Diffusion and light-induced drift in stellar atmospheres

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1 Chemically peculiar stars
2 Diffusion theory
3 Description of stellar plasma
4 Radiative acceleration
5 Stratification of chemical elements
6 Isotopic anomalies in CP stars
7 Light-induced drift
8 Evolutionary modelling of isotope separation
9 Conclusions
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 $\sim$1–2 dex;
  - He-weak stars with isotopic anomaly – overabundance of $^3$He;
  - He-rich stars (21 000 – 30 000 K), $N_{\text{He}}/N_{\text{H}} \sim 0.5$ (norm $\sim 0.1$). Most massive CP stars.
Abundance anomalies

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

![Graph showing abundance anomalies for HgMn star HD 175640](image)

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).

Element Stratification in Stars: 40 Years of Atomic Diffusion.
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

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

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

Chapman-Enskog theory

Burgers’ theory

Diffusion theory: description of stellar plasma

Main equations

Diffusion velocity

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

General equation of diffusion velocity

\[ v_1 - v_2 = -\frac{N_2^2}{N_1 N_2} D_{12} \left\{ \nabla \ln \frac{N_1}{N} + \frac{N_1 N_2 (m_2 - m_1)}{N \rho} \nabla \ln P - \frac{\rho_1 \rho_2}{P \rho} (F_1 - F_2) + \frac{D_T}{D_{12}} \nabla \ln T \right\} \]

Concentration  Pressure  Forces  Temperature

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;
\( \rho_1, \rho_2 \) mass densities of particles 1 and 2, \( \rho_i = m_i N_1, \rho = \rho_1 + \rho_2 \);
\( D_{12} \) 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 ≡ accelerations.

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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:

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

$$\frac{\partial \rho_i}{\partial t} + \nabla (\rho_i v_i) = 0 \quad (1)$$
Diffusion theory: description of stellar plasma

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 $a_{i}^{\text{rad}}$, 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 $g \sim 10^4$ cm/s$^2$!
Radiative acceleration

Generic expression for radiative acceleration

\[ a_{j}^{\text{rad}} = \frac{\pi}{m_{j}c} \int_{0}^{\infty} \sigma_{\nu} F_{\nu} \, d\nu \]

where \( \sigma_{\nu} \) is absorption cross-section and \( \pi F_{\nu} \) 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 \( j \):

\[ a_{j}^{ul} = \frac{\pi}{m_{j}c} X_{j,l} \int_{0}^{\infty} \sigma_{\nu,ul} F_{\nu} \, d\nu = \frac{\pi}{m_{j}c} X_{j,l} \int_{0}^{\infty} \sigma_{ul}^{0} V(u_{\nu}, a) F_{\nu} \, d\nu \]

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; \( V(u_{\nu}, a) \) is Voigt function.

Radiative acceleration of element \( i \) in simplest approximation is given by

\[ a_{i}^{bb} = \frac{\pi}{m_{i}c} \sum_{j \in i} X_{j} \sum_{l,u > l} X_{j,l} \int_{0}^{\infty} \sigma_{ul}^{0} V(u_{\nu}, a) F_{\nu} \, d\nu \]

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 $j$:

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

The term $y_k$ represents the momentum taken away by the eject electron.
Radiative accelerations in stellar 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 & Stift 2008 – stratification in magnetic stars.
Stratified model atmospheres

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**BUT**
Simulations of the abundance anomalies require:
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Simulations of the abundance anomalies require:

- computation of the time-dependent formation of stratification, because diffusion is non-linear process
Stratified model atmospheres

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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
- $M = 0.61M_\odot$
- $T_{\text{eff}} = 12,400$ K
- $\approx 30$ Myr after ZAHB

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 – \(^3\text{He}\) in star 3 Cen A – Sargent & Jugaku, 1961

- **Hg**: 1962 W.P. Bidelman – HST (HR7775, \(\chi\) Lupi) – 2003 Dolk et al. (31 HgMn stars) ...

- **Pt**: 1973 Dworetsky & 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.

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 $^{199}\text{Hg}$ and $^{201}\text{Hg}$, the stable, odd-A isotopes.
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?
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.

- 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
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 $a^{\text{LID}}$ additional to usual radiative acceleration $a^{\text{rad}}$ (Aret & Sapar 2002, Astron. Nachr. 323, 1, 21).
- The expression for $a^{\text{LID}}$ is similar to the formula for $a^{\text{rad}}$ but instead of Voigt function its derivative relative to wavelength is to be used.
- Efficiency of LID $\varepsilon$ 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 $l \rightarrow u$

\[
\begin{align*}
    a^\text{LID}_j &= \varepsilon q \frac{\pi}{m_i c} \int_0^\infty X_{j,l} \sigma_{ul}^0 \frac{\partial V(u_\nu, a)}{\partial u} F_\nu d\nu \\
    \varepsilon &= \frac{C_u - C_l}{A_u + C_u} \\
    q &= \frac{m_j \nu_T c}{2 h\nu} = \frac{m_j \nu_T}{2} : \frac{h\nu}{c}
\end{align*}
\]

- $C_u$ 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

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Computation of LID

Acceleration due to b-b transitions including LID effect

\[ a_{bb}^j \Rightarrow a_{bb^+}^j = a_{bb}^j + a_{bb}^{LID} \]

\[ V(u, a) \Rightarrow V(u, a) + \varepsilon q \frac{\partial V(u, a)}{\partial u} \]

- 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 \((R = 5\,000\,000, \text{ corresponding Doppler shift 60 m/s})\) 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.
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:
- \( \log g = 4, T_{\text{eff}} = 9500, 10750 \text{ ja } 12000 \text{ K} \)
- \( C^0_{\text{Hg}} = \text{solar, solar+3 dex ja solar+5 dex} \)

Initial state:
- Homogeneous abundance of Hg throughout the atmosphere;
- Solar (terrestrial) ratios of isotope abundances.
Evolutionary modelling of isotope separation

**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

Mass flow $\rho V$

$C_0 =$ solar+5dex  
T = 10 750 K  
$\Delta t = 1 \text{ yr}$

Click on figure to play movie

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Time-dependent stratification of isotopes in CP stars

Mass flow $\rho V$

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

$T = 10750 \text{ K}$, $\Delta t = 1 \text{ yr}$
Evolution of isotope concentrations $\log\left(\frac{C_i}{C_0}\right)$

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

$T = 10\ 750\ K$  
$\Delta t = 1\ yr$

Click on figure to play movie
Evolutionary modelling of isotope separation

Evolution of isotope concentrations $\log\left(\frac{C_i}{C_0}\right)$

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

$T = 10,750\text{ K}$

$\Delta t = 1\text{ yr}$

Click on figure to play movie
Evolution of isotope concentrations $\log(C_i/C_0)$

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

$6500$ K

$T = 10\,750\,\text{K}$

$\Delta t = 1\,\text{yr}$

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Evolutionary modelling of isotope separation

Atmosphere with microturbulence

Final equilibrium isotope separation profiles

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

\[
\begin{align*}
\text{T} &= 10\,750\,\text{K} & \log g &= 4.0 & \rho^0 &= \text{solar+5dex} \\
\end{align*}
\]

\[
\begin{align*}
\log C_i^- & \quad \log \tau \quad \text{for } i = 198, 199, 200, 201, 202, 204 \\
\end{align*}
\]
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

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

\[ \Delta t = 1 \, \text{yr} \]

Click on figure to play movie
Dependence on effective temperature

\[ \log \left[ \frac{C_i}{C_0} \right] \]

\[ \log \tau \]

- Time = 210 yrs (\( \Delta t = 1 \) yr)
  - \( T_{\text{eff}} = 9500 \) K – fastest
  - \( T_{\text{eff}} = 10750 \) K
  - \( T_{\text{eff}} = 12000 \) K – slowest

Higher \( T_{\text{eff}} \) – higher collision rates – smaller diffusion velocity
Dependence on initial abundance of mercury

Concentrations after 10 yrs

Model atmospheres:

- $T_{\text{eff}} = 10\,750\,\text{K}$, $\log g = 4$
- $V \sin i = 0$
- $C_0 = \text{solar}$
- $C_0 = \text{solar + 3 dex}$
- $C_0 = \text{solar + 5 dex}$
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

\[
\begin{array}{c}
\log \left( \frac{C_i}{C_0} \right) \\
\log \tau
\end{array}
\]

With hyperfine splitting

\[
\begin{array}{c}
\log \left( \frac{C_i}{C_0} \right) \\
\log \tau
\end{array}
\]
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
Appendix

Structure of SMART

General structure of programme SMART

Initial block
- Initialization
- Read model
- Start arrays
- Read linelist

Main block
- Saha
- Continuous absorption
- Line absorption
- Spectrum

Specific tasks
- Relaxational NLTE
- Diffusion
- Model correction
- Clump acceleration
- Limb darkening

Output
- Next time step
- Next correction

Common data

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