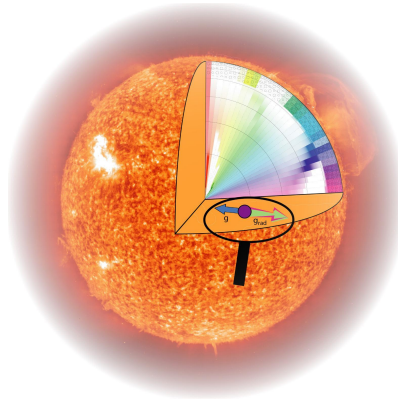


# Atomic diffusion

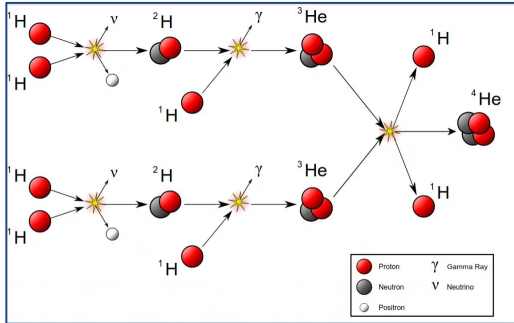


Morgan Deal  
LUPM, University of Montpellier

What can affect chemical elements in the Sun?

# What can affect chemical elements in the Sun?

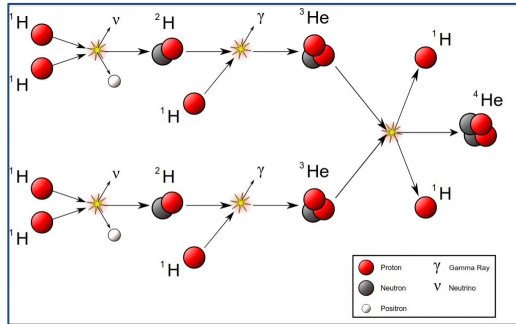
## Nuclear reactions



- PP chain
- CNO cycle
- Proton capture
- ...

# What can affect chemical elements in the Sun?

## Nuclear reactions



- PP chain
- CNO cycle
- Proton capture
- ...

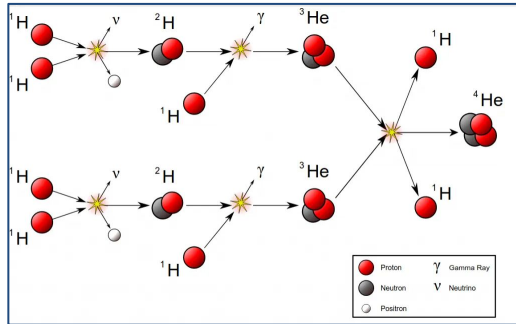
## Accretion



- From a companion
- Planet engulfment
- Protoplanetary disk
- ...

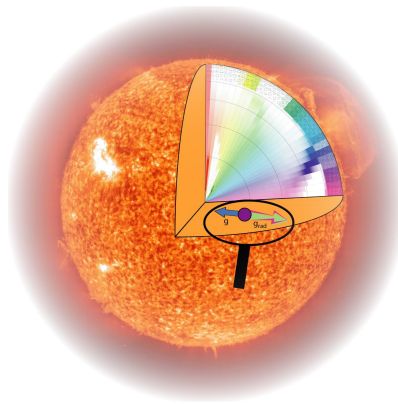
# What can affect chemical elements in the Sun?

## Nuclear reactions



- PP chain
- CNO cycle
- Proton capture
- ...

## Internal transport



- Convection
- Rotation induced mixing
- **Atomic diffusion**
- ...

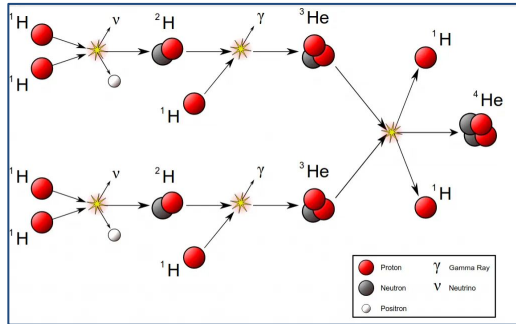
## Accretion



- From a companion
- Planet engulfment
- Protoplanetary disk
- ...

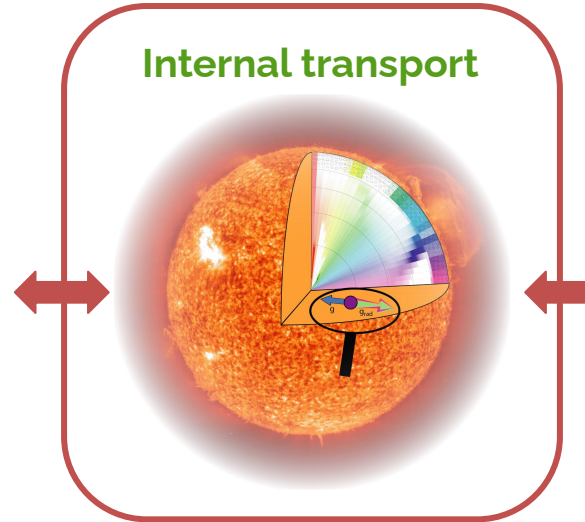
# What can affect chemical elements in the Sun?

## Nuclear reactions



- PP chain
- CNO cycle
- Proton capture
- ...

## Internal transport



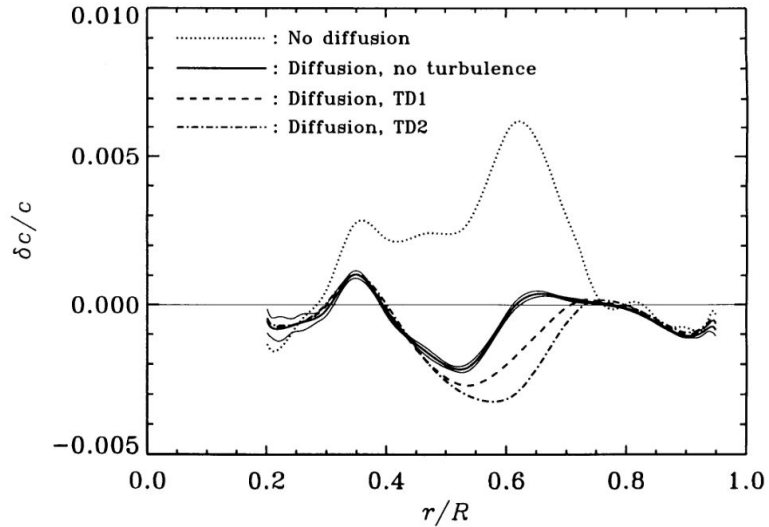
- Convection
- Rotation induced mixing
- **Atomic diffusion**
- ...

## Accretion

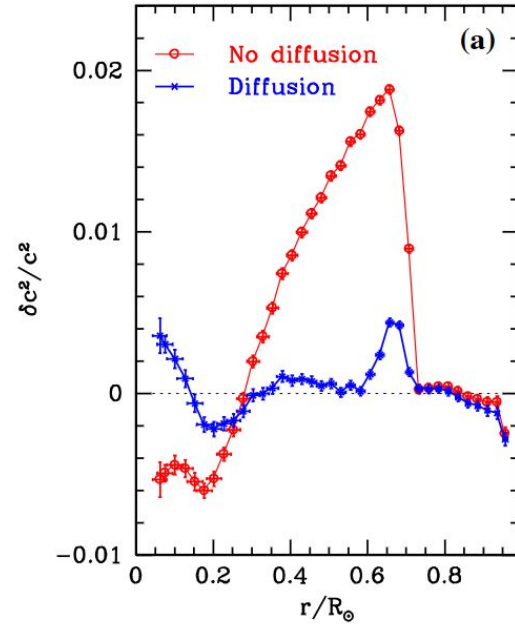


- From a companion
- Planet engulfment
- Protoplanetary disk
- ...

- Sun (Bahcall & Pinsonneault 1992; Bahcall+1995; Christensen-Dalsgaard+1996; Richard+1996; Ciaccio+1997; Gabriel 1997; Morel+1997; Brun+1998; Elliott 1998; Turcotte+1998b; .).

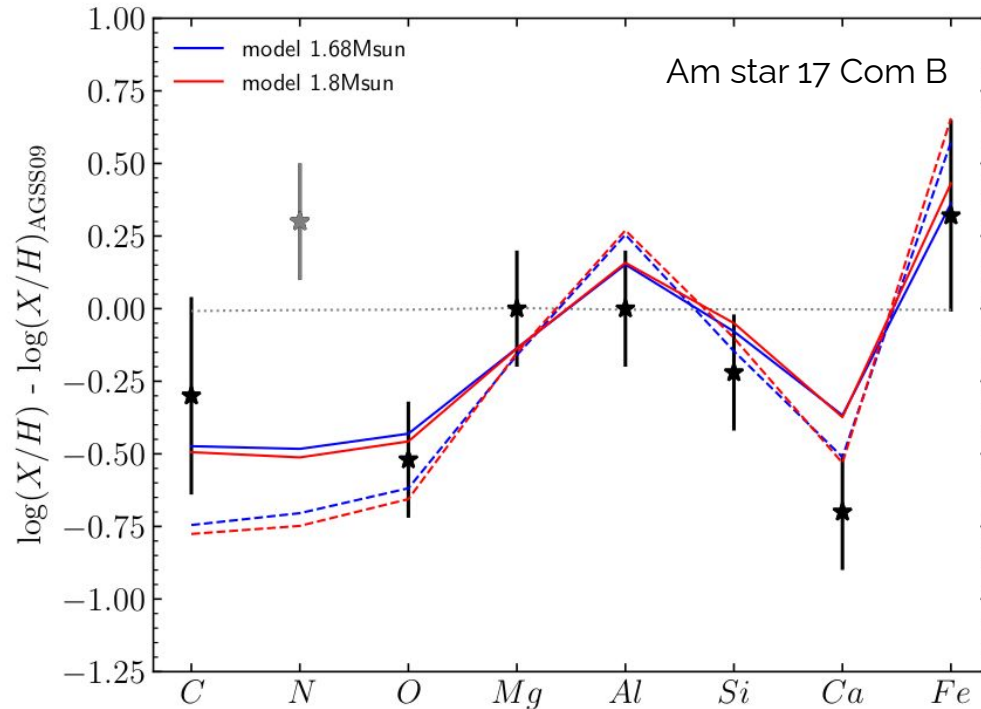


Christensen Dalsgaard+ 1993



Basu 2016

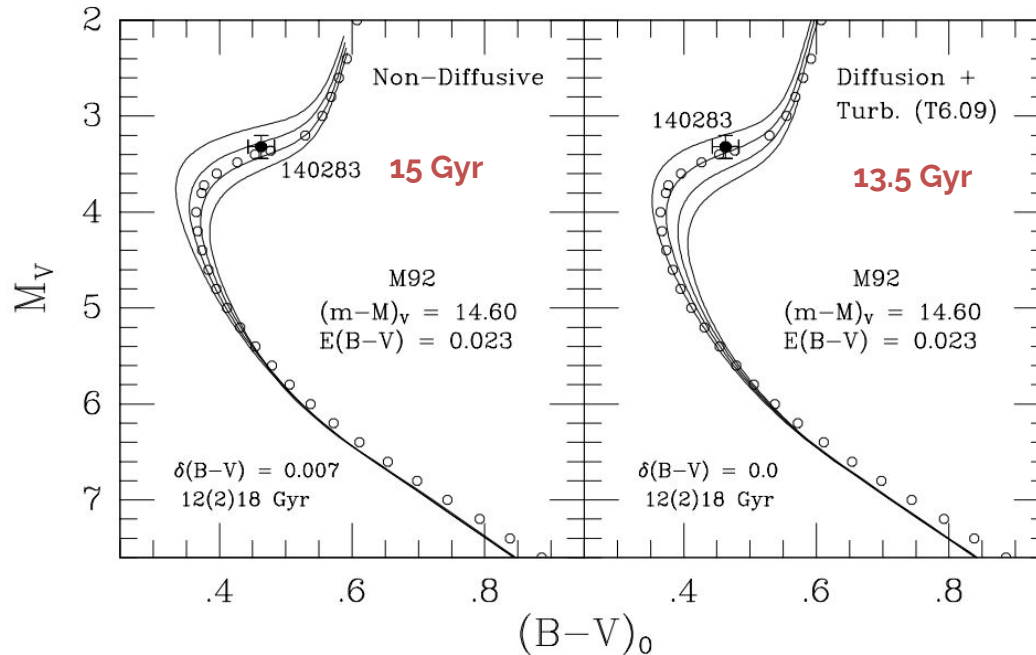
- **Sun** (Bahcall & Pinsonneault 1992; Bahcall+1995; Christensen-Dalsgaard+1996; Richard+1996; Ciaccio+1997; Gabriel 1997; Morel+1997; Brun+1998; Elliott 1998; Turcotte+1998b; .).
- **CP stars** (Praderie 1967; Michaud 1970a; Watson 1970, 1971; .).



Deal & Monier 2020

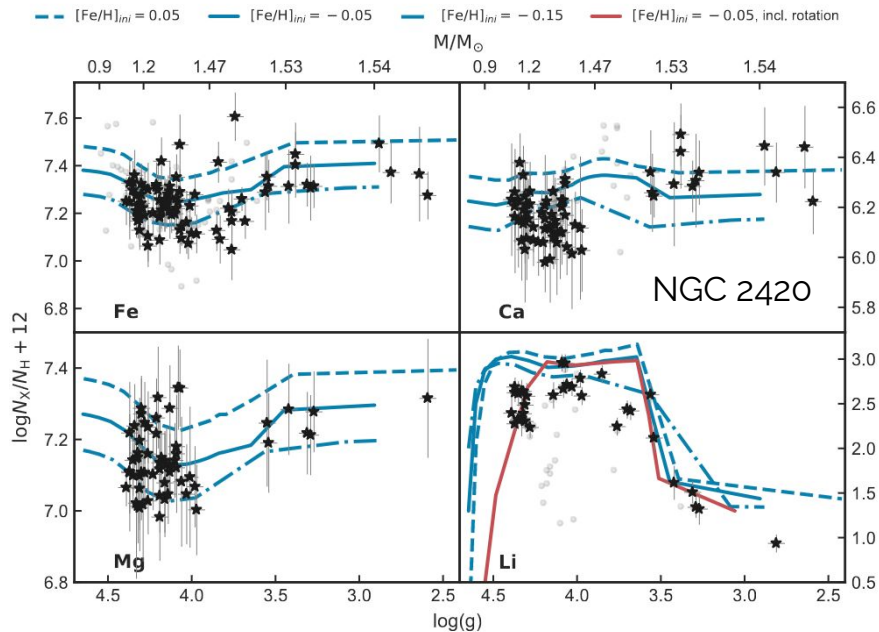


- **Sun** (Bahcall & Pinsonneault 1992; Bahcall+1995; Christensen-Dalsgaard+1996; Richard+1996; Ciaccio+1997; Gabriel 1997; Morel+1997; Brun+1998; Elliott 1998; Turcotte+1998b; .).
- **CP stars** (Praderie 1967; Michaud 1970a; Watson 1970, 1971; .).
- **Clusters:** - Lower ages when atomic diffusion is taken into account



VandenBerg+2002

- **Sun** (Bahcall & Pinsonneault 1992; Bahcall+1995; Christensen-Dalsgaard+1996; Richard+1996; Ciaccio+1997; Gabriel 1997; Morel+1997; Brun+1998; Elliott 1998; Turcotte+1998b; ..).
- **CP stars** (Praderie 1967; Michaud 1970a; Watson 1970, 1971; ..).
- **Clusters:** - Lower ages when atomic diffusion is taken into account



- **Abundance trends** (Korn+2007; Norlander+2012; Gruyters+2013,+2016; Bertelli Motta+2015; Dotter+2017; Souto+2018; Semenova+2020; ..)

Semenova+2020

## Diffusion equation

$$\rho \frac{\partial X_i}{\partial t} = \frac{1}{r^2} \frac{\partial}{\partial r} \left[ r^2 \rho \boxed{D_{\text{turb}}} \frac{\partial X_i}{\partial r} \right] - \frac{1}{r^2} \frac{\partial}{\partial r} \left[ r^2 \rho \boxed{v_i} \right] + A_i m_p \left[ \sum_j (r_{ji} - r_{ij}) \right]$$

↓ ↓ ↓

Turbulent processes Atomic diffusion Nuclear reactions

## Diffusion velocities (trace element)

$$v_i = D_{ip} \left[ -\frac{\partial \ln X_i}{\partial r} + \frac{A_i m_p}{kT} (g_{rad,i} - g) + \frac{(\bar{Z}_i + 1) m_p g}{2kT} + \kappa_T \frac{\partial \ln T}{\partial r} \right]$$

↓ ↓

Radiative acceleration      Gravitational settling

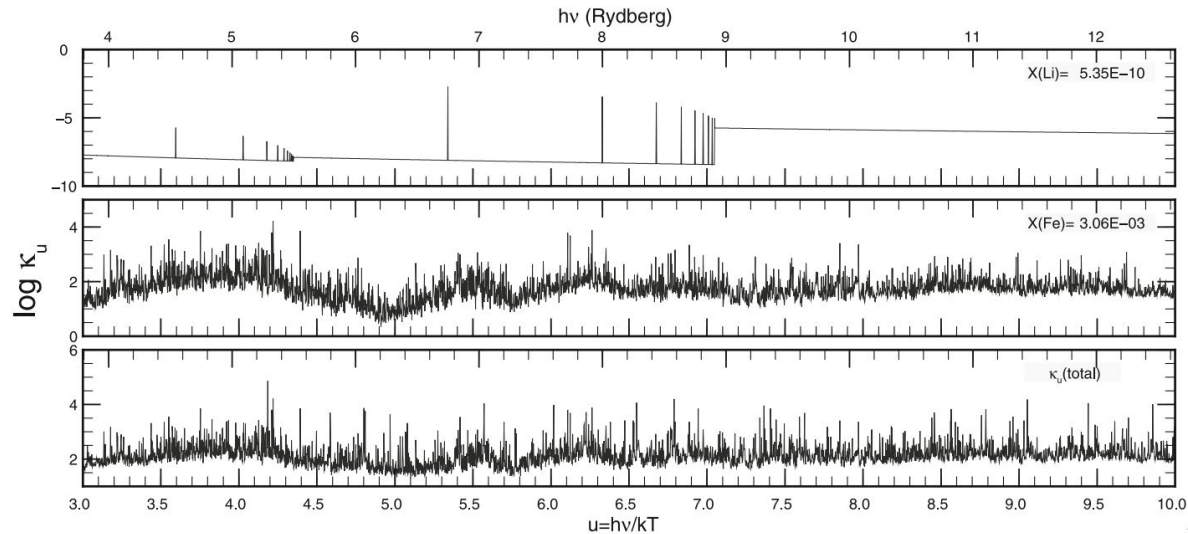
$$D_{ip} \propto \frac{1}{Z_i^2}$$

**Partial ionisation** is crucial for atomic diffusion computations !

# Radiative acceleration

$$g_{rad,i} = \frac{1}{4\pi r^2} \frac{L\kappa_R}{cX_i} \int_0^\infty \frac{\kappa_{u,i}}{\kappa_{u,tot}} \mathcal{P}(u) du$$

Monochromatic opacities

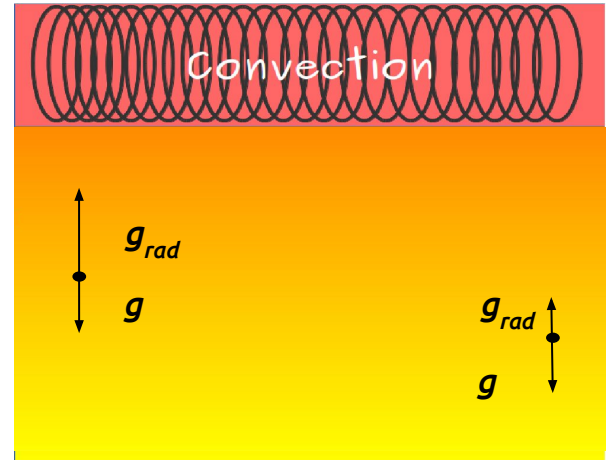


Richer & Michaud 2005

Atomic diffusion is efficient in radiative zones

$$D_{\text{conv}} \approx 10^{13} \text{ cm}^2 \cdot \text{s}^{-1}$$

$$D_{\text{He}} \approx 3.6 \text{ cm}^2 \cdot \text{s}^{-1}$$

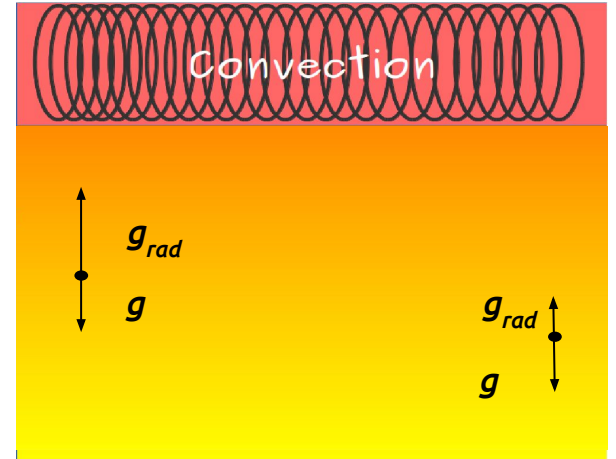
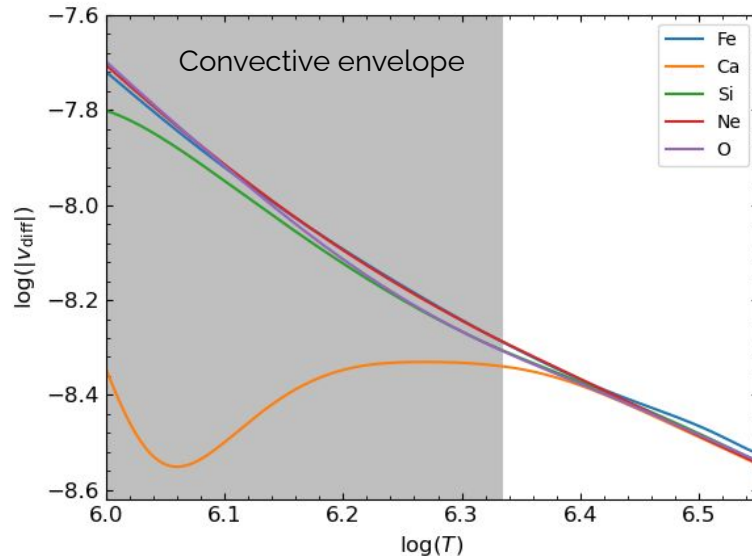


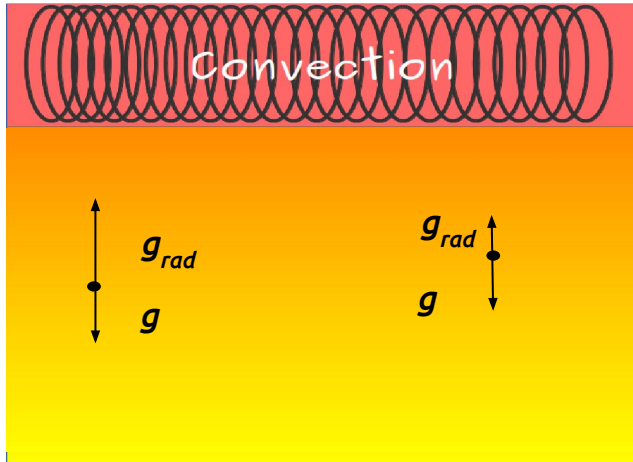
Atomic diffusion is efficient in radiative zones

$$D_{\text{conv}} \approx 10^{13} \text{ cm}^2 \cdot \text{s}^{-1}$$

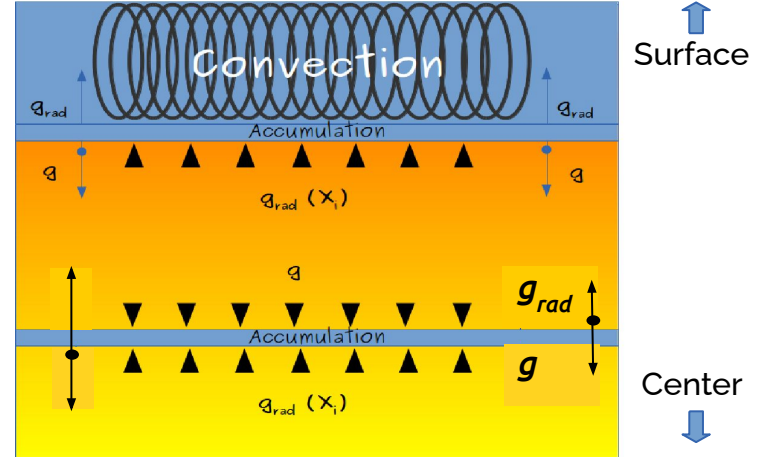
$$D_{\text{He}} \approx 3.6 \text{ cm}^2 \cdot \text{s}^{-1}$$

It is more efficient close to the surface





Leads to accumulation of some elements



These effects are different **for each element** and depend on :

- the **abundance** of the element
- the **ionisation state**
- the **photon flux**

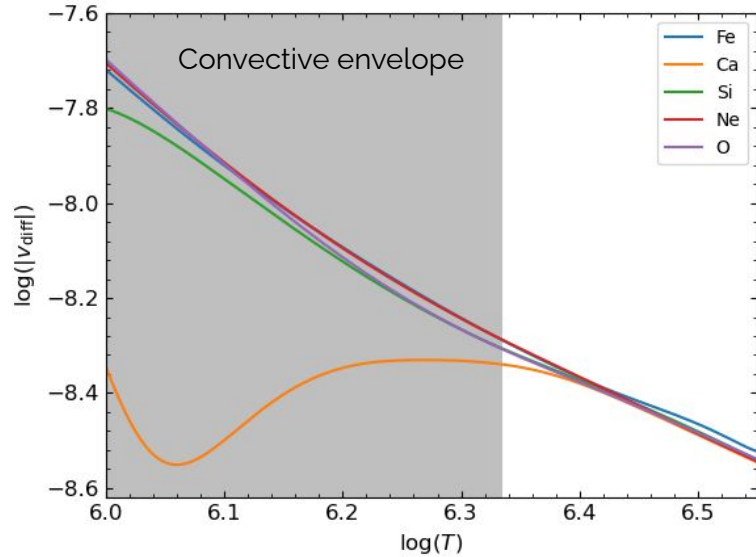


**Direct influence** on stellar **structure** and **surface abundances**

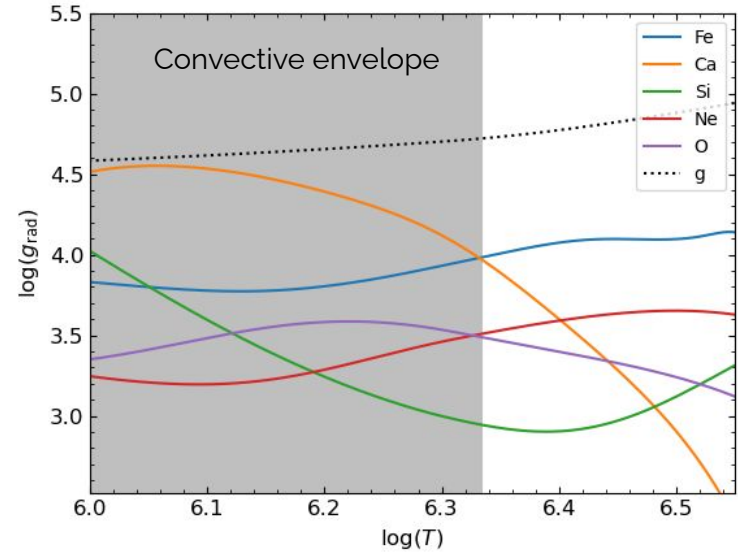


# Radiative accelerations in the Sun

Velocities

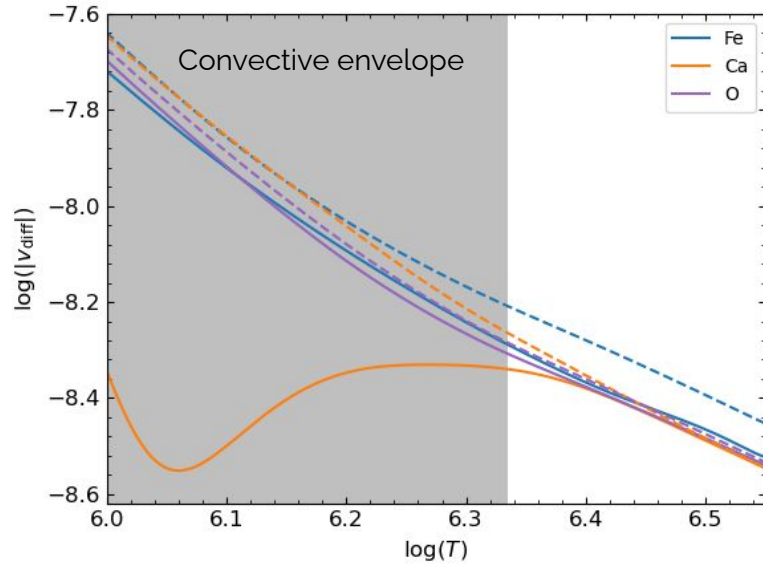


radiative accelerations

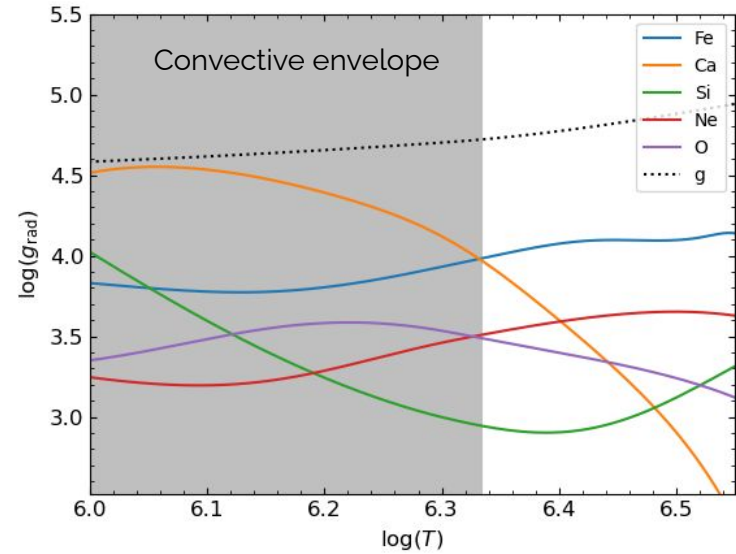


# Radiative accelerations in the Sun

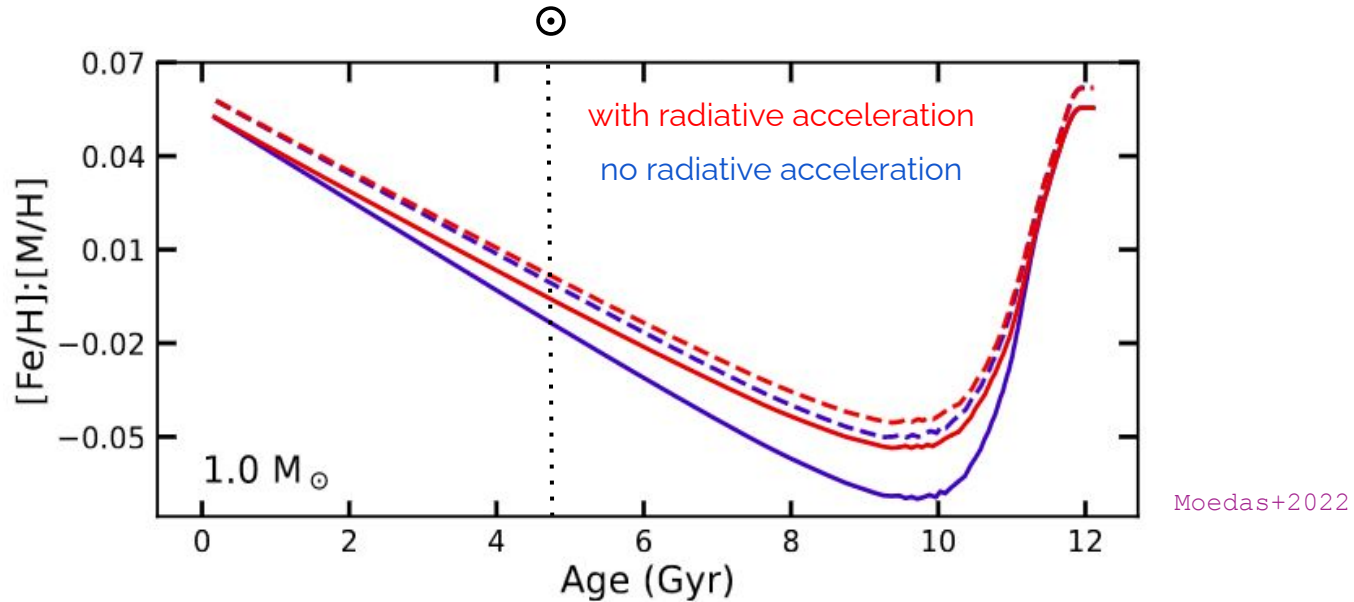
## Velocities



## radiative accelerations



# Evolution of the surface abundances of solar models



Even if  $g > g_{\text{rad}}$ , radiative accelerations have an impact on solar models

# Possible impact of iron opacity increase on iron $g_{\text{rad}}$ (toy model)

Iron opacity underestimated by 30-400% at the  
bottom of the CE of the Sun ([Bailey+2015](#))

## Possible impact of iron opacity increase on iron $g_{\text{rad}}$ (toy model)

Iron opacity underestimated by 30-400% at the  
bottom of the CE of the Sun (Bailey+2015)

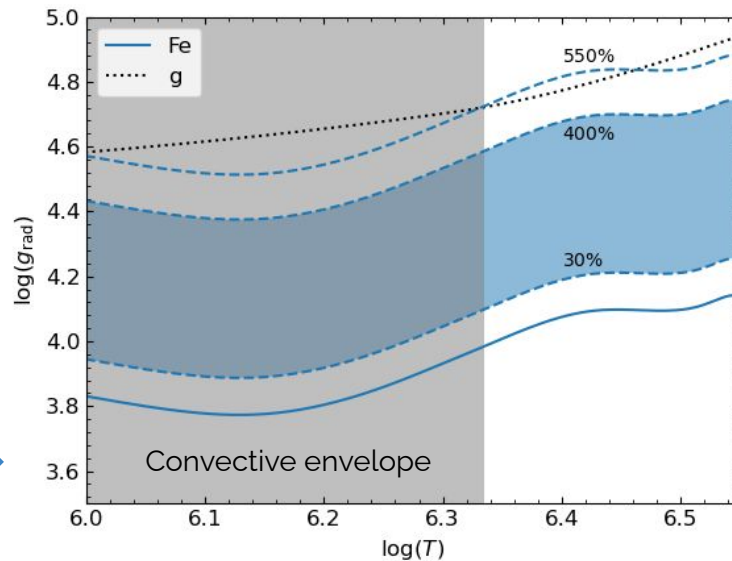
The determination of  $g_{\text{rad}}$  requires the full spectra  
and current theoretical computations cannot (**yet!**)  
explain it

# Possible impact of iron opacity increase on iron $g_{\text{rad}}$ (toy model)

Iron opacity underestimated by 30-400% at the bottom of the CE of the Sun (Bailey+2015)

The determination of  $g_{\text{rad}}$  requires the full spectra and current theoretical computations cannot (**yet!**) explain it

If we assume that the whole spectra is affected in the same way (**which is not the case!**)



# Implementation in stellar evolution codes

## Diffusion velocities

(for mixture of metals)

- Burger 1969
  - Chapman & Cowling 1970
  - Michaud & Proffitt 1993
  - Thoul+1994
-

# Implementation in stellar evolution codes

## Diffusion velocities

(for mixture of metals)

- Burger 1969
  - Chapman & Cowling 1970
  - Michaud & Proffitt 1993
  - Thoul+1994
- 

## Radiative accelerations

- direct use of atomic data (for atmospheres)
  - use of opacity tables with fixed frequency grids (Montréal/Montpellier code, Turcotte+1998; OPCD, Seaton 2005)
  - Single-Valued Parameter approximation (LeBlanc & Alecian 2004, 2020)
-



# Implementation in stellar evolution codes

## Diffusion velocities

(for mixture of metals)

- [Burger 1969](#)
  - [Chapman & Cowling 1970](#)
  - [Michaud & Proffitt 1993](#)
  - [Thoul+1994](#)
- 

## Radiative accelerations

- direct use of atomic data (for atmospheres)
  - use of opacity tables with fixed frequency grids (Montréal/Montpellier code, [Turcotte+1998](#); OPCODE, [Seaton 2005](#))
  - Single-Valued Parameter approximation ([LeBlanc & Alecian 2004,2020](#))
- 

## Opacities

- **OP** monochromatic opacities (OPCODE, [Seaton 2005](#))
- **OPAL** monochromatic opacities (Montpellier/Montréal code, not public)
- **SCO-RCG** monochromatic opacities (Ni, [Hui-Bon-hoa+2022](#), not public)
- **OPLIB** monochromatic opacities ([Colgan+2016](#))

# Implementation in stellar evolution codes

CESTAM  
Montpellier/Montréal code  
TGECC  
MESA

## Diffusion velocities (for mixture of metals)

- + + + - Burger 1969
- + - Chapman & Cowling 1970
- + - Michaud & Proffitt 1993
- + - Thoul+1994

---

- direct use of atomic data (for atmospheres)

## Radiative accelerations

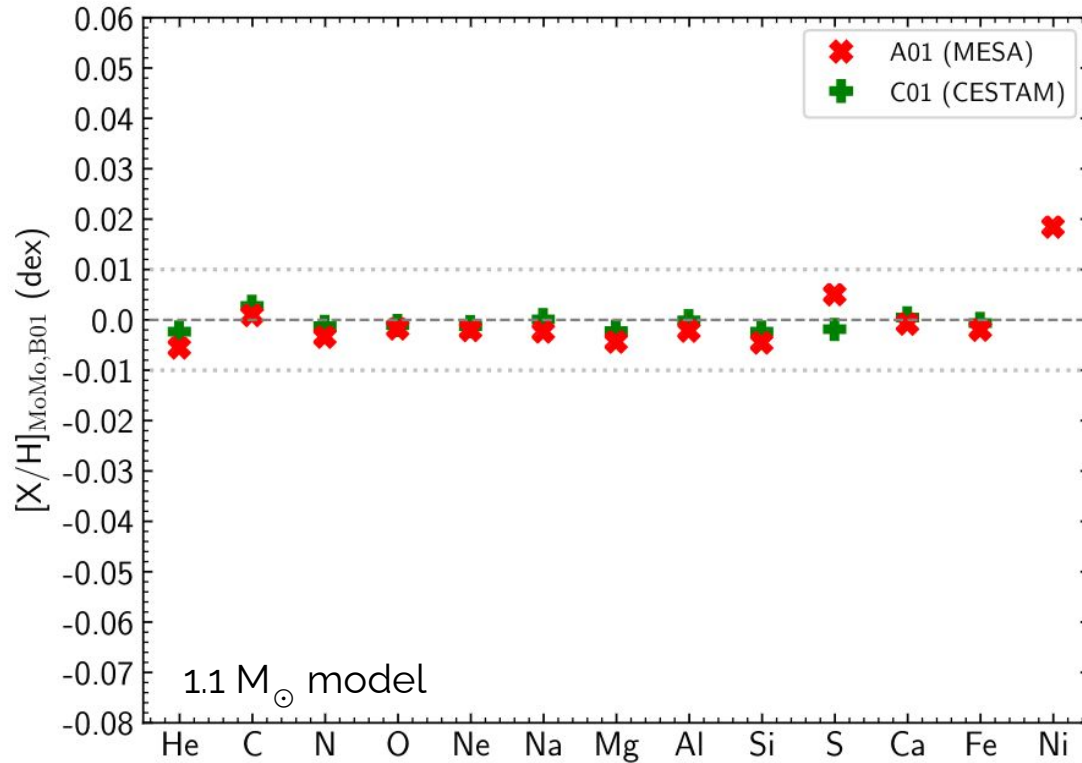
- + + - use of opacity tables with fixed frequency grids (Montréal/Montpellier code, Turcotte+1998; OPCD, Seaton 2005)
- + + + - Single-Valued Parameter approximation (LeBlanc & Alecian 2004, 2020)

---

## Opacities

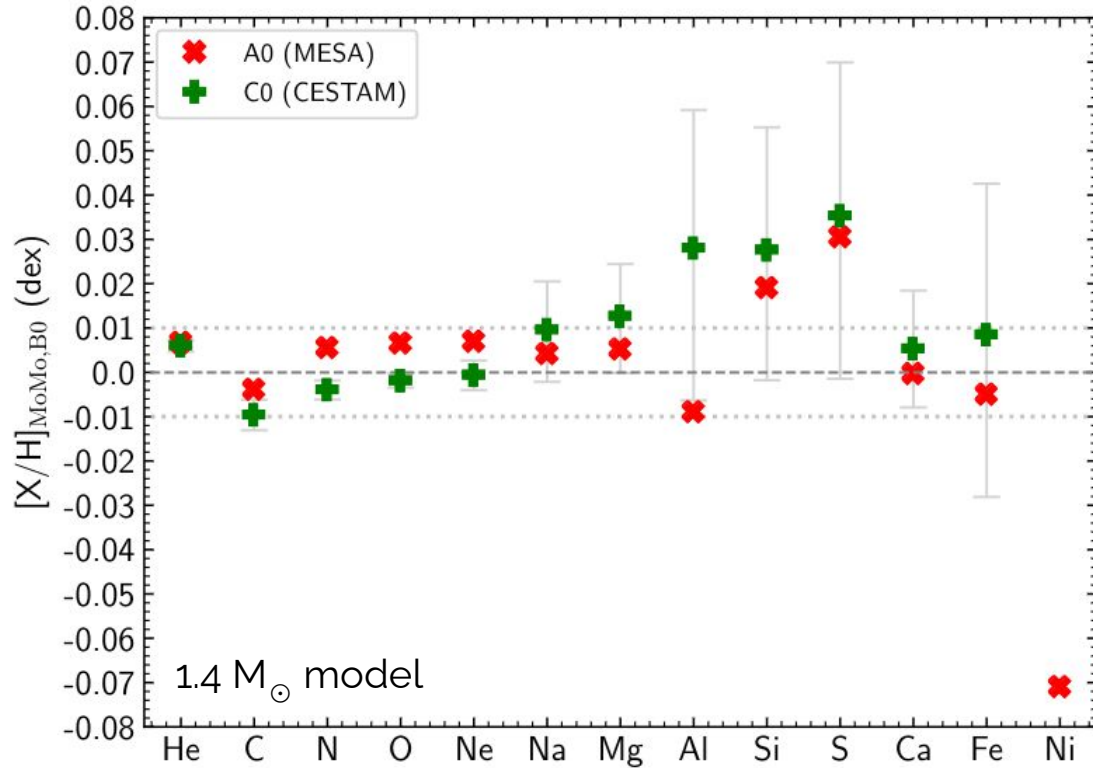
- + + + - **OP** monochromatic opacities (OPCD, Seaton 2005)
- + - **OPAL** monochromatic opacities (Montpellier/Montréal code, not public)
- + - **SCO-RCG** monochromatic opacities (Ni, Hui-Bon-hoa+2022, not public)
- **OPLIB** monochromatic opacities (Colgan+2016)

# Comparisons between codes



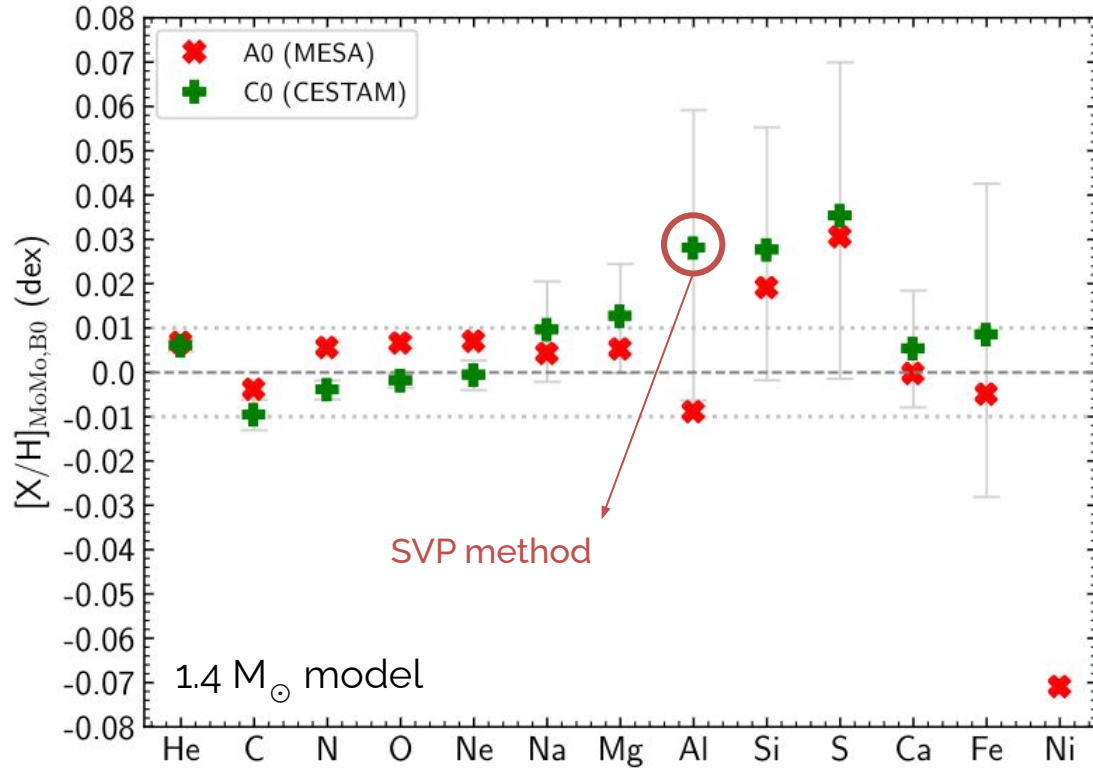
Campilho+2022

# Comparisons between codes



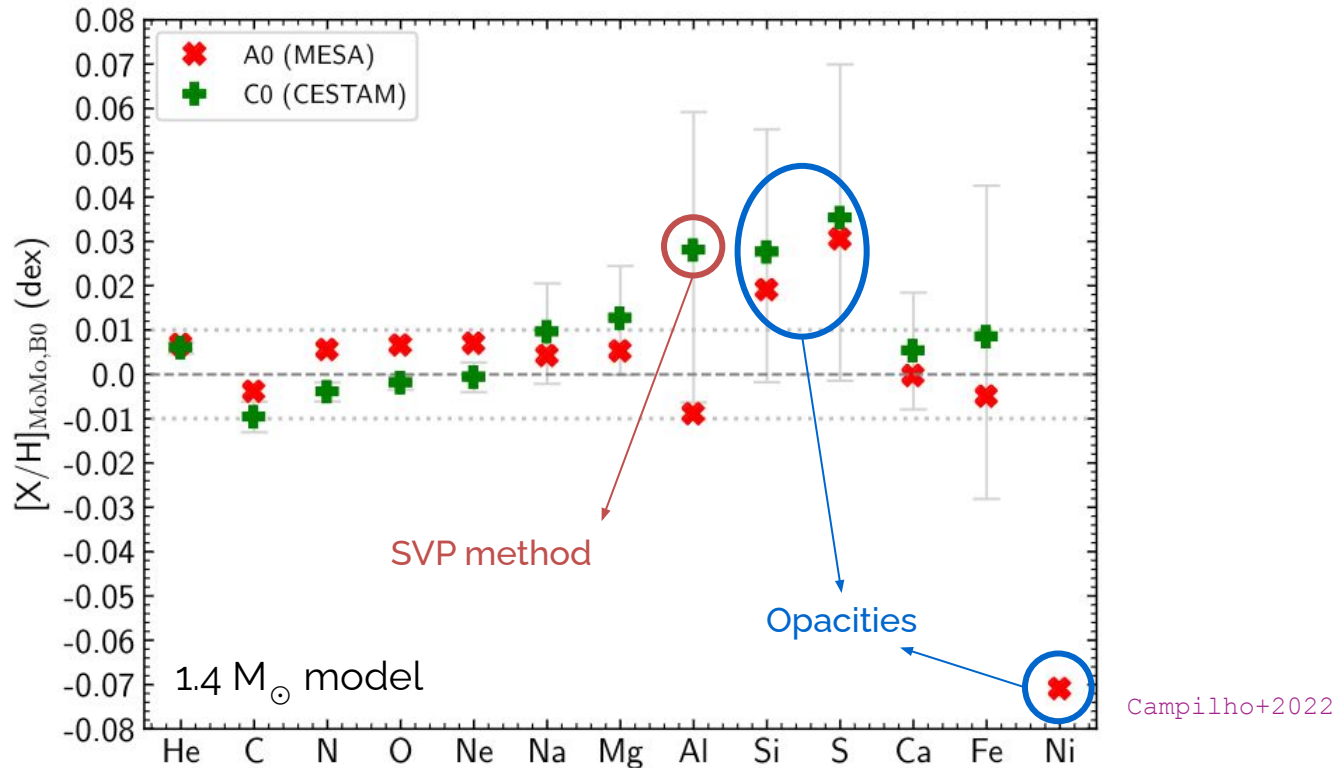
Campilho+2022

# Comparisons between codes



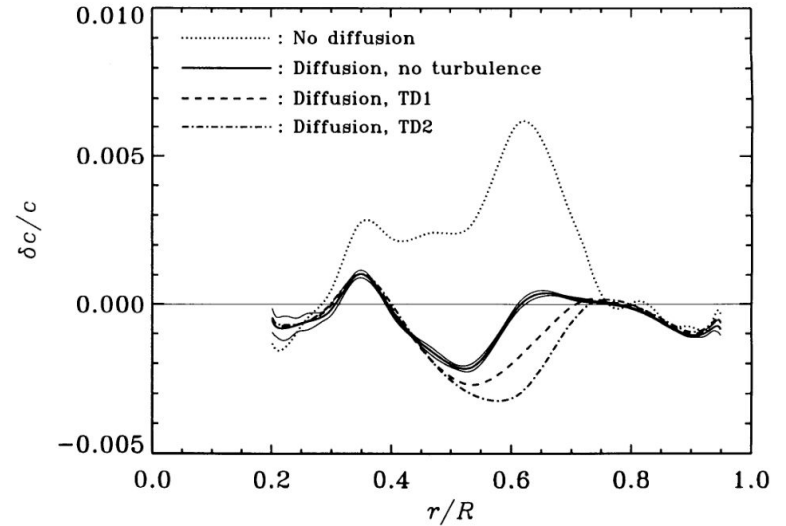
Campilho+2022

# Comparisons between codes



# Additional transport processes

Solar models including **atomic diffusion** show a **better agreement** with helioseismology



Christensen Dalsgaard+ 1993

## Additional transport processes

Solar models including **atomic diffusion** show a **better agreement** with helioseismology

But **Li** and **Be** abundances cannot be explained by atomic diffusion **alone (helium too!)**

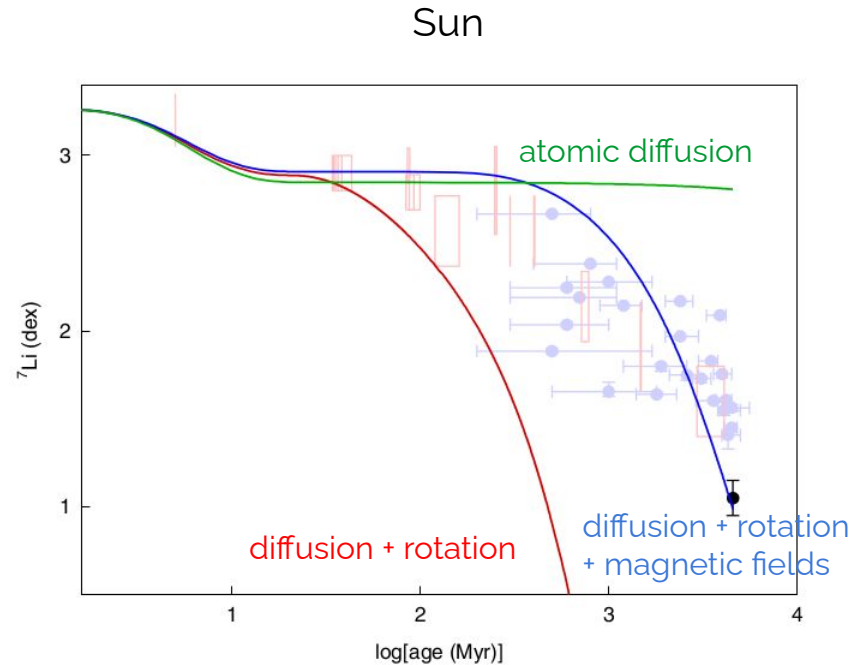


# Additional transport processes

Solar models including **atomic diffusion** show a **better agreement** with helioseismology

But **Li** and **Be** abundances cannot be explained by atomic diffusion **alone (helium too!)**

Need for **additional transport processes**



Eggenberger+2022

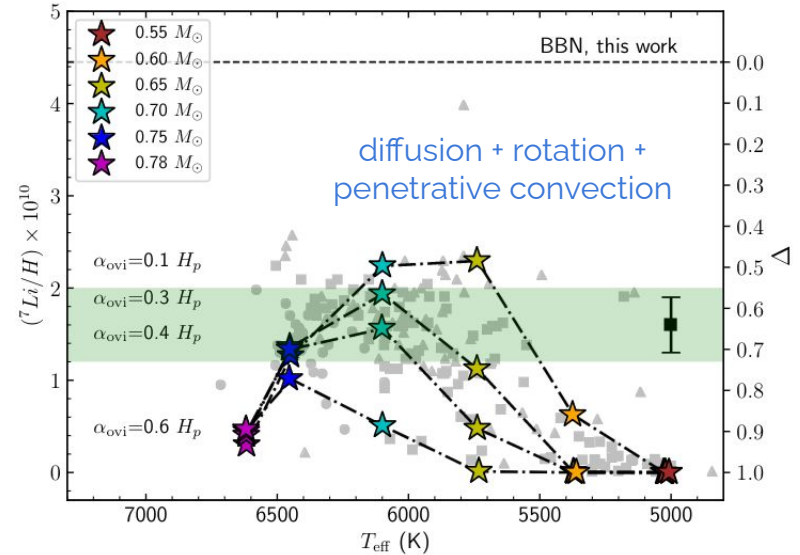
# Additional transport processes

Solar models including **atomic diffusion** show a **better agreement** with helioseismology

But **Li** and **Be** abundances cannot be explained by atomic diffusion **alone (helium too!)**

Need for **additional transport processes**

Pop. II stars



Deal+2021

# What should we use for solar models?

## Diffusion velocities

(for mixture of metals)

- [Burger 1969](#)
  - [Chapman & Cowling 1970](#)
  - [Michaud & Proffitt 1993](#)
  - [Thoul+1994](#)
- 

## Radiative accelerations

- direct use of atomic data (for atmospheres)
  - use of opacity tables with fixed frequency grids (Montréal/Montpellier code, [Turcotte+1998](#); OPCODE, [Seaton 2005](#))
  - Single-Valued Parameter approximation ([LeBlanc & Alecian 2004,2020](#))
- 

## Opacities

- **OP** monochromatic opacities (OPCODE, [Seaton 2005](#))
- **OPAL** monochromatic opacities (Montpellier/Montréal code, not public)
- **SCO-RCG** monochromatic opacities (Ni, [Hui-Bon-hoa+2022](#), not public)
- **OPLIB** monochromatic opacities ([Colgan+2016](#))

# What should we use for solar models?

## Diffusion velocities

(for mixture of metals)

- [Burger 1969](#)
  - [Chapman & Cowling 1970](#)
  - [Michaud & Proffitt 1993](#)
  - [Thoul+1994](#)
- 

## Radiative accelerations

- direct use of atomic data (for atmospheres)
  - use of opacity tables with fixed frequency grids (Montréal/Montpellier code, [Turcotte+1998](#); OPCD, [Seaton 2005](#))
  - Single-Valued Parameter approximation ([LeBlanc & Alecian 2004,2020](#))
- 

## Opacities

- **OP** monochromatic opacities (OPCD, [Seaton 2005](#))
- **OPAL** monochromatic opacities (Montpellier/Montréal code, not public)
- **SCO-RCG** monochromatic opacities (Ni, [Hui-Bon-hoa+2022](#), not public)
- **OPLIB** monochromatic opacities ([Colgan+2016](#))

# What should we use for solar models?

## Diffusion velocities

(for mixture of metals)

- [Burger 1969](#)
  - [Chapman & Cowling 1970](#)
  - [Michaud & Proffitt 1993](#)
  - [Thoul+1994](#)
- 

## Radiative accelerations

- direct use of atomic data (for atmospheres)

- use of opacity tables with fixed frequency grids (Montréal/Montpellier code, [Turcotte+1998](#); OPCODE, [Seaton 2005](#))

- Single-Valued Parameter approximation ([LeBlanc & Alecian 2004,2020](#))
- 

## Opacities

- **OP** monochromatic opacities (OPCODE, [Seaton 2005](#))
- **OPAL** monochromatic opacities (Montpellier/Montréal code, not public)
- **SCO-RCG** monochromatic opacities (Ni, [Hui-Bon-hoa+2022](#), not public)
- **OPLIB** monochromatic opacities ([Colgan+2016](#))

# What should we use for solar models?

## Diffusion velocities

(for mixture of metals)

- [Burger 1969](#)
  - [Chapman & Cowling 1970](#)
  - [Michaud & Proffitt 1993](#)
  - [Thoul+1994](#)
- 

## Radiative accelerations

- direct use of atomic data (for atmospheres)

- use of opacity tables with fixed frequency grids (Montréal/Montpellier code, [Turcotte+1998](#); OPCODE, [Seaton 2005](#))

- Single-Valued Parameter approximation ([LeBlanc & Alecian 2004,2020](#))
- 

## Opacities



- **OP** monochromatic opacities (OPCODE, [Seaton 2005](#))
- **OPAL** monochromatic opacities (Montpellier/Montréal code, not public)
- **SCO-RCG** monochromatic opacities (Ni, [Hui-Bon-hoa+2022](#), not public)
- **OPLIB** monochromatic opacities ([Colgan+2016](#))

# What should we use for solar models?

## Diffusion velocities

(for mixture of metals)

- [Burger 1969](#)
- [Chapman & Cowling 1970](#)
- [Michaud & Proffitt 1993](#)
- [Thoul+1994](#)

## Radiative accelerations

- direct use of atomic data (for atmospheres)

- use of opacity tables with fixed frequency grids (Montréal/Montpellier code, [Turcotte+1998](#); OPCODE, [Seaton 2005](#))

- Single-Valued Parameter approximation ([LeBlanc & Alecian 2004,2020](#))

## Opacities



- **OP** monochromatic opacities (OPCODE, [Seaton 2005](#))

- **OPAL** monochromatic opacities (Montpellier/Montréal code, not public)

- **SCO-RCG** monochromatic opacities (Ni, [Hui-Bon-hoa+2022](#), not public)

- **OPLIB** monochromatic opacities ([Colgan+2016](#))

## Conclusions

- Atomic diffusion is an **important ingredient of solar models**
- **Radiative accelerations play a role**, but small compare to gravitational settling
- **Opacity revisions** may have a significant impact on radiative accelerations ...
- ... which may help to **reconcile models and observations**
- Atomic diffusion is only **one of the transport processes** acting in the Sun

Thank you for your attention !