega = \omega - \omega_{mn}$ , ( $|\Omega| \ll \omega, \omega_{mn}$ ). Molecules that have absorbed radiation

change the kinetic cross sections. Simultaneously with the stimulated transitions there is a competitive process—radiative decay of the excited level with frequency  $\Gamma_m$ . Thus, the gas phase can be interpreted as a binary mixture consisting of the particles with equal masses  $m$  but different cross sections. Stimulated transitions and radiative decay of the excited levels lead to the exchange of molecules between excited and unexcited components.

The state of the such gas mixture can be described by distribution functions of excited  $f_m$  and unexcited  $f_n$  molecules. Let us introduce the cylindrical coordinate system  $x, \varphi, z$ . After that the distribution functions in the case of stationary gas state satisfy the following kinetic equations [12]:

$$\begin{aligned} \mathbf{v}_\perp \frac{\partial f_n}{\partial \mathbf{x}} &= \frac{1}{2} \Gamma_m \chi(\mathbf{v})(f_m - f_n) + \Gamma_m f_m + S_n, \\ \mathbf{v}_\perp \frac{\partial f_m}{\partial \mathbf{x}} &= -\frac{1}{2} \Gamma_m \chi(\mathbf{v})(f_m - f_n) - \Gamma_m f_m + S_m, \\ \chi(\mathbf{v}) &= \frac{4|G_{mn}|^2 \Gamma}{\Gamma_m [\Gamma^2 + (\Omega - kv_z)^2]}, \quad G_{mn} = \frac{E_0 d_{mn}}{2\hbar}, \quad v_\perp^2 = v_x^2 + v_\varphi^2. \end{aligned} \tag{1}$$

Here  $\mathbf{v}_\perp$  and  $\mathbf{x}$  are two-dimensional molecular velocity and radius vector respectively in the plane perpendicular to the axis of the capillary,  $\Gamma_m$  is the rate of radiative decay of the excited level,  $\Gamma$  is the homogeneous width of absorption line of molecular transition  $m - n$ ,  $S_n$  and  $S_m$  are Boltzmann collision integrals of molecules in ground and excited state respectively,  $E_0$  is the amplitude of the electrical field in the light wave,  $\hbar$  is the Planck’s constant,  $d_{mn}$  is the dipole matrix element of  $m - n$  transition,  $G_{mn}$  is the Rabi frequency;  $\chi(\mathbf{v})$  is the probability of absorption per unit time for molecules with a given velocity  $\mathbf{v}$ . In the environments with low optical depth or at relatively small distances the velocity of gas drift is believed to be independent of the longitudinal coordinate  $z$ . It’s also assumed that the radiation intensity is independent of the transverse coordinate.

As boundary conditions for (1) let us assume specularly-diffuse model, according to which the some fraction  $1 - \varepsilon_i$  of the particles of  $i$ th species is reflected specularly, and fraction  $\varepsilon_i$  of the particles is scattered diffusely with the Maxwell velocity distribution function. Neglecting the inelastic collisions of the gas particles with the wall one can obtain:

$$\begin{aligned} f_i^+(\mathbf{v}) &= \varepsilon_i f_i^s(\mathbf{v}) + (1 - \varepsilon_i) f_i^-(\mathbf{v} - 2(\mathbf{v} \cdot \mathbf{n})\mathbf{n}), \quad \mathbf{v} \cdot \mathbf{n} > 0 \\ f_i^s &= \frac{n_i^s}{\pi^{3/2} \bar{v}^3} \exp\left(-\frac{v^2}{\bar{v}^2}\right) \\ \bar{v} &= \left(\frac{2k_B T}{m_0}\right)^{1/2}, \quad i = m, n. \end{aligned} \tag{2}$$

Here  $\mathbf{n}$  is the unit vector normal to the boundaries and pointing towards the wall, indexes “-”, “+”, “s” relate correspondingly to the particles impinging the surface of the capillary, reflected specularly and diffusively,  $m_0$  is the mass of particles,  $k_B$  is the Boltzmann constant,  $T$  is average temperature of the system,  $\bar{v}$  is the most probable molecular speed. For the general case, the phenomenological coefficients  $\varepsilon_i$  are different ( $\varepsilon_m \neq \varepsilon_n$ ).

Taking into account that the parameter ( $|\chi(\mathbf{v})| \ll 1$ ) is small, which corresponds to the low intensity radiation, it can be assumed that the concentration of excited particles is considerably smaller in comparison with the concentration of unexcited particles ( $n_m \ll n_n$ ). In the such case the state of each component is supposed to be slightly disturbed from

equilibrium. Consequently velocity distribution functions can be written in the form of the perturbed Maxwellian distributions:

$$f_i(\mathbf{x}, \mathbf{v}) = f_{i0}[1 + h_i(\mathbf{x}, \mathbf{v})], \quad \|h_i(\mathbf{x}, \mathbf{v})\| \ll 1, \tag{3}$$

where

$$f_{i0} = \frac{n_{i0}}{\pi^{3/2}\bar{v}} \exp\left(-\frac{v}{\bar{v}}\right)^2,$$

$n_{i0}$ —equilibrium numerical density of particles in the  $i$ th state,  $h_i$ —unknown perturbation function,  $\|h_i\|$ —norm of function  $h_i$  in the velocity space. It should be noted that the linearization of the distribution function around the resonant value of the molecular velocity can appear to be the unreasonable approximation. However, it can be neglected at calculating the macroscopic value [13].

Let us consider only elastic collisions between the molecules. Taking into account the mentioned above suggestions we can use the linearized collision integral for the kinetic equation (1) of third order developed by McCormack [10]:

$$\begin{aligned} &c_{\perp} \left( \cos\theta \frac{\partial h_i}{\partial r} - \frac{\sin\theta}{r} \frac{\partial h_i}{\partial \theta} \right) + R_i (h_i - \beta_i \Gamma_{mi} h_m) \\ &= c_z R_i \psi_i + \beta_i R_i \Gamma_{mi} + \frac{1}{2} R_i \Gamma_{mi} \chi(\mathbf{v}) \left( \frac{n_j - n_i}{n_i} \right) \\ &(i, j) = m, n, i \neq j, \beta_n = \frac{n_m}{n_n}, \beta_m = -1, \end{aligned} \tag{4}$$

where

$$\begin{aligned} R_i &= \frac{r_0}{\bar{v}} (\gamma_{ii} + \gamma_{ij}), \quad \mathbf{c} = \frac{\mathbf{v}}{\bar{v}}, \quad \Gamma_{mi} = \frac{\Gamma_m}{\gamma_{ii} + \gamma_{ij}}, \quad \mathbf{r} = \frac{\mathbf{x}}{r_0}, \\ \psi_i &= 2[u_i - \varphi_{ij}^{(1)}(u_i - u_j) - \varphi_{ij}^{(2)}(H_i - H_j)] \\ &+ 4c_{\perp} \cos\theta [(1 - \varphi_{ii}^{(3)} + \varphi_{ii}^{(4)} - \varphi_{ij}^{(3)})\Pi_{izr} + \varphi_{ij}^{(4)}\Pi_{jzr}] \\ &+ \frac{4}{5} \left( c_{\perp}^2 - \frac{5}{2} \right) \left[ (1 - \varphi_{ii}^{(5)} + \varphi_{ii}^{(6)} - \varphi_{ij}^{(5)})H_i + \varphi_{ij}^{(6)}H_j - \frac{5}{2}(u_i - u_j)\varphi_{ij}^{(2)} \right], \\ \varphi_{mn}^{(k)} &= \frac{v_{mn}^{(k)}}{\gamma_{mm} + \gamma_{mn}}, \quad c_{\perp}^2 = c_r^2 + c_{\varphi}^2, \quad c_r = c_{\perp} \cos\theta, \quad c_{\varphi} = c_{\perp} \sin\theta \\ u_i &= U_i/\bar{v} = \pi^{-3/2} \int \exp(-c^2) c_z h_i d\mathbf{c}, \\ \Pi_{izr} &= P_{izr}/2p_i = \pi^{-3/2} \int \exp(-c^2) c_z c_r h_i d\mathbf{c}, \\ H_i &= q_i/p_i\bar{v} = \pi^{-3/2} \int \exp(-c^2) c_z (c^2 - 5/2) h_i d\mathbf{c}. \end{aligned} \tag{5}$$

Here  $R_i$  is the gas rarefaction parameter, which is proportional to the inverse Knudsen number  $Kn$ ;  $U_i, P_{ixz}, q_i, p_i$ —macroscopic flow velocity, shear stress, heat flux and pressure respectively for  $i$ th species,  $\gamma_{ii}, \gamma_{ij}$ —collision frequencies between the particles of  $i$ th

species and between the particles of  $i$ th and  $j$ th species respectively. Expressions for frequencies  $v_{ij}^{(k)}$  through the Chapman-Cowling integrals are presented in Appendix.

Boundary conditions (2) for the linearized case (3) take a form:

$$h_i^+(r = 1, \mathbf{c}) = (1 - \varepsilon_i)h_i^-(r = 1, \mathbf{c}) + \varepsilon_i \left( \frac{n_i^s - n_{i0}}{n_{i0}} \right) \quad i = m, n. \tag{6}$$

The second term in the right hand side doesn't depend on the molecular velocities and, consequently, doesn't give the contribution to the macroscopic flow velocity, stress tensor and heat flux. So, in the following consideration it can be omitted. The term which is proportional to  $n_i^s - n_{i0}$  connects with the distribution of the scattered molecules and doesn't depend on the distribution function related to impinging molecules. The second term in (6) appeared after transformation of the distribution function  $f_i^s$  in (2) into the distribution function  $f_{i0}$  in (3).

The experiments carried out by [14, 15] show that the relative difference between the diameters of excited and unexcited particles ( $\sigma_m$  and  $\sigma_n$  respectively) is approximately 1 %. Moreover, the coefficients of specularly-diffuse reflection are different slightly. Thus, in the theory two small parameters can be introduced:

$$\frac{|\Delta\sigma|}{\sigma_n} \ll 1, \quad \Delta\sigma = \sigma_m - \sigma_n, \quad |\Delta\varepsilon| = |\varepsilon_n - \varepsilon_m| \ll 1. \tag{7}$$

The linearization of the task in small parameters (7) and the subsequent selection of the terms, which are proportional to  $\Delta\varepsilon$  and  $\Delta\sigma/\sigma_n$ , give the possibility to diminish the number of varying parameters and separate the surface and bulk mechanisms of LIHT and LID. The general expressions for the local gas drift  $I$  and heat flux  $q$  take a form:

$$\begin{aligned} I &= n_n U_n + n_m U_m = \frac{n\Gamma_m r_0}{2\sqrt{\pi}} \left( G_1 \Delta\varepsilon + G_2 \frac{\Delta\sigma}{\sigma_n} \right), \\ q &= q_n + q_m = \frac{p\Gamma_m r_0}{2\sqrt{\pi}} \left( Q_1 \Delta\varepsilon + Q_2 \frac{\Delta\sigma}{\sigma_n} \right). \end{aligned} \tag{8}$$

Here  $n = n_n + n_m$  and  $p = nk_B T$  are the numerical density and gas pressure respectively. Dimensionless kinetic coefficients  $G_1$ ,  $Q_1$  and  $G_2$ ,  $Q_2$  characterizing the surface and bulk mechanisms of LID and LIHT depend on the radial coordinate  $r$ , gas rarefaction parameter  $R \equiv R_n$ , frequency parameter  $\Gamma_{mn}$  and accommodation coefficient  $\varepsilon_n$  of molecules in a ground state.

The average fluxes can be defined as

$$\begin{aligned} \langle I \rangle &= 2 \int_0^1 I r dr = \frac{n\Gamma_m r_0}{2\sqrt{\pi}} \left( \langle G_1 \rangle \Delta\varepsilon + \langle G_2 \rangle \frac{\Delta\sigma}{\sigma_n} \right), \\ \langle q \rangle &= 2 \int_0^1 q r dr = \frac{p\Gamma_m r_0}{2\sqrt{\pi}} \left( \langle Q_1 \rangle \Delta\varepsilon + \langle Q_2 \rangle \frac{\Delta\sigma}{\sigma_n} \right). \end{aligned} \tag{9}$$

### 3 Method of Solution

To diminish the number of independent variables and simplify the calculations let us introduce the reduced distribution functions:

$$\begin{aligned} \Phi_i &= \frac{1}{\sqrt{\pi}} \int_{-\infty}^{+\infty} c_z h_i \exp(-c_z^2) dc_z, \\ F_i &= \frac{1}{\sqrt{\pi}} \int_{-\infty}^{+\infty} c_z \left( c^2 - \frac{5}{2} \right) h_i \exp(-c_z^2) dc_z. \end{aligned} \tag{10}$$

Expressions (5) for partial dimensionless velocities, stress shears and heat fluxes take a form:

$$\begin{aligned} u_i &= \frac{1}{\pi} \int_0^\infty c_\perp \exp(-c_\perp^2) dc_\perp \int_{-\pi}^\pi \Phi_i d\theta, \\ \Pi_{izr} &= \frac{1}{\pi} \int_0^\infty c_\perp^2 \exp(-c_\perp^2) dc_\perp \int_{-\pi}^{+\pi} \cos \theta \Phi_i d\theta, \\ H_i &= \frac{1}{\pi} \int_0^\infty c_\perp \exp(-c_\perp^2) dc_\perp \int_{-\pi}^\pi F_i d\theta. \end{aligned} \tag{11}$$

Multiplying (4) successively by  $1/\sqrt{\pi}c_z \exp(-c_z^2)$  and  $1/\sqrt{\pi}c_z(c^2 - 5/2) \exp(-c_z^2)$  and integrating the final expressions over  $dc_z$  one can obtain:

$$\begin{aligned} c_\perp \left( \cos \theta \frac{\partial \Phi_i}{\partial r} - \frac{\sin \theta}{r} \frac{\partial \Phi_i}{\partial \theta} \right) + R_i (\Phi_i - \beta_i \Gamma_{mi} \Phi_m) \\ = R_i \psi_i^{(1)} + \frac{1}{2\sqrt{\pi}} R_i \Gamma_{mi} \chi_1 \left( \frac{n_j - n_i}{n_i} \right), \end{aligned} \tag{12}$$

$$\begin{aligned} c_\perp \left( \cos \theta \frac{\partial F_i}{\partial r} - \frac{\sin \theta}{r} \frac{\partial F_i}{\partial \theta} \right) + R_i (F_i - \beta_i \Gamma_{mi} F_m) \\ = R_i \psi_i^{(2)} + \frac{1}{2\sqrt{\pi}} R_i \Gamma_{mi} ((c_\perp^2 - 5/2)\chi_1 + \chi_3) \left( \frac{n_j - n_i}{n_i} \right), \end{aligned} \tag{13}$$

where

$$\begin{aligned} \psi_i^{(1)} &= \frac{1}{\sqrt{\pi}} \int_{-\infty}^{+\infty} c_z^2 \exp(-c_z^2) \psi_i dc_z, \\ \psi_i^{(2)} &= \frac{1}{\sqrt{\pi}} \int_{-\infty}^{+\infty} c_z^2 \left( c^2 - \frac{5}{2} \right) \exp(-c_z^2) \psi_i dc_z, \\ \chi_k &= \int_{-\infty}^{+\infty} c_z^k \exp(-c_z^2) \chi(c_z) dc_z. \end{aligned} \tag{14}$$

In the case of inhomogeneous absorption line ( $\Gamma \ll k\bar{v}$ ), which is typical for gases, the integral absorption parameter  $\chi_k$  is equal to

$$\chi_k = \frac{4\pi}{k\bar{v}} \left( \frac{\Omega}{k\bar{v}} \right)^k \frac{|G_{mn}|^2}{\Gamma_m} \exp \left[ - \left( \frac{\Omega}{k\bar{v}} \right)^2 \right]. \tag{15}$$

In the case of the homogeneous absorption line ( $|\Omega|, \Gamma \gg k\bar{v}$ )

$$\chi_1 = \frac{4\sqrt{\pi}\Omega(k\bar{v})\Gamma}{\Gamma_m} \left( \frac{|G_{mn}|}{\Omega^2 + \Gamma^2} \right)^2, \quad \chi_3 = 1.5 \chi_1. \tag{16}$$

Boundary conditions (6) for functions  $\Phi_i$  and  $F_i$  take the following form:

$$\begin{aligned}\Phi_i(r=1, \cos\theta < 0) &= (1 - \varepsilon_i)\Phi_i(r=1, \cos\theta > 0), \\ F_i(r=1, \cos\theta < 0) &= (1 - \varepsilon_i)F_i(r=1, \cos\theta > 0).\end{aligned}\tag{17}$$

Inhomogeneous terms of linear integro-differential equations (12) and (13) are the linear combination of independent values  $\chi_1$  and  $\chi_3$ . Consequently, the general solutions of these equations must have the analogous structure, i.e.

$$\Phi_i = \Phi_{i1}\chi_1 + \Phi_{i3}\chi_3, \quad F_i = F_{i1}\chi_1 + F_{i3}\chi_3.\tag{18}$$

Macroscopic values (11) and kinetic coefficients in (8) can be written as

$$\begin{aligned}u_i &= u_{i1}\chi_1 + u_{i3}\chi_3, & \pi_{ixz} &= \pi_{ixz1}\chi_1 + \pi_{ixz3}\chi_3, & H_i &= H_{i1}\chi_1 + H_{i3}\chi_3, \\ G_i &= G_{i1}\chi_1 + G_{i3}\chi_3, & Q_i &= Q_{i1}\chi_1 + Q_{i3}\chi_3, & i &= 1, 2.\end{aligned}\tag{19}$$

Kinetic coefficients averaged over the capillary cross section

$$\langle G_i \rangle = \langle G_{i1} \rangle \chi_1 + \langle G_{i3} \rangle \chi_3, \quad \langle Q_i \rangle = \langle Q_{i1} \rangle \chi_1 + \langle Q_{i3} \rangle \chi_3, \quad i = 1, 2.\tag{20}$$

Substituting expressions (18) in (12) and (13) and equating the factor at values  $\chi_1$  and  $\chi_3$  one can obtain the following equations for  $\Phi_{ik}$  and  $F_{ik}$ :

$$\begin{aligned}c_{\perp} \left( \cos\theta \frac{\partial \Phi_{i1}}{\partial r} - \frac{\sin\theta}{r} \frac{\partial \Phi_{i1}}{\partial \theta} \right) + R_i (\Phi_{i1} - \beta_i \Gamma_{mi} \Phi_{m1}) \\ = R_i \psi_{i1}^{(1)} + \frac{1}{2\sqrt{\pi}} R_i \Gamma_{mi} \left( \frac{n_j - n_i}{n_i} \right), \\ c_{\perp} \left( \cos\theta \frac{\partial \Phi_{i3}}{\partial r} - \frac{\sin\theta}{r} \frac{\partial \Phi_{i3}}{\partial \theta} \right) + R_i (\Phi_{i3} - \beta_i \Gamma_{mi} \Phi_{m3}) = R_i \psi_{i3}^{(1)},\end{aligned}\tag{21}$$

and

$$\begin{aligned}c_{\perp} \left( \cos\theta \frac{\partial F_{i1}}{\partial r} - \frac{\sin\theta}{r} \frac{\partial F_{i1}}{\partial \theta} \right) + R_i (F_{i1} - \beta_i \Gamma_{mi} F_{m1}) \\ = R_i \psi_{i1}^{(2)} + \frac{1}{2\sqrt{\pi}} R_i \Gamma_{mi} \left( c_{\perp}^2 - \frac{5}{2} \right) \left( \frac{n_j - n_i}{n_i} \right), \\ c_{\perp} \left( \cos\theta \frac{\partial F_{i3}}{\partial r} - \frac{\sin\theta}{r} \frac{\partial F_{i3}}{\partial \theta} \right) + R_i (F_{i3} - \beta_i \Gamma_{mi} F_{m3}) \\ = R_i \psi_{i3}^{(2)} + \frac{1}{2\sqrt{\pi}} R_i \Gamma_{mi} \left( \frac{n_j - n_i}{n_i} \right).\end{aligned}\tag{22}$$

Here  $\psi_{ik}^{(1)}$  and  $\psi_{ik}^{(2)}$  can be derived from  $\psi_i^{(1)}$  and  $\psi_i^{(2)}$  by the replacements  $u_i \rightarrow u_{ik}$ ,  $\Pi_{izr} \rightarrow \Pi_{izrk}$ ,  $H_i \rightarrow H_{ik}$ .

Boundary conditions (6) for functions  $\Phi_{ik}$  and  $F_{ik}$  taking into account expressions (10) and (18) can be written as:

$$\begin{aligned} \Phi_{ik}(r = 1, \cos \theta < 0) &= (1 - \varepsilon_i)\Phi_{ik}(r = 1, \cos \theta > 0), \\ F_{ik}(r = 1, \cos \theta < 0) &= (1 - \varepsilon_i)F_{ik}(r = 1, \cos \theta > 0), \quad k = 1, 3. \end{aligned} \tag{23}$$

The effective collision frequency for particles in a ground state  $\gamma_n = \gamma_{nm} + \gamma_{nm} \approx \gamma_{nn}$  can be taken by analogy with the BGK model in a form  $\gamma_n = p/\eta$  ( $p$  is a gas pressure,  $\eta$  is coefficient of dynamic viscosity). For hard spherical molecules  $\eta = \rho \bar{v} l / \sqrt{\pi}$ , where  $l$ —mean free path. Thus, the gas rarefaction parameter connects with the Knudsen number  $Kn$  in the following way

$$R \equiv R_n = \frac{\sqrt{\pi}}{2Kn}, \quad Kn = \frac{l}{r_0}.$$

For numerical solution of (21) and (22) with boundary conditions (23) let us apply the discrete velocity method. In this method the continuum spectrum  $0 < c_{\perp} < \infty, 0 < \theta < 2\pi$  was replaced by  $N_c$  number of discrete velocities  $c_{\perp j}$  and  $N_{\theta}$  number of discrete values  $\theta_q$  correspondingly. In the physical space, the distance between the plates ( $0 \leq r \leq 1$ ) was divided into  $N_r$  equal intervals.

The derivatives in (21) and (22) were presented by finite-differences. The following iteration scheme was used

1. The initial values of macroscopic quantities  $u_{ik}, \Pi_{izr k}, H_{ik}$  was set and from (21) and (22) the values of  $\Phi_{ik}$  and  $F_{ik}$  functions presented by finite-differences were calculated.
2. The obtained functions  $\Phi_{ik}$  and  $F_{ik}$  were taken to calculate the new values of  $u_{ik}, \Pi_{izr k}, H_{ik}$  according to expressions (11).
3. Further, we went to step 1 and used the calculated values of  $u_{ik}, \Pi_{izr k}, H_{ik}$  to obtain the values of functions  $\Phi_{ik}$  and  $F_{ik}$  on the following iteration.

As initial approximation the equilibrium gas state was taken

$$u_{ik} = 0, \quad \Pi_{izr k} = 0, \quad H_{ik} = 0.$$

The convergence criterion for the iterative process has been set equal to  $10^{-6}$ .

The values of all physical variables (11) in the point  $i$  of the physical space were calculated in accordance with the Gaussian quadrature formulas:

$$\begin{aligned} u_i^k &= \frac{1}{\pi} \sum_{j=1}^{N_c} \sum_{q=1}^{N_{\theta}} \Phi_i^{kj q} W_j \Delta \theta, \\ \Pi_{izr}^k &= \frac{1}{\pi} \sum_{j=1}^{N_c} \sum_{q=1}^{N_{\theta}} \Phi_i^{kj q} W_j \Delta \theta \cos \theta_q, \\ H_i^k &= \frac{1}{\pi} \sum_{j=1}^{N_c} \sum_{q=1}^{N_{\theta}} F_i^{kj q} W_j \Delta \theta, \end{aligned} \tag{24}$$

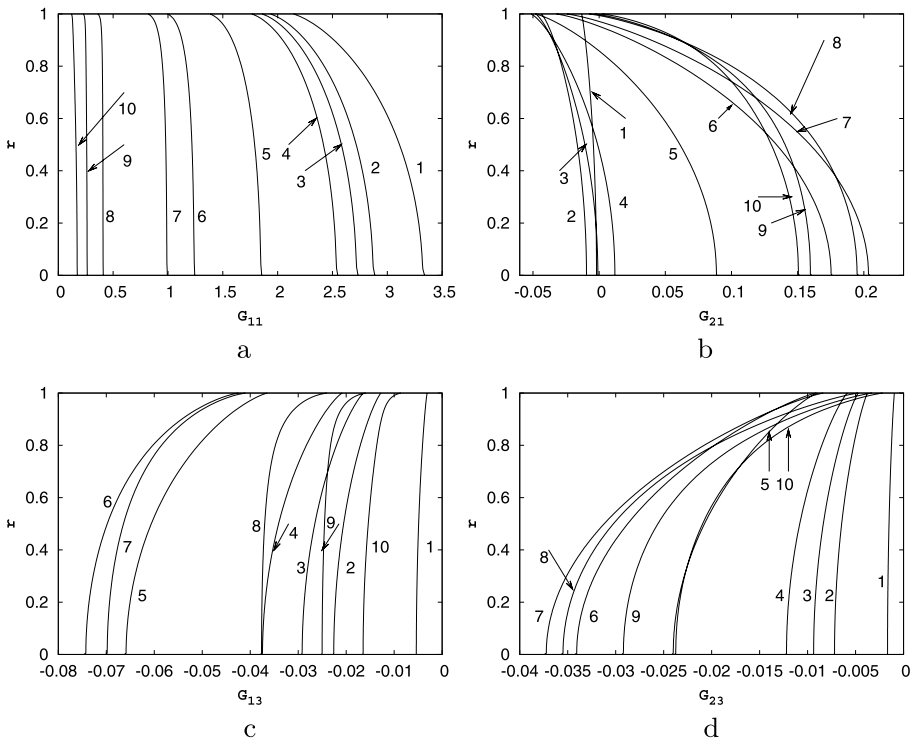
where  $W_j$ —Gaussian weight for  $c_{\perp j}$  discrete velocity value. For the calculations we used  $N_c = 20$  Gaussian nodes,  $N_{\theta}$  was taken equal to 400 and  $N_r = 200$ .



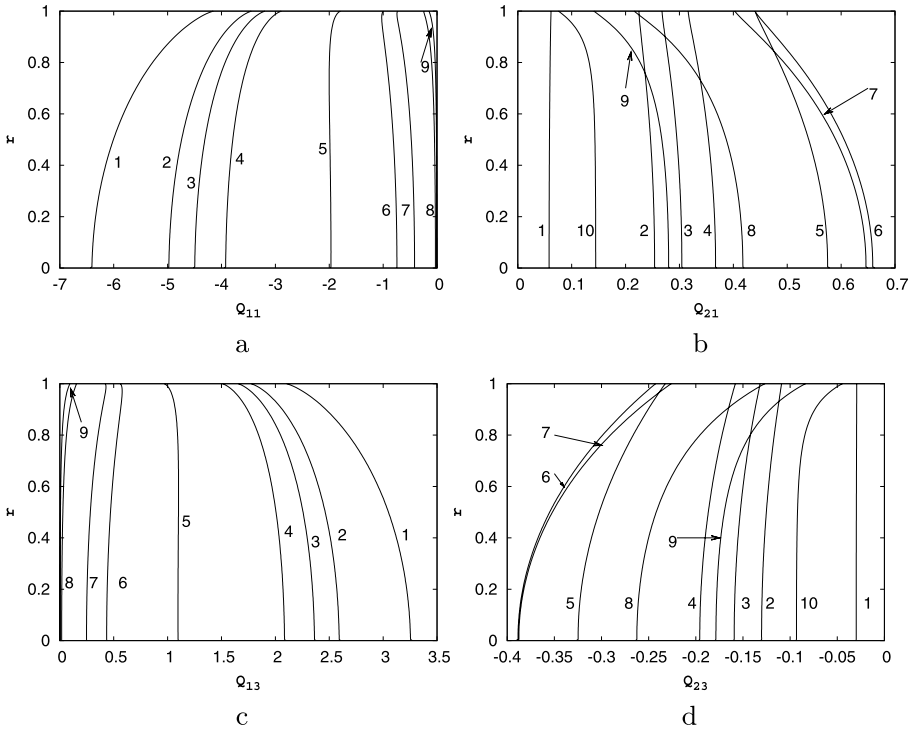
### 4 Results and Discussions

The numerical calculations support the conclusion that LID of one-component gas is possible only in confined systems, whereas LIHT can take place in unbounded gas as well. It was shown that LIHT can occur at the values of  $0 < |\Omega|/(k\bar{v}) < 3$ . The effect is more evident at  $|\Omega|/(k\bar{v}) \approx 1.0$  and vanishes at  $|\Omega|/(k\bar{v}) > 3$  due to failure of resonant conditions.

Figure 1 gives the information about the surface ( $G_{11}$  and  $G_{13}$ ) and bulk ( $G_{21}$  and  $G_{23}$ ) components of the dimensionless LID velocity in the capillary cross section. It should be noted that coefficients  $G_{11}$  and  $G_{21}$  give the main contribution to surface and bulk LID respectively whereas the contribution of  $G_{13}$  and  $G_{23}$  to LID is considerably small. The surface component of LID  $G_{11}$  at  $R > 1$  is seen to be a constant value along the radius of the capillary. It can be concluded that the gas viscosity doesn't influence on the magnitude of LID velocity. It's interesting to examine the evolution of bulk component of gas flow velocity  $G_{21}$  at the transition from the free molecular to continuum regime (Fig. 1b). At small values of  $R$ , the magnitude of  $G_{21}$  depends weakly on the radial coordinate  $r$ . At  $R > 0.1$  the structure of bulk LID started to be more complex. Near the capillary axis there is a formation of flow "kernel" directed to one side while in the near wall region the gas moves in opposite direction. The existence of oppositely directed flux connects with the fact that at intermediate values of  $R$  the flux of excited particles in near wall region is larger than that of unexcited particles. At the axis the situation is absolutely opposite. In a near free molecular regime ( $R \leq 0.1$ ) at positive values of finite detuning,  $\Omega > 0$ , bulk



**Fig. 1** Profiles of dimensionless velocity of LID in dependence on the rarefaction parameter  $R$  at  $\Gamma_{mn} = 0.01$  and  $\epsilon_n = 1$  (1— $R = 0.01$ , 2—0.05, 3—0.07, 4—0.1, 5—0.3, 6—0.7, 7—1, 8—3, 9—5, 10—10)

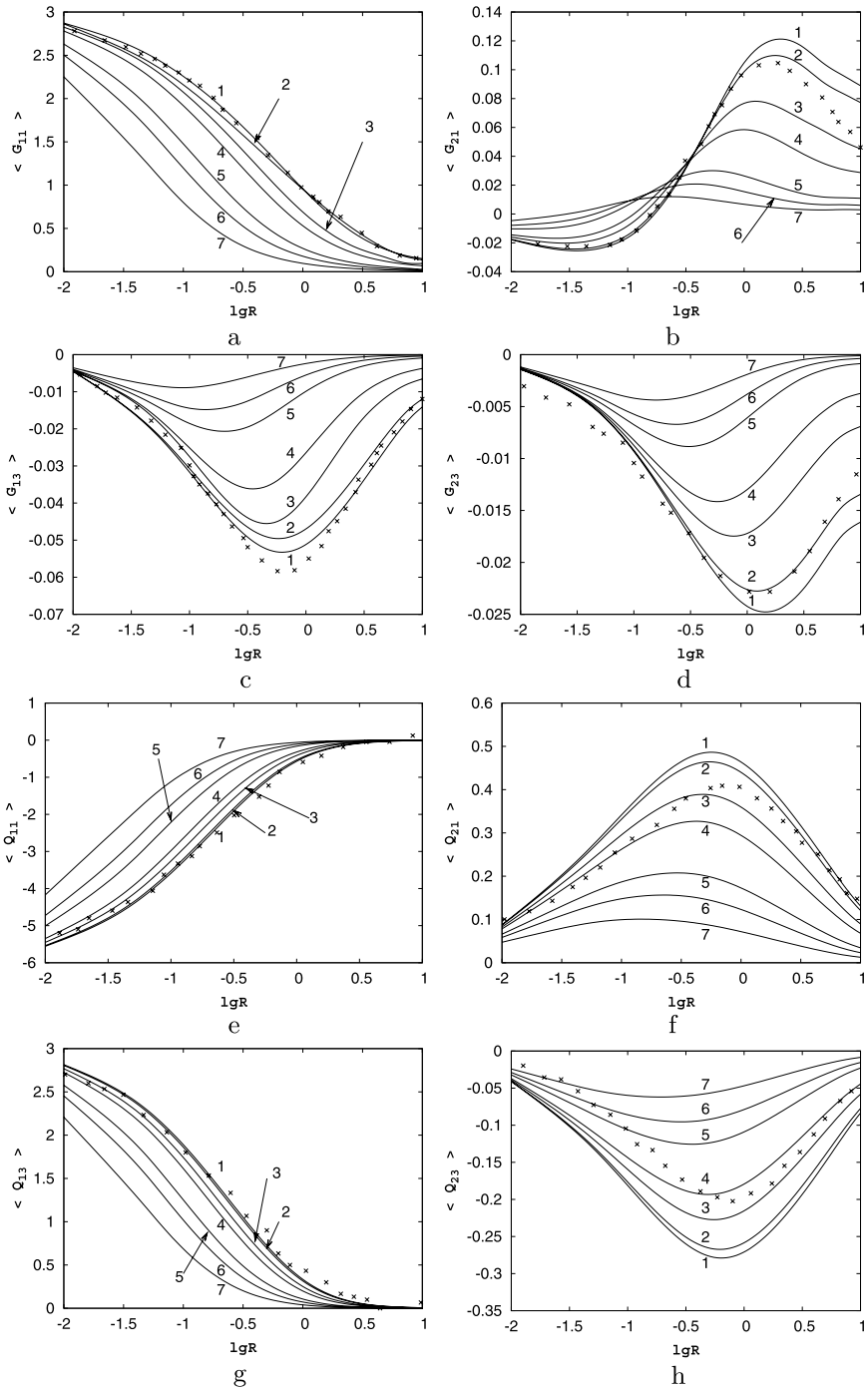


**Fig. 2** Profiles of dimensionless heat flux in dependence on the rarefaction parameter  $R$  at  $\Gamma_{mn} = 0.01$  and  $\varepsilon_n = 1$  ( $1-R = 0.01$ ,  $2-0.05$ ,  $3-0.07$ ,  $4-0.1$ ,  $5-0.3$ ,  $6-0.7$ ,  $7-1$ ,  $8-3$ ,  $9-5$ ,  $10-10$ )

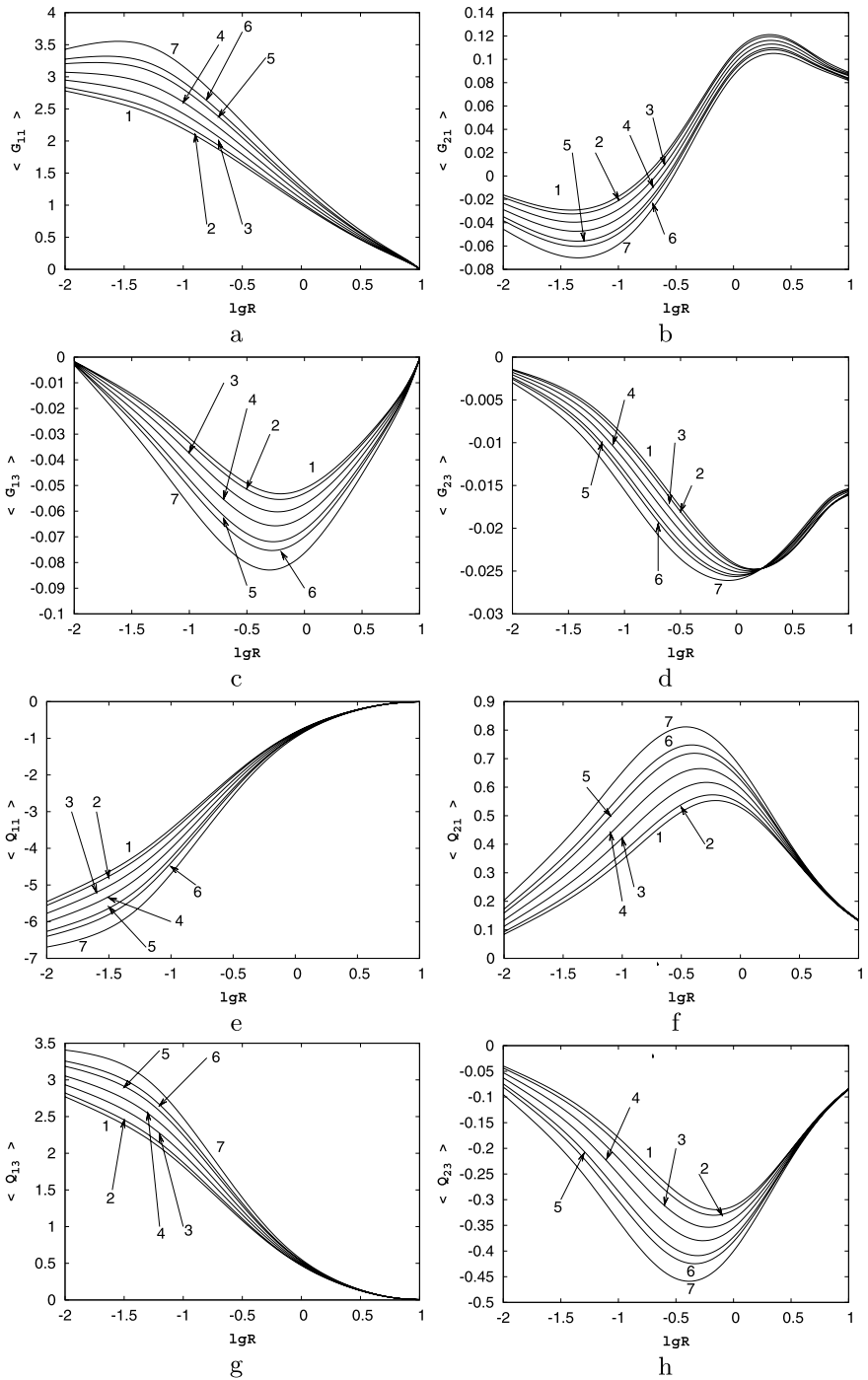
component of LID, defined mainly by the kinetic coefficient  $G_{21}$ , is directed oppositely to the wave-vector  $\mathbf{k}$ . Moreover, in a near wall region the value of  $G_{21}$  is larger than at the axis of capillary (concave profile). In the slip flow regime ( $R \geq 10$ ) the direction of bulk component at  $\Omega > 0$  coincides with the direction of wave-vector  $\mathbf{k}$  and its value increases when moving away from the capillary surface (convex profile). Thus, in a transitional regime the change of the gas flow direction occurs.

The profiles of the heat flux in dependence on the values of gas rarefaction parameter  $R$  at  $\Gamma_{mn} = 0.01$  and  $\varepsilon_n = 1$  are presented on figures Fig. 2. Obviously, the surface LIHT is directed oppositely to the surface LID. Especially at  $R > 0.7$  LIHT has more large value at the capillary wall than at the axis, but at  $R < 0.7$  the opposite situation occurs. Bulk components of LIHT characterized by the coefficients  $Q_{21}$  and  $Q_{23}$  are approximately homogeneous in the capillary cross section (Fig. 2b, d).

On Fig. 3a, c, e, g the dependencies of the average kinetic coefficients over the capillary cross section  $\langle G_{11} \rangle$ ,  $\langle G_{13} \rangle$ ,  $\langle Q_{11} \rangle$ ,  $\langle Q_{13} \rangle$  on the gas rarefaction parameter  $R$  at different values of frequency parameter  $\Gamma_{mn}$  are presented. These coefficients characterizing the surface mechanism of LID and LIHT respectively are the constant-sign functions of the gas rarefaction parameter  $R$ . So that the directions of surface components of LID and LIHT are determined only by the signs of the difference of the accommodation coefficients  $\Delta\varepsilon$  and detuning of radiation frequency from the center of the absorption line  $\Omega$ . For example, if  $\Delta\varepsilon > 0$ , in the case of inhomogeneous absorption line ( $\Gamma \ll k\bar{v}$ ) the direction of surface



**Fig. 3** Average kinetic coefficients over the capillary cross section as functions of the gas rarefaction parameter  $R$  at  $\varepsilon_n = 1$  and different values of frequency parameter  $\Gamma_{mn}$  ( $1-\Gamma_{mn} = 0.01, 2-0.1, 3-0.5, 4-1, 5-3, 6-5, 7-10$ , dots—Bubnov-Galerkin method [11])



**Fig. 4** Average kinetic coefficients over the capillary cross section as functions of the gas rarefaction parameter  $R$  at  $T_{mn} = 0.01$  and different values of the accommodation coefficient  $\varepsilon_n$  ( $1 - \varepsilon_n = 1, 2 - 0.98, 3 - 0.94, 4 - 0.9, 5 - 0.86, 6 - 0.84, 7 - 0.8$ )

flux of LID at  $\Omega > 0$  coincides with the direction of the light beam, but at  $\Omega < 0$  they are oppositely directed.

It's evident that at transition from the free molecular to continuum regime the values of coefficients  $\langle G_{11} \rangle$ ,  $\langle Q_{11} \rangle$ ,  $\langle Q_{13} \rangle$  decrease monotonically, but the value of coefficient  $\langle G_{13} \rangle$  reaches the maximum at intermediate values of rarefaction parameter  $R$ .

The decrease of the coefficients responsible for surface LID and LIHT at increase of the frequency parameter  $\Gamma_{mn}$  and any fixed value of  $R$  can be explained by the decrease of excited particles quantity due to collisions with the capillary wall. In a such way with increase of the rarefaction parameter ( $R \approx 1$ ) the coefficients  $\langle G_{11} \rangle$ ,  $\langle G_{13} \rangle$ ,  $\langle Q_{11} \rangle$ ,  $\langle Q_{13} \rangle$  decreases in 5 times. It would be noted that results of work presented here are in a good agreement with the results of work [11] obtained in approximation  $\Gamma_{mn} \ll 1$ .

The dependencies of kinetic coefficients  $\langle G_{21} \rangle$ ,  $\langle G_{23} \rangle$ ,  $\langle Q_{21} \rangle$ ,  $\langle Q_{23} \rangle$  characterizing bulk mechanism of LID and LIHT on rarefaction parameter  $R$  at different values of frequency parameter  $\Gamma_{mn}$  are shown on Fig. 3b, d, f, h.

At any fixed value of  $\Gamma_{mn}$  the dependencies of these kinetic coefficients on  $R$  have the nonmonotone behaviour. Furthermore, all of these coefficients, except for  $\langle G_{21} \rangle$ , are constant-sign functions of the gas rarefaction parameter. The magnitudes of coefficients  $\langle G_{23} \rangle$ ,  $\langle Q_{21} \rangle$ ,  $\langle Q_{23} \rangle$  reach the maximum for values of  $R$  in the range from 0.3 to 1 depending on the value of  $\Gamma_{mn}$ . Coefficient  $\langle G_{21} \rangle$  is changeable-sign function of rarefaction parameter  $R$ . The value of  $\langle G_{21} \rangle$  reaches the minimum value at  $R \approx 0.07$ , maximum— $R \approx 1-3$ . It changes the sign in transitional regime in the range of  $0.3 < R < 0.7$  depending on the parameter  $\Gamma_{mn}$ . It means that the direction of the bulk component of LID is defined not only by the signs of  $\Omega$  and difference  $\Delta\sigma$  of the effective diameters of excited and unexcited particles but also by the gas pressure in a capillary. This effect was discussed in detail for the case of  $\Gamma_{mn} \ll 1$  in the work [8] when the inversion value of  $R$  was fixed.

On Fig. 3 it's seen that with increase of the value of  $\Gamma_{mn}$ , i.e. decrease of the number of collisions experienced by the excited particle before its deactivation, the values of kinetic coefficients decrease. For example, increasing value of  $\Gamma_{mn}$  from 0.01 to 10 decreases the coefficients  $\langle Q_{21} \rangle$ ,  $\langle Q_{23} \rangle$  approximately in 5 times, and coefficients  $\langle G_{21} \rangle$ ,  $\langle G_{23} \rangle$ —over orders of magnitude. In limit  $\Gamma_{mn} \rightarrow \infty$  all excited particles would be deactivated until the interactions. In such limit, the bulk mechanism of LID and LIHT vanishes.

On Fig. 4 the dependencies of kinetic coefficients on the rarefaction parameter  $R$  at  $\Gamma_{mn} = 0.01$  and different values of coefficient of specularly-diffuse reflection  $\varepsilon_n$  of molecules in a ground state were presented. It's obvious that decrease of  $\varepsilon_n$  leads to the increase of all kinetic coefficients. Particularly, the decrease of the accommodation coefficient  $\varepsilon_n$  from 1 to 0.84 can increase the kinetic coefficients by 30–60%. Let us note that such dependence takes place only in transitional and free molecular regimes  $R \leq 1$ . In the slip flow regime at  $R > 5$  the kinetic coefficients depend very slightly on the accommodation coefficient  $\varepsilon_n$ .

**Acknowledgement** This research was supported in part by the Russian Foundation for Basic Research (Grant No. 09-01-00052).

## Appendix

Expressions for frequencies  $v_{ij}^{(n)}$  in terms of Chapman-Cowling integrals are defined by the form of the intermolecular interaction potential [10],

$$v_{ij}^{(1)} = \frac{8}{3} n_j \Omega_{ij}^{11}, \quad v_{ij}^{(2)} = \frac{4}{3} n_j \left( \frac{2}{5} \Omega_{ij}^{12} - \Omega_{ij}^{11} \right),$$

$$\begin{aligned}
 v_{ij}^{(3)} &= \frac{4}{5} n_j \left( \frac{10}{3} \Omega_{ij}^{11} + \Omega_{ij}^{22} \right), & v_{ij}^{(4)} &= \frac{4}{5} n_j \left( \frac{10}{3} \Omega_{ij}^{11} - \Omega_{ij}^{22} \right), \\
 v_{ij}^{(5)} &= \frac{8}{15} n_j \left( \Omega_{ij}^{22} + \frac{55}{8} \Omega_{ij}^{11} \frac{5}{2} \Omega_{ij}^{12} + \frac{1}{2} \Omega_{ij}^{13} \right), \\
 v_{ij}^{(6)} &= \frac{8}{15} n_j \left( -\Omega_{ij}^{22} + \frac{55}{8} \Omega_{ij}^{11} - \frac{5}{2} \Omega_{ij}^{12} + \frac{1}{2} \Omega_{ij}^{13} \right).
 \end{aligned}$$

The values of Chapman-Cowling integrals  $\Omega_{ij}^{sr}$  within the framework of the hard-sphere model are calculated by the formula [10]

$$\Omega_{ij}^{sr} = \left( \frac{\pi k_B T}{m} \right)^{1/2} \sigma_{ij}^2 \frac{1}{2} (r+1)! \left[ 1 - \frac{1+(-1)^s}{2(s+1)} \right],$$

where  $\sigma_{ij} = (\sigma_{ii} + \sigma_{jj})/2$  is the effective radius of interaction of particles of sort  $i$  and  $j$ . Within the framework of the same hard-sphere model, the particles collision frequency is written as

$$\gamma_{ij} = \frac{16}{5} n_j \sigma_{ij}^2 \left( \frac{\pi k_B T}{m} \right)^{1/2}.$$

## References

1. Gel'mukhanov, F.K., Shalagin, A.M.: Light-induced diffusion of gasses. JETP Lett. **29**, 711–713 (1979)
2. Gel'mukhanov, F.K., Shalagin, A.M.: Theory of optically induced diffusion of gases. Sov. Phys. JETP **51**, 839–846 (1980)
3. Rautian, S.G., Shalagin, A.M.: Kinetics Problems of Non-linear Spectroscopy. North-Holland, Amsterdam (1991)
4. Ghiner, A.V., Stockman, M.I., Vaksman, M.A.: Surface light-induced drift of a rarefied gas. Phys. Lett. A **96**, 79–82 (1983)
5. Chermnyaninov, I.V., Chernyak, V.G.: Slip of a gas in a field of optical radiation. J. Eng. Phys. Thermophys. **55**, 1343–1345 (1988)
6. Dykhne, A.M., Starostin, A.N.: Theory of the drift motion of molecules in a resonant infrared-radiation field. Zh. Eksp. Teor. Fiz. **79**, 1211–1227 (1980)
7. Vaksman, M.A., Gainer, A.V.: Theoretical analysis of the motion of a dense gas which interacts with a wall during velocity-selective excitation. J. Exp. Theor. Phys. **52**, 23–29 (1980)
8. Chernyak, V.G., Vintovkina, E.A., Chermnyaninov, I.V.: Optically induced drift of single-component gas in capillaries. Zh. Eksp. Teor. Fiz. **76**, 768–774 (1993)
9. Chernyak, V.G., Subbotin, E.A.: Theory of light-induced drift of a one-component gas in a capillary. Zh. Eksp. Teor. Fiz. **81**, 122–128 (1995)
10. McCormack, F.J.: Construction of linearized kinetic models for gaseous mixtures and molecular gases. Phys. Fluids **16**, 2095–2105 (1973)
11. Chermnyaninov, I.V., Chernyak, V.G., Vilisova, E.A.: Light-induced heat and mass transfer in a single-component gas in a capillary. J. Exp. Theor. Phys. **105**, 511–519 (2007)
12. Gel'mukhanov, F.K., Il'Ichov, L.V.: Transfer phenomena in a gas interacting with light. Khim. Fis. **3**, 1544–1554 (1984)
13. Gel'mukhanov, F.K., Il'Ichov, L.V., Shalagin, A.M.: Kinetic theory of light-induced drift of gas particles. Physica A **137**, 502–530 (1986)
14. Van der Meer, G.J., Hoogeveen, R.W.M., Hermans, L.J.F., Chapovsky, P.L.: Light-induced drift of CH3F in noble gases. Phys. Rev. A **39**, 5237–5242 (1989)
15. Chapovsky, P.L., Van der Meer, G.J., Smeets, J., Hermans, L.J.F.: Alternative approach to light-induced drift in molecular gases. Phys. Rev. A **45**, 8011–8018 (1992)