Exercises plan

- Part 0: stand-alone chemical network with KROME
- Part 1: adding chemistry to PROTO
- Part 2: adding thermal processes to PROTO
- **Part 3: adding photochemistry to PROTO**
- Part 4: playing with surface chemistry

Problem 2: Adding Photochemistry

Aims of this exercise

1. add photochemistry to the chemical network
2. enable photobins in KROME
3. tell to KROME what is your photochemistry metric
4. tell to KROME what is the radiation flux in each bin
5. use KROME to get gas and dust opacity

- KROME is capable of using xsecs form files
- add water photodissociation rates to network (see table)
- download H_2O xsec(s) from SWRI database (see talk)
- copy as `H2O.dat` in the SWRI folder of KROME (surprise)

20. $H_2O + \gamma$	$\rightarrow$	$H + OH$	`@xsecs=SWRI`
21. $H_2O + \gamma$	$\rightarrow$	$H_2O^+ + e^-$	`@xsecs=SWRI`

- `@xsec=SWRI` is your rate
- wrap reactions in `@photo_start` and `@photo_stop` (see CR)

Pre-processor stage

- `nenergy` in `proto_commons.f90` determines KROME bins
- set bins using `-photoBins=NBINS` options
- re-run KROME pre-processor with the new options
- copy the usual suspect (`krome_all.f90`) and all `swri*.dat` to PROTO folder

Compilation/run stage

- set the photobin metric[1] using `krome_set_photobinE_lr`
- set the amount of radiation per energy bin[2] `krome_set_photoBinJ`
- compile, run, and plot H_2O (cfr. with Fig. 6)

[1] same for all cells, and determined by PROTO
[2] each cell has a different flux

Opacity in KROME

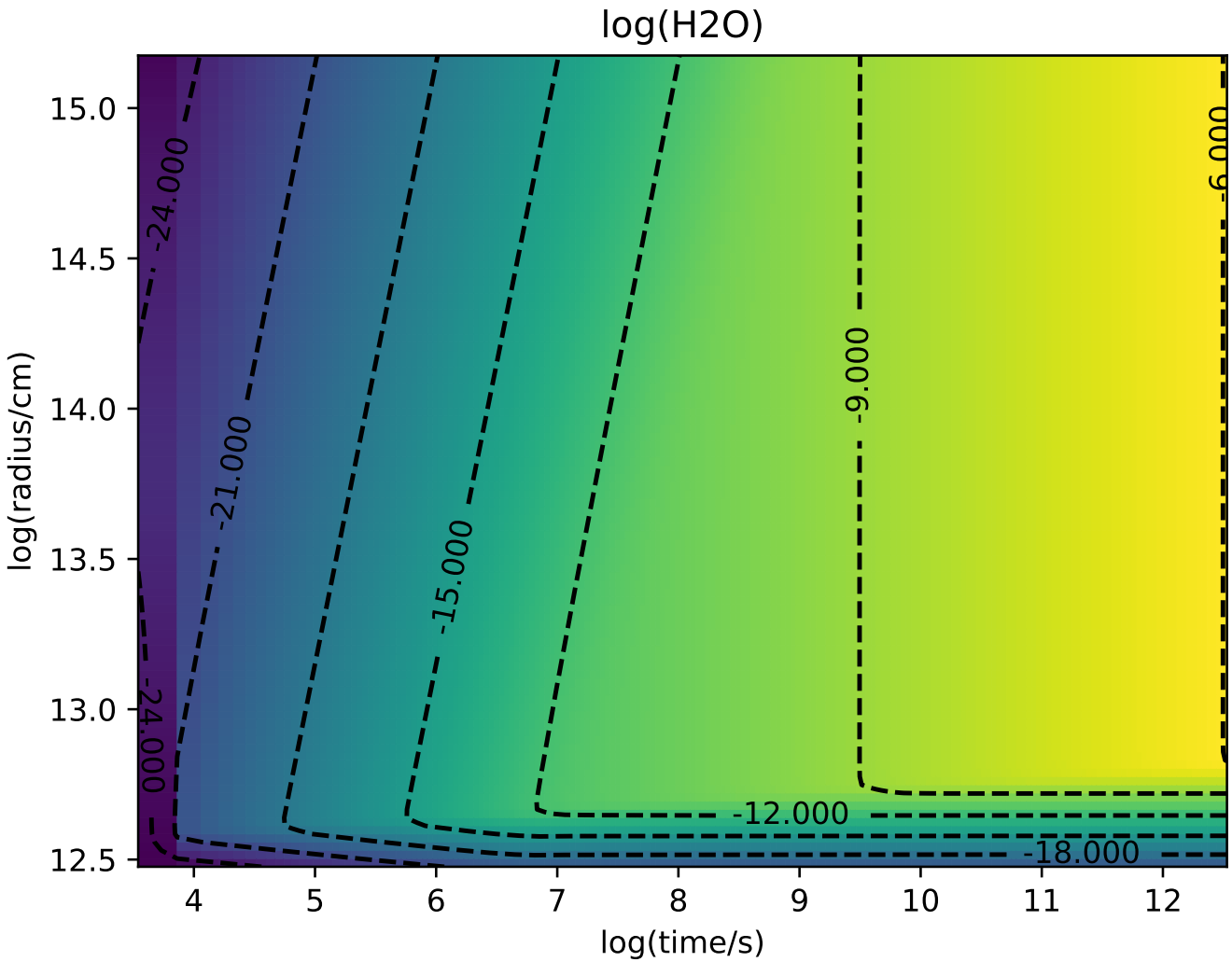
- KROME provides gas and dust opacity
- gas opacity is self-consistent (see slides), but not effective here
- dust opacity can be loaded from file (see below) using `krome_load_opacity_table` in `init_chemistry`

Opacity file

- use opacity file from Draine's website

PROTO gets opacity from KROME

- Each cell get the energy-dependent opacity from KROME using `krome_get_opacity_size_d2g` in `solve_chemistry`


log(H2O)
log(radius/cm)
log(time/s)
15.0
14.5
14.0
13.5
13.0
12.5
4
5
6
7
8
9
10
11
12
-24.000
-21.000
-15.000
-9.000
-6.000
-12.000
-18.000

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Plan

- Add water sticking and evaporation
- Play around with $T = T_{dust}$ to understand what is going on

22. H_2O	$\rightarrow$	H_2O_{dust}	`krate_stickSi`
23. H_2O_{dust}	$\rightarrow$	H_2O	`krate_evaporation`

Table: Surface chemistry reactions and corresponding rates.

Adsorption

$X \rightarrow X_{dust}$

$$k_a = \frac{\pi v_g S \int a^2 \varphi(a)\,\mathrm{d}a}{4/3\pi\rho_0 \int a^3 \varphi(a)\,\mathrm{d}a}$$

- momenta $\langle a^2 \rangle$ and $\langle a^3 \rangle$
- if $\varphi(a) \propto a^p \rightarrow$ analytical
- $p = -3.5$
- $\rho_0 = 3$ g cm^{-3}
- $a_{min} = 5 \times 10^{-7}$ cm
- $a_{max} = 2.5 \times 10^{-5}$ cm
- $\mathcal{D} = 10^{-2}$
- $v_g = \sqrt{8 k_B T / \pi m_X}$
- $S(T, T_d) =$ some function
- `1,CO,CO_dust,krate_stickSi(n, idx_CO, Tdust)`

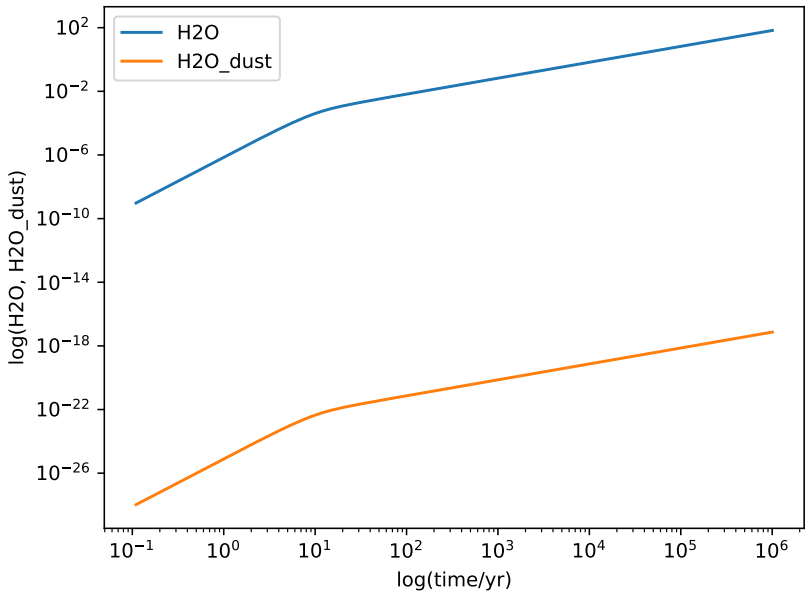
Desorption

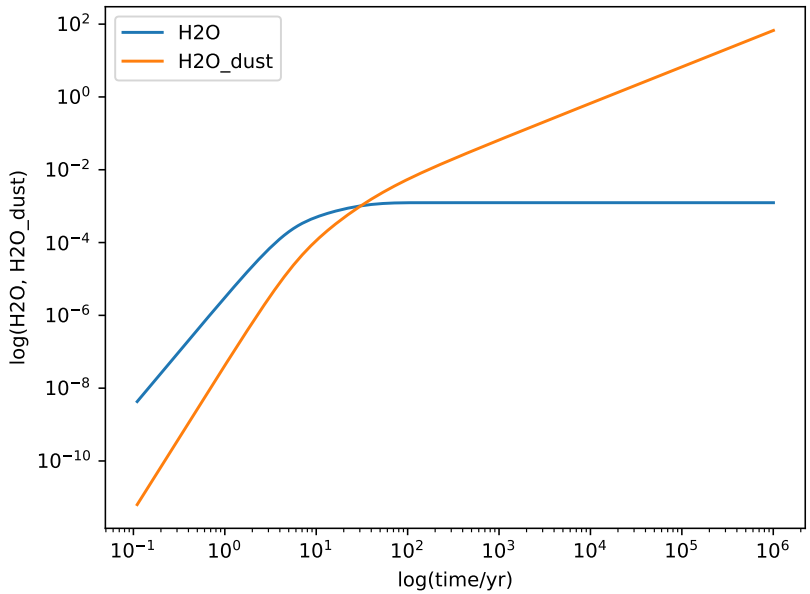
$X_{dust} \rightarrow X$

$$k_e = \nu_0 \exp\left(-\frac{E_i}{k_B T_d}\right)$$

```
2,CO_dust,CO,krate_evaporation(n, idx_CO, Tdust)
```

10^3 K vs 50 K





*y*scale!

$50, 85, 10^2, 10^3$ K, try also 80 K to compare with 85 K.

GOOD WORK!