# The Role of Light-Induced Drift in Diffusion of Heavy Metals and their Isotopes in CP Stars: an Example of Mercury

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## 1. General picture

More than a decade ago the problem of the role of light-induced drift (LID) in diffusion of chemical elements and their isotopes in the envelopes and atmospheres of quiescent CP stars has been brought up by Atutov & Shalagin (1988) and Nasyrov & Shalagin (1993) and studied by some investigators (LeBlanc & Michaud 1993; Sapar & Aret 1995; Proffitt et al. 1999; Aret & Sapar 2002). A main difficulty of the problem is that it demands very precise input physics. High-precision isotopic and superfine splitting of spectral lines is necessary to describe adequately the overlap of spectral lines what has a crucial meaning for generation of LID. Superfine splitting due to nuclear spin takes place for isotopes with odd number of baryons and we have obtained the data only recently. We had spectral line data only for HgI to HgIII to model the separation of mercury in quiescent stellar atmosphere, but we hope that the data is sufficient to generate in general the realistic picture of diffusion due to LID.

Diffusion coefficient due to LID is strongly dependent on the difference of impact cross-sections for the ground state and different excited states of ions. This problem is still open and needs essential improvement. We assumed that impact cross-section is determined by the contribution due to core polarisability and its contribution outside the Debye sphere.

In reality the atmospheres are not the absolutely quiescent ones. Essential disturbances which can change drastically the picture are stellar wind, meridional circulation due to stellar rotation, macro- and microturbulence and magnetic fields. For the present we can model the abundance evolution in absolutely quiescent stellar atmospheres. We believe that mean trends of the process will remain the same also in the presence of the microturbulent mixing of the stellar matter although the time scales should grow several orders of magnitude.

On the example of mercury we show that LID gives an essential contribution to diffusion of heavy elements in the atmospheres of CP stars, especially to the separation of isotopes. Generally LID for heavy elements causes sedimentation of lighter isotopes and levitation of the heavier ones. Early stages of the computed evolution of the isotope separation are shown on the colored maps. The computations of the evolutionary model atmosphere sequences have been made using a FORTRAN program SMART, composed by the authors. The short, handy and consumer-oriented program is mentioned for modelling of stellar atmospheres, for study of physical processes in them and for computation of stellar spectra.

The light-induced drift can be described in terms of equivalent acceleration (Aret & Sapar 2002), which gives additional contribution to the conventional radiative acceleration. For transitions from a lower quantum state $l$ to the upper quantum state $u$ the acceleration due to LID can be reduced to

$$a^d_{ul} = qD\frac{\pi}{c}\int\limits_0^\infty \sigma^0_{ul}\frac{\partial W(u_\nu, a)}{\partial u_\nu}F_\nu d\nu. \tag{4}$$

In this formula $\sigma^0_{ul}$ is the total transition cross-section per gram of the isotope studied, the large number $q$ is determined by the ratio of the mean thermal momentum of the particle to the momentum of the absorbing photon, namely $q = Mv_Tc/2h\nu$, and the efficiency of LID $D = (C_u - C_v)/(A_u + C_u)$, where the quantities $C$ are the collision frequencies for the particles in the quantum states given by subscript and $A_u$ is the frequency of spontaneous transitions from the upper state. Further, $W$ is the Voigt function with dimensionless argument $u_\nu$ defined by $u_\nu = (\nu - \nu_0)/(\Delta\nu_D)$ and the parameter of the Voigt profile $a = \Gamma/(4\pi\Delta\nu_D)$. The main problem, which remains unsolved with sufficient strictness is finding the expressions of the collision frequencies $C$.

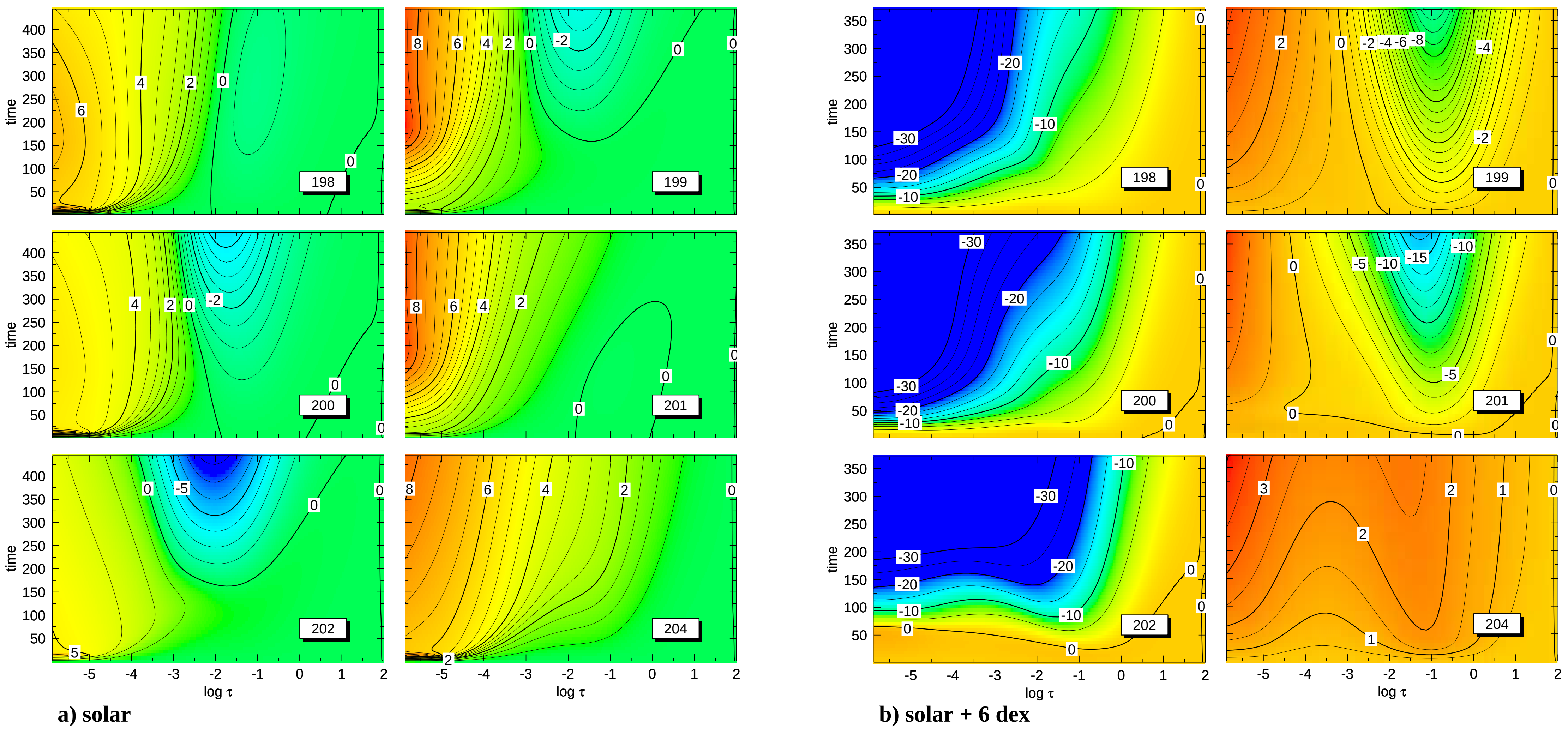
The long-range Coulomb interaction between ions and the hard-sphere collision model for the neutral atoms have been used as in the paper by Gonzales et al. (1995). To take into account the contribution of the core to the cross-section of Debye sphere we have accepted that the interaction force due to the atomic polarisability is proportional to $r^{-5}$ and consequently the integral contribution of the core is proportional to $r^{-4}$. Additionally we have assumed that the contribution of the core to the collision cross-section of ions is characterized by the factor

$$\phi_j = (1 - \delta_{0j})D_0^2/D_j^2, \tag{5}$$

where $D_j$ is the diffusion coefficient and its subscript is the ionization stage. The radius of the core in the hard-sphere model have been taken to correspond to the effective main quantum number in the hydrogenic approximation. In this assumption the total diffusion coefficient of the LID for the sum of ions $j$ is

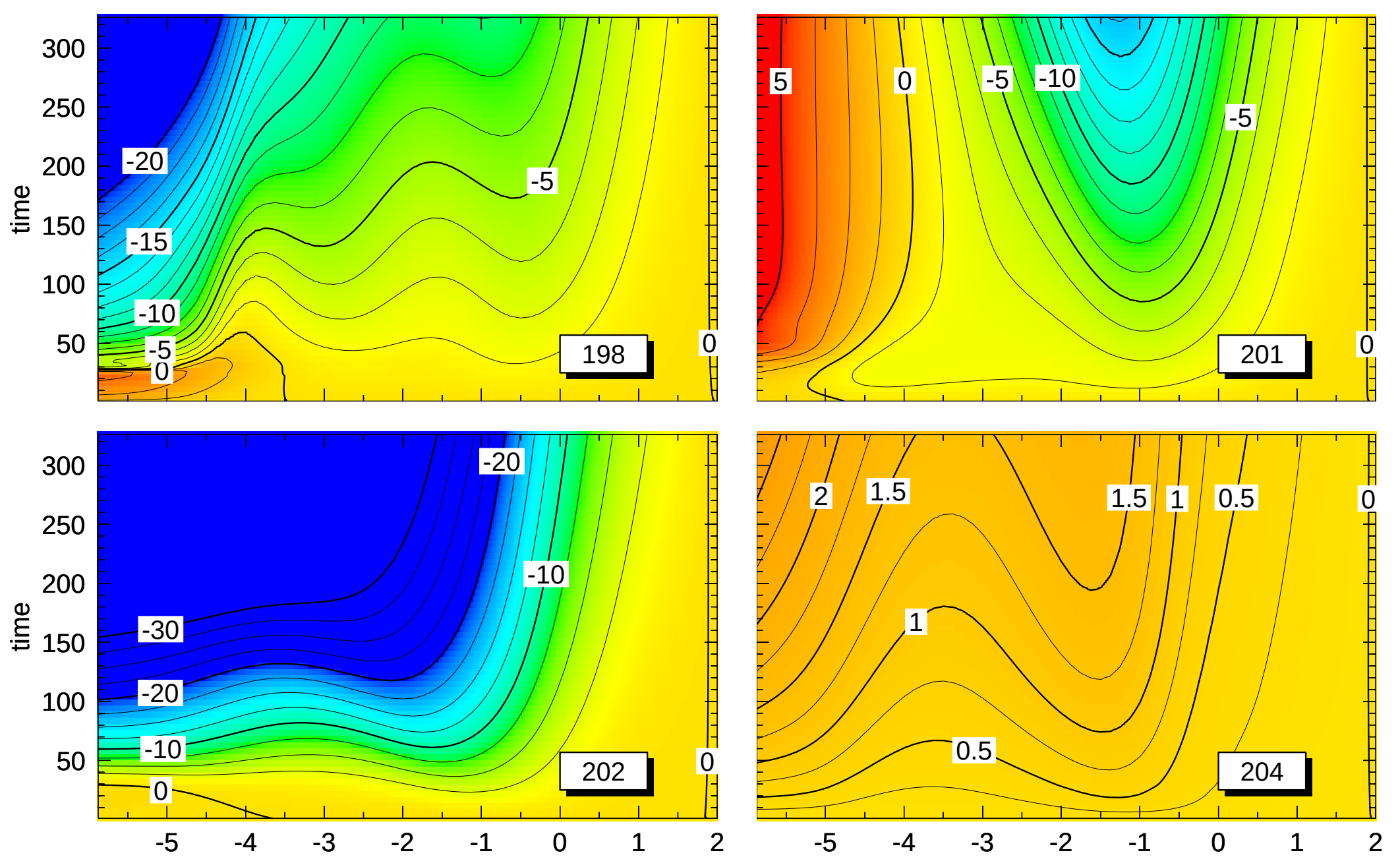
$$\Delta_i = \sum_j (D_0\phi_j + D_j)X_j. \tag{6}$$

where $X_j$ is the ionization rate corresponding to the subscript.



**a) solar**

**b) solar + 6 dex**



**c) HR 7775**

**Figure 1.** Evolutionary changes of abundances of Hg isotopes relative to their initial abundances: $\log C_i$.
Atomic weights of Hg isotopes are shown in panels. Initial abundances: a) solar, b) solar + 6 dex, c) HR7775. Time steps $dt_{solar+6} = dt_{\rm HR7775} = 100\ dt_{solar}$
According to our estimates the turbulent mixing should decelerate the diffusion processes from about 1000 times in the outer layers to millions times in the deepest layer. Note that radiative acceleration is dominant at low abundances and in the outer layers and LID at high abundances and in deeper layers.

## 2. Segregational evolution of heavy metal isotope abundances

Diffusional segregation of isotopes of chemical elements is based on the equations of continuity and of the diffusion velocity. The equation of continuity in the case of the plane-parallel stellar atmosphere for the ratio $C_i$ of abundance (concentration) to its initial value for isotope $i$ of the chemical element studied is reduced to the form suitable for the model computations:

$$\frac{d\ln C_i}{dt} = \nu_i + \left(\frac{d\ln\mu}{dn}\right)^{-1}\left(\frac{d\nu_i}{dn} + \nu_i\frac{d\ln C_i}{dn}\right), \qquad \nu_i = \frac{\rho V_i}{\mu}, \tag{1}$$

where $\rho$ is the total density and $\mu$ is the total column density of the stellar atmosphere. All the derivatives are relative to the number of model atmosphere layer $n$. The quantity $\nu_i$ can be termed as the localized flow, the second term takes into account its gradient and the third – the gradient of $\ln C_i$. All spacial derivatives have been computed using the 4th order polynomials of the Lagrange interpolation formula for equal argument differences $\Delta n = 1$.

The expression for the diffusion velocity in a quiescent stellar atmosphere in its most simple form (ignoring the thermal diffusion) is

$$V_i = a_it_i - \Delta_i\frac{d\ln\rho C_i}{dr}, \tag{2}$$

where $t_i$ is the free flight time between collisions and $a_i$ is the total acceleration due to gravity, light pressure and LID. The free flight time $t_i$ for isotope $i$ has been estimated from formula $\Delta_i = kTt_i/M_i$. The formulae for the diffusion coefficients $\Delta_i$ were taken from the paper by J.-F. Gonzalez et al. (1995) and averaged duely over the ionization stages. Thus we find

$$\frac{d\ln\rho C_i}{dn} = -\frac{M_ia_i\mu}{kT\rho}\frac{d\ln\mu}{dn}. \tag{3}$$

Acceleration $a_i$ depends on the value of $C_i$ and therefore this equation can be solved only iteratively. In our opinion the main physical process which evokes the evolutionary segregation of isotopes in the atmospheres of quiescent stellar atmospheres is LID. Namely in the asymmetrical spectral lines the radiative excitation rate and thus also the free-flight paths of atomic species depend on the direction of their radial thermal velocity. This asymmetry in excitation rates evokes the LID.

**Table 1.** Adopted isotopic composition

| | $^{198}$Hg | $^{199}$Hg | $^{200}$Hg | $^{201}$Hg | $^{202}$Hg | $^{204}$Hg |
|---|---|---|---|---|---|---|
| solar, % | 9.97 | 16.87 | 23.10 | 13.18 | 29.89 | 6.87 |
| HR7775, % | 0.10 | 0.00 | 0.00 | 0.40 | 37.50 | 62.00 |

Presence of turbulence essentially changes the process of diffusion and macroturbulence cancels the diffusion at all. As it has been shown by E. Schatzman (1969), the influence of microturbulence on the diffusion can be expressed as an additional diffusion coefficient in the expression of the diffusion velocity, namely in this case

$$V_i = a_it_i - (\Delta_i + D_T)\frac{d\ln\rho C_i}{dr}, \qquad D_T = \alpha\left(\frac{kT}{M}\right)^{3/2}\frac{1}{g}, \tag{7}$$

where $D_T$ is the coefficient of turbulent diffusion. Unfortunately we do not have realistic physical picture to estimate the value of $D_T$. However, to fit it to the observations in tentative computations we assumed that the characteristic microturbulence velocity is of the order of the mean thermal velocity of heavy atomic particles and the characteristic height is of the order $H = kT/MG$. We included a freely adjustable coefficient $\alpha$ and thus obtained the expression for $D_T$ given above. Consequently, $D_T \gg \Delta_s$, and as a result, the equilibrium gradient of $|\ln C_i|$ is essentially smaller than in the case of ideally quiescent stellar atmosphere. The time scale for evolution in the presence of microturbulent mixing is many dex slower than in the quiescent atmospheres and corresponding picture should be essentially more realistic.

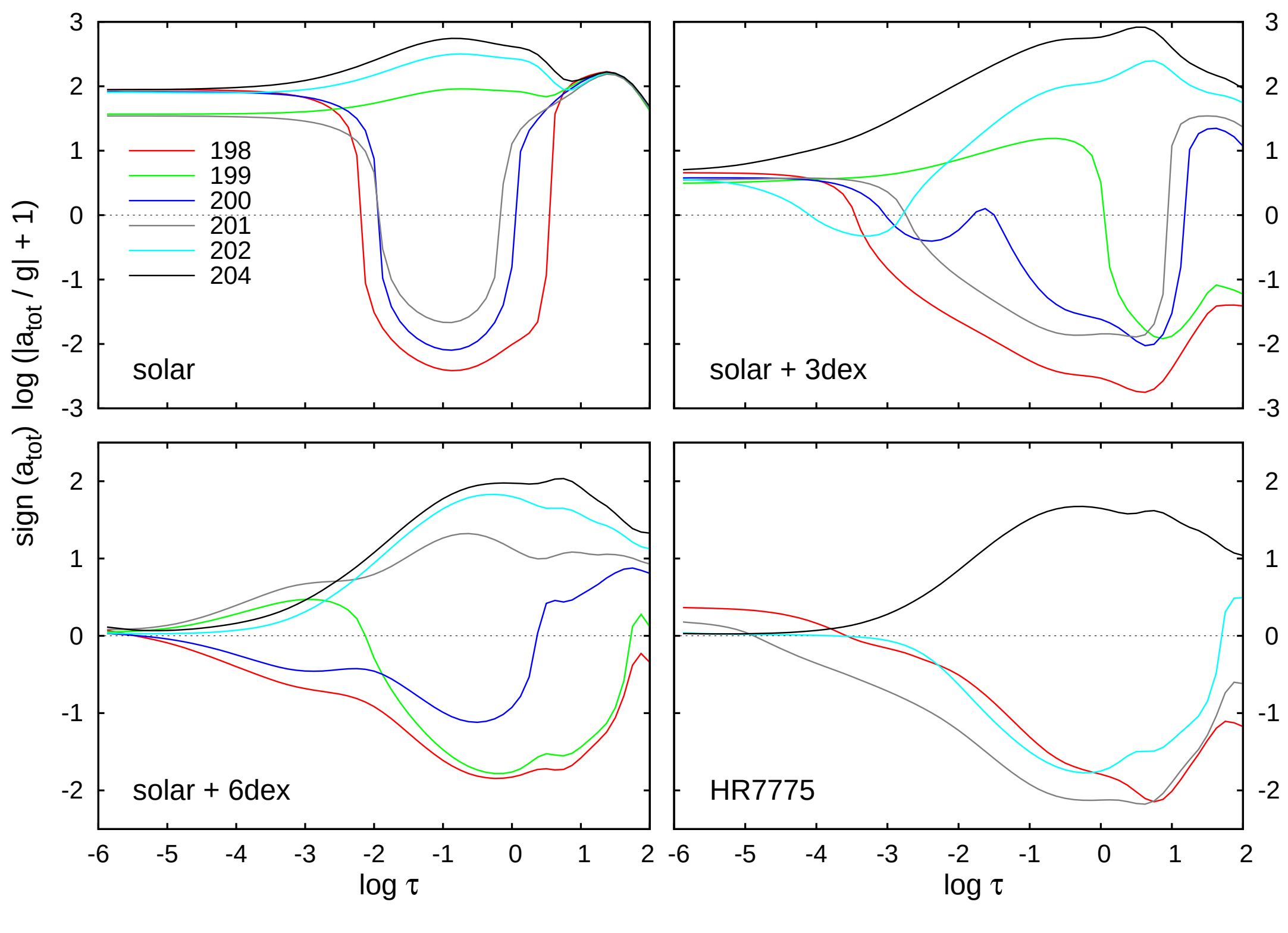


**Figure 2.** The ratio $a_{tot}/g$ in modified logarithmic scale at the initial time for different Hg abundances shown in panels. Acceleration $a_{tot} = a_{rad} + a_{LID}$.

## 3. Input data and results of evolution modelling

Spectral line data were taken from the lists of Kurucz (CD18) and Vienna data base VALD. Isotopic splitting for most of Hg lines was calculated using relative shifts according to Striganov and Dontsov (1955). Hyperfine and isotopic structure and oscillator strengths of Hg lines available in papers by Proffitt et al. (1999) and Smith (1997) were used to improve our line list. Total number of HgI-III lines used in calculations was 99 including 8 resonance lines. We adopted solar abundance and isotopic mixture by Anders & Grevesse (1989) and isotopic mixture of HR7775 from paper by Dolk et al. (2003) (Table 1). We used solar mercury abundance $\log N_{\rm Hg}$= -10.91 and $\log N_{\rm Hg}$= solar + 6 for HR7775 (on the scale where $\log N_{\rm H}$= 0). All calculations were carried out for the model atmosphere with parameters $T_{eff} = 10750, \log g = 4, V\sin i = 0, V_{turb} = 0$, corresponding to the star HR7775.

For all isotopes the initial values $C_i = 1$. The boundery values of velocities at the outermost layer were assumed to be zero, i.e. the lack of stellar wind was assumed. At the bottom of stellar atmosphere the isotope flows were linearly extrapolated. The NLTE effects and presence of magnetic field were ignored in the modelling. The process of Hg isotope separation was calculated for the cases of initial solar, solar+3 dex, solar+6 dex and HR7775 abundances of mercury isotopes. Evolutionary changes in the quiescent stellar atmospheres are proceeding very rapidly, especially in outer layers. Diffusion processes in the case of initial solar abundances turned out to be about 100 times slower than in atmosphere with $\log N_{\rm Hg} = \rm solar + 6dex$.

Early stages of evolution in the quiescent atmosphere are shown in Fig. 1. Radiative acceleration is dominant at low abundances because then the weak mutual influence of Hg lines cannot produce any essential asymmetry of spectral line profiles, the same holds for outer layers where the electrons of excited states return to lower states before they collide (Figs. 2, 3). In the beginning of the evolution process in the star with solar abundances of mercury isotopes the radiative drive is dominant (Fig. 2) causing rise of abundance of all Hg isotopes. In outer layers this process is much faster than in deeper layers of atmosphere (Fig. 1a). With increasing of the Hg abundance the role of LID also increases causing levitation of heavier and sedimentation of lighter isotopes. This process is well seen in Fig. 1b where calculations were started with $\log N_{\rm Hg} = \rm solar + 6dex$. In the model atmosphere where only two heaviest isotopes are present the LID causes sedimentation of $^{202}$Hg and levitation of $^{204}$Hg (Fig. 1c). Superfine splitting of spectral lines of odd isotopes mixes the order of spectral lines of different isotopes what evokes more complicated picture of evolutionary changes of isotope abundances.

## 4. Main conclusions

We conclude that LID is important for diffusional segregation of isotopes of heavy elements. The concept of quiescent atmospheres can explain general picture of LID phenomenon in CP stars. To describe realistically the CP star atmospheres the mixing due to microturbulence must be taken into account and the computations for stellar atmospheres must be extended with the diffusion modelling in the stellar envelopes. For mercury and similarly for other heavy chemical elements the LID phenomenon causes the levitation of the heaviest isotope and generally sedimentation of the lighter ones. The phenomenon of diffusion is essentially more complicated if the hyperfine splitting of spectral lines of isotopes with odd number of baryons is present. Non-trivial isotope anomalies are observed in many mercury-manganese CP star atmospheres, the genesis of which demands special additional studies. Presence of observed isotopic anomalies suggests that abundances of Hg isotopes may vary throughout the CP star atmosphere. This assumption is supported also by observations which give dramatically different abundances derived from lines of different ionization stages in the assumption of homogeneous chemical composition and LTE modelling. This feature could be explained in terms of variable abundances throughout the stellar atmospheres.

Results of present work are the preliminary ones and essential further efforts are needed to get adequate detailed picture of physical processes generating the puzzling observed Hg spectral line profiles in HgMn star spectra.

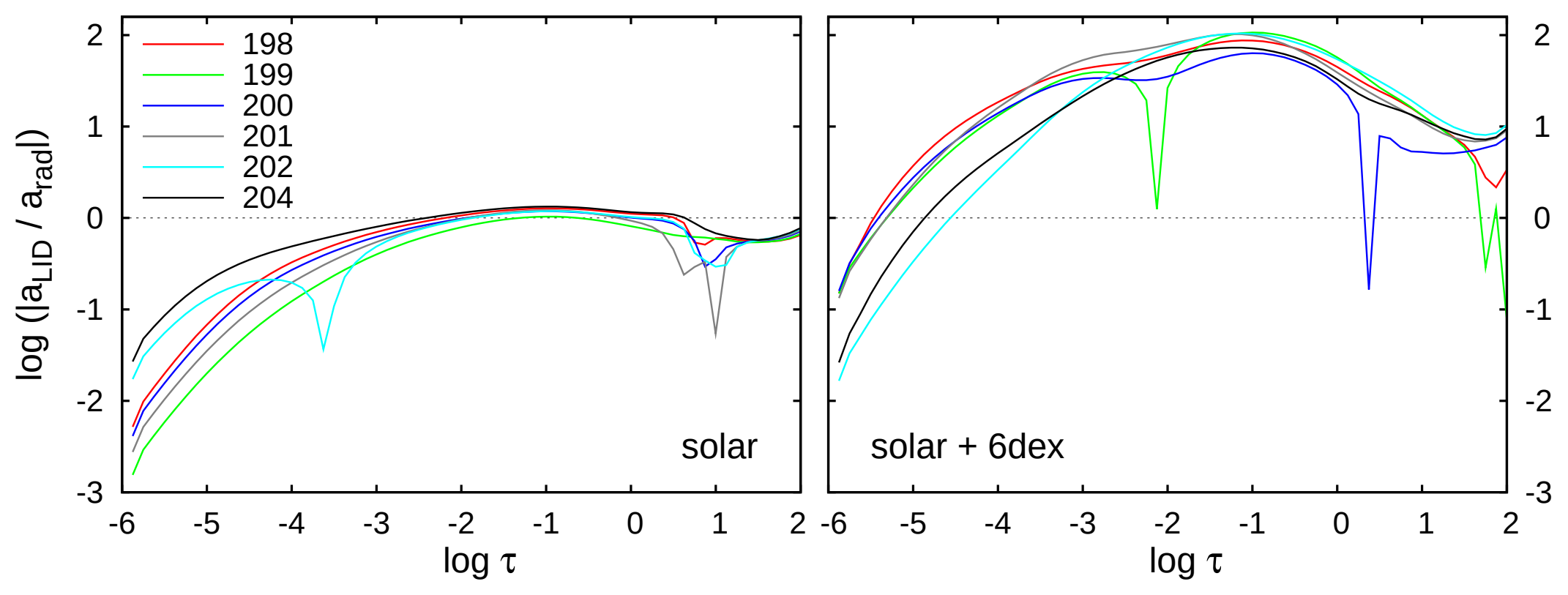


**Figure 3.** Initial ratios of accelerations $a_{LID}/a_{rad}$ for solar and solar+6 dex abundances of Hg isotopes. Radiative acceleration is dominant at low abundances and in the outer layers and LID at high abundances and in deeper layers.

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