Segregation of isotopes of heavy metals due to light-induced drift: results and problems

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Nature of LID

- Light-induced drift (LID) has been suggested by Atutov and Shalagin (1988) as a mechanism causing isotopic anomalies in CP stars.
- LID appears due to asymmetry of radiative flux in spectral lines.
- LID can be described as acceleration a_{LID} additional to usual radiative acceleration a_{rad}.
- The expression for a_{LID} is similar to the formula for a_{rad} but instead of Voigt function its derivative relative to wavelength is to be used.
- Effectiveness of LID depends on probability of particle to stay in the upper state until the next collision.

Separation of isotopes due to LID

- Asymmetry of flux in overlapping isotope lines generates different accelerations to isotopes, yielding segregation of isotopes.
- Isotopic spectral line splitting is similar in most spectral lines and thus the effect of LID is cumulative.
- LID causes rising of isotope with red–shifted line and sinking of isotope with blue–shifted line.
- For heavy elements effect of field shift (due to nuclear volume) dominates over the mass shift. Thus spectral lines of heavier isotopes are shifted to longer wavelengths.
- Hyperfine splitting of spectral lines of isotopes with odd number of nucleons is irregular relative to isotopic splitting. This complicates the picture of diffusional segregation.

Separation of mercury isotopes

- LID generally causes subsequent sinking the lighter isotopes and rising of the heavier ones, leaving finally only the heaviest isotope in the atmosphere.
- Computation of LID demands high–precision spectral data and high–resolution ($R = 5\ 000\ 000$, corresponding Doppler shift 60 m/s) model computations.
- Collision cross-sections for particles determine effectiveness of LID and thus precise data are necessary. Unfortunately the data are since of low exactness.
- Isotope segregation in higher atmospheric layers proceeds essentially quicker than in the deeper ones due to large differences in mean free flight times.

Main formulae for LID

Main formulae for LID used in computations are given in our poster

- Diffusion coefficient by Gonzalez et al.(1995) has been used.
- LID efficiency has been computed using long–range Coulomb interaction between ions, the hard core impact model for neutrals and extension of the model outside the Debye sphere for ion–neutral impacts.
- Boundary conditions were specified by using the Lagrange 4th order interpolation polynomials.

Software – program SMART

Spectra and Model Atmospheres by Radiative Transfer

1. SMART has been composed by the authors for modelling stellar atmospheres and studying different physical processes in them.
    - SMART is a compact and simple software;
    - FORTRAN 77 code has been refactored to Fortran 90.
2. Evolutionary segregation of mercury isotopes in quiescent atmospheres of CP stars has been computed.
    - calculation of 1 time step takes approx 16 min on PC (CPU 3.2 GHz, 2 GB RAM)

Initial data

- Model atmospheres have been computed with SMART using moderate spectral resolution (R=30 000) sampling.
- Continuous spectrum has been used in almost traditional way. Inglis–Teller type formula have been used to smooth transitions from high-excitation spectral line series to corresponding continua.
- Spectral line data from Kurucz file `gfhyperall.dat` have been used.
- Spectral line data for Hg have been compiled from different sources. Isotopic and hyperfine splitting of spectral lines has been analyzed.
  Line list contains about 700 resonance and low excitation spectral lines for HgI, HgII and HgIII

Evolutionary scenarios for Hg isotopes

Evolution of stratification of Hg isotopes have been computed for some initial abundances and effective temperatures.

- Initial state
  - Homogeneous abundance of Hg throughout the atmosphere;
  - Solar (terrestrial) ratios of isotope abundances.
- The stellar wind and the microturbulence, both reducing or even cancelling the diffusional segregation of isotopes were ignored.
- The longest evolutionary sequence (500 time steps, à 1 year) has been computed for model atmosphere with parameters $T_{eff} = 10\,750$ K and $\log g = 4$.

List of computed evolutionary scenarios

Model atmospheres with $\log g = 4$ and $V \sin i = 0$ have been accepted for all computed evolutionary scenarios

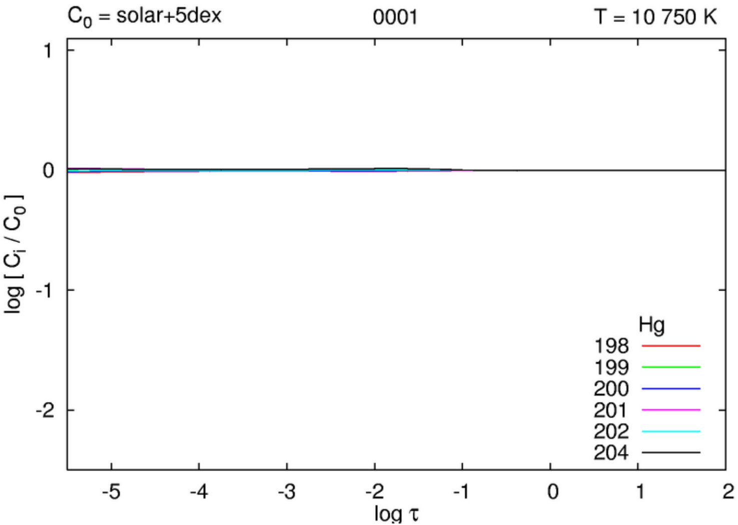
- $T_{eff} = 9500$ K
  - C_0 = solar + 5dex, $\Delta t = 1$ year
- $T_{eff} = 10750$ K
  - * C_0 = solar + 5dex, $\Delta t = 1$ year
  - † C_0 = solar + 3dex, $\Delta t = 0.1$ year
  - C_0 = solar, $\Delta t = 0.01$ year
- $T_{eff} = 12000$ K
  - C_0 = solar + 5dex, $\Delta t = 1$ year
  - C_0 = solar + 3dex, $\Delta t = 0.1$ year
  - C_0 = solar, $\Delta t = 0.01$ year

For the same set of model atmospheres the evolutionary scenarios for Hg have been computed ignoring influence of lines of all other elements

*longest time sequence (500 steps)

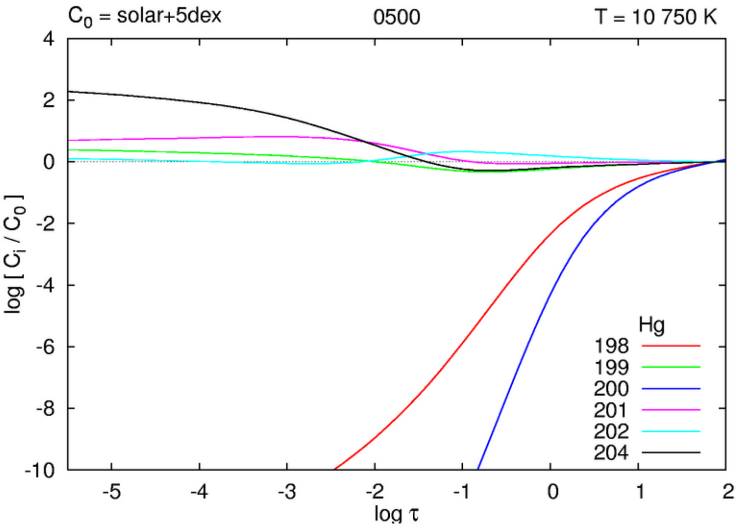
†both with and without hyperfine splitting of Hg lines

Evolution of concentrations $\log(C_i/C_0)$



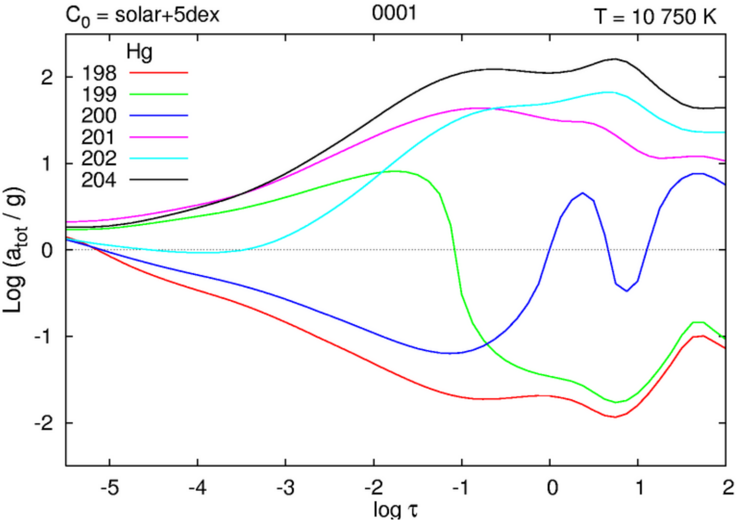
Change of y-axis at timestep 120 [-2.5 : 1] → [-10 : 4]

Evolution of concentrations $\log(C_i/C_0)$



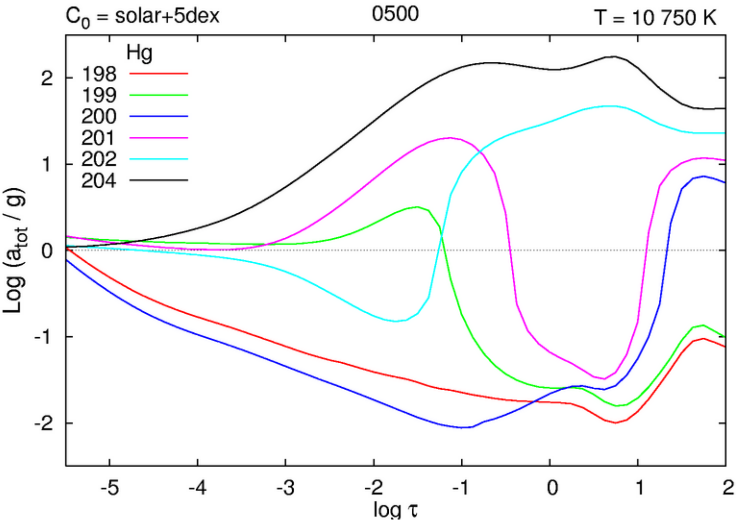
Change of y-axis at timestep 120 [-2.5 : 1] → [-10 : 4]

Evolution of acceleration $a_{tot} = a_{rad} + a_{LID}$



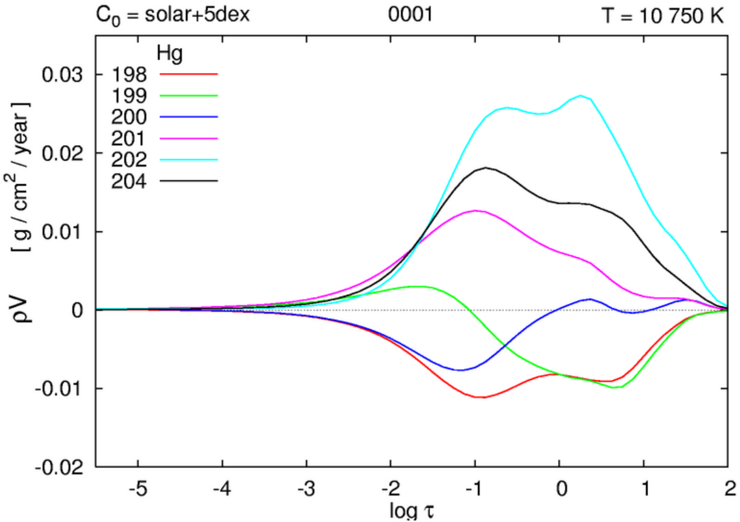
Modified logarithmic scale $\mathrm{sign}(a)\log\left(\left|\frac{a}{g}\right|+1\right)$

Evolution of acceleration $a_{tot} = a_{rad} + a_{LID}$

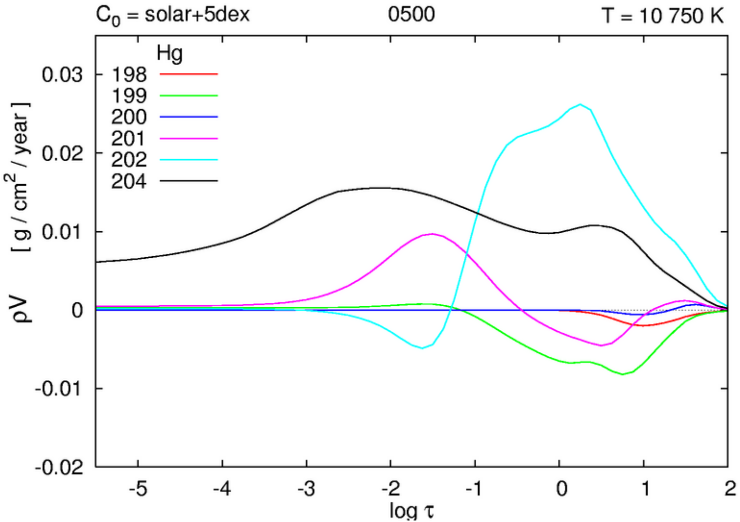


Modified logarithmic scale $\operatorname{sign}(a)\log\left(\left|\frac{a}{g}\right|+1\right)$

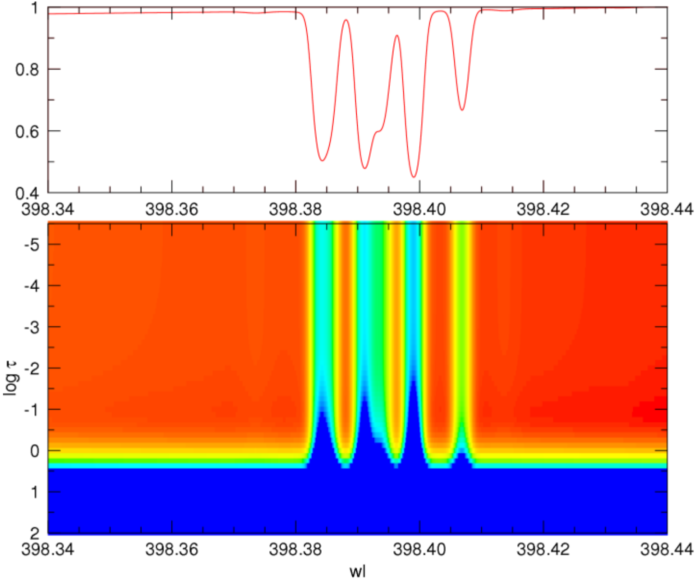
Evolution of mass flow ρV



Evolution of mass flow ρV



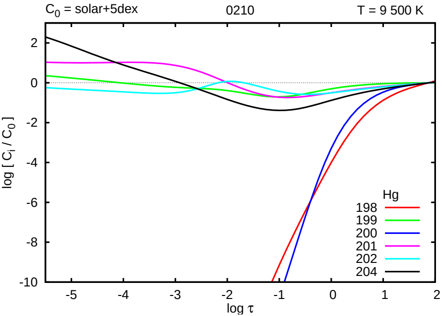
$T_{eff} = 10750$ K, $\log g = 4$, C_0 = solar + 5dex, $\Delta t = 1$ year

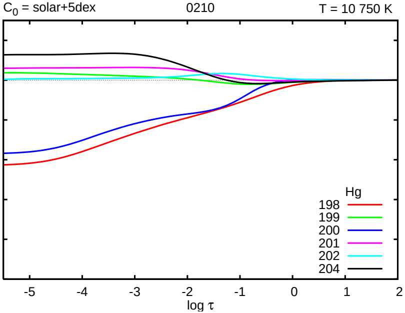


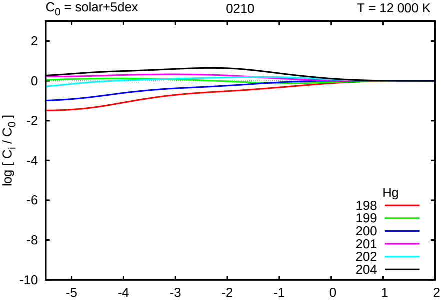
Temperature influence on the evolution

Compare Hg abundance evolution in model atmospheres with $\log g = 4$, $V \sin i = 0$ and C_0 = solar + 5dex

- $T_{\mathit{eff}} = 9500$ K — fastest segregation
- $T_{\mathit{eff}} = 10750$ K
- $T_{\mathit{eff}} = 12000$ K — slowest segregation



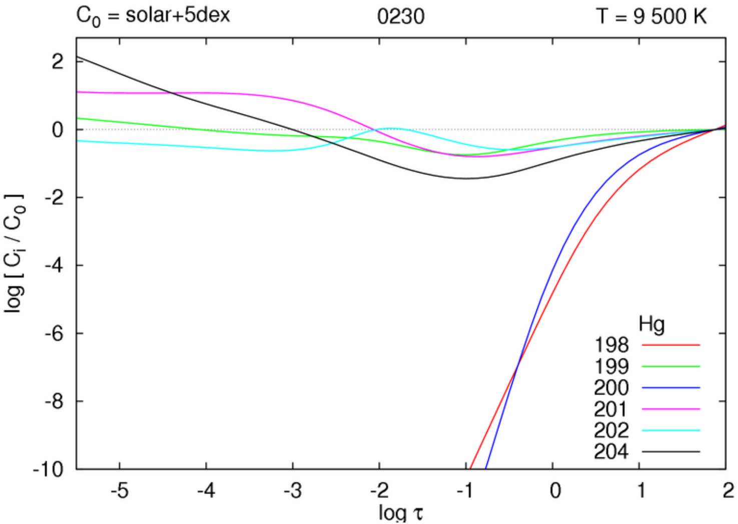




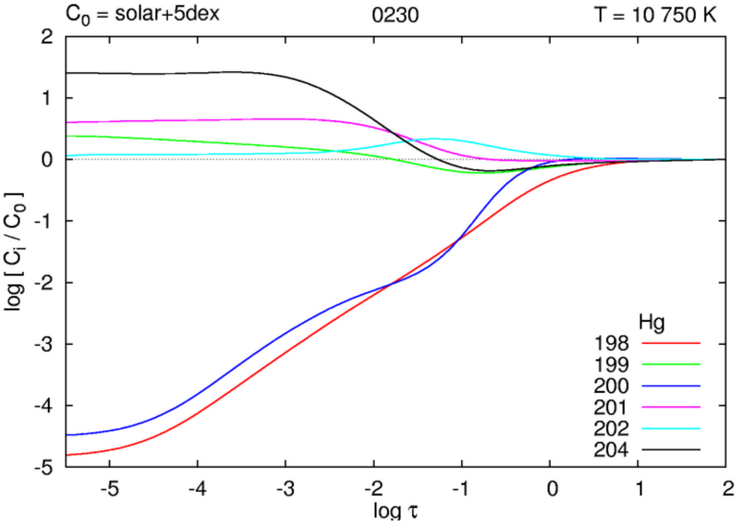
time = 210 years ($\Delta t = 1$ year)

- $T_{eff} = 9500$ K — fastest
- $T_{eff} = 10750$ K
- $T_{eff} = 12000$ K — slowest

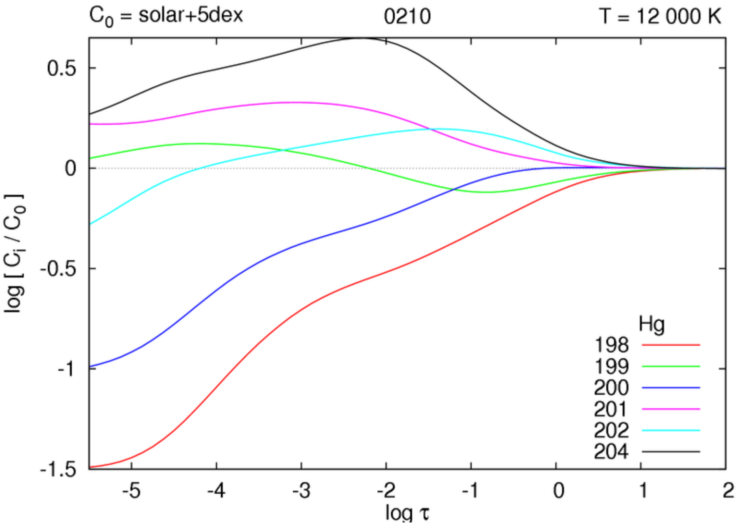
Evolution of concentrations $\log(C_i/C_0)$ at T = 9 500 K



Evolution of concentrations $\log(C_i/C_0)$ at T = 10 750 K



Evolution of concentrations $\log(C_i/C_0)$ at T = 10 750 K



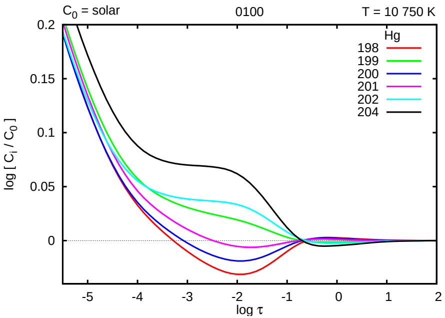
Influence of initial Hg abundance on the evolution

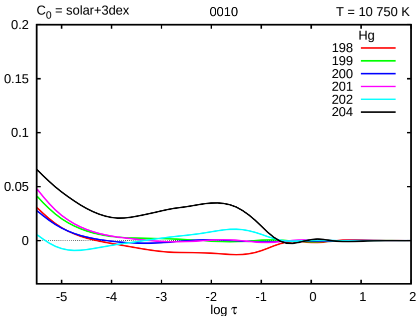
Compare Hg abundance evolution in model atmospheres with
$T_{eff} = 10\,750\ K$, $\log g = 4$, $V \sin i = 0$

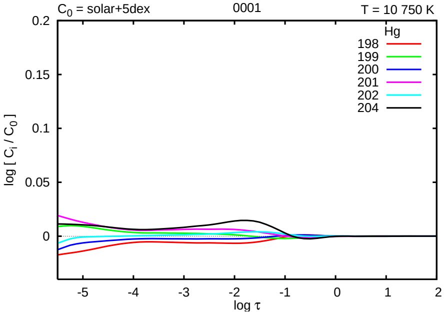
- C_0 = solar
  a_{rad} dominates, abundances of all isotopes grow fast
  time step Δt = 0.01 year

- C_0 = solar + 3dex
  a_{rad} dominates on the surface, a_{LID} – in deeper layers
  time step Δt = 0.1 year

- C_0 = solar + 5dex
  a_{LID} dominates, separation of isotopes starts immediately
  time step Δt = 1 year

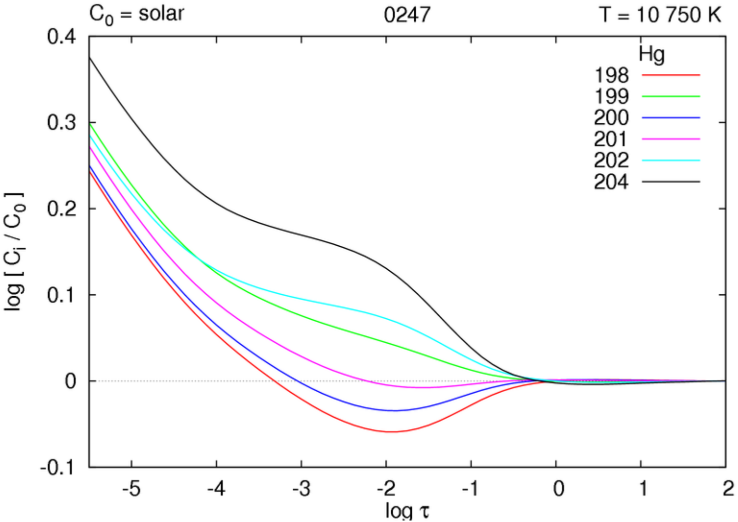






Concentrations at time = 1 year

Evolution of concentrations $\log(C_i/C_0)$ with C_0 = solar

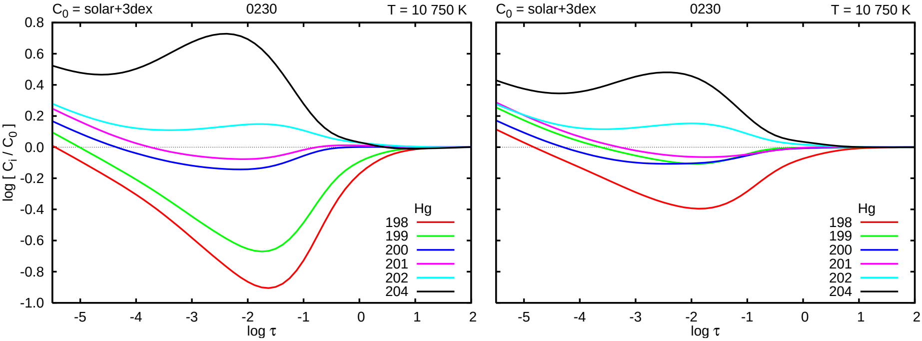


Influence of the hyperfine splitting of Hg lines

Concentration at time step 230

Without hyperfine splitting

With hyperfine splitting



Main conclusions

- Computed evolutionary sequences of isotope segregation can help to explain the observed unusual ratios of isotopes of heavy elements in the atmospheres of CP stars, including vertical abundance profiles.
- Radiative acceleration is dominant at solar abundance of Hg, role of LID increases with increase of Hg abundance and it becomes dominant at abundance $\sim$ solar + 5dex.
- Separation of isotopes starts in the outer rarefied layers and propagates into the deeper layers.
- Separation time scale increases essentially with effective temperature.
- Lighter isotopes with even number of nucleons sink rapidly.
- Hyperfine splitting of spectral lines decelerates and weakens the diffusional segregation of isotopes.

Problems for future investigations

Several improvements are required to calculate realistic evolutionary scenarios:

- more complete and accurate data of spectral line strengths and their damping constants;
- more exact cross–sections for different impact processes;
- more realistic time scales by including processes slowing down the diffusion (turbulence, stellar wind);
- more stable algorithms for time integration;
- the physically more adequate initial data and inner boundary conditions. This requires expanding of calculations of diffusion processes deeper into stellar envelope*.

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*Segregation of Hg isotopes in deeper layers of stellar envelope is probably ineffective because isotopic splitting is larger for higher ions and isotopic lines do not overlap.

Future plans

We are planning:

- to compute more realistic evolutionary scenarios and longer time sequences for mercury;
- to include stellar wind into evolutionary computations (corresponding formulae are given in our poster);
- to investigate the possibilities of physically motivated inclusion of diffusion coefficient corresponding to turbulence;
- to calculate evolution scenarios for calcium isotopes;
- to elaborate new more stable algorithms, which enable longer time steps;
- to parallelize the code;
- to develop an apply a mathematical method, which enables to find the final equilibrium isotope distribution.

Program SMART: capabilities and restrictions

Spectra and Model Atmospheres by Radiative Transfer

Authors: Arved Sapar, Raivo Poolamäe and Anna Aret (Tartu Observatory)

1. Stellar atmospheres of O, B and A spectral classes (9 000 – 40 000 K)
2. Capabilities:
    - Stellar spectra – radiative flux through the stellar atmosphere
    - Stellar models – by iterative correction of initial model
    - Diffusive separation of elements and isotopes in CP stars
    - Relaxational formation of NLTE
    - Accelerations of clumps in stellar wind
    - Spectra of rotating stars and eclipsing binaries
    - Radiative transfer in lines in stellar wind
3. Restrictions:
    - plain-parallel and static stellar atmosphere
    - chemically homogeneous atmosphere
    - LTE
    - no molecules