Chemical modeling of C/O ratio in protoplanetary disks

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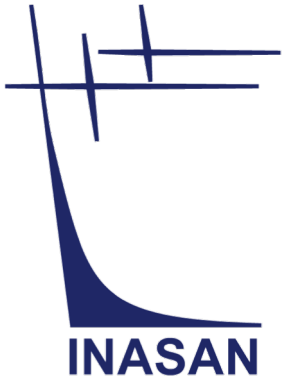
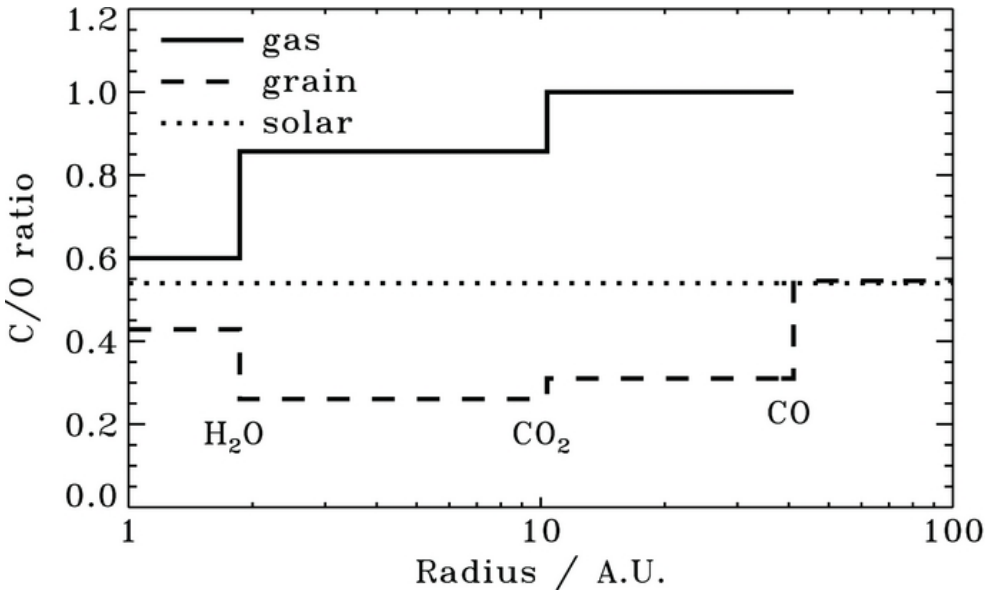


The Periodic Table through Space and Time
Saint-Petersburg
2019

Carbon-to-oxygen ratio

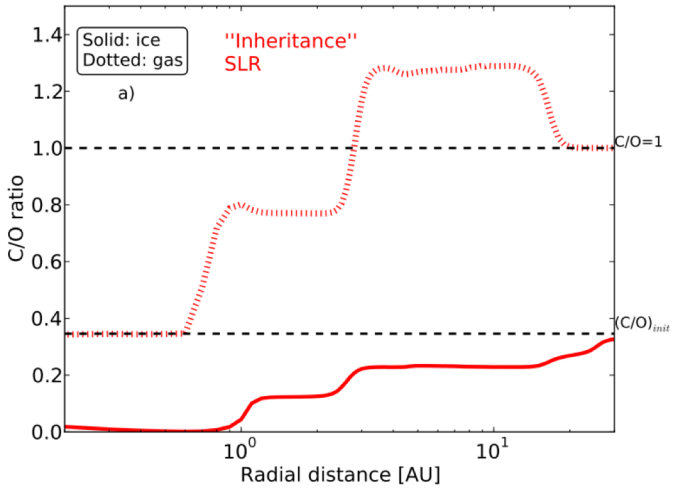
- C/O > 1 is observed in atmospheres of exoplanets (Swain+09, Madhusudhan+11) and in gas phase in protoplanetary disks (Bergin+16, Semenov+18, Cleeves+18)
- Carbon excess can appear in gas and ice phases due to redistribution of major volatiles
- Possible connection to planet formation mechanisms

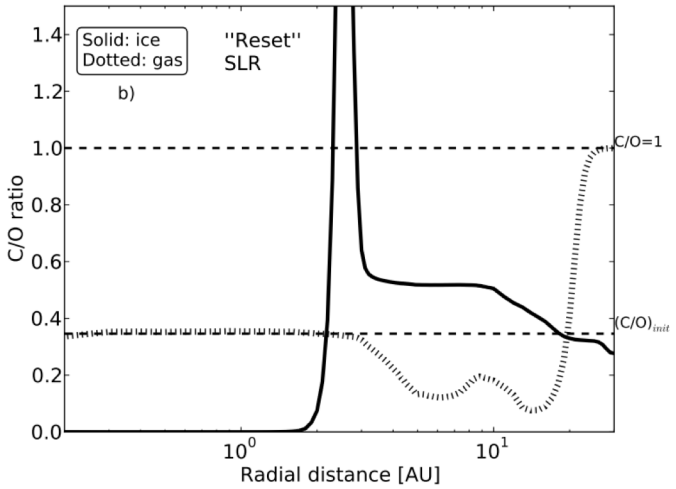


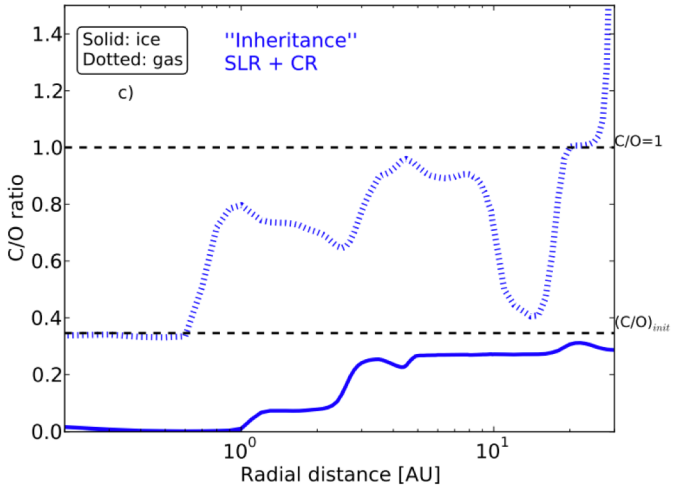
Öberg+11

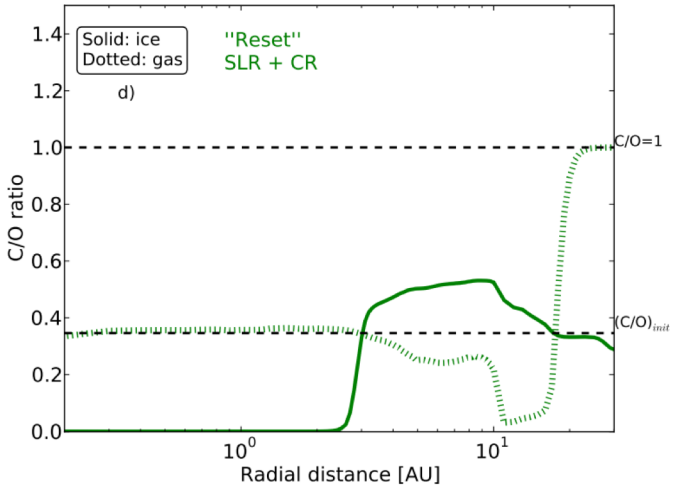
C/O in gas and in ice is affected by snowlines of major volatiles

Mordasini+16, Eistrup+18, Cridland+19









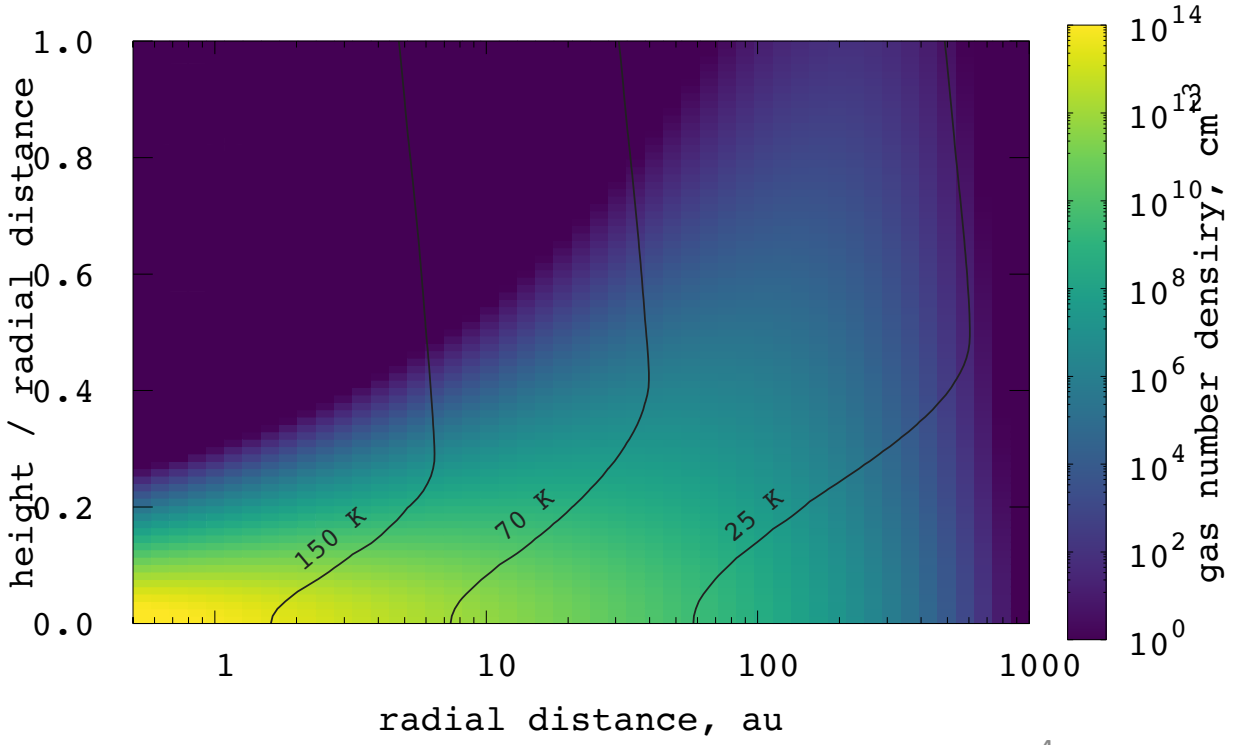
Eistrup+16

ANDES model

- Non-equilibrium astrochemical code ANDES by Akimkin+13 is used to calculate chemical evolution of the disk.
- Axially-symmetric disk model
- Hydrostatic equilibrium in vertical direction
- Modified ALCHEMIC reactions network (Semenov & Wiebe 2011) with 650 species and 7803 reactions including surface chemistry.

Main model parameters are:
stellar mass $M_{\bigstar}$, disk mass M_{disk}, disk characteristic radius R_c, initial chemical composition

Example of disk structure in ANDES



Model parameters

- We run a number of models with different parameters
- Reference initial elemental composition is “low metals”
- Models with higher C.

Parameter	Values
$M_\star, M_\odot$	0.3, 0.5, 1.0, 1.5, 2.5
$M_{disk}, \% M_\star$	0.1, 0.3, 1, 3, 10
R_c, au	20, 50, 100

low metals
by Lee+98
C/O=0.4

H_2	0.499
He	0.09
H	0.002
C	7.3(-5) 1.408(-4) 2.112(-4)
N	2.14(-5)
O	1.76(-4)
S	8(-8)

Eistrup+16,
C/O=0.35

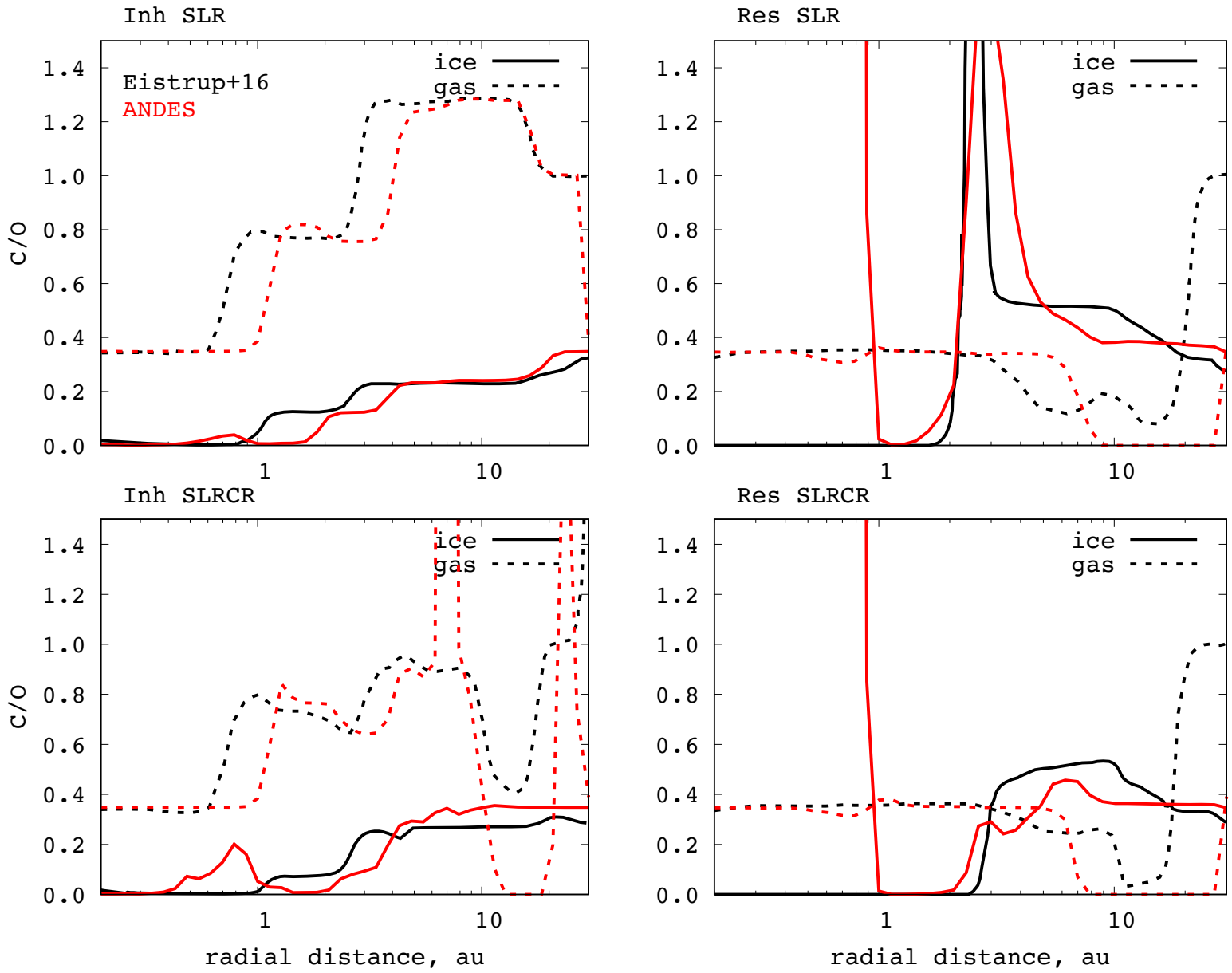
H_2	0.5
He	9.8(-2)
H	9.1(-5)
C	1.8(-4)
N	6.2(-5)
O	5.2(-4)
S	6(-6)

+ molecular abundances from Eistrup+16

Benchmarking with Eistrup+16

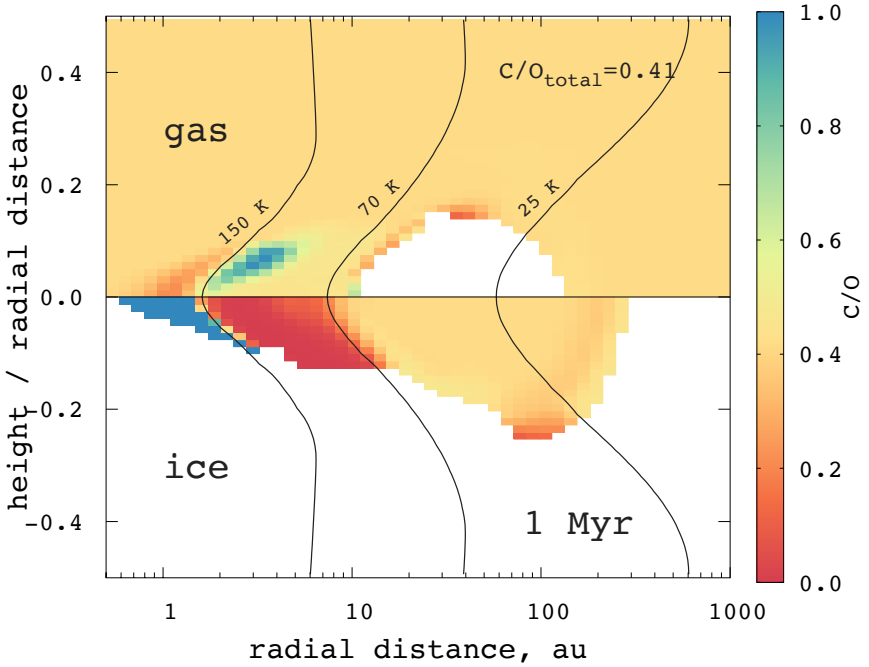
~ the same physical structure

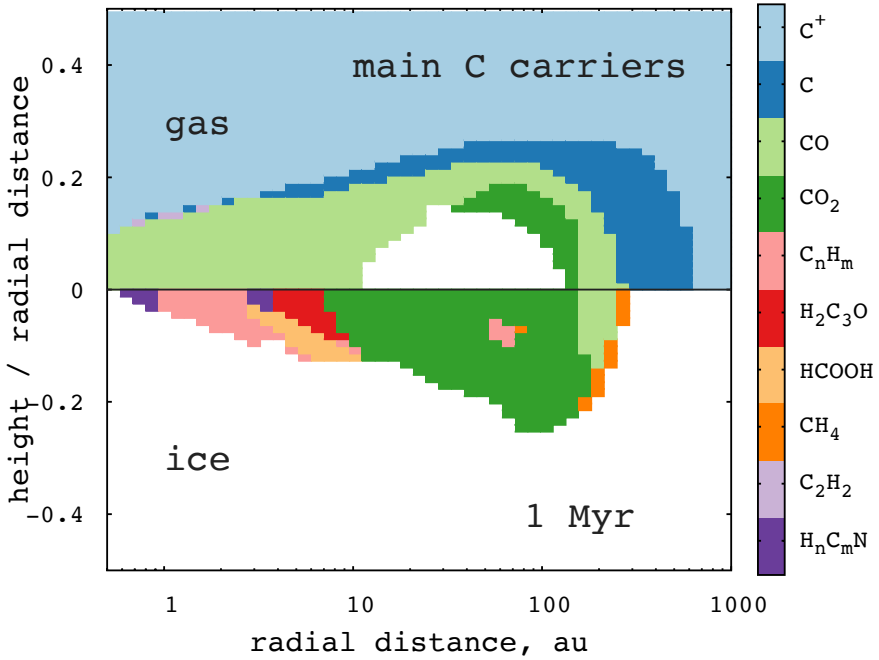
different chemical network

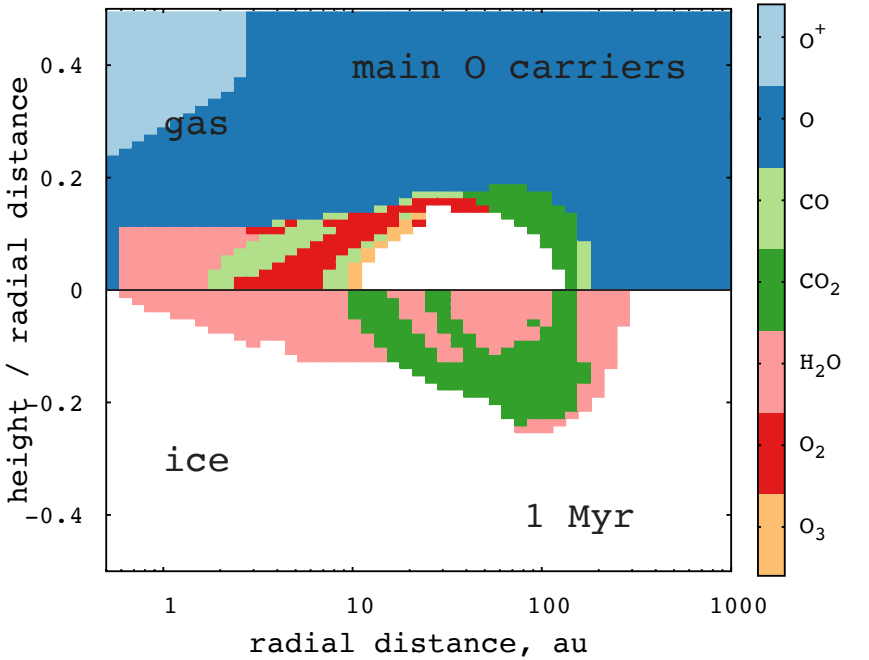


Reference model

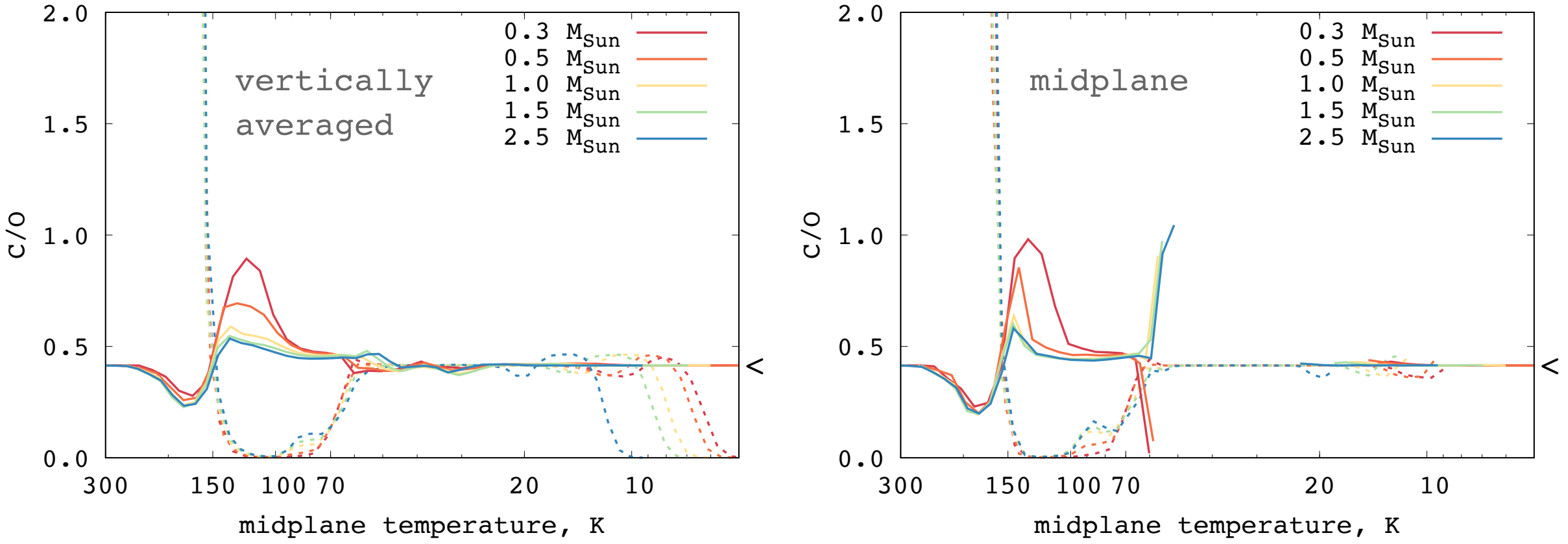
$M_{disk} = 0.01 M_{\odot}$
$M_{\bigstar} = 1 M_{\odot}$
$R_c = 50$ au
Elemental initial composition with C/O=0.41 (low metals by Lee+98)







C/O in disks with different stars



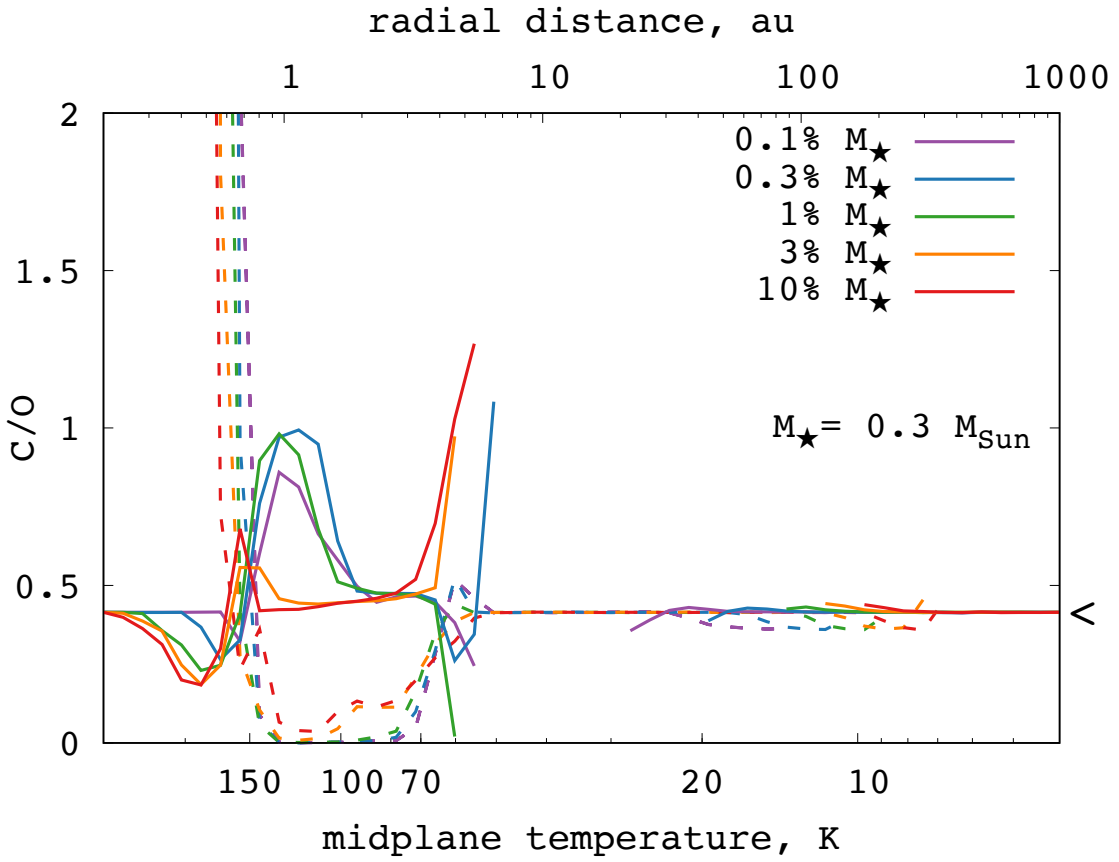
C/O in gas (solid lines) and in ice (dashed lines)

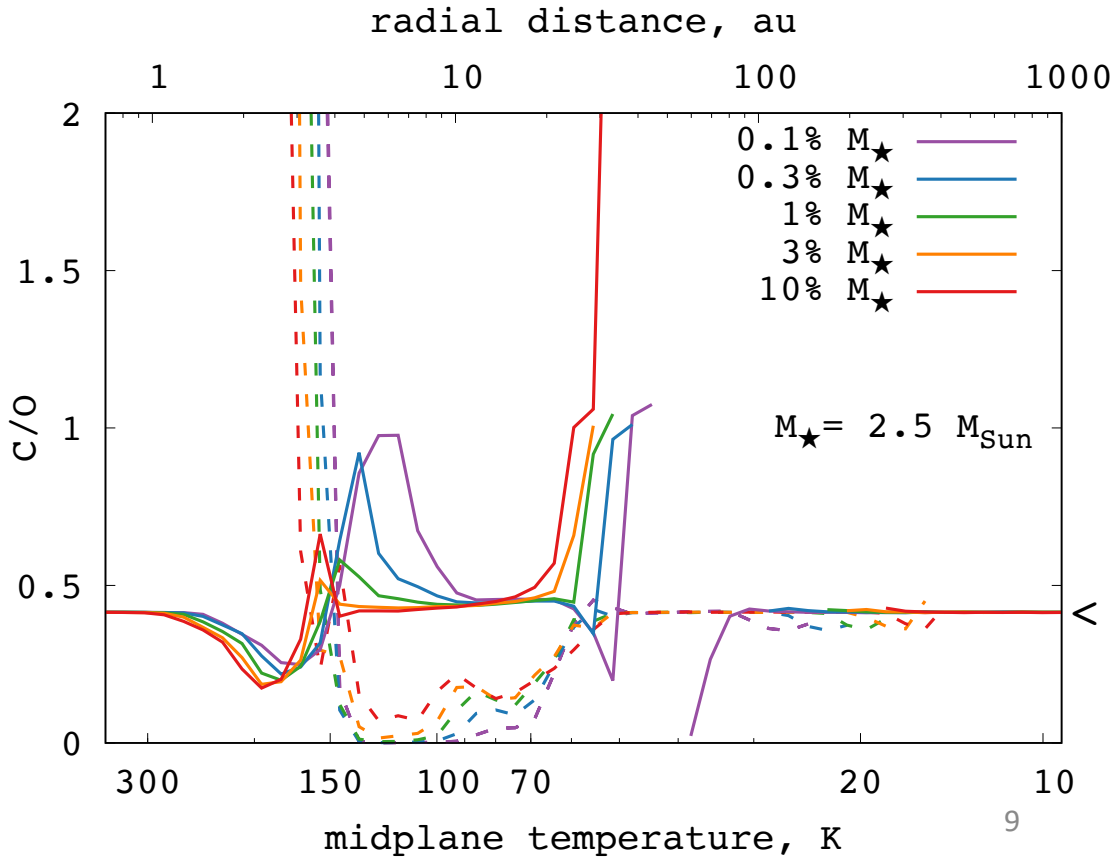
C/O in gas phase is close to 1:

- around 1 au in models with low-mass disks around low-mass stars
- between 20-30 au in models with massive disks around massive stars

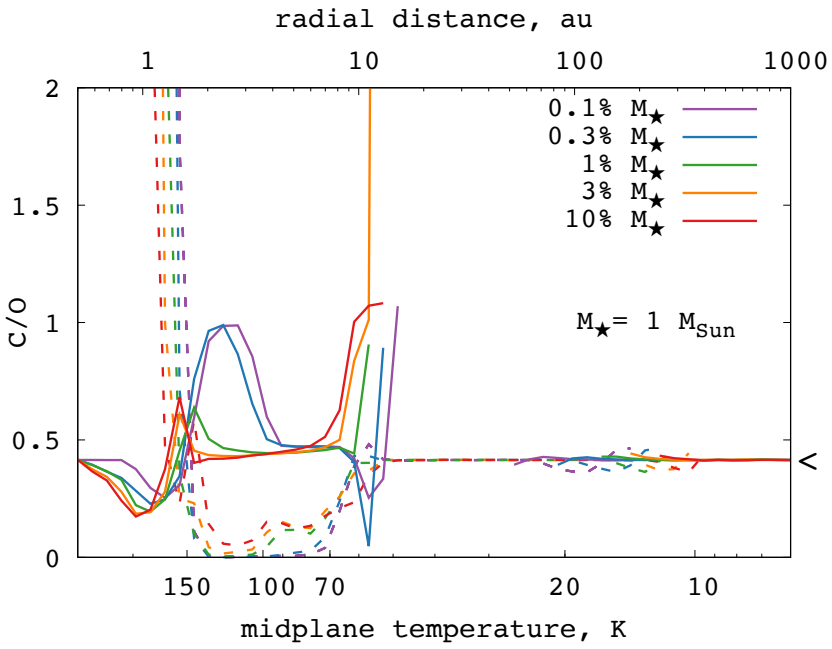
C/O in ice phase is exceeds 1:

- in the inner hot region of disks

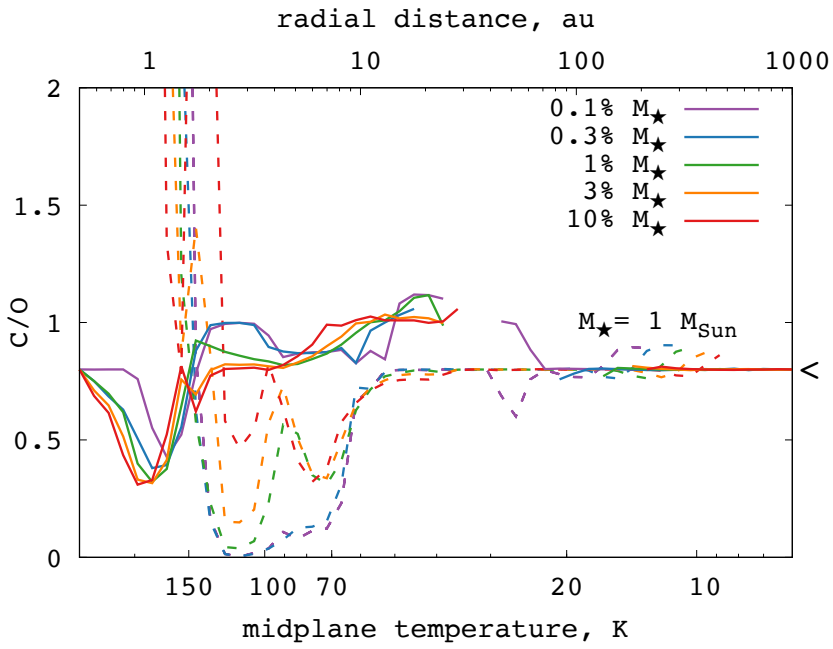




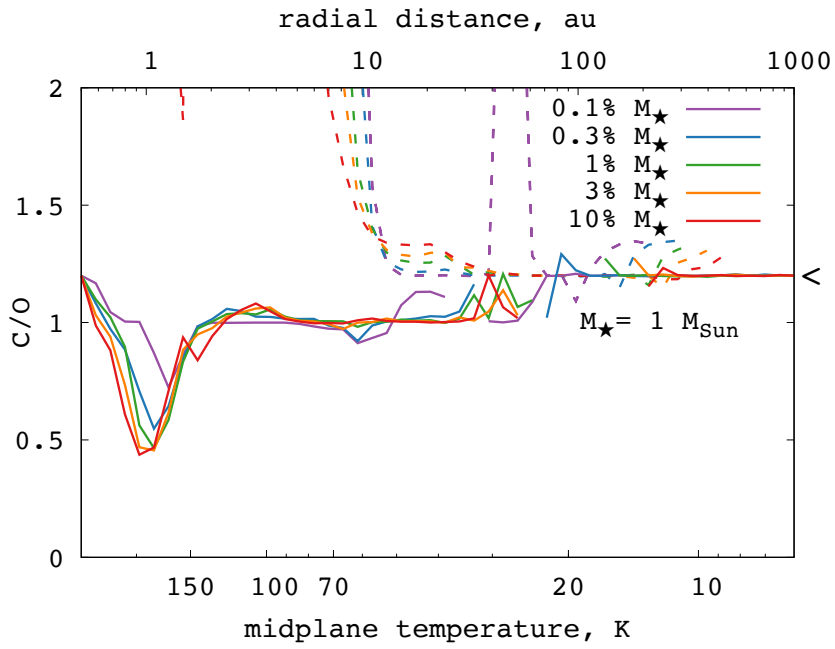
Initial metallicities



C/O=0.41

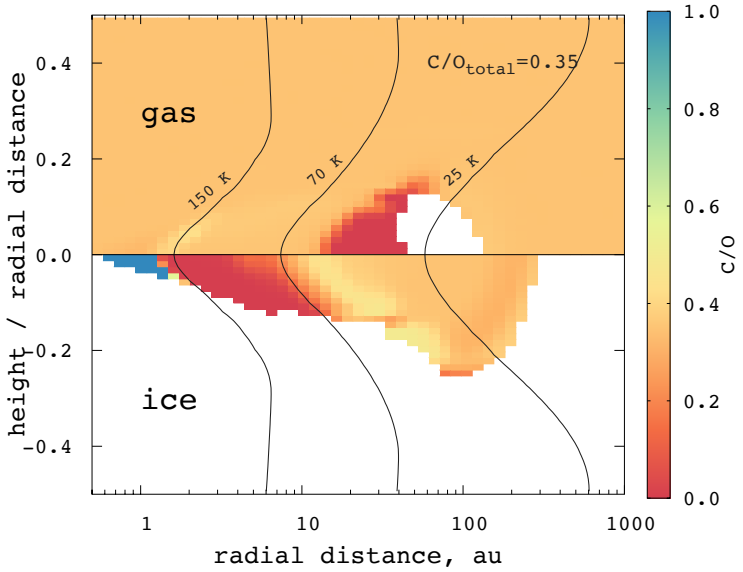


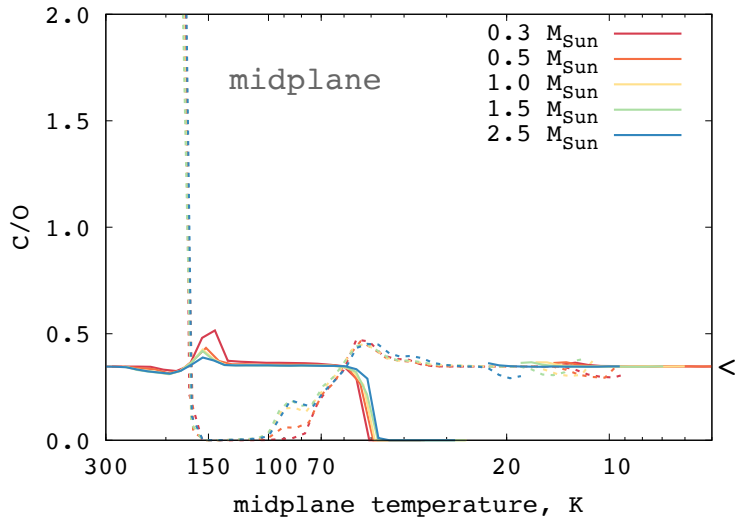
C/O=0.8



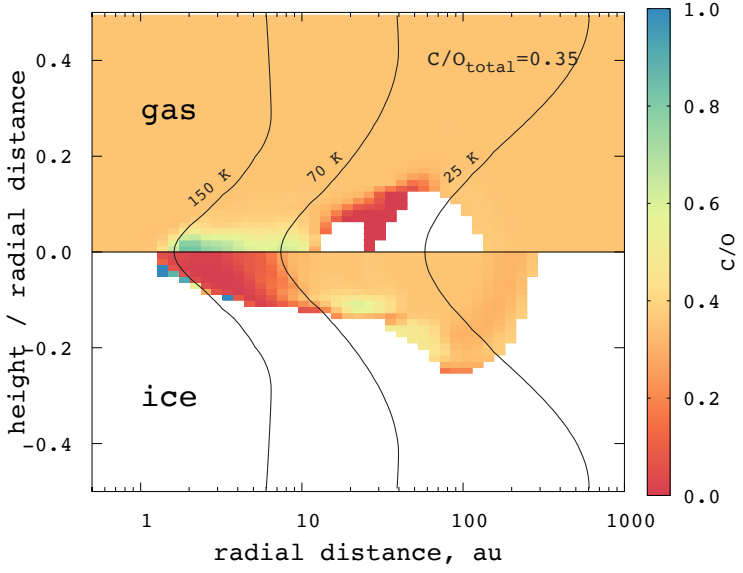
C/O=1.2

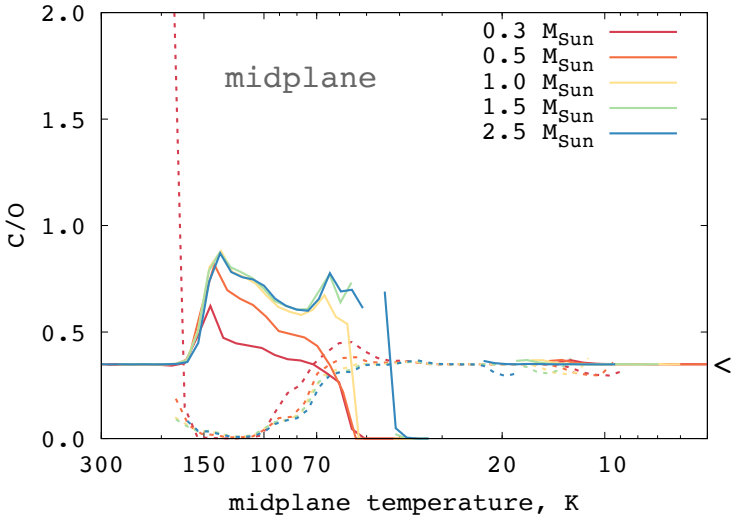
Atomic
initial composition





Molecular
initial composition





initial abundances from Eistrup+16

Molyarova et al. in prep.

Conclusions

- C/O in the disc midplane changes sharply around the snowlines of water and carbon dioxide. Gas-phase processes affect C/O as well
- Carbon and oxygen have very low midplane abundances in the gas in the bulk of protoplanetary disc (outside CO_2 snowline).
- C/O variations in the midplane are larger than in vertically averaged C/O.
- C/O in the gas phase tends to reach 1 in the inner regions (right outside the water snowline) of the least massive discs around the least massive stars, as well as at 10–20 au in more massive discs.

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