The chemistry of water in regions of high mass star formation

Floris van der Tak (*MPIfR Bonn*)

Malcolm Walmsley *(Osservatorio di Arcetri)*
Fabrice Herpin *(Observatoire de Bordeaux)*
Cecilia Ceccarelli *(Observatoire de Grenoble)*

Why chemistry?

Sensitive to temperature, density etc

probe physical components (disk, outflow, ...)

"typical" molecules

Sensitive to time

estimate chemical ages

Why water ?

- Cornerstone of oxygen chemistry (in top 3)
- Potential major gas coolant
- Expected to be widespread

Making Water

- Ion-molecule reactions: cold gas phase

  O^{+}... H_3O^{+} ... H_2O

- Grain surface reactions: cold dust grains

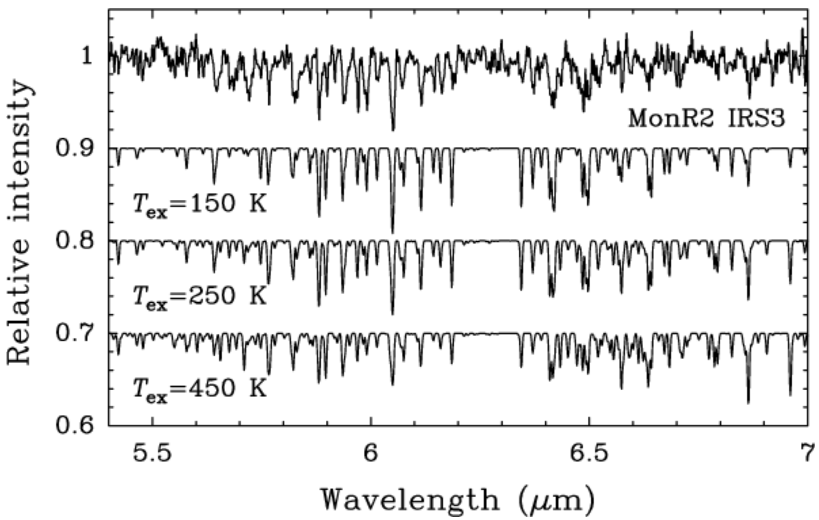
  $O + 2H = H_2O$

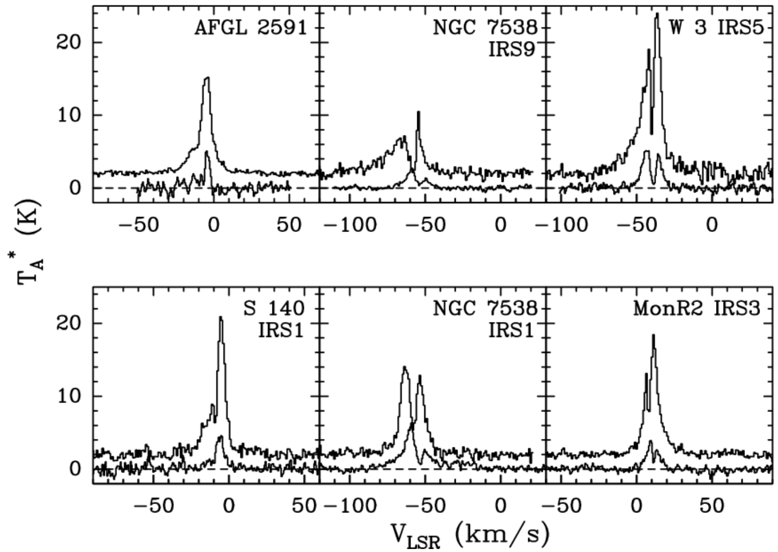
- Neutral-neutral reactions: warm / hot gas phase

  O (H_2, H) OH (H_2, H) H_2O

Previous Water Observations

- ISO-SWS: $H_2O/H_2 \sim 10^{-4.5}$ (gas phase & solid state absorption)
- SWAS: $H_2O/H_2 \sim 10^{-8.5}$ (emission on ~arcmin scale)
- Ground-based: (mostly) 22 & 183 GHz masers
  (hard to extract abundance)

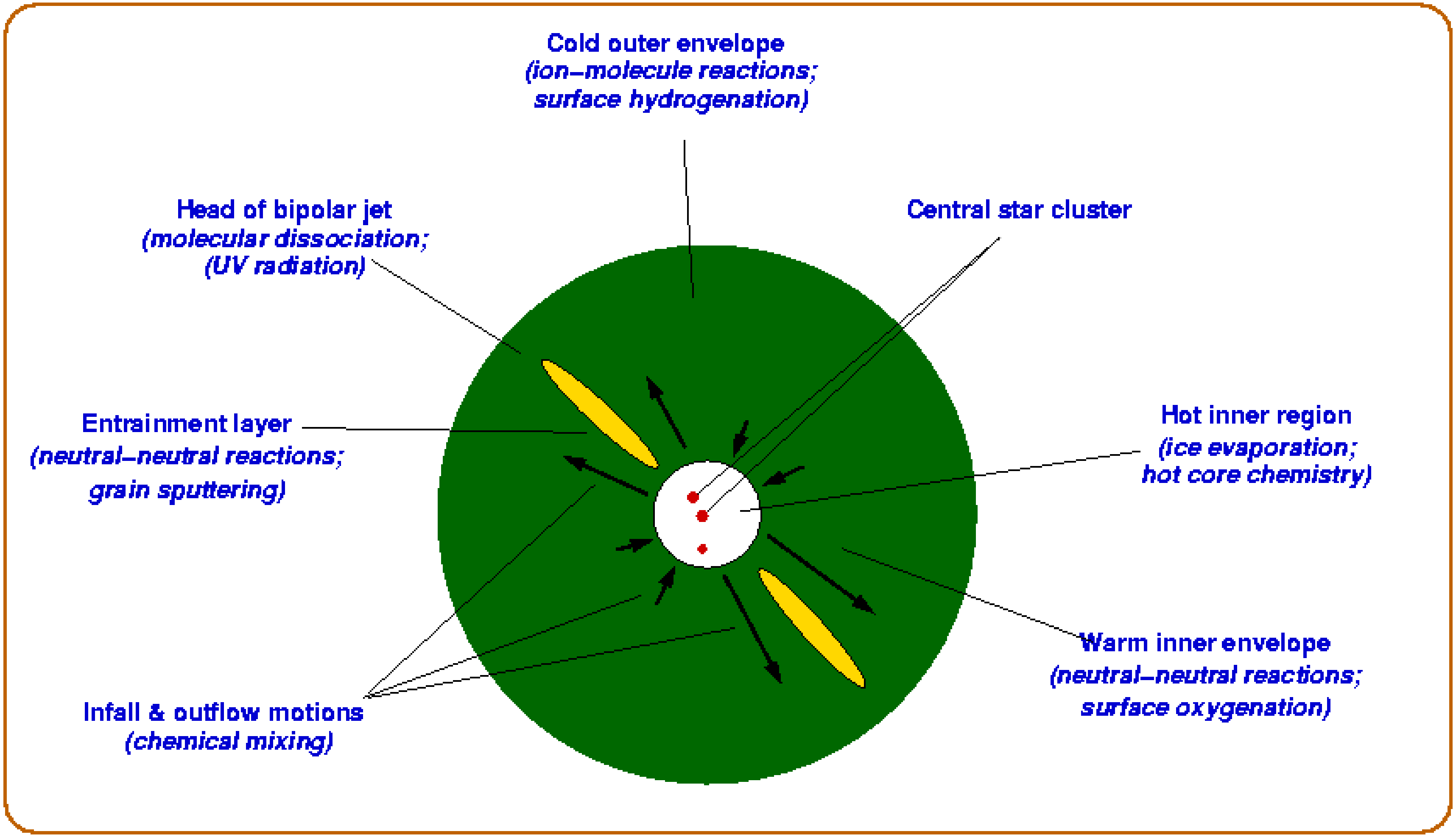




(Snell et al;
Boonman et al)

Highly variable (unlike CO) ...but where is it?

So where is it? Everywhere !



Need high spatial & spectral resolution data:
Ground-based observations

Observed Lines

Species	Transition	Freq	E_{up}	Telescope	Beam	Use
p-$H_2{}^{18}O$	3_{13}-2_{20}	203.41	204	IRAM	12”	warm H_2O
HDO	1_{10}-1_{11}	80.58	47	IRAM	30”	
HDO	3_{12}-2_{21}	225.90	168	IRAM	11”	excitation &
HDO	2_{11}-2_{12}	241.56	95	JCMT	21”	deuteration
HDO	1_{01}-0_{00}	464.92	22	JCMT	12”	
SO_2	$12_{0,12}$-$11_{1,11}$	203.39	49	IRAM	12”	shock chem
CH_3OH	5_{-1}-4_0	84.52	40	IRAM	30”	ice mantles

The Sample: 8 objects

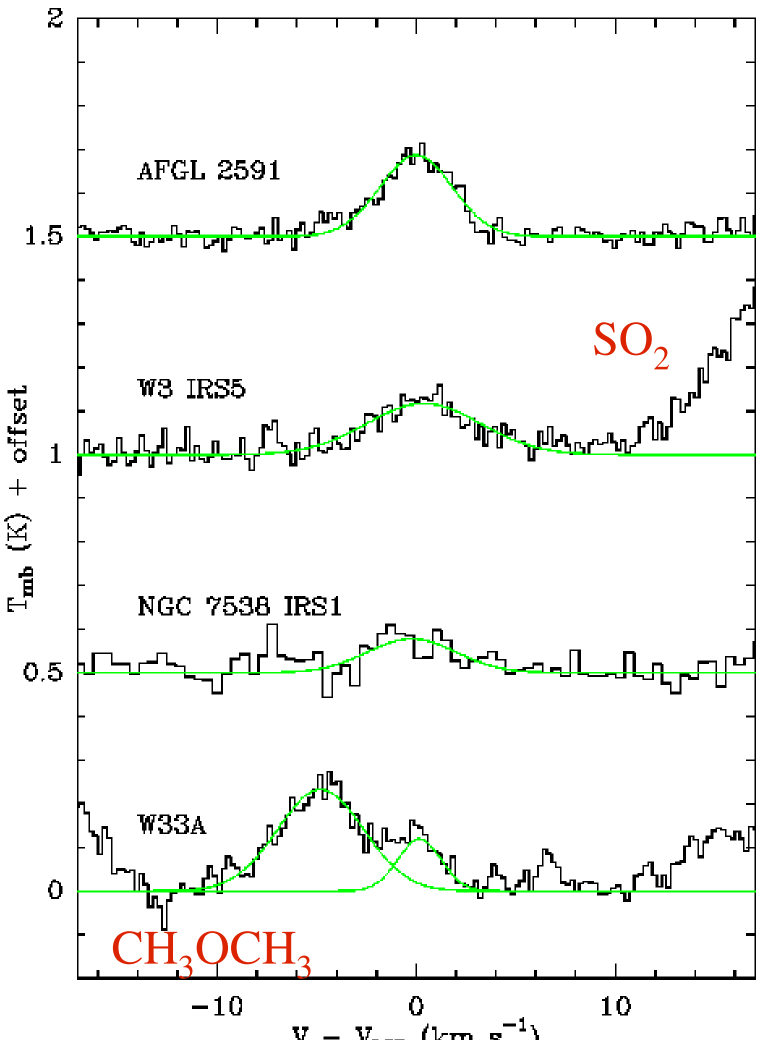
- L = 2 x 10^3 - 2 x 10^5 L_0
- d = 1 - 4 kpc
- M = 30 - 1100 M_0 within ~0.1 pc (~arcmin)
- Bright in mid-IR: compare with ISO
- Weak in radio: pre-UCHII stage
- Submm spectra:
  - evolution from cold to warm envelope related to M/L
  - stage before "hot core"

IRAM 30m spectra: 50% detected

- Detected sources have most warm gas

  Not just excitation effect:
- HDO detected in same sources

p-$H_2{}^{18}O$ 203.4 GHz



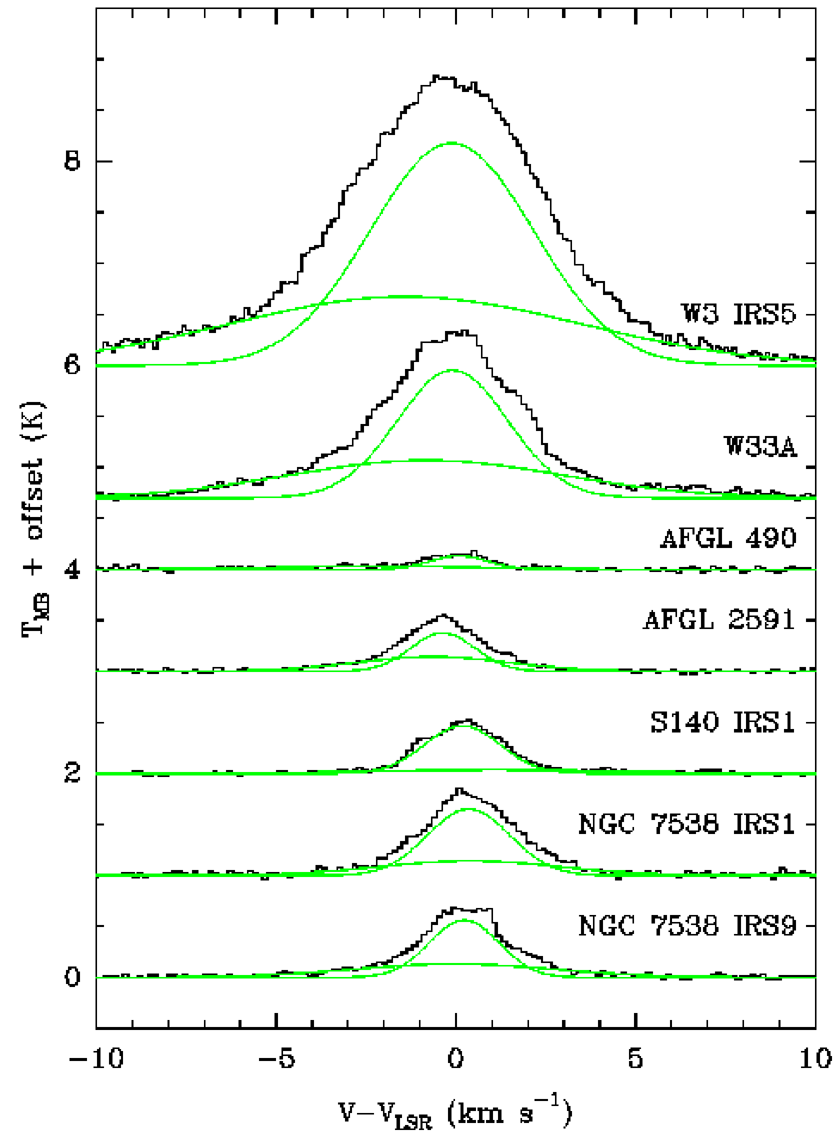
Line profiles of CH_3OH and SO_2

- 20-50% of line flux in outflow

similar fraction as for CS, SO

- desorption of grain mantles:

half mechanical, half radiative?



Excitation & Column density

T_{rot}(HDO) ~ 110 K

assuming source size <12 - 18”

$N(H_2O)$ ~ 2 x 10^{17} cm^{-2}

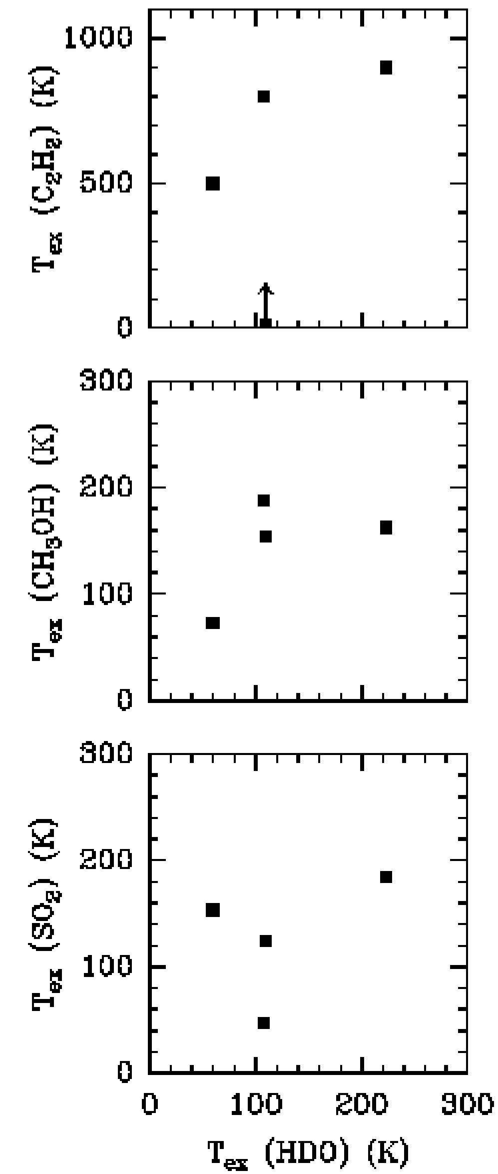
similar to ISO: extended over >1” (1000 AU)

N(HDO) ~ 2 x 10^{14} cm^{-2}

HDO/H_2O higher in colder sources,

and consistent with solid state obs.

But T_{rot}>> T_{chem}: molecules “stored”

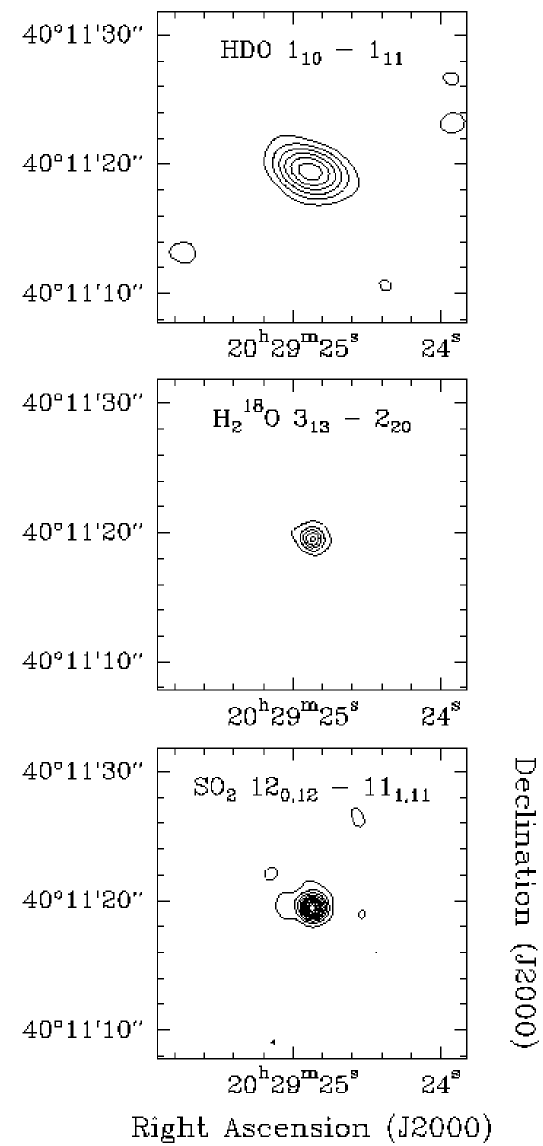


Bure maps of AFGL 2591

Compact emission: size 500 - 1000 AU
C+D config: beam 1.2 & 4.0”

Line width similar to single dish value:
kinematically same gas

All of single-dish flux recovered:
no extended halo resolved out



Estimating abundances

Divide $N(H_2O)$ by $N(H_2)$: ~10^{-6}, but:

ignores beam size mismatch

ignores excitation gradients

assumes uniform distribution

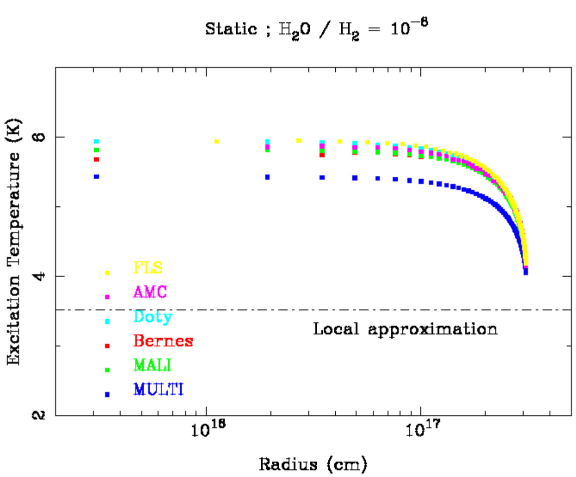
Model line emission with Monte Carlo program

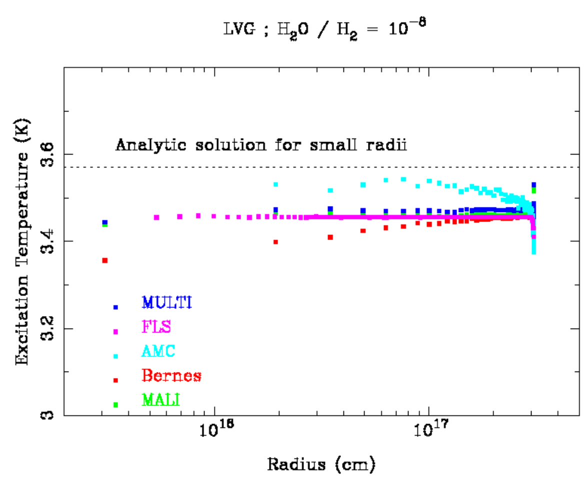
Ratran (Hogerheijde & van der Tak 2000)

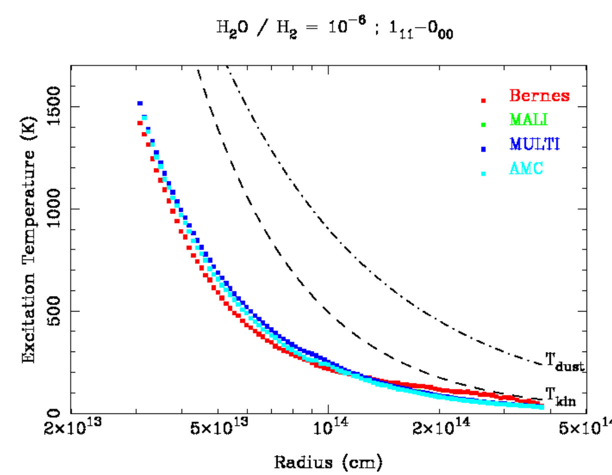
molecular data: Schöier et al (2005)

dust properties: Ossenkopf & Henning (1994)

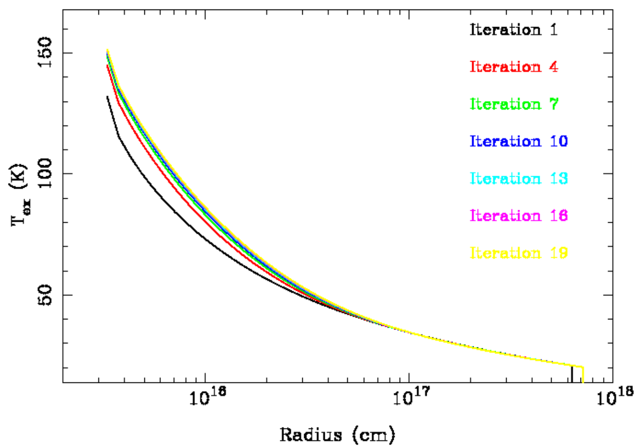
temperature & density profiles: Van der Tak et al (2000)







Abundance profiles of H_2O & HDO



Constant abundance models:

HDO / H_2 ~ 10^{-8}, H_2O / H_2 ~ 10^{-5}

But emitting region 4-5” FWHM ...

Jump models:

H_2O / H_2 ~ 1.2-2.0 x 10^{-4} (SWAS: ~ 10^{-6})

Jump at T=100-115 K point

HDO / H_2 ~ from 10^{-9} to 10^{-7}

Similar jumps seen in SO_2 and CH_3OH

Water is mostly evaporated ice

Future directions

- Ground-based studies of non-ISO sources
  - effect of *L*, *M*, geometry, ...
  - resolve abundance enhancements (ALMA)
- Space-based THz spectroscopy (*Herschel*)
  - good handle on excitation & *o/p* ratio
  - abundances in **each** chemical zone
  - extend to low-mass sources

Further Reading

- Monte Carlo program:

  http://www.mpifr-bonn.mpg.de/staff/fvandertak/ratran/

- Molecular database:

  http://www.strw.leidenuniv.nl/~moldata/

- Water benchmark:

  http://www.mpifr-bonn.mpg.de/staff/fvandertak/H2O/