

### The chemical composition: relative mass abundances



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- stellar matter (relatively) simple, because of high  $T$  &  $P$  no chemical compounds, and **atoms are completely ionized** in most parts of star.
- Def:  $X_i = X_i(m, t)$  is fraction of unit mass of **nuclei  $i$**  such that
  - Normalization:  $\sum_i X_i = 1$ ,  $(0 \leq m \leq M)$ .
    - stellar mass
    - depth coordinate
  - with  $m_i$  being the particle number / unit volume and  $m_i$  (not to be mixed with depth-coordinate  $m$ ) being the mass of nuclei  $i$
- (rel.) abundances by mass:  $X_i = \frac{m_i n_i}{\rho}$ .
- convention:  $X \equiv X_H, Y \equiv X_{He}, Z \equiv 1 - X - Y$ .
  - "metals" (incl. C, N, O, ...)

### The chemical composition: relative mass abundances

- convention:  $X \equiv X_H, Y \equiv X_{He}, Z \equiv 1 - X - Y$ .
- young stars and in envelopes of most star:  
 $X = 0.65 \dots 0.75, Y = 0.30 \dots 0.25, Z = 0.05 \dots 0.0001$ .

Abundances for 200902290001 composition:

Element	abundance	relative metal	number fraction	mass fraction	atomic mass
He	100(0)	.....	.....	0.00260	4.00260
Li	100(0)	.....	.....	.....	.....
Be	100(0)	.....	.....	.....	.....
B	100(0)	.....	.....	.....	.....
C	100(0)	.....	.....	.....	.....
N	100(0)	.....	.....	.....	.....
O	100(0)	.....	.....	.....	.....
F	100(0)	.....	.....	.....	.....
Ne	100(0)	.....	.....	.....	.....
Na	100(0)	.....	.....	.....	.....
Mg	100(0)	.....	.....	.....	.....
Al	100(0)	.....	.....	.....	.....
Si	100(0)	.....	.....	.....	.....
P	100(0)	.....	.....	.....	.....
S	100(0)	.....	.....	.....	.....
Cl	100(0)	.....	.....	.....	.....
Ar	100(0)	.....	.....	.....	.....
K	100(0)	.....	.....	.....	.....
Ca	100(0)	.....	.....	.....	.....
Ti	100(0)	.....	.....	.....	.....
V	100(0)	.....	.....	.....	.....
Cr	100(0)	.....	.....	.....	.....
Fe	100(0)	.....	.....	.....	.....
Co	100(0)	.....	.....	.....	.....
Ni	100(0)	.....	.....	.....	.....

Asplund et al. (2009) solar composition  $Z_{\text{sun}} = 0.0134$

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	$Z_s$	$Z_s/X_s$
Califan et al. (2009)	$0.0156 \pm 0.0011$	0.0213
Hondek & Gough (2011)	$0.0142 \pm 0.0005$	0.0186
Asplund et al. (2009)	0.0134	0.0181

Sun

- during late evolutionary stages this picture becomes more complicated and more  $X_i$  need to be defined; in relative massive stars **electron capture** destroys all elements  $\rightarrow$  **only neutrons**.
- note advantage of  $X_i(m, t)$ :  $X_i(r, t)$  would lead to immediate change of all  $X_i$  and dependent functions with an expansion or compression of the star.

The chemical composition: **variation with time t**

**Radiative regions** (no mixing and for now diffusion is also neglected):

— **only nuclear transmutations can alter** (create/destroy)  $X_i(m, t)$ :

$$\frac{\partial X_i}{\partial t} = \frac{m_i}{\rho} \left[ \sum_j r_{ji} - \sum_k r_{ik} \right], \quad i = 1 \dots I$$

transformation of element  $j$  into  $i$ ;  
creation of element  $i$  total nr. of elements  
transformation of element  $i$  into  $k$ ;  
destruction of element  $i$

where  $r_{ji}$  is the **nuclear reactions rate** (reactions per unit volume and time) that transforms nuclei  $j$  to  $i$ .

- note  $r_{ji}$  (and  $r_{ij}$ ) **give directly the change of  $n_i$  per second.**

The chemical composition: **variation with time t**

reaction  $p \rightarrow q$  connected with a release of energy  $\epsilon_{pq}$ .

— energy generation rate  $\epsilon$  per unit mass  $\propto r_{pq}$

$$\epsilon = \sum_{p,q} \epsilon_{pq} = \frac{1}{\rho} \sum_{p,q} r_{pq} \epsilon_{pq}$$

- We introduce energy generated from transforming **one mass unit  $m_p$  of nucleus type  $p$  into  $q$**

$$q_{pq} = \frac{\epsilon_{pq}}{m_p}, \quad \text{(energy release per unit mass when element  $p$  is converted into element  $q$ )}$$

and rewrite equation for the time-dependence of  $X_i$  in terms of  $\epsilon$ :

$$\frac{\partial X_i}{\partial t} = \sum_j \frac{\epsilon_{ji}}{q_{ji}} - \sum_k \frac{\epsilon_{ik}}{q_{ik}}$$

The chemical composition: **variation with time t**

Equation for the time-dependence of  $X_i$  in terms of  $\epsilon$ :

$$\frac{\partial X_i}{\partial t} = \sum_j \frac{\epsilon_{ji}}{q_{ji}} - \sum_k \frac{\epsilon_{ik}}{q_{ik}},$$

which represents a **system of  $I$  differential equations** ("nuclear reactions network").

- For "simple" evolution phases a single equation is sufficient, such as for hydrogen burning with an overall  $\epsilon = \epsilon_H$ , i.e.

$$\frac{\partial X}{\partial t} = -\frac{\epsilon_H}{q_H} \quad \text{with } \partial Y / \partial t = -\partial X / \partial t,$$

where  $q_H$  is the energy release per unit mass when hydrogen is converted into helium.

- similar to nuclear time scale  $\tau_n = E_n / L$ , time scales  $\tau_{X_i}$  for every individual nuclear burning can be defined. Because nuclear energy reservoir  $E_n \propto \int X_i dm \implies \tau_n = \tau_{X_i}$  for exhaustion of element  $i$ .

The chemical composition: **diffusion**  
(microscopic effects that can change chemical composition)

Gradients in chemical **concentration, temperature and pressure** cause **diffusion** of elements which **either tends to smooth out differences (concentration diffusion) or make heavier elements to migrate to either higher  $T$  or  $P$ .**

Concentration diffusion:

- concentration  $c$  of particles of a certain species:  $c := \frac{n_i}{n} \cdot \text{total number density}$

number density of species  $i$  total number density  
 $n_i$   $n$   
diffusion coefficient

— **flux  $j_D$  of concentration (Fick's 1st law):**  $j_D = -D \nabla c$ .

The chemical composition: **diffusion**

Concentration diffusion:

**flux  $j_D$  of concentration** (Fick's 1<sup>st</sup> law):  $j_D = -D \nabla c$ .

- to obtain an order-of-magnitude estimate of the characteristic diffusion time scale  $\tau_D$  we use

$$j_D = c v_D \rightarrow v_D = -\frac{D}{c} \nabla c,$$

diffusion velocity

and continuity equation  $\frac{\partial c}{\partial t} = -\nabla \cdot j_D$  to obtain

$$\frac{\partial c}{\partial t} = \nabla \cdot (D \nabla c) \xrightarrow{\text{constant } D} \frac{\partial c}{\partial t} = D \nabla^2 c \rightarrow \tau_D \simeq \frac{S^2}{D}$$

characteristic length of variation of  $c$

The chemical composition: **diffusion**

All three diffusion types can be formally written as

$$v_D = -\frac{1}{c} D (\nabla c + k_T \nabla \ln T + k_P \nabla \ln P).$$

coefficients of order unity

Combined effect of concentration and temperature diffusion:

- we assume  $\nabla T$  perpendicular to x-y plane in cartesian coordinates.  
 - particle flux ( $j = cv$ ) in +z direction is then

$$j^+ = \frac{1}{6} c (-\ell) \bar{v} (-\ell),$$

$\ell$ ...particle mean free path

from integration (averaging) of  $(\cos)^2$  over (unit) solid angle (1 hemisphere)

where mean velocity  $\bar{v}$  and concentration  $c$  are taken at  $z = -\ell$ , the location of the particle's last encounter before entering the x-y plane.

The chemical composition: **diffusion**

Combined effect of concentration and temperature diffusion:

- particle flux ( $j = cv$ ) in +z direction is  $j^+ = \frac{1}{6} c (-\ell) \bar{v} (-\ell)$ .

- particle flux in +z and -z direction is

$$j^\pm = \frac{1}{6} \left( c(0) \mp \frac{\partial c}{\partial z} \ell \right) \left( \bar{v}(0) \mp \frac{\partial \bar{v}}{\partial z} \ell \right),$$

in which we expanded  $c$  and  $\bar{v}$  about  $z = 0$  to first order.

→ net flux:  $j = j^+ - j^- = -\frac{1}{3} \left( \frac{\partial c}{\partial z} \ell \bar{v} + \frac{\partial \bar{v}}{\partial z} \ell c \right)$ ,

which in general does not vanish, i.e. we have obtained Fick's law.

The chemical composition: **diffusion**

Combined effect of concentration and temperature diffusion:

net flux:  $j = j^+ - j^- = -\frac{1}{3} \left( \frac{\partial c}{\partial z} \ell \bar{v} + \frac{\partial \bar{v}}{\partial z} \ell c \right)$ . (a)

The relative diffusion velocity  $v_{D1} - v_{D2}$  between two types of particles (1,2) with fluxes  $j_1, j_2$  and concentrations  $c_1, c_2$  is

$$v_{D1} - v_{D2} = \frac{j_1}{c_1} - \frac{j_2}{c_2}.$$

molecular weight of particle type  $i$

→ insert (a) into (b) and using  $\bar{v}_i = (3RT/\mu_i)^{1/2}$  leads to

$$v_{D1} - v_{D2} = -\frac{D}{c_1 c_2} \left( \frac{\partial c_1}{\partial z} + k_T \frac{\partial \ln T}{\partial z} \right).$$

concentration + temperature diffusion

The chemical composition: **diffusion**

Combined effect of **concentration** and **temperature diffusion**:

$$v_{D1} - v_{D2} = -\frac{D}{c_1 c_2} \left( \frac{\partial c_1}{\partial z} + k_T \frac{\partial \ln T}{\partial z} \right)$$

In a mixture of two species ( $i = 1, 2$ )  $D$  and  $k_T$  have the form (Landau, Lifshitz, vol. 6, 1987)

$$D = \frac{1}{3} (c_2 \ell_1 \bar{v}_1 + c_1 \ell_2 \bar{v}_2) = \left( \frac{3kT}{3} \right)^{1/2} (c_2 \ell_1 \mu_1^{-1/2} + c_1 \ell_2 \mu_2^{-1/2}),$$

$$k_T = \frac{1}{2} \frac{\ell_1 \sqrt{\mu_2} - \ell_2 \sqrt{\mu_1}}{\ell_1 c_2 \sqrt{\mu_2} + \ell_2 c_1 \sqrt{\mu_1}} c_1 c_2 (c_2 - c_1),$$

where  $\ell_1$  and  $\ell_2$  are the mean free paths of the two species, and  $0 < |k_T| \lesssim 1$ .  $k_T > 0$  for a H-He gas mixture.

The chemical composition: **diffusion**

Combined effect of **concentration** and **temperature diffusion**:

$$v_{D1} - v_{D2} = -\frac{D}{c_1 c_2} \left( \frac{\partial c_1}{\partial z} + k_T \frac{\partial \ln T}{\partial z} \right),$$

$$D = \frac{1}{3} (c_2 \ell_1 \bar{v}_1 + c_1 \ell_2 \bar{v}_2) = \left( \frac{3kT}{3} \right)^{1/2} (c_2 \ell_1 \mu_1^{-1/2} + c_1 \ell_2 \mu_2^{-1/2}),$$

$$k_T = \frac{1}{2} \frac{\ell_1 \sqrt{\mu_2} - \ell_2 \sqrt{\mu_1}}{\ell_1 c_2 \sqrt{\mu_2} + \ell_2 c_1 \sqrt{\mu_1}} c_1 c_2 (c_2 - c_1).$$

→  $D$  is of order:  $D \approx \left( \frac{3kT}{3} \right)^{1/2} \ell \approx \frac{1}{3} v^* \ell$ .

for pure temperature diffusion:  $\text{sign}(v_D) = -\text{sign}(\partial \ln T / \partial z)$ .

-e.g., with  $v_D = v_H - v_{He} > 0$  → hydrogen diffuses in the direction of lower temperature, i.e. “upwards” in the star.

The chemical composition: **diffusion**

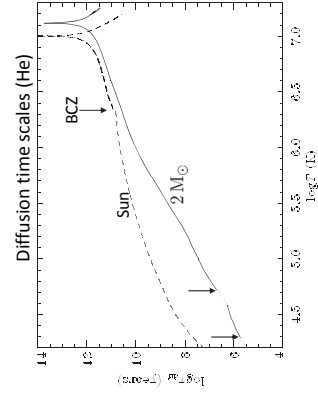
Combined effect of **concentration** and **temperature diffusion**:

$$v_{D1} - v_{D2} = -\frac{D}{c_1 c_2} \left( \frac{\partial c_1}{\partial z} + k_T \frac{\partial \ln T}{\partial z} \right),$$

$$D \approx \left( \frac{3kT}{3} \right)^{1/2} \ell \approx \frac{1}{3} v^* \ell.$$

- For central solar region ( $T \approx 10^7$  K,  $\rho \approx 100$  g cm<sup>-3</sup>):  
 $\ell \approx 10^{-8}$  cm and  $D \approx 6$  cm<sup>2</sup> s<sup>-1</sup>,  $S \approx R_\odot \approx 10^{11}$  cm

→  $\tau_D \approx S^2/D \approx 10^{13}$  years  $>$  age<sup>Universe</sup>,  
 yet diffusion is important for solar evolution  
 (from testing models against helioseismology) !!



Aerts, Christensen-Dalsgaard, Kurtz(2010)  
 Figure 3.2

The chemical composition: **diffusion**

Combined effect of **concentration**, **temperature** & **pressure diffusion**:

The chemical composition: **diffusion**

Pressure diffusion (gravitational settling):

- Diffusion in isothermal layers exist due to  $\nabla P \neq 0$ .

- Here we only consider isothermal layer in hydrostatic equilibrium with a two-component ( $i = 1, 2$ ) perfect gas:

$$H_{P_i} = \frac{P_i}{g \rho_i} = \frac{\mathfrak{R}T}{g \mu_i}, \quad \text{where } dP_i/dz = -g\rho_i; \quad P_i = \mathfrak{R}\rho_i T / \mu_i.$$

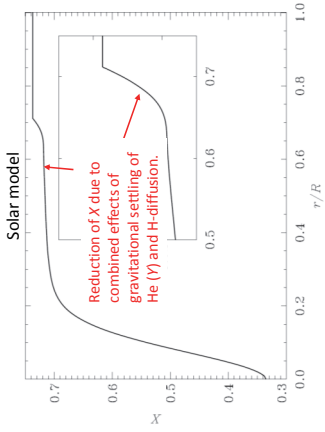
- because concentration  $c_i \propto P_i \propto \exp(-z/H_{P_i})$

→ component with larger  $\mu_i$  "falls off" faster with  $z$ , i.e. **heavier element "moves below" lighter one.**

- with  $|k_P| \simeq |k_T| \simeq 1$  gravitational settling typically takes also a long time, but **is not unimportant, for example, in our Sun!**

The chemical composition: **diffusion**

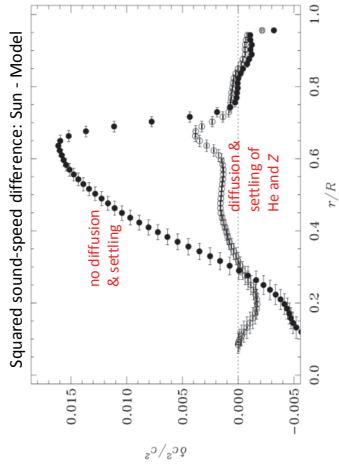
Combined effect of all diffusion effects:



Christensen-Dalsgaard, Di Mauro (2007)

The chemical composition: **diffusion**

Combined effect of all diffusion effects:



Christensen-Dalsgaard, Di Mauro (2007)

The chemical composition: **diffusion**

- from the continuity equation for concentration  $c$  and use of the definition of the (total) diffusion velocity  $v_D$ , one can derive the following expression when **using  $X_i$  instead of  $c$**  (Thoul et al. 1994):

$$\frac{\partial X_i}{\partial t} = - \frac{1}{\rho r^2} \frac{\partial}{\partial r} \left[ r^2 X_i T^{5/2} \left( A_P(i) \frac{\partial \ln p}{\partial r} + A_T(i) \frac{\partial \ln T}{\partial r} + \underbrace{\sum_{k \neq i, \text{He}^4} A_k(i) \frac{\partial \ln C_k}{\partial r}}_{\text{because of mass and charge conservation}} \right) \right].$$

because of mass and charge conservation

- additional effect of **radiative levitation**: coupling of radiation field to partially ionized atoms results in a **net upward force**, counteracting downward gravitational settling, which can lead to **strong variations of  $X_i$  at stellar surface.**

The chemical composition: **variation with time t**

**Convective regions:**

- Mixing due to turbulent motion is **very fast** (years to minutes) compared to **nuclear time scale**, i.e. within convection zone (CZ)

$$\frac{\partial X_i}{\partial m} = 0,$$

i.e. composition remains homogeneous.

The graph shows the chemical composition  $X_i$  on the vertical axis and mass  $m$  on the horizontal axis. A horizontal line at  $X_i = \bar{X}_i$  spans from mass  $m_1$  to  $m_2$ , labeled as the convection zone (CZ). Outside this zone, the composition varies with mass.

The chemical composition: **variation with time t**

**Convective regions:**

The graph shows the chemical composition  $X_i$  on the vertical axis and mass  $m$  on the horizontal axis. A step change in composition occurs at masses  $m_1$  and  $m_2$ , defining the convection zone (CZ). The composition is constant at  $\bar{X}_i$  within the CZ but changes at the boundaries. Labels  $X_{i22}$ ,  $\bar{X}_i$ , and  $X_{i11}$  are shown on the vertical axis.

- Locations  $m_1$  and  $m_2$  can change with time  $t$  and so does  $\bar{X}_i(t)$ :  
 change due to nuclear reactions  
 change due to boundaries moving into inhomogeneous composition (dredge-up).

$$\frac{\partial \bar{X}_i}{\partial t} = \frac{1}{m_2 - m_1} \times \left( \int_{m_1}^{m_2} \frac{\partial X_i}{\partial t} dm + \frac{\partial m_2}{\partial t} (X_{i2} - \bar{X}_i) - \frac{\partial m_1}{\partial t} (X_{i1} - \bar{X}_i) \right)$$

The chemical composition: **variation with time t**

**Convective regions:**

- For very fast nuclear transmutations (very short  $t_n$ ) “instantaneous” mixing is no longer valid.
- **Convective mixing is treated as a diffusive process** with diffusion velocities  $v_m$  estimated from the mixing-length ( $\ell_m$ ) approach, i.e. an additional term such as (Langer et al. 1985)

$$\frac{\partial}{\partial r} \left[ D_c \frac{\partial X_i}{\partial r} \right] = \frac{\partial}{\partial r} \left[ \left( \frac{1}{3} v_m \ell_m \right) \frac{\partial X_i}{\partial r} \right],$$

is added to the equation for  $\partial X_i / \partial t$ , where  $D_c$  is typically orders of magnitude larger than the diffusion constants  $D$ ,  $k_t$  and  $k_p$  for concentration, temperature and pressure diffusion.