

Diffusion and light-induced drift in stellar atmospheres

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Chemically peculiar stars

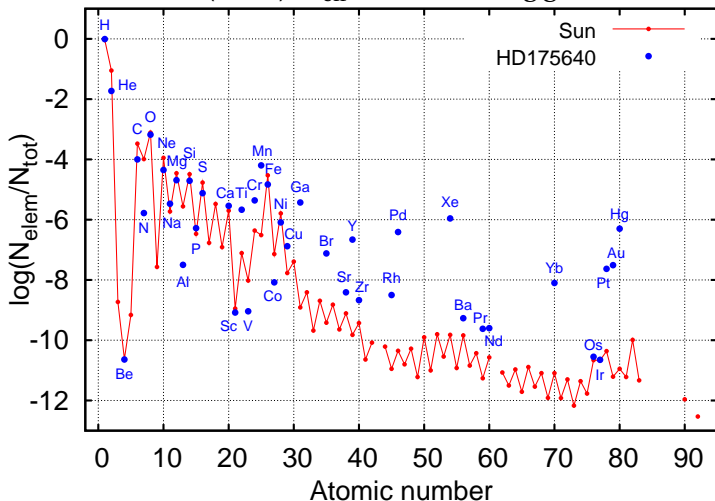
Chemically peculiar (CP) stars are early type main-sequence stars with distinctly unusual abundances of certain elements.

Classification of CP stars by G. Preston (1974, ARA&A, 12, 257)

- **CP1**: Am stars (7 000 – 10 000 K, F5 – A4), Ca and/or Sc deficiency, enhanced heavy metals. Non-variable, non-magnetic. Many in binaries.
- **CP2**: Ap stars (8 000 – 15 000 K, F0 – B5), enhanced Si, Cr, Sr, Eu et al. (+3...+6 dex). Magnetic, variable stars with abundance spots.
- **CP3**: HgMn stars (10 000 – 15 000 K, A2 – B8), enhanced heavy metals: Hg (up to 6 dex), Mn etc. He, Al, Zn, Ni, Co deficiency. Isotopic anomalies. Non-variable, non-magnetic stars with very slow rotation, 50% in binaries.
- **CP4**: He stars
 - He-weak stars (14 000–21 000 K), He deficiency ~ 1 – 2 dex;
 - He-weak stars with isotopic anomaly – overabundance of ^3He ;
 - He-rich stars (21 000 – 30 000 K), $N_{\text{He}}/N_{\text{H}} \sim 0.5$ (norm ~ 0.1).
Most massive CP stars.

Abundance anomalies

HgMn star HD 175640 (B9 V): $T_{\text{eff}}=12\,000\text{ K}$, $\log g=3.95$



Castelli & Hubrig 2004, A&A 425, 263

Causes of the anomalies

Several hypotheses have been advanced:

- interior nucleosynthesis in a post-main-sequence phase of evolution (Fowler et al 1965)
- surface contamination of a normal star by a supernova companion (Guthrie 1967)
- selective magnetic accretion of interstellar matter (Havnes & Conti 1971)
- radiative-driven diffusion in stellar atmospheres (Michaud 1970)
 - anomalous abundances appear due to stratification of elements in stellar atmosphere, the bulk composition of the entire star is normal;
 - stratification of elements forms due to atomic diffusion. It is determined by competition between **gravitational and radiative forces**;
 - Microscopic diffusion only works in quiet atmospheres (i.e. convection and turbulence, mass loss and meridional flows are weak enough).

Articles on history: EAS Publications Series, Vol. 17 (2005).

Element Stratification in Stars: 40 Years of Atomic Diffusion.

Description of stellar plasma

Main assumptions:

- Plasma can be considered as dilute gas, i.e. the ideal gas equation of state applies ($P = NkT$)
- Maxwellian velocity distributions
- Same temperature for all ions and electrons
- Diffusion velocities are much smaller than thermal velocities
- Collisions are dominated by classical interactions between two point particles
- Diffusion of every trace element is treated separately
- No magnetic fields

Boltzmann equation: commonly used formalisms

Descriptions of stellar plasma are all based on the Boltzmann equation

Boltzmann equation for species i

$$\frac{df_i}{dt} \equiv \frac{\partial f_i}{\partial t} + \mathbf{v}_i \cdot \frac{\partial f_i}{\partial \mathbf{r}} + \dot{\mathbf{v}}_i \cdot \frac{\partial f_i}{\partial \mathbf{v}_i} = \text{Coll}(f_i)$$

where $f_i = f_i(\mathbf{r}, \mathbf{v}, t)$ distribution function of species i ;
 $\text{Coll}(f_i)$ collision term



Chapman-Enskog theory

Chapman, S. and Cowling, T. G.:
 The mathematical theory of
 non-uniform gases. Cambridge:
 University Press, 1970



Burgers' theory

Burgers, J. M.: Flow Equations
 for Composite Gases. New
 York: Academic Press, 1969

Comparison: Thoul, A., Montalbán, J., 2007, EAS Publ. Series 26, 25

Diffusion velocity

Diffusion velocity for mixture of two gases in presence of external forces
(Chapman & Cowling, Ch. 14)

General equation of diffusion velocity

$$v_1 - v_2 = -\frac{N^2}{N_1 N_2} D_{12} \left\{ \underbrace{\nabla \ln \frac{N_1}{N}}_{\text{Concentration}} + \underbrace{\frac{N_1 N_2 (m_2 - m_1)}{N \rho} \nabla \ln P}_{\text{Pressure}} - \underbrace{\frac{\rho_1 \rho_2}{P \rho} (F_1 - F_2)}_{\text{Forces}} + \underbrace{\frac{D_T}{D_{12}} \nabla \ln T}_{\text{Temperature}} \right\}$$

where v_1, v_2 mean velocities of particles 1 and 2

N_1, N_2 number densities of particles 1 and 2, $N = N_1 + N_2$

m_1, m_2 masses of particles 1 and 2;

ρ_1, ρ_2 mass densities of particles 1 and 2, $\rho_i = m_i N_i$, $\rho = \rho_1 + \rho_2$;

D_{12} diffusion coefficient;

D_T thermal diffusion coefficient;

P gas pressure $P = P_1 + P_2$;

T temperature;

F_1, F_2 external forces on particles 1 and 2 per unit mass \equiv accelerations

Diffusion velocity

We assume in the stellar atmosphere:

- hydrostatic equilibrium: $\nabla P = \rho_1 F_1 + \rho_2 F_2$
- diffusion of trace element in buffer gas: $N_1 \ll N_2$
- thermal diffusion can be neglected, because $\nabla \ln T \ll \nabla \ln P$.

In this approximation, general equation of diffusion velocity reduces to:

Equation of diffusion velocity in stellar atmosphere

$$v_1 = -D_{12} \left(\nabla \ln N_1 - \frac{m_1}{kT} F_1 \right)$$

Equation of continuity

Equation of continuity for ion j of element i

$$\frac{\partial \rho_{i,j}}{\partial t} + \nabla(\rho_{i,j} v_{i,j}) = \dot{\rho}_{i,j}$$

where $\rho_{i,j} = m_i N_{i,j}$ density of ion j with mass m_i ;
 $v_{i,j}$ diffusion velocity of ion j
 $\dot{\rho}_{i,j}$ source term due to ionization and recombination

For element i holds $\sum_{j \in i} \dot{\rho}_{i,j} = 0$ and we obtain:

Equation of continuity for element i

$$\frac{\partial \rho_i}{\partial t} + \nabla(\rho_i v_i) = 0 \quad (1)$$

Main equations in plane-parallel model atmosphere

Equation of continuity for element i

$$\frac{\partial \rho_i}{\partial t} + \frac{\partial(\rho_i v_i)}{\partial r} = 0$$

Diffusion in non-magnetic stellar atmosphere is mainly determined by competing gravity g and radiative acceleration a_i^{rad} , thus $F_i = a_i^{\text{rad}} - g$ and we obtain:

Equation of diffusion velocity

$$v_i = D_i \left(\frac{m_i}{kT} (a_i^{\text{rad}} - g) - \frac{d \ln N_i}{dr} \right)$$

In main sequence stars $a_i^{\text{rad}} \sim 0 - 10^7$, while $g \sim 10^4 \text{ cm/s}^2$!

Radiative acceleration

Generic expression for radiative acceleration

$$a_j^{\text{rad}} = \frac{\pi}{m_j c} \int_0^\infty \sigma_\nu \mathcal{F}_\nu d\nu$$

where σ_ν is absorption cross-section and $\pi \mathcal{F}_\nu$ is total monochromatic flux.

In atmospheres of CP stars radiative levitation acts primarily through **bound-bound atomic transitions**. For transition $l \rightarrow u$ of ion j :

$$a_j^{\text{ul}} = \frac{\pi}{m_j c} X_{j,l} \int_0^\infty \sigma_{\nu,ul} \mathcal{F}_\nu d\nu = \frac{\pi}{m_j c} X_{j,l} \int_0^\infty \sigma_{ul}^0 V(u_\nu, a) \mathcal{F}_\nu d\nu$$

where $X_{j,l}$ is state l population fraction; $\sigma_{ul}^0 = \frac{\pi e^2 f_{ul}}{m_e c \Delta \nu_D}$ is photon absorption cross-section in line; $V(u, a)$ is Voigt function.

Radiative acceleration of element i in simplest approximation is given by

$$a_i^{\text{bb}} = \frac{\pi}{m_i c} \sum_{j \in i} X_j \sum_{l, u > l} X_{j,l} \int_0^\infty \sigma_{ul}^0 V(u_\nu, a) \mathcal{F}_\nu d\nu$$

Total acceleration should be obtained taking into account redistribution of momentum among the various ionization states.

Calculation of radiative acceleration

Main ingredients for computing radiative acceleration: cross-sections, populations, photon fluxes – more or less similar to those needed for synthetic spectra, but

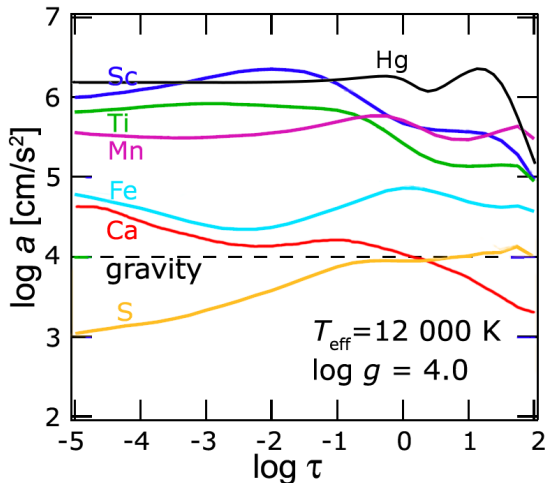
- Different selection criteria for atomic transitions: main contributors to the integral at any depth (not limited to the line forming region)
- All layers should be considered, even very deep, which implies higher ionization degrees than usually taken
- Bound-free interactions can contribute significantly

For bound-free transitions from level l of ion $j - 1$, which benefits to ion j :

$$a_j^{\text{bf}} = \frac{\pi}{m_j c} \sum_l \frac{N_{j-1,l}}{N_j} \int_0^\infty (1 - y_l) \sigma_{j-1,l,\infty} \mathcal{F}_\nu d\nu$$

The term y_k represents the momentum taken away by the eject electron.

Radiative accelerations in stellar atmospheres



LTE radiative accelerations for a solar abundance of each element in the plane-parallel static atmosphere. Hui-Bon-Hoa et al. 2002, Sapar et al. 2008

Stratified model atmospheres

Model atmospheres with equilibrium stratification of elements ($v_i = 0$):

- Dreizler & Wolf 1999 – for white dwarfs;
- Hui-Bon-Hoa et al. 2000 – for blue-horizontal branch stars (based on PHOENIX atmospheric code);
- LeBlanc & Monin 2004 – for Ap stars (more recent version of previous model);
- Alecian & Stiff 2008 – stratification in magnetic stars.

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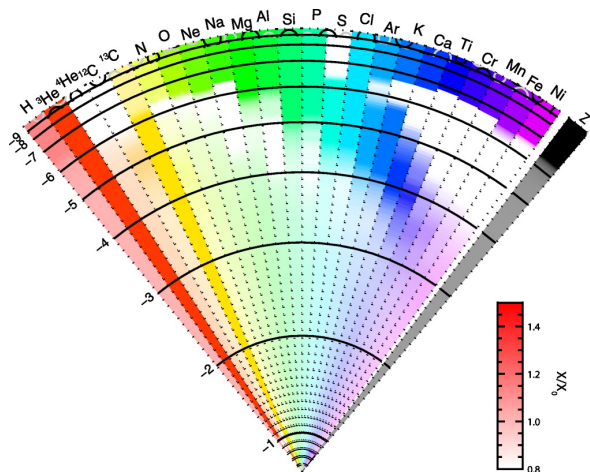
BUT

Simulations of the abundance anomalies require:

- computation of the **time-dependent** formation of stratification, because diffusion is non-linear process
- taking into account exchange of each element with the interior of the star (given by **stellar evolution models** with diffusion).

Stellar evolution models with diffusion

Radiative-driven diffusion causes stratification of chemical elements also in stellar interiors



Evolutionary model:
HB star

$$M = 0.61M_{\odot},$$

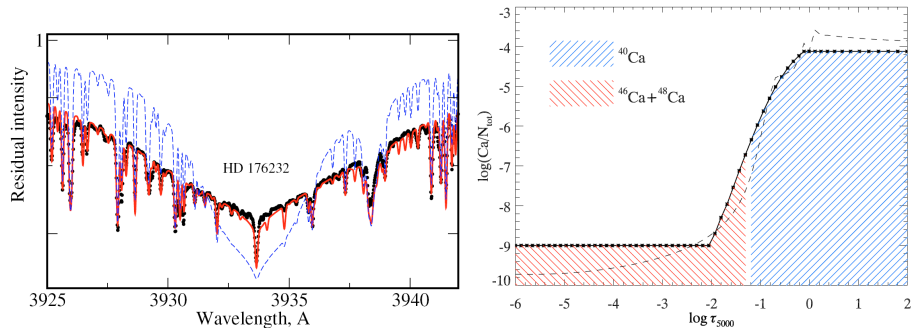
$$T_{\text{eff}} = 12\,400\text{ K}$$

≈ 30 Myr after ZAHB

Michaud, Richer & Richard, 2008 ApJ, 675, 1223

Observational evidence of element stratification

Deviation of observed in CP stars line profiles from those expected in homogeneous atmosphere provide strong observational evidence for an existence of abundance stratification.



Comparison between the observed profiles (black) of the Ca II 3933 Å line and calculations with the stratified (red) and homogeneous (blue) Ca distributions for Ap star HD176232. Vertical stratification and isotopic separation of Ca derived for HD176232 are shown on the right panel. (Ryabchikova et al 2008, A&A 480, 811).

Isotopic anomalies in CP stars

Isotopic anomaly \equiv isotope abundance ratios differ from solar ones

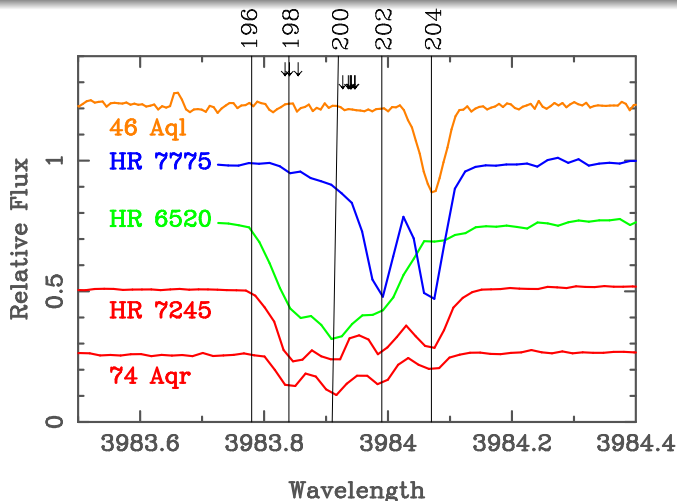
Very high-resolution spectra with high signal-to-noise ratio are necessary to obtain isotope abundances

First observation – ^3He in star 3 Cen A – Sargent & Jugaku, 1961

- **Hg**: 1962 W.P. Bidelman – HST (HR7775, χ Lupi) – 2003 Dolk et al. (31 HgMn stars) ...
- **Pt**: 1973 Dworesky & Vaughan – 1995–99 HST – 1999 ESO VLT, 5 HgMn stars (Hubrig et al.) ...
- **Ca**: 2004 ESO VLT (Castelli & Hubrig) – 2007 Cowley et al. (22 HgMn, 27 Ap, 18 other CP star)...
- **Li**: 1964 Herbig – 2007 Polosukhina & Shavrina ...
- **Xe**: 2007 Castelli & Hubrig
- **Tl**: 1996 HST, Leckrone et al.

Overview: Cowley, Hubrig, Castelli 2008, Contrib. Astron. Obs. Skalnaté Pleso 38, 291

Isotopic anomaly of mercury in CP stars



UVES spectra of the $\lambda 3984$ region in 5 HgMn stars. Vertical lines indicate the wavelengths of the stable, even-A isotopes, indicated above the plot. Short arrows indicate the hyperfine components of ^{199}Hg and ^{201}Hg , the stable, odd-A isotopes.

Isotopic anomalies in CP stars

Anomalies vary significantly from star to star, but there is a tendency:

- Heavy elements: heavier isotopes are overabundant
- Light elements: lighter isotopes are overabundant

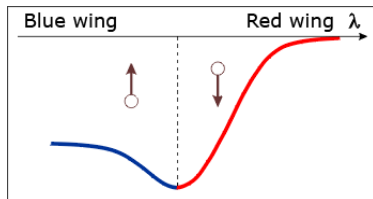
Radiative acceleration is almost the same for all isotopes of given element.

What causes separation of isotopes?

Physics of the light-induced drift

Light-induced drift (LID) has been suggested by Atutov and Shalagin (1988) as a mechanism causing isotopic anomalies in CP stars.

LID is generated by absorption in a spectral line with asymmetrical profile



Upward flow of particles

Radiative flux < Radiative flux

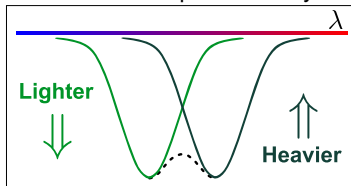
Number of excited particles < Number of excited particles

Mobility > Mobility

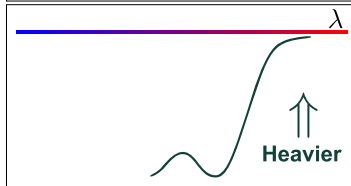
- Larger flux in the red wing \Rightarrow upward flow of particles
- Larger flux in the blue wing \Rightarrow downward flow of particles
- Resulting LID (sum over all lines) is essential only if there is a **systematic asymmetry** in spectral lines

Light-induced drift of isotopes

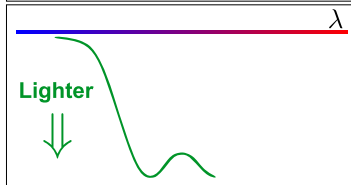
Spectral lines of isotopes of heavy element



Isotopes with slightly shifted energy levels have **overlapping** spectral lines, giving **systematically similar asymmetry** in line profiles. For heavy elements spectral lines of heavier isotopes are shifted to longer wavelengths.



Heavier isotope has larger flux in the red wing
Heavier isotope rises



Lighter isotope has larger flux in the blue wing
Lighter isotope sinks

Separation of isotopes due to LID

- 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
 - Heavy elements (nuclear volume isotope shift):
sinking of the lighter isotopes and rising of the heavier ones;
 - Light elements (nuclear mass isotope shift):
sinking of the heavier isotopes and rising of the lighter ones.
- Hyperfine splitting of spectral lines of isotopes with odd number of nucleons is irregular relative to isotopic splitting. This complicates the picture of diffusional separation.

Main formulae for LID

- LID can be described as acceleration a^{LID} additional to usual radiative acceleration a^{rad} (Aret & Sapar 2002, Astron. Nachr. 323, 1, 21).
- 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.
- Efficiency of LID ε depends on difference of collision frequencies in upper and lower state and on probability of particle to stay in the upper state until the next collision.

Light-induced drift in line $l \rightarrow u$

$$a_j^{LID} = \varepsilon q \frac{\pi}{m_i c} \int_0^{\infty} X_{j,l} \sigma_{ul}^0 \frac{\partial V(u_\nu, a)}{\partial u} \mathcal{F}_\nu d\nu \quad (2)$$

$$\varepsilon = \frac{C_u - C_l}{A_u + C_u} \quad q = \frac{m_j v_T c}{2 h \nu} = \frac{m_j v_T}{2} : \frac{h \nu}{c}$$

- C_u ja C_l are collision frequencies for particles in upper and lower state
- A_u is frequency (probability) of spontaneous transitions from the upper state

Computation of LID

Acceleration due to b-b transitions including LID effect

$$a_j^{bb} \Rightarrow a_j^{bb+} = a_j^{bb} + a_j^{LID}$$
$$V(u, a) \Rightarrow V(u, a) + \varepsilon q \frac{\partial V(u, a)}{\partial u}$$

- Effect of LID is largest in stellar atmosphere, it is ineffective in stellar interiors and outer layers;
- Computation of LID of heavy elements demands high-resolution ($R = 5\,000\,000$, corresponding Doppler shift 60 m/s) synthetic spectra at all depths;
- Statistical representation of opacities (like opacity sampling) cannot be used, opacities should be calculated line by line;
- Radiative flux has to be obtained through the detailed resolution of the radiative transfer equation.

Program SMART

Spectra and Model Atmospheres by Radiative Transfer

A. Sapar, A. Aret, R. Poolamäe – Tartu Observatory, Estonia

Model atmospheres of O, B and A stars (9 000 – 40 000 K)

Static, plane-parallel, LTE

Fortran 90, Windows and Linux

Minimum PC configuration: 2 GB RAM, 2 GHz CPU

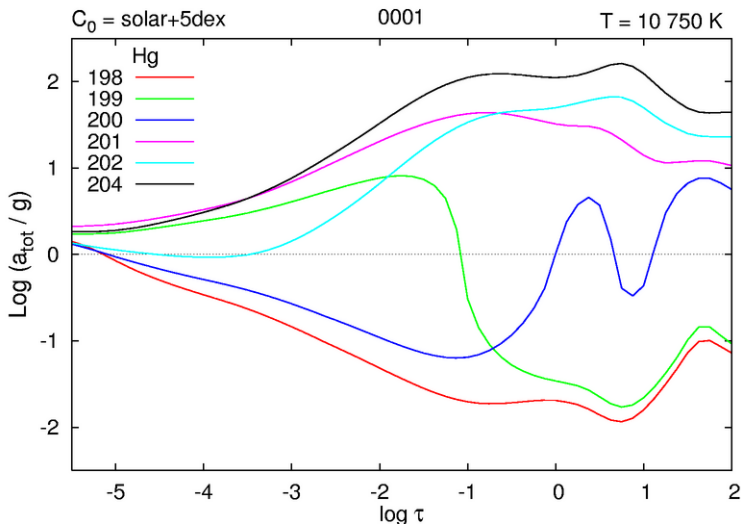
Evolutionary separation of mercury isotopes has been computed in quiescent atmospheres of CP stars:

- $\log g = 4$, $T_{\text{eff}} = 9\,500, 10\,750$ ja $12\,000$ K
- $C_{\text{Hg}}^0 = \text{solar}$, solar+3 dex ja solar+5 dex

Initial state:

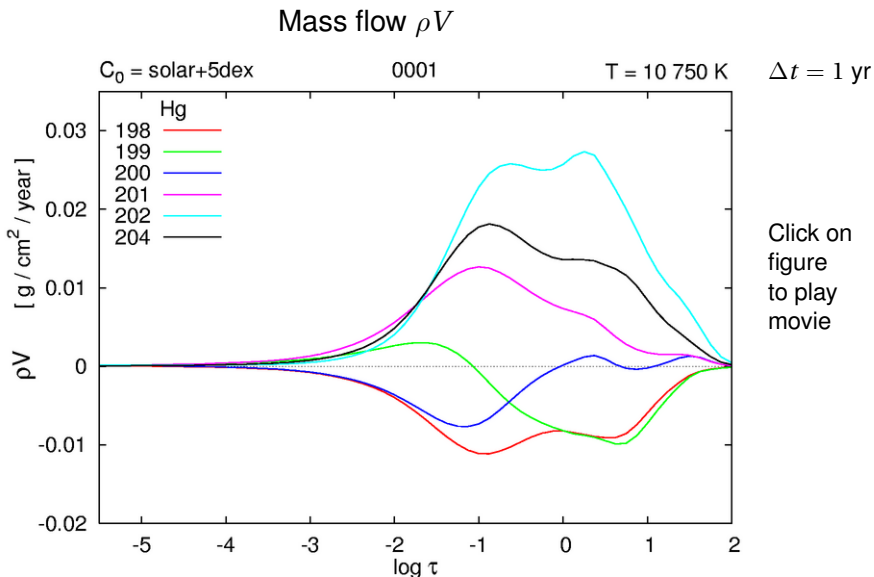
- Homogeneous abundance of Hg throughout the atmosphere;
- Solar (terrestrial) ratios of isotope abundances.

Acceleration $a_j^{\text{tot}} = a_j^{\text{bb}} + a_j^{\text{LID}}$ of mercury isotopes

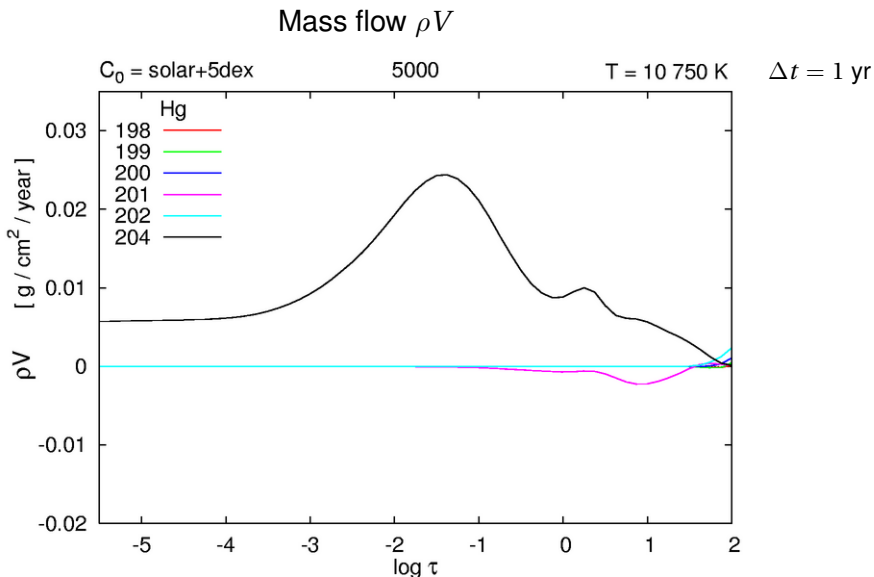


Modified logarithmic scale $\text{sign}(a) \log \left(\left| \frac{a}{g} \right| + 1 \right)$

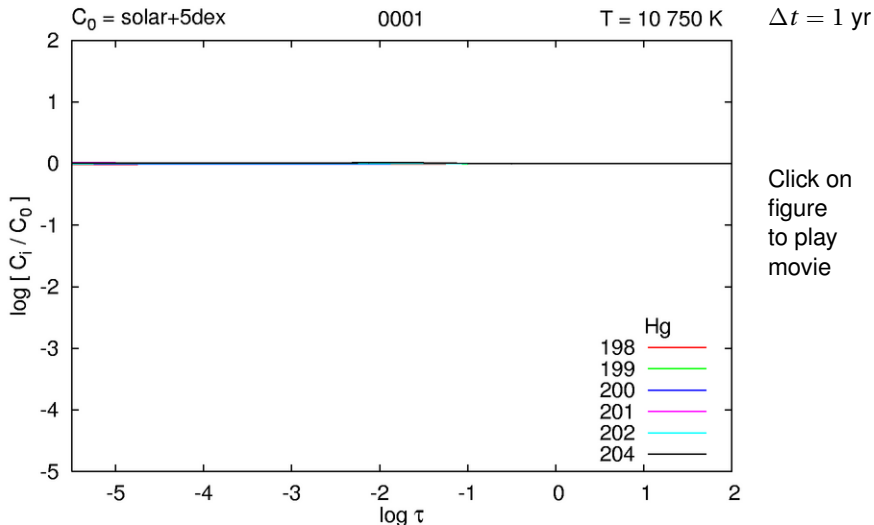
Time-dependent stratification of isotopes in CP stars

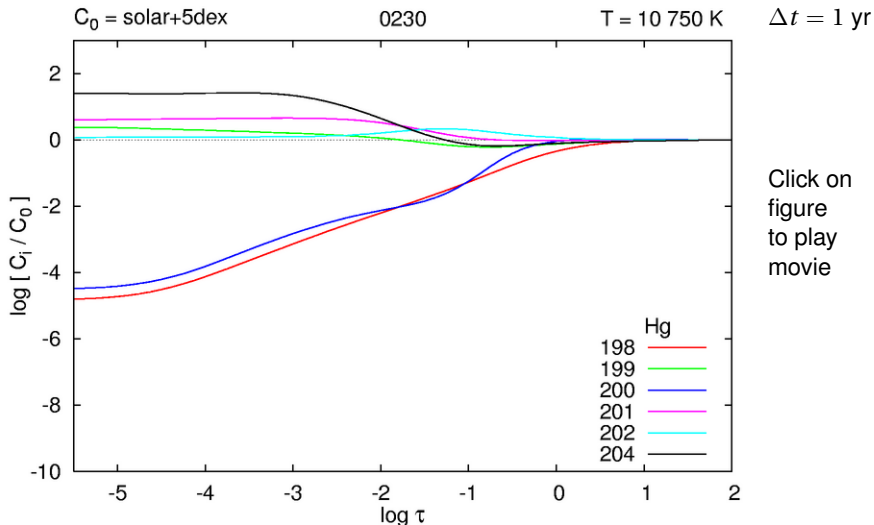


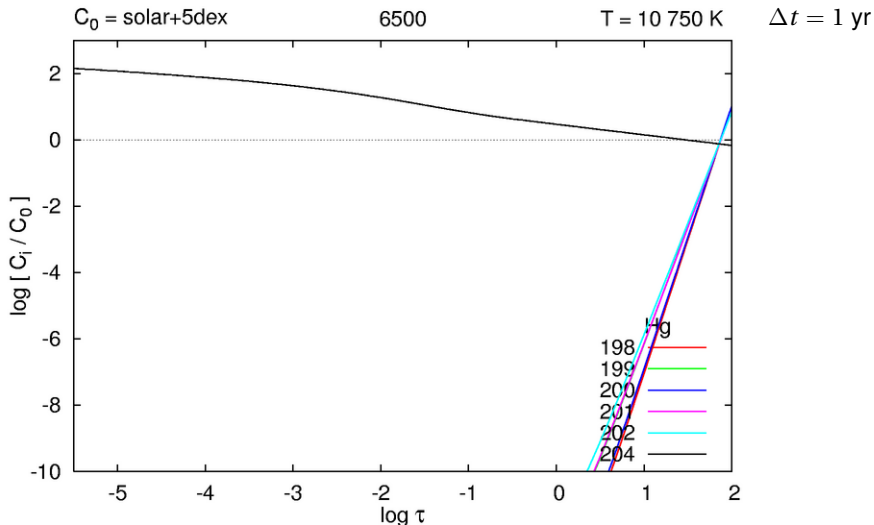
Time-dependent stratification of isotopes in CP stars



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



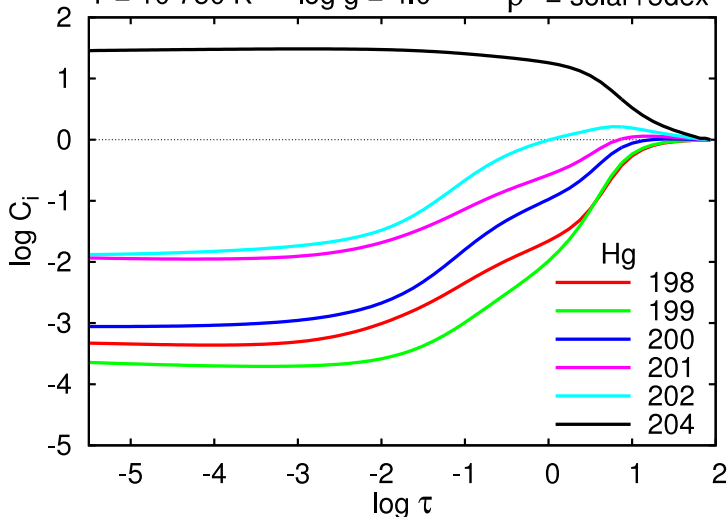
Evolution of isotope concentrations $\log(C_i/C_0)$ 

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

Final equilibrium isotope separation profiles

Atmosphere with microturbulence $D_{\text{turb}} = 50 \times D_{\text{atom}}$

$T = 10\,750\text{ K}$ $\log g = 4.0$ $\rho^0 = \text{solar}+5\text{dex}$

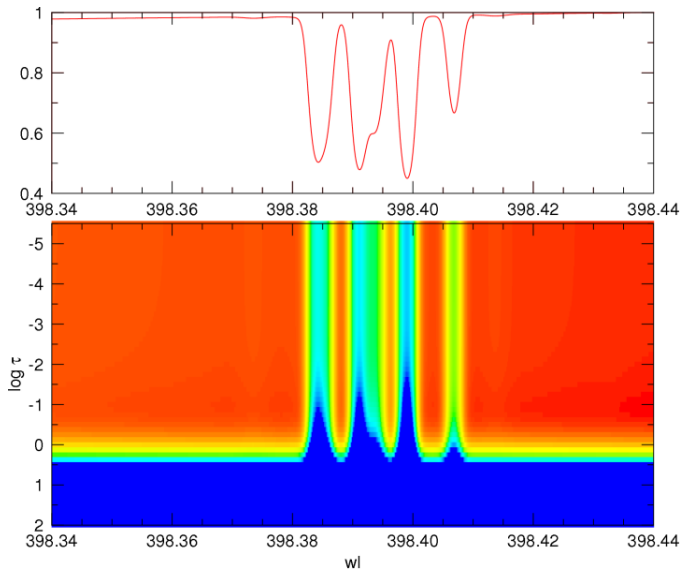


Conclusions

- Atomic diffusion is a mechanism responsible for abundance anomalies in CP stars;
- Diffusional separation of chemical elements occurs in stellar atmospheres only if the macroscopic motions are weak enough;
- Stratification of elements is mainly determined by competition between gravitational and radiative forces;
- Separation of isotopes takes place due to LID:
 - Heavy elements: heavier isotopes rise, lighter isotopes sink
 - Light elements: lighter isotopes rise, heavier isotopes sink
- LID is most effective in stellar atmospheres, it is not important in outer layers and in stellar interiors;
- Hyperfine splitting of spectral lines decelerates separation of isotopes and makes the picture more complicated;
- Microturbulence slows down the diffusion and reduces abundance gradients.

Evolution of HgII 3984 Å line

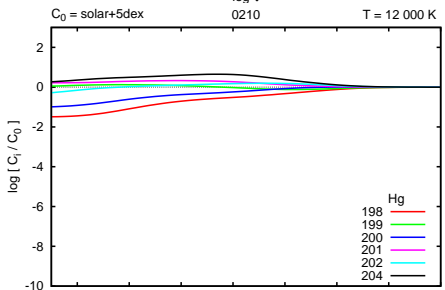
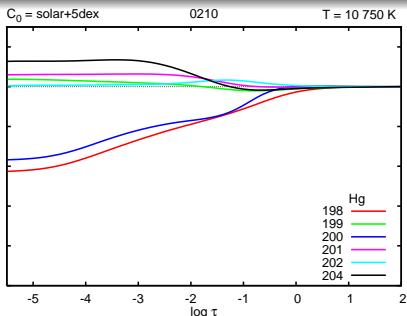
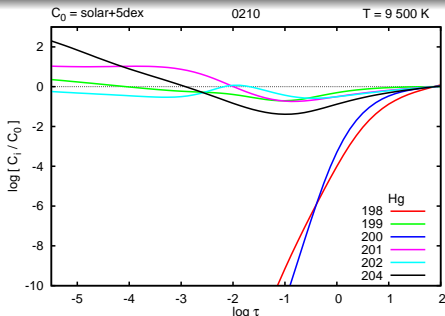
$T_{eff} = 10750$ K, $\log g = 4$, $C_0 = \text{solar} + 5\text{dex}$



$\Delta t = 1$ yr

Click on
figure
to play
movie

Dependence on effective temperature

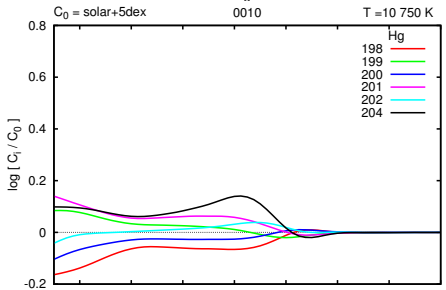
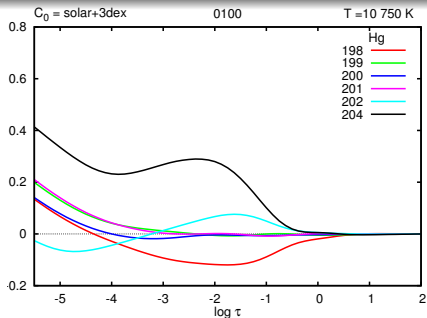
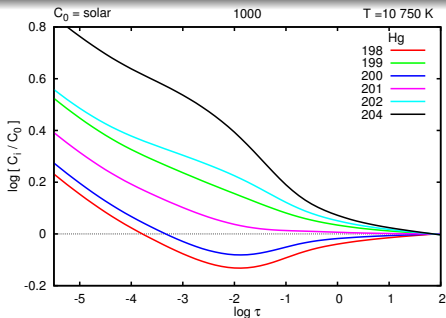


time = 210 yrs ($\Delta t = 1$ yr)

- $T_{\text{eff}} = 9\,500\text{ K}$ – fastest
- $T_{\text{eff}} = 10\,750\text{ K}$
- $T_{\text{eff}} = 12\,000\text{ K}$ – slowest

Higher T_{eff} – higher collision rates –
smaller diffusion velocity

Dependence on initial abundance of mercury



Concentrations after 10 yrs

Model atmospheres:

$T_{\text{eff}} = 10\,750\text{ K}$, $\log g = 4$,

$V \sin i = 0$

– $C_0 = \text{solar}$

– $C_0 = \text{solar} + 3\text{ dex}$

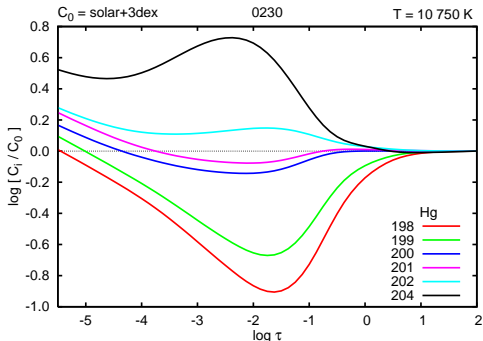
– $C_0 = \text{solar} + 5\text{ dex}$

Influence of the hyperfine splitting of Hg lines

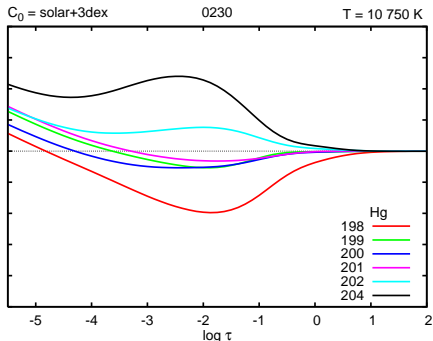
Concentration at time step 230

$$T_{\text{eff}} = 10\,750 \text{ K}, \log g = 4, C_0 = \text{solar} + 3 \text{ dex}$$

Without hyperfine splitting



With hyperfine splitting



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

General structure of programme SMART

