Constraining the accretion regions of meteorites via astrochemical modelling of protoplanetary disks

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The Beginning

- This project springs from "A divergent heritage for complex organics in Isheyevo lithic clasts" synergy project (van Kooten et al., 2017, GCA, 205, 119).
- Isheyevo is a CH/CB carbonaceous chondrite with two noticeably different lithologies but a continuous transition between the two.
  - It contains pristine lithic clasts that can be categorised as either hydrated (H) or weakly hydrated (A).
  - The A-clasts are ^{15}N-enriched ($^{15}\mathrm{N}/\mathrm{N} = 0.004 - 0.006$) relative to the H-clasts ($^{15}\mathrm{N}/\mathrm{N} = 0.0039 - 0.0043$).
  - There are $^{15}\mathrm{N}/\mathrm{N}$ hotspots reaching ~ 0.022.
  - $\mathrm{D}/\mathrm{H} = (1.1 - 1.3) \times 10^{-4}$ for the A-clasts and $\mathrm{D}/\mathrm{H} = (1.2 - 1.6) \times 10^{-4}$ for the H-clasts.

Image credit: D. Weir's meteoritestudies.com

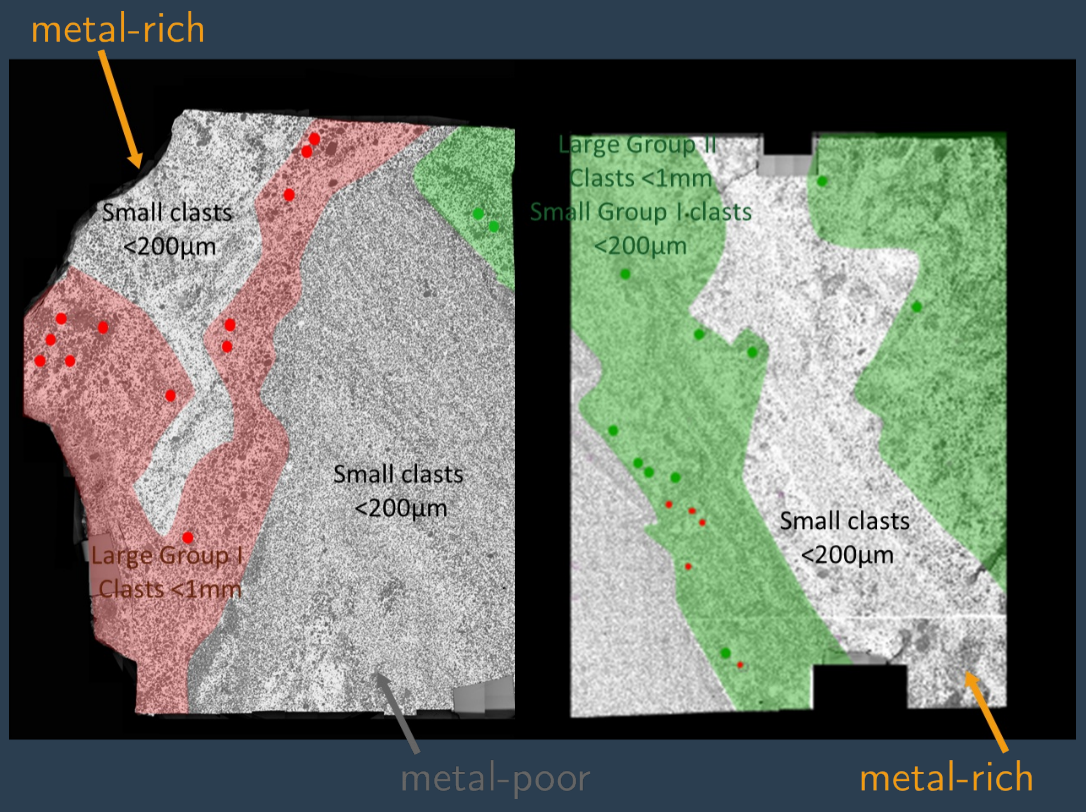
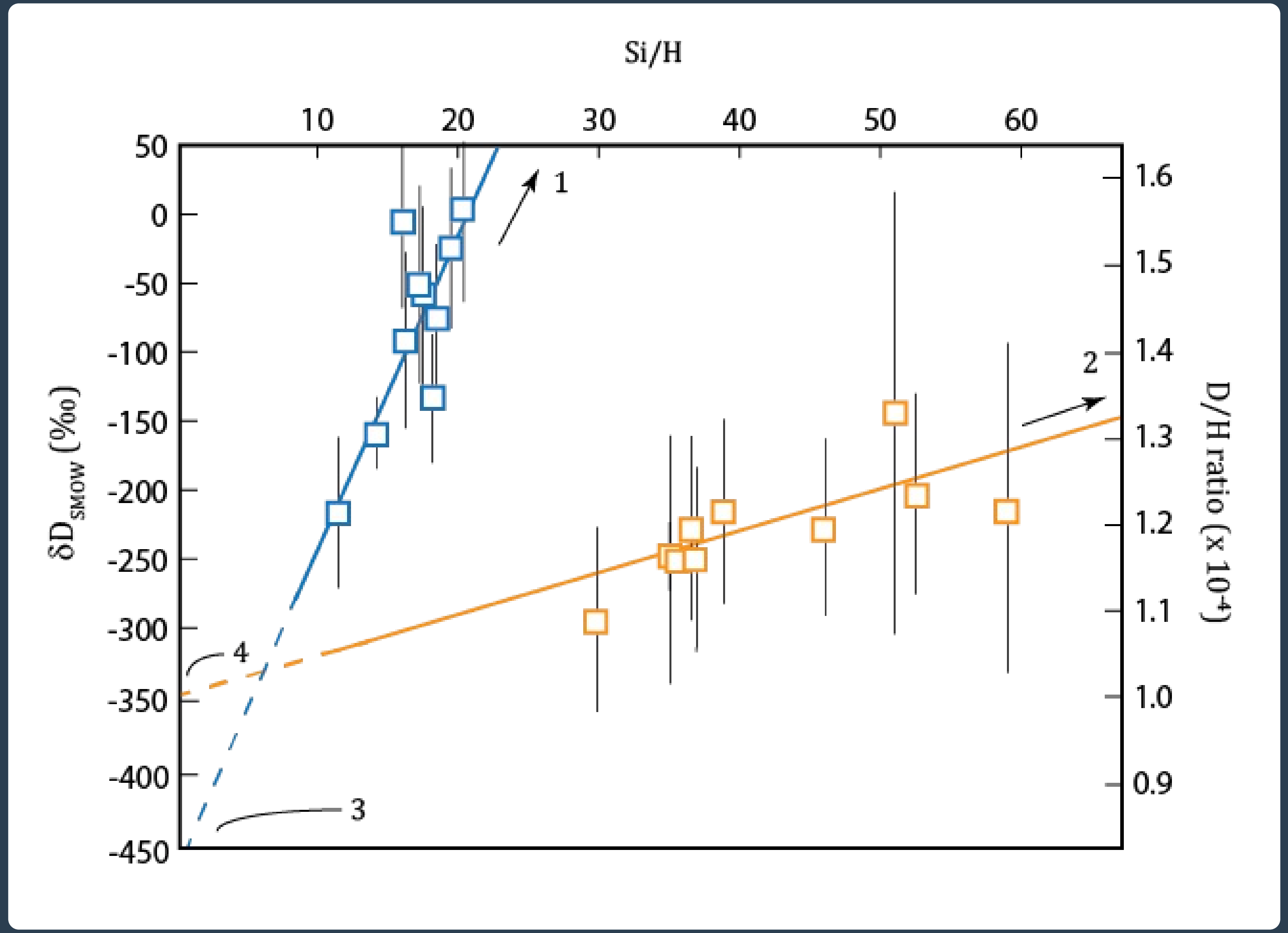
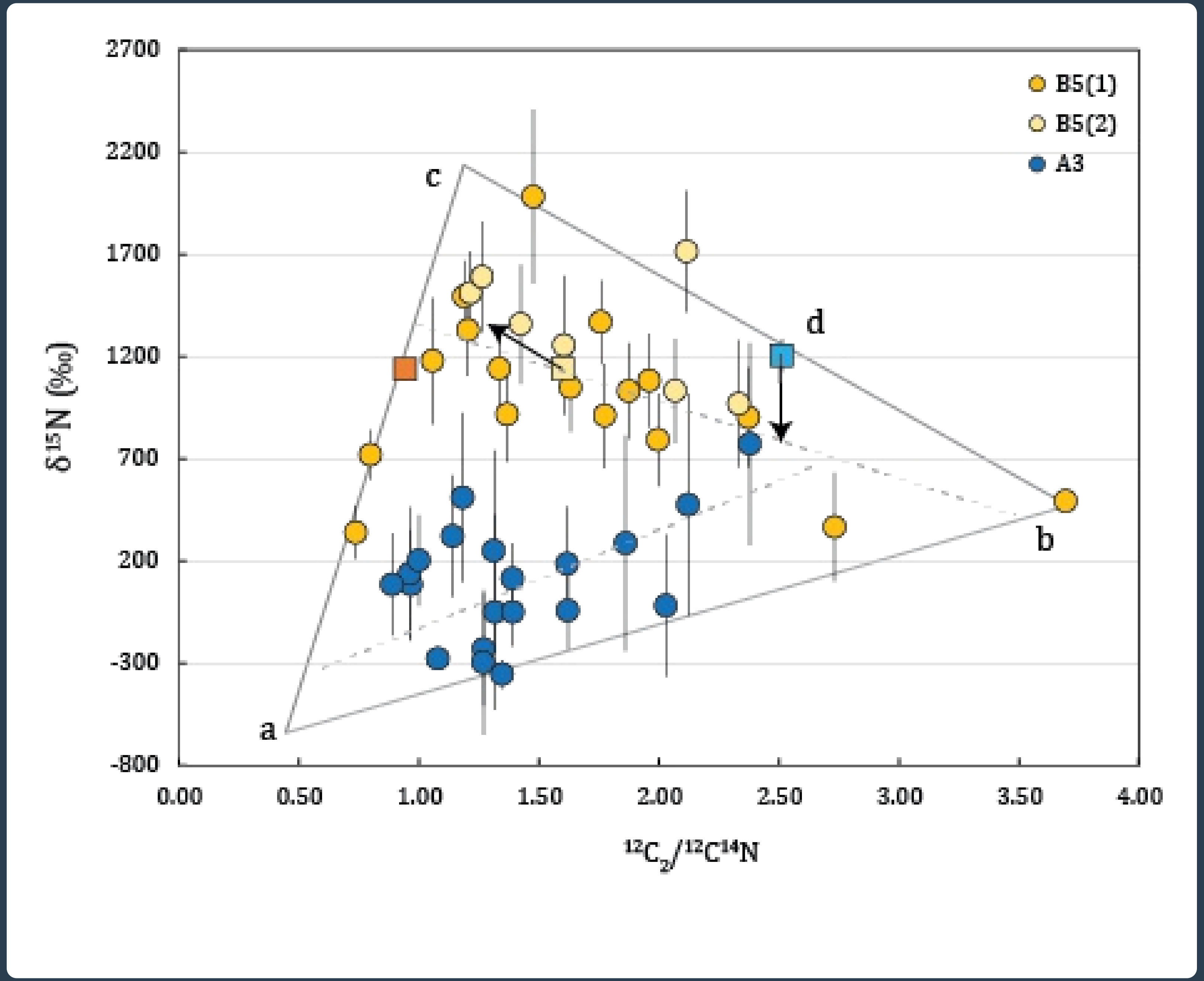


Image credit: Elishevah van Kooten

Isotopic Trends in Isheyevo

van Kooten et al. (2017)

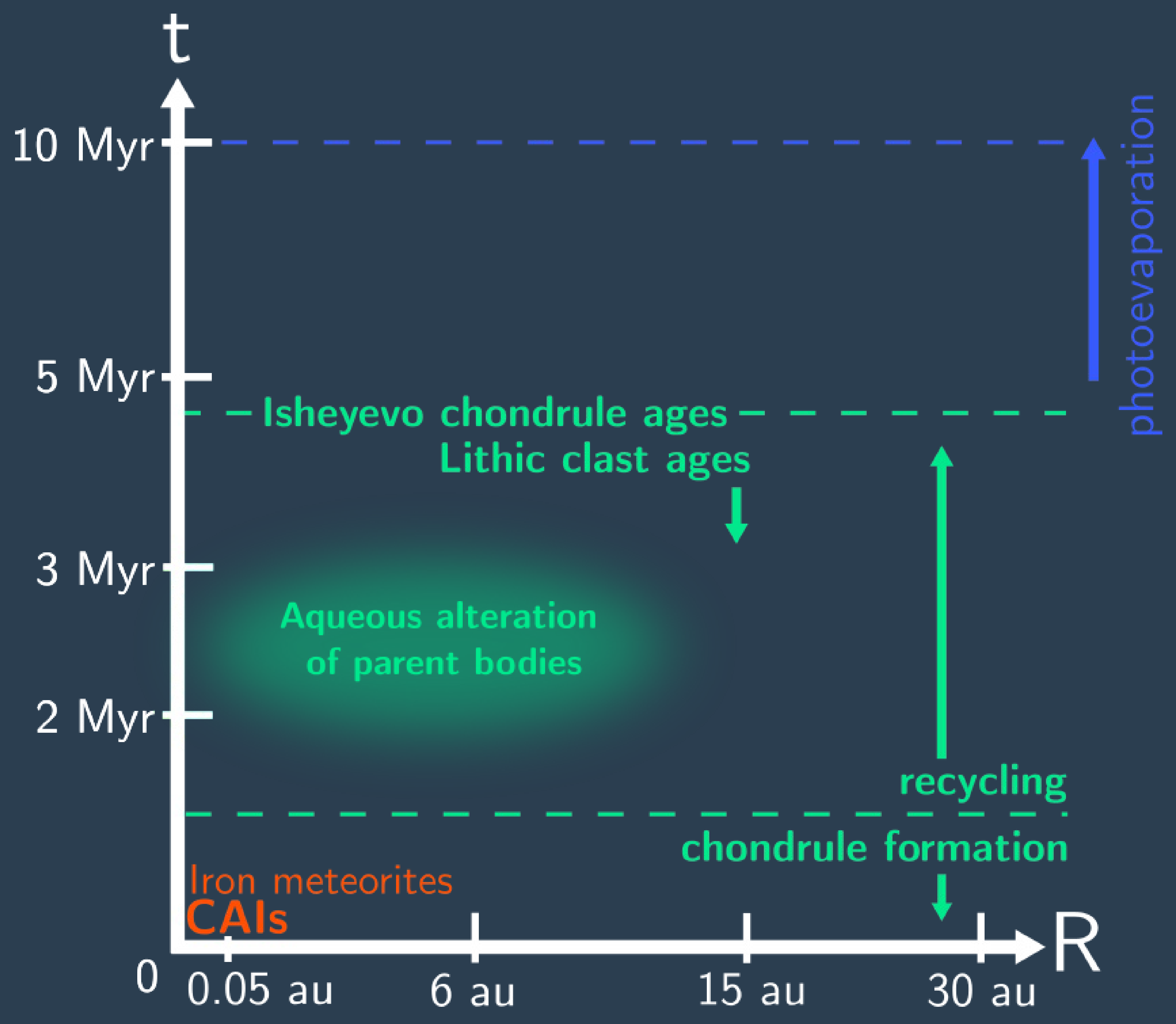




⟵ increasing hydration

- A-clasts: orange; H-clasts: blue.
- $\delta^{15}\mathrm{N} = \left(\frac{^{15}\mathrm{N}/\mathrm{N}_{\mathrm{meas}}}{^{15}\mathrm{N}/\mathrm{N}_{\mathrm{air}}} - 1\right) \times 1000$

Can we constrain the accretion regions of meteorite parent bodies?



- To understand Isheyevo, one can invoke heterogeneous accretion.
- Perhaps the accretion of the different lithologies occurred at different space-times in the Solar System.
- How can we place constraints?
  - Let's use Chemistry!
  - Isotopic ratios are commonly measured in meteorites.
  - We will assume that volatiles end up in meteorite parent bodies via freeze-out.

Approach

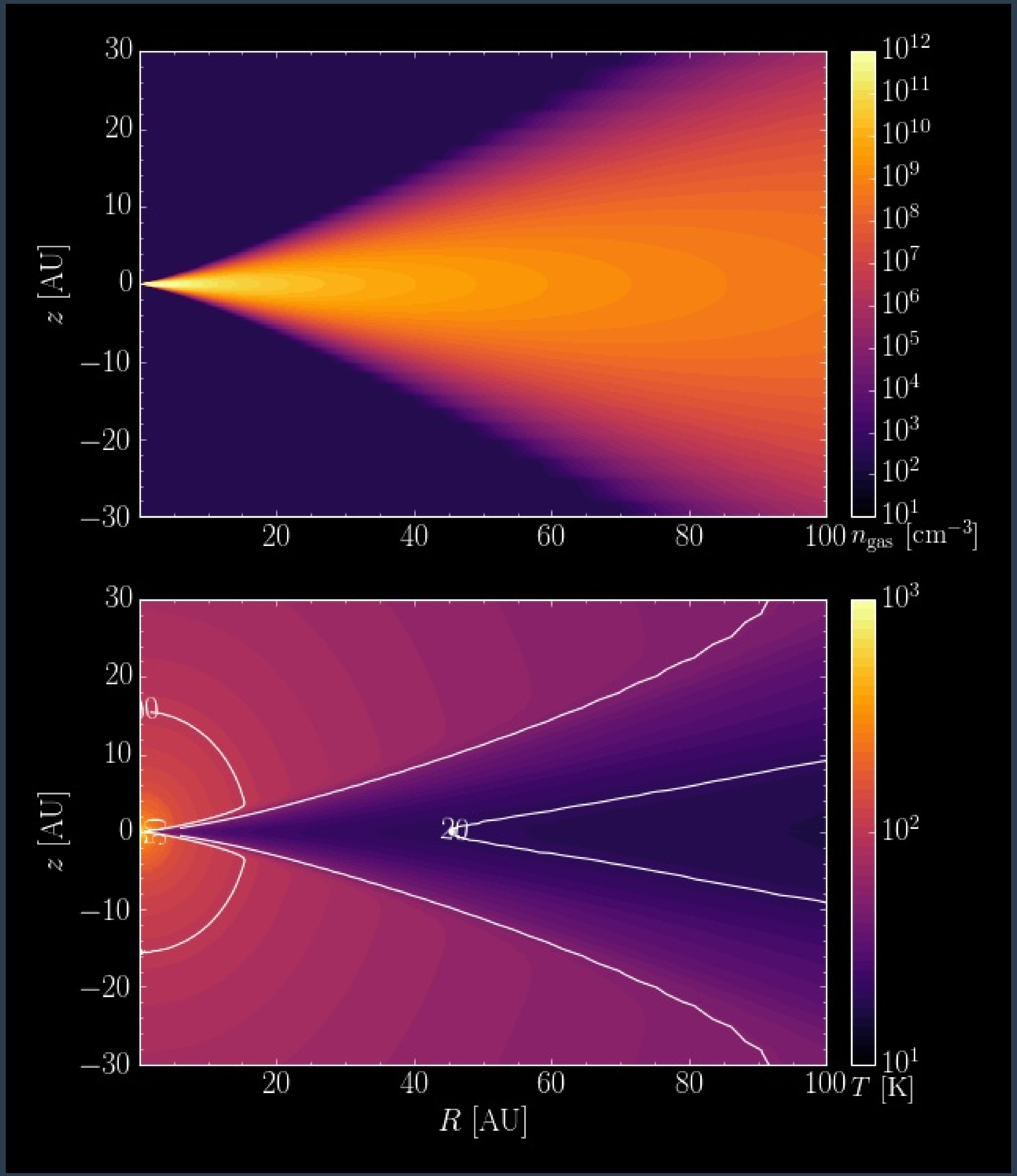
How can we learn about the chemical structure of the PPD?

1. Radiative transfer: Hyperion (http://www.hyperion-rt.org)
   - Dust radiative transfer incl. isotropic scattering and internal viscous heating (single grain size; no settling).
   - Temperature-dependent mean opacities from Semenov et al. (2003), Ferguson et al. (2005).
   - Dust sublimation is accounted for in the opacities.
   - Hard work courtesy of Søren Frimann.
2. Non-equilibrium chemisitry: KROME (http://kromepackage.org)
   - The KIDA database network is used (http://kida.obs.u-bordeaux1.fr/), modified for $^{15}\mathrm{N}, \mathrm{D}$, isotope fractionation (Roueff et al., 2015), ice accretion/thermal desorption (Charnley, Rodgers & Ehrenfreund 2001; Rodgers & Charnley, 2003) and simplified photochemistry.
     - The network is "isotopologised" $(\mathrm{D}, \mathrm{D}_2, \mathrm{D}_3, {}^{15}\mathrm{N}$, but not ${}^{15}\mathrm{N}_2, \mathrm{D}_4)$; isotopologized reaction rates determined by "statistical approach" (Millar et al., 1989).
     - Binding energies for thermal desorption "scraped" from the literature.
     - There are 1341 chemical species (including 56 ice species) and more than 53400 reactions.
   - The DOCMAKE tool is used to explore the network, examine reaction rates and produce integrated photochemical rates (with cross-sections from the Leiden database).

3. The glue: **SLiPPD** (Snow Lines in Protoplanetary Disks) Python package.

> - https://bitbucket.org/perrybothron/slippd
> - Sets up and invokes Hyperion and KROME in succession or individually in serial or in parallel (MPI).
> - Visualisation and analysis scripts are provided.
> - For a given network, you can calculate the chemical fluxes of reactions over a range of densities and temperatures.
> - Between RT iterations, hydrostatic equilibrium is re-calculated and the density adjusted.
> - It will become public once a paper is submitted (also the chemical network).

Parameterised Disk Structure



$$\rho(R, z) = \rho_0 \left(\frac{R_0}{R}\right)^{-2.3} \exp\left(-\frac{R}{R_0}\right) \exp\left[-\frac{1}{2}\left(\frac{z}{h(R)}\right)^2\right]$$

- Internal viscous heating is included:

  $\Gamma_{\mathrm{visc}} = \frac{9}{4}\alpha P \Omega_{\mathrm{Kep}}$

  $\alpha = 10^{-3}$

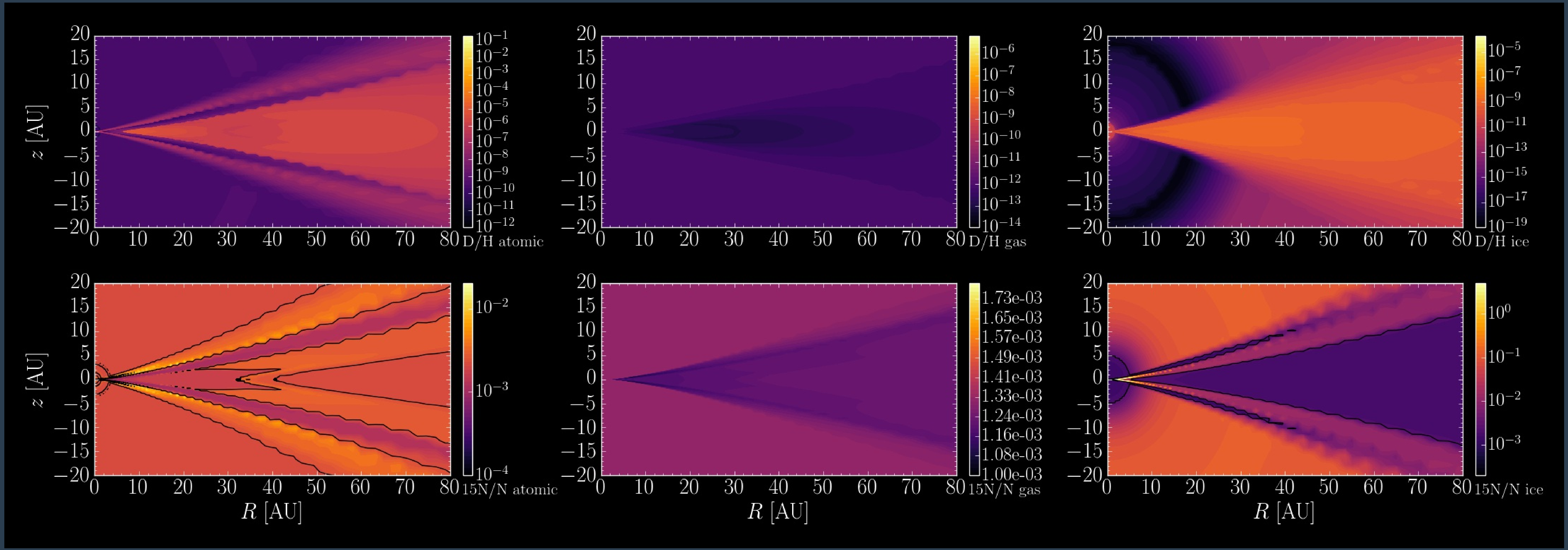
  $M_{\mathrm{disk}} = 0.01 M_\odot, M_* = 1.0 M_\odot$

  $T_{\mathrm{eff}} = 4339\ \mathrm{K}, R_* = 1.78 R_\odot$

- Constant gas-to-dust ratio of 100.
- Dust sublimation accounted for via temperature-dependent opacities.

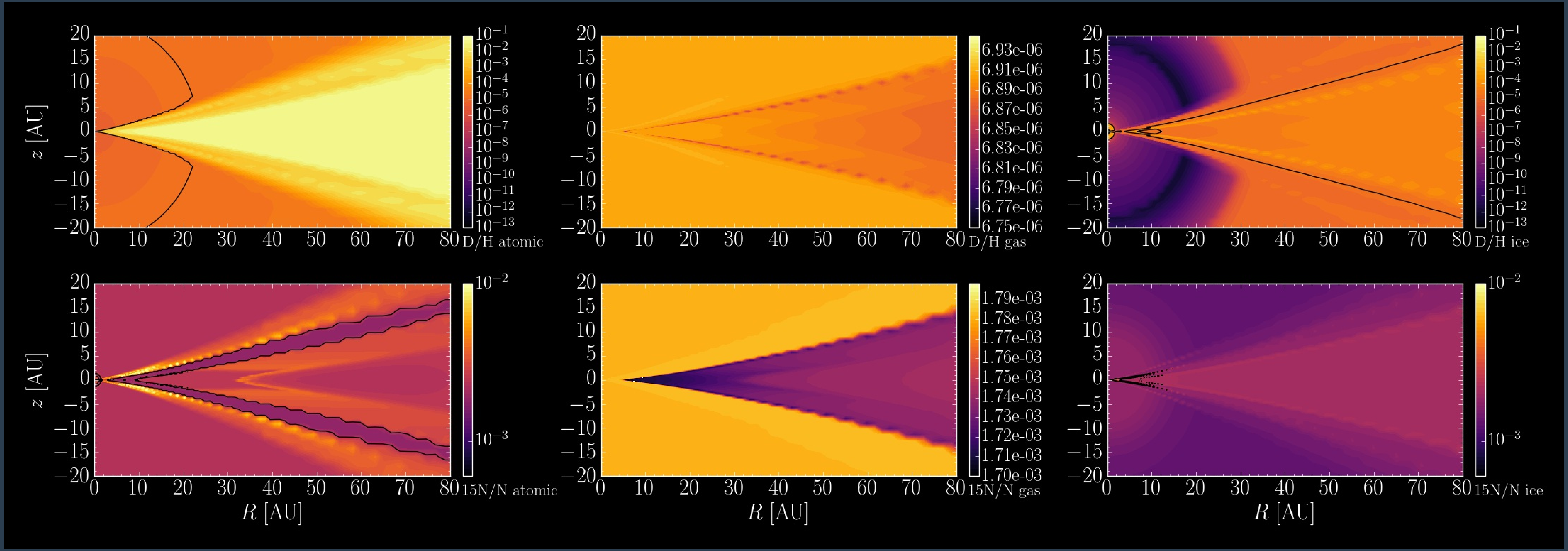
The Middle: Preliminary Results

After 2.5 Myr of chemical evolution



Initial conditions are from Bruderer et al. (2009).

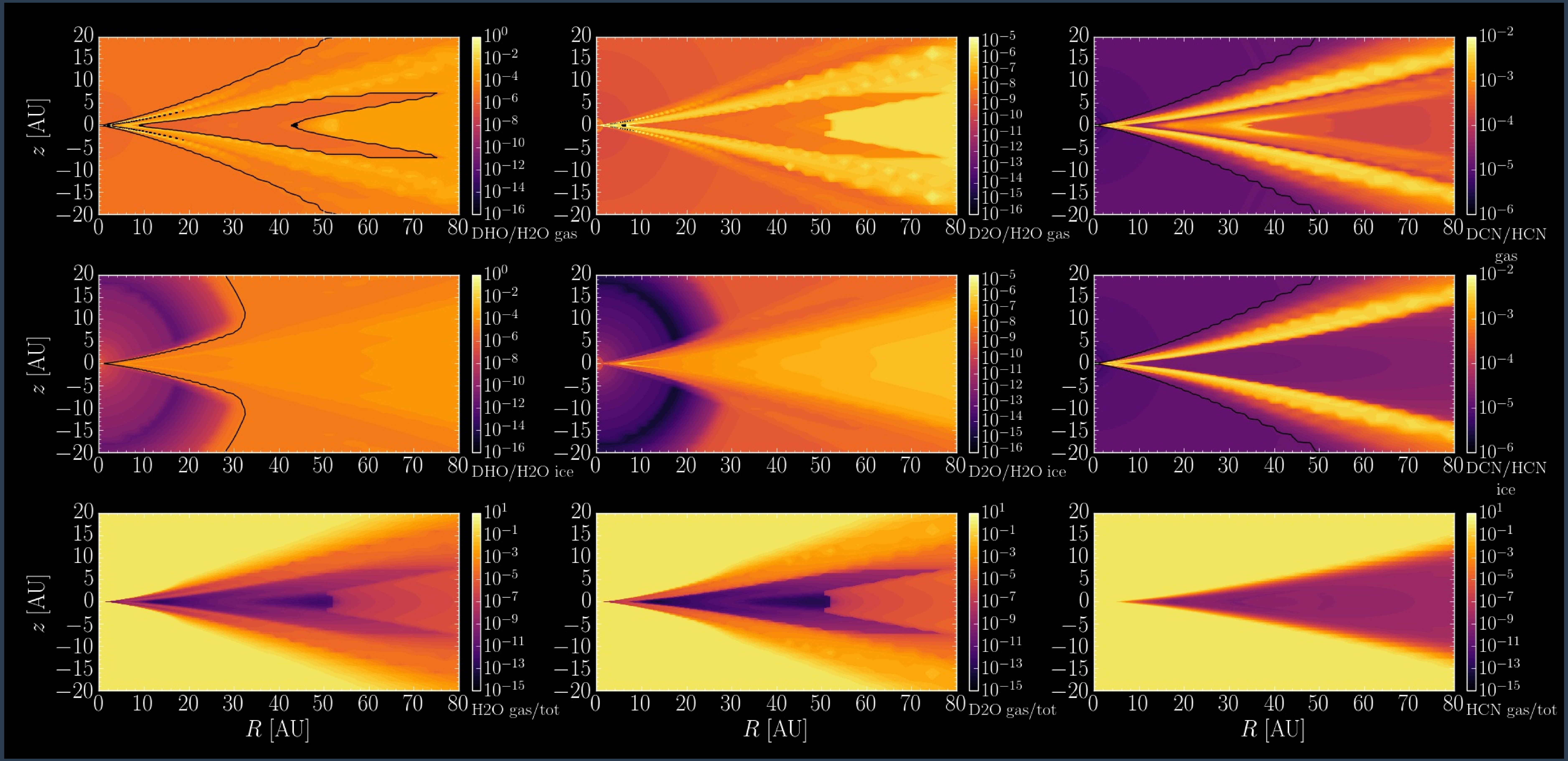
Now with isotopologised initial abundances



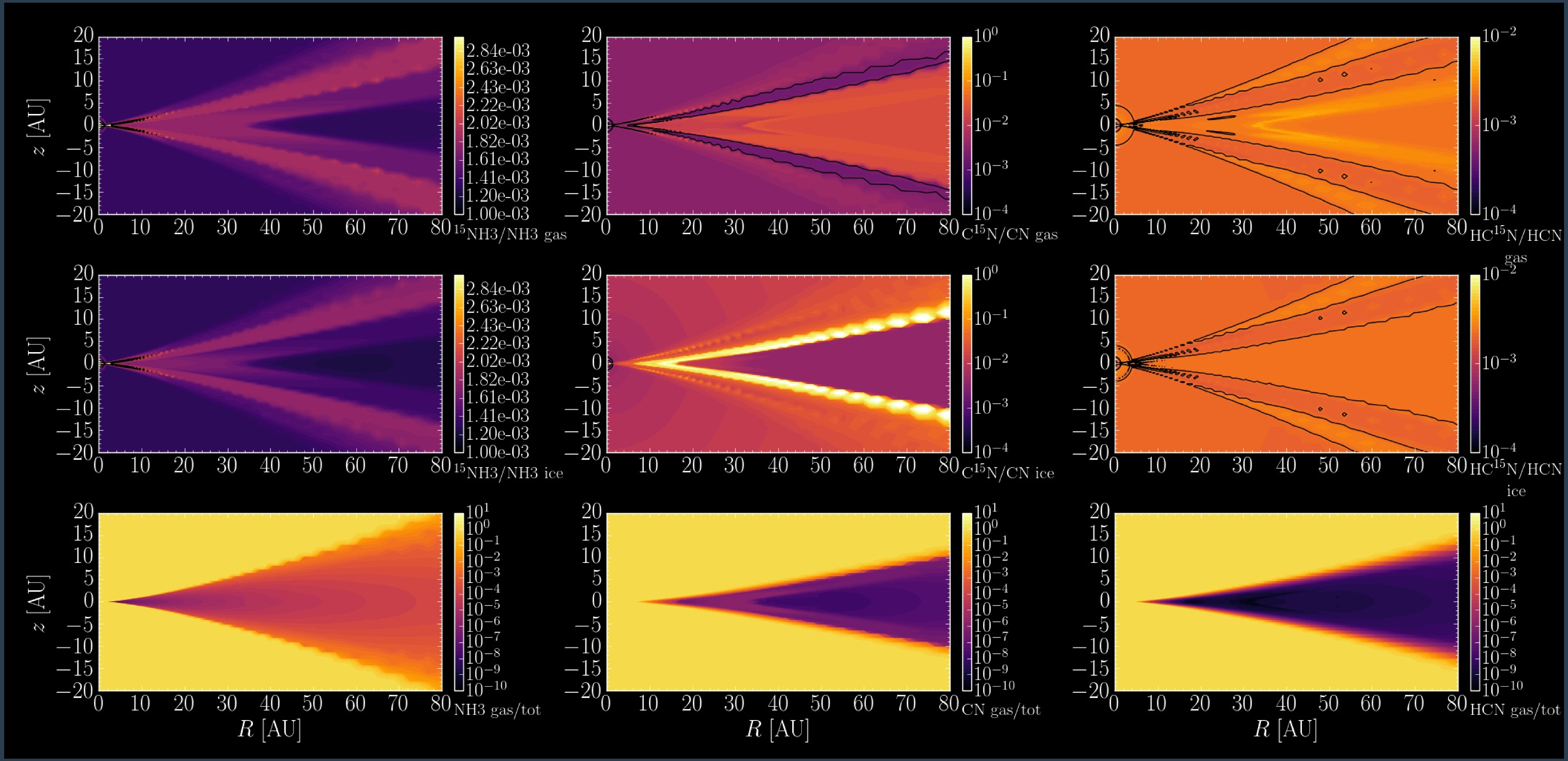
Freeze-out timescale $\propto n^{-1}T^{-1/2}$

Desorption timescale $\propto \exp(-E_{\mathrm{b}}/T)$

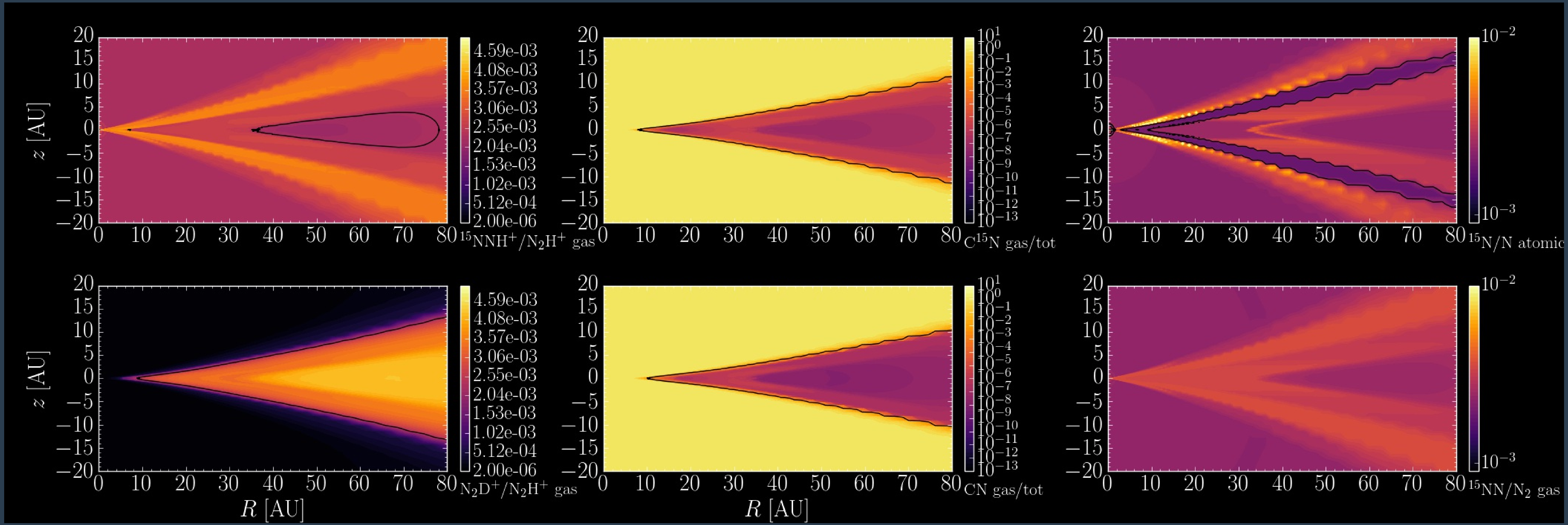
D-bearing molecules



^{15}N -bearing molecules

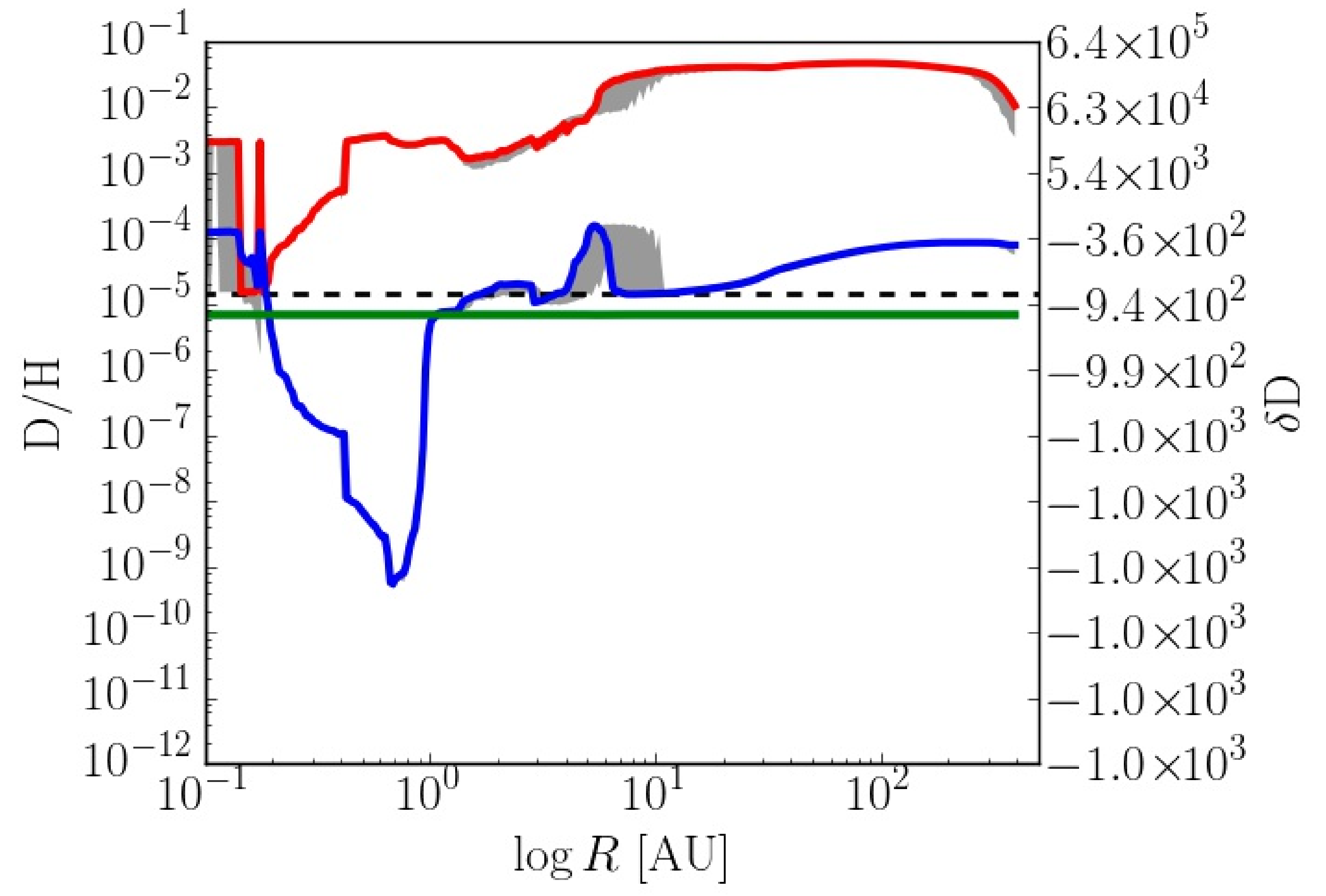


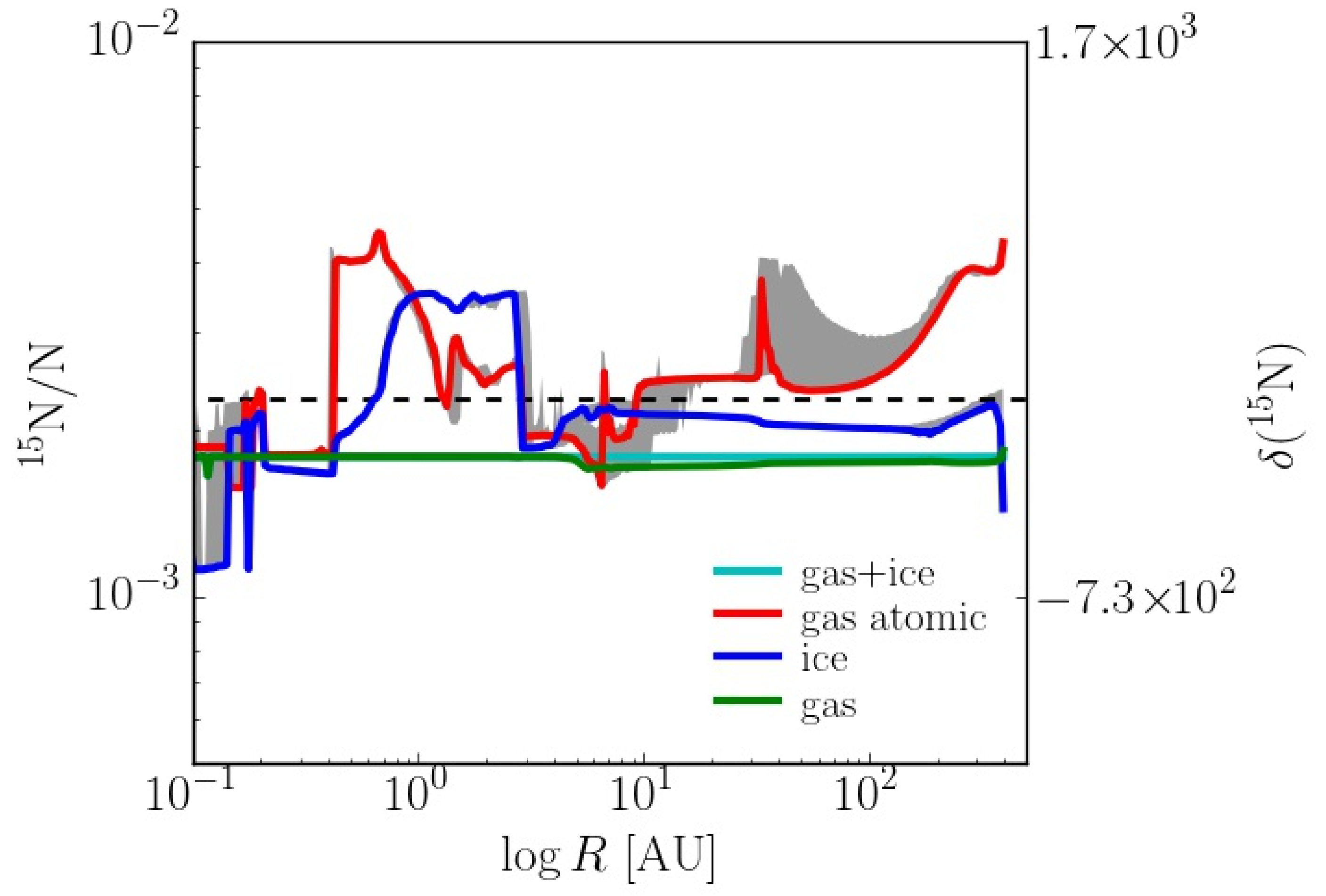
More!

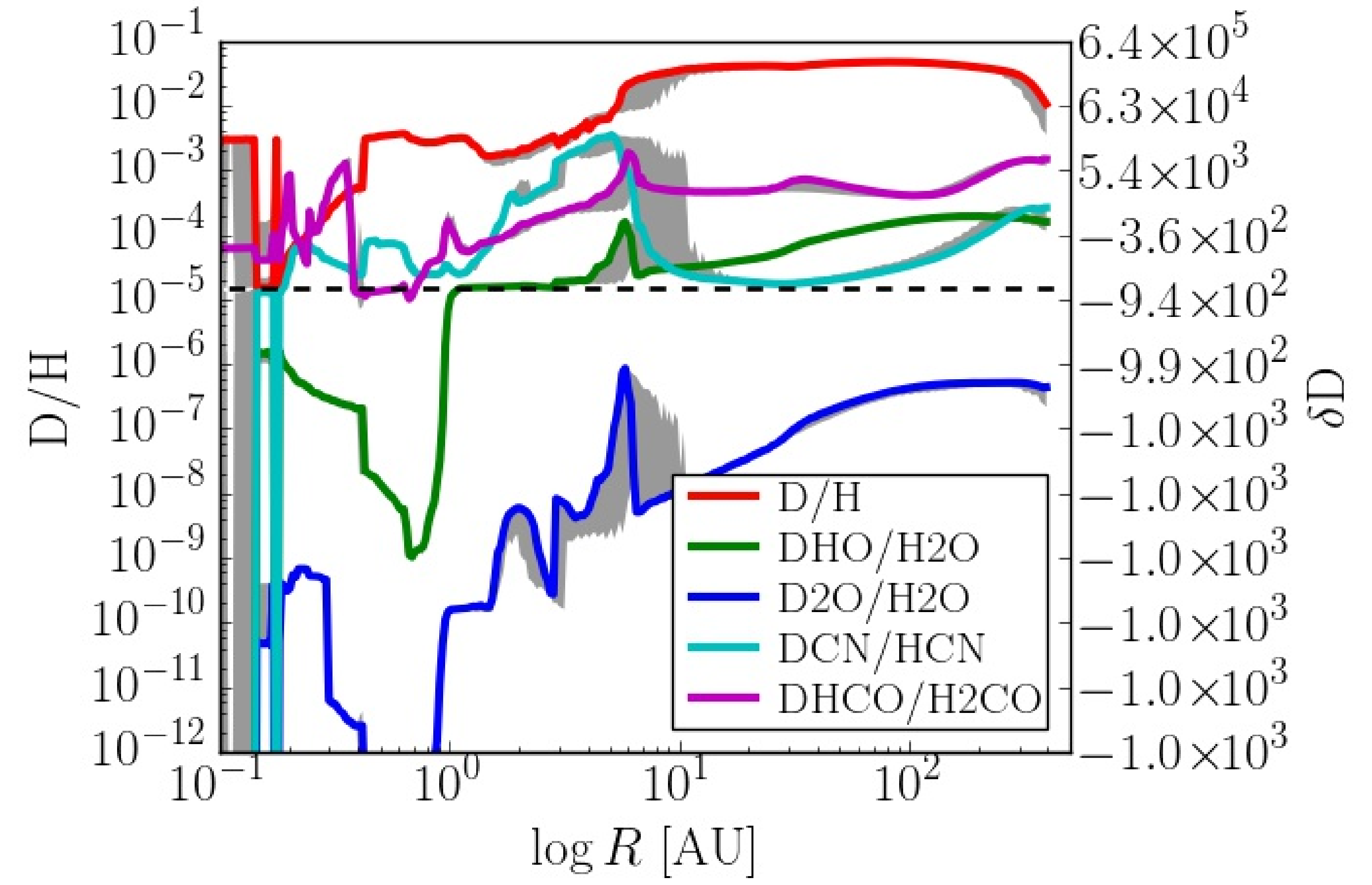


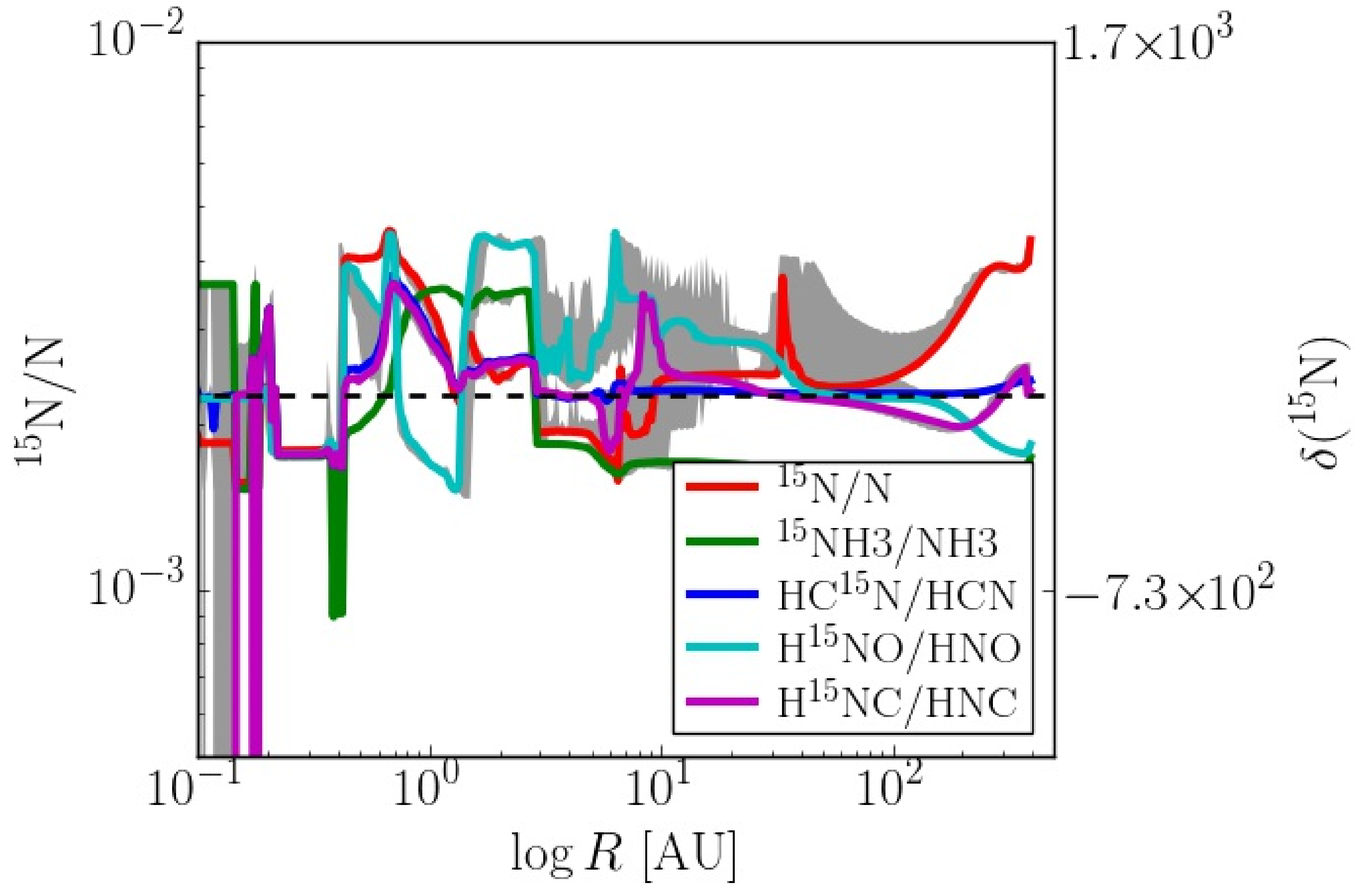
z [AU]
R [AU]
^{15}NNH$^+$/N$_2$H$^+$ gas
C^{15}N gas/tot
^{15}N/N atomic
N$_2$D$^+$/N$_2$H$^+$ gas
CN gas/tot
^{15}NN/N$_2$ gas

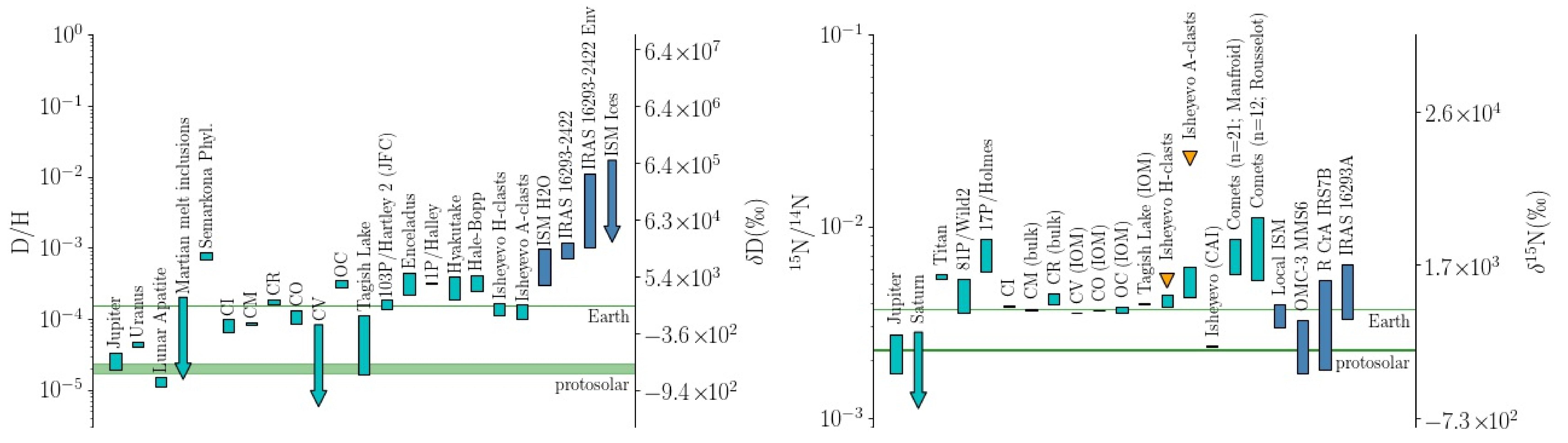
In the midplane











D/H
10^0
10^{-1}
10^{-2}
10^{-3}
10^{-4}
10^{-5}
Jupiter
Uranus
Lunar Apatite
Martian melt inclusions
Semarkona Phyl.
CI
CM
CR
CO
CV
OC
Tagish Lake
103P/Hartley 2 (JFC)
Enceladus
1P/Halley
Hyakutake
Hale-Bopp
Isheyevo H-clasts
Isheyevo A-clasts
ISM H2O
IRAS 16293-2422
IRAS 16293-2422 Env
ISM Ices
Earth
protosolar
6.4×10^7
6.4×10^6
6.4×10^5
6.3×10^4
5.4×10^3
-3.6×10^2
-9.4×10^2
δD(‰)
$^{15}N/^{14}N$
10^{-1}
10^{-2}
10^{-3}
Jupiter
Saturn
Titan
81P/Wild2
17P/Holmes
CI
CM (bulk)
CR (bulk)
CV (IOM)
CO (IOM)
OC (IOM)
Tagish Lake (IOM)
Isheyevo H-clasts
Isheyevo A-clasts
Isheyevo (CAI)
Comets (n=21; Manfroid)
Comets (n=12; Rousselot)
Local ISM
OMC-3 MMS6
R CrA IRS7B
IRAS 16293A
Earth
protosolar
2.6×10^4
1.7×10^3
-7.3×10^2
$\delta^{15}N$(‰)

The End (for now)

- The variation of $\mathrm{D/H}$ and $^{15}\mathrm{N/N}$ ratios in different ice species as a function of radius is not simple.
- Recall the values in Isheyevo:
  > - A-clasts: $^{15}\mathrm{N/N} = 0.004 - 0.006; \mathrm{D/H} = (1.1 - 1.3) \times 10^{-4}$.
  > - H-clasts: $^{15}\mathrm{N/N} = 0.0039 - 0.0043; \mathrm{D/H} = (1.2 - 1.6) \times 10^{-4}$;
  > - Hotspots: $^{15}\mathrm{N/N} \sim 0.022$.
- Overall, the results are in reasonable agreement with the range of Solar System measurements, including the Isheyevo clasts, but we do not reach the hotspot values.

Wish List

- What would dust surface chemistry do?
- Via LIME, generate synthetic observations for different disks.
- Add heating and cooling to temperature calculation (CR heating, photoelectric heating, etc.).

Thank you for your attention!

This presentation uses hovercraft (https://hovercraft.readthedocs.io/), impress.js (http://impress.github.io/impress.js) and the Bootswatch Superhero theme (https://bootswatch.com/).