A comprehensive ionization chemical network for protoplanetary disks

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Introduction

Ionization plays a critical role in the gas dynamics of protoplanetary disks (PPDs) as it determines how well the gas are coupled with magnetic field and whether magnetorotational instability (MRI) will operate.

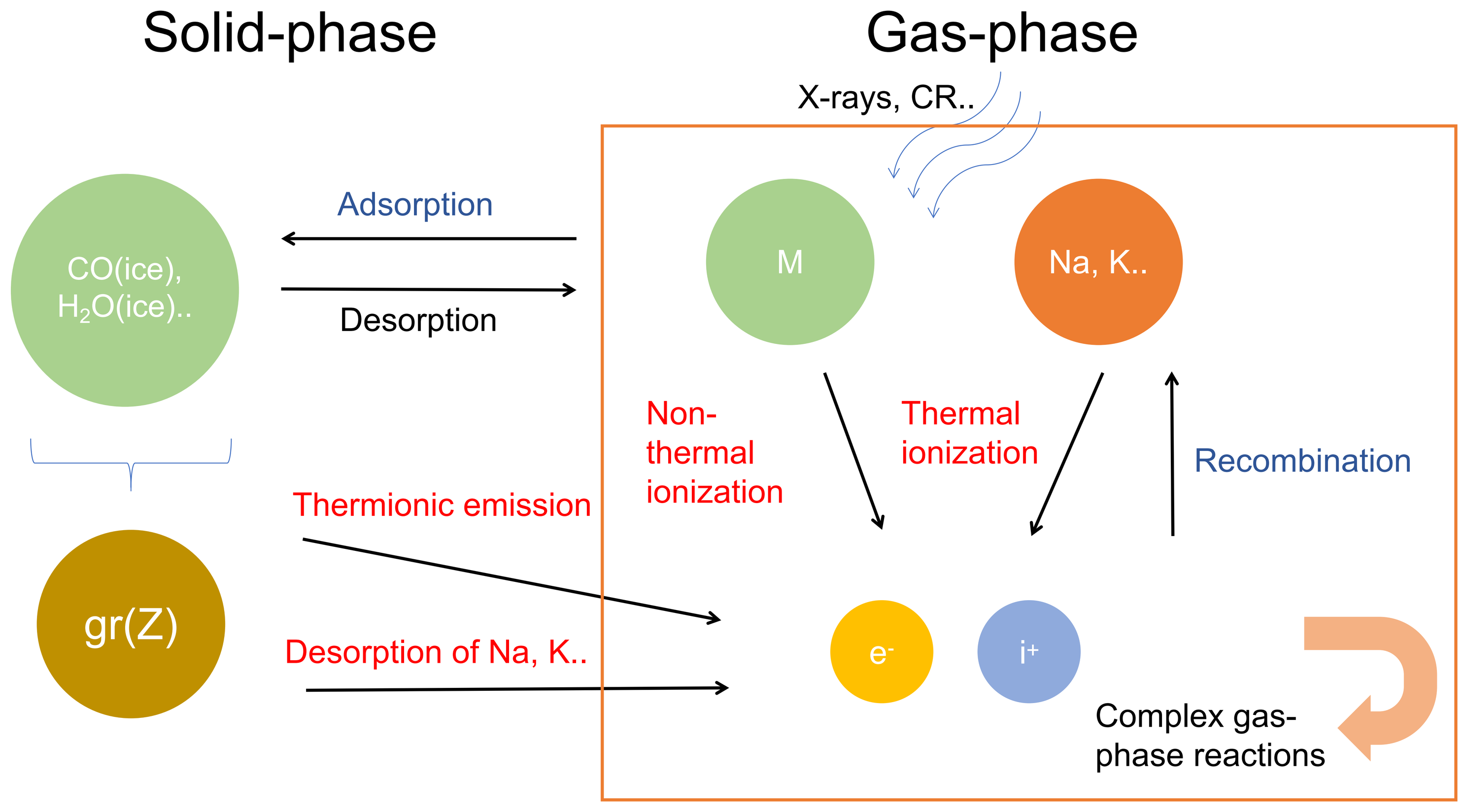
For the bulk regions of protoplanetary disks, the temperature is low and the dominant ionization sources are non-thermal ones, such as X-rays and cosmic-rays. The ionization level is low and the MRI is largely suppressed.

However, for the innermost regions, the temeperature surpasses the threshold of ~1000K to trigger thermal ionization of alkali species and dust thermionic emission. The ionization level goes high and the MRI is likely to revive. The transition region is commonly referred to as the the deadzone inner boundary and suggested to be a preferred location for planet formation.

To better understand the complex ionization processes in PPDs, we develop a comprehensive ionization chemical network that accounts for both thermal and non-thermal ionization.

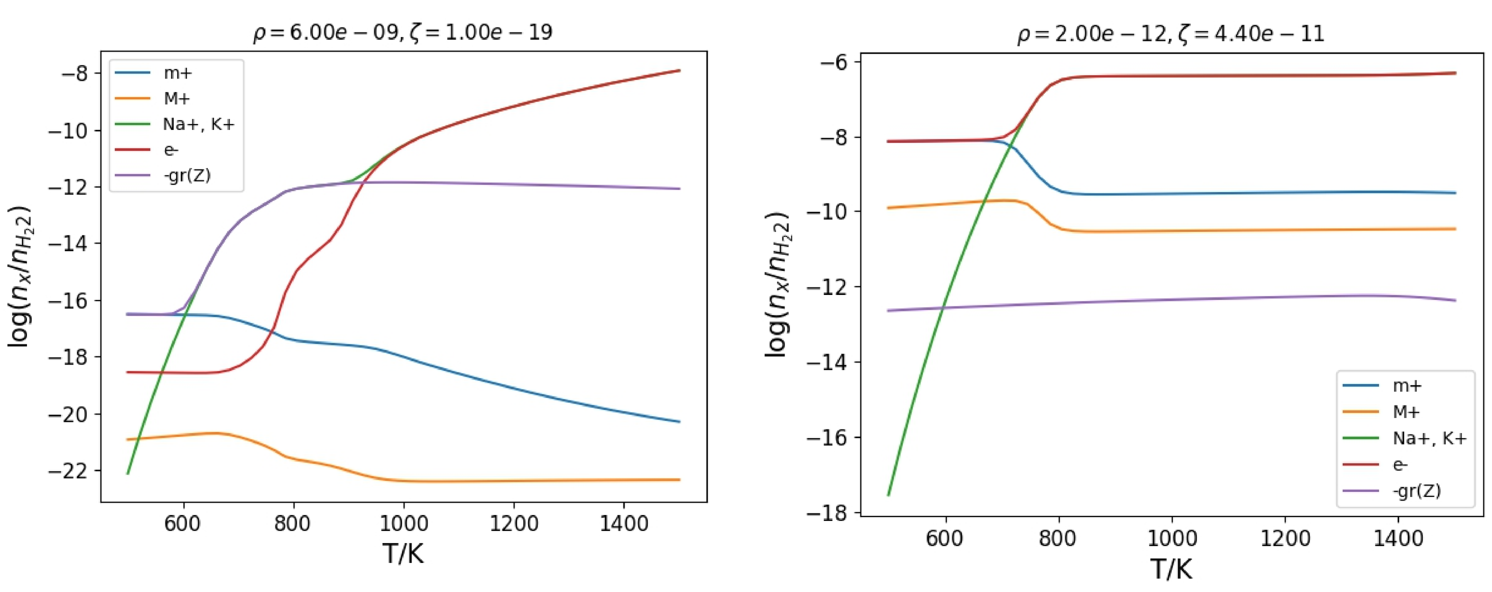
Using this model, we calculate the ionization fraction and the resulting magnetic diffusivities throughout the full range of physical conditions present in PPDs and discuss the implications on the gas dynamics of the innermost disk regions.

The chemical network



Our chemical network is established by incorporating the works of Ilgner & Nelson 2006 and Desch & Turner 2015. It includes ~170 species and ~2400 reactions.

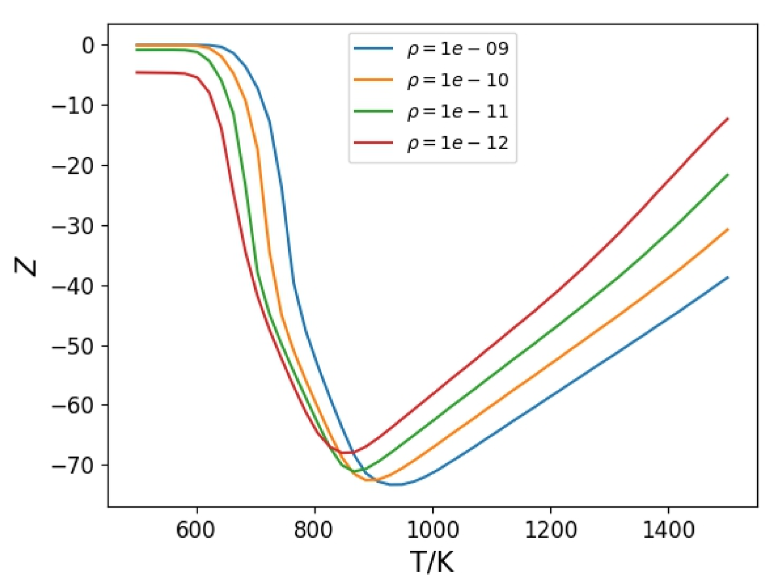
1. Complex gas-phase reactions drawn from updated UMIST12 database (McElroy et al. 2013)
2. Adsorption and desorption of gas-phase species on dust grains
3. Non-thermal ionization effects (X-rays, cosmic-rays and decay of shor-lived radioactive nuclei)
4. Thermal ionization of alkali species (Na, K)
5. Dust thermionic emission



Here we show how the **abundances of charged species** vary with temperature with fixed density and non-thermal ionization rate.

Left (midplane): $\rho=6\times10^{-9}$ g cm^{-3} ($n_{H2}=1.3\times10^{15}$ cm^{-3}), $\zeta=1\times10^{-19}$ s^{-1}.

Right (upper layer): $\rho=2\times10^{-12}$ g cm^{-3} ($n_{H2}=4.3\times10^{11}$ cm^{-3}), $\zeta=4.4\times10^{-11}$ s^{-1}.

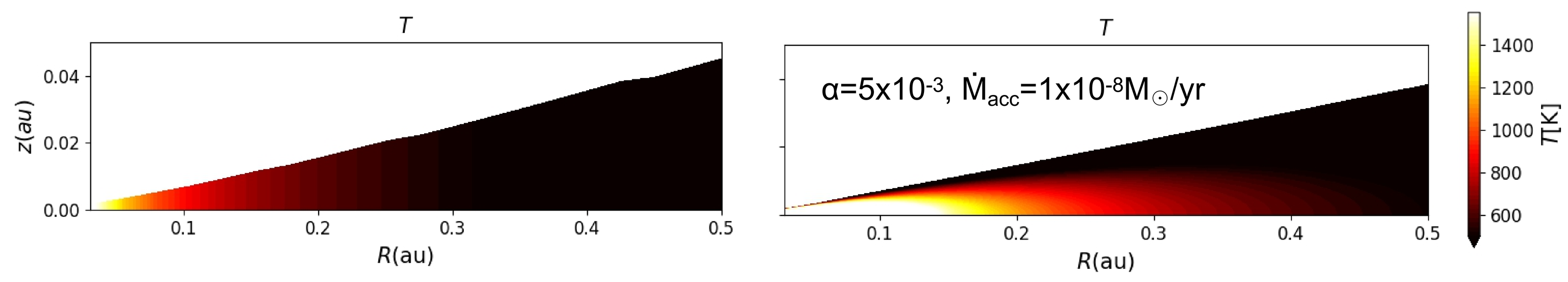


Dust mean charge is shown.

1. Grains can be highly charged when ionization fraction is high.
2. Instead of treating differently charged grains as separate entities, the dust mean charge is calculated.
3. This approach enables us to simplify the analysis while still capturing the behavior of a range of grain charges.

Model setup

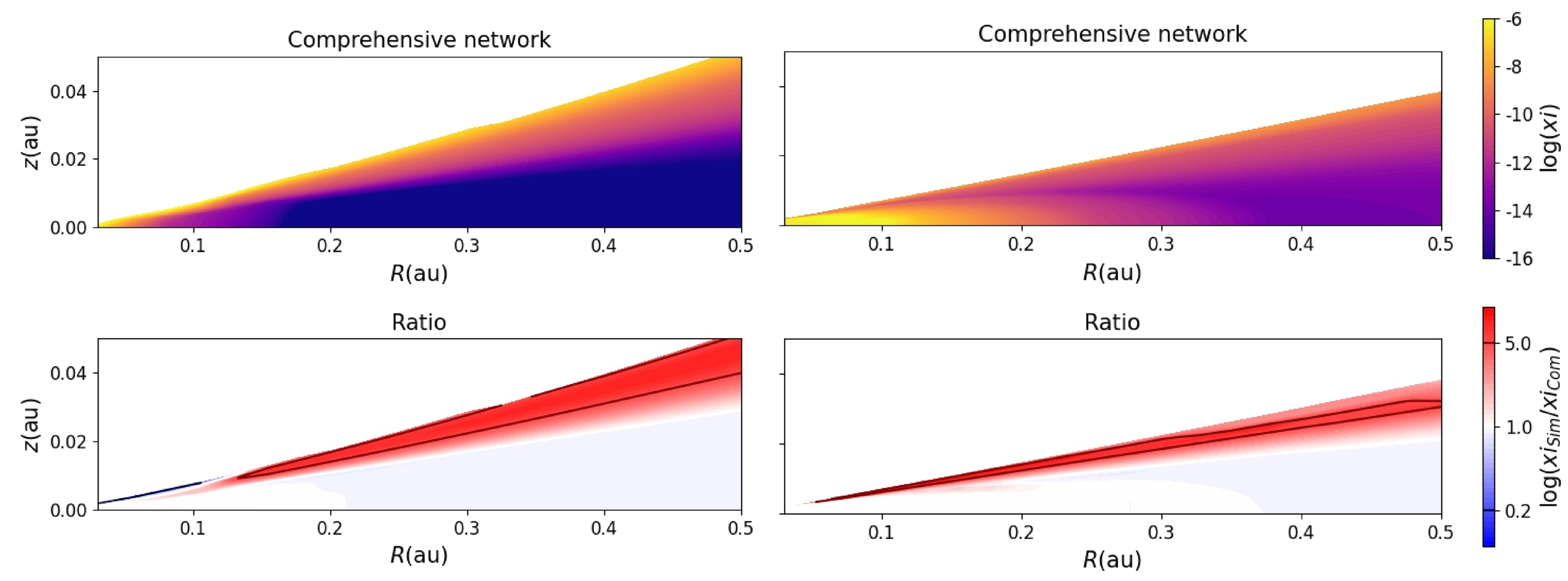
We apply our network to two disk models:



MMSN-like disk: Surface density = 500g cm^{-2} r_{au}^{-1}, T = 280K $r_{au}^{-0.5}$

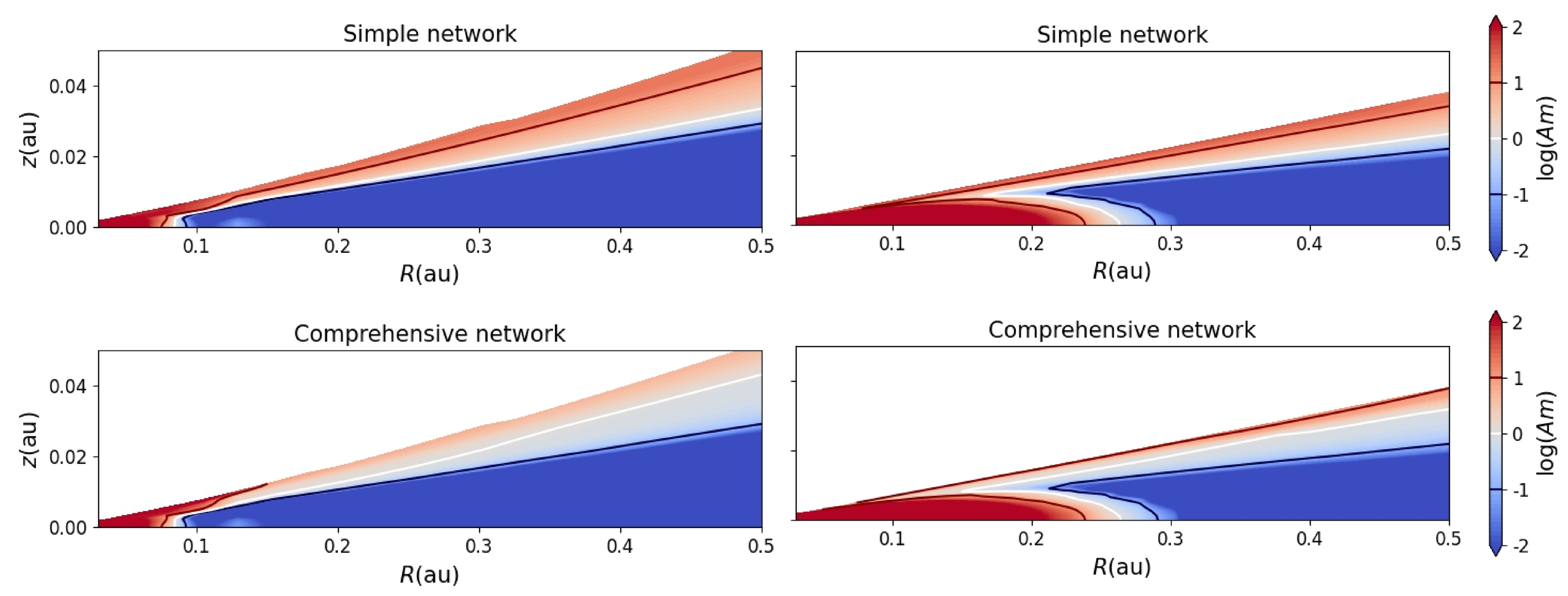
α disk: Surface density = 175g cm^{-2} $r_{au}^{-0.6}$, T calculated with analytical solution of radiative transfer (Mori et al. 2019)

Results



Here we present the **ionization fraction** calculated from our comprehensive network and the **ratio** between the simple and comprehensive ones.

1. The upper layer is strongly ionized by non-thermal sources. And the ionization fraction of midplane rises rapidly where temperature reaches ~1000K and triggers thermal ionization.
2. The major difference between simple and comprehensive network lies in upper layers. The simple network results in ~5 times higher ionization fraction than the comprehensive one, which would destabilize the surface layer that would otherwise be stable.



Ambipolar Elsasser number (Am) is shown to predict the MRI-active region. When Am < ~1, the MRI is substantially damped by Ambipolar diffusion.

1. The simple network shows an MRI-unstable surface layer while comprehensive shows a more stable one.
2. At ~0.25au in the α disk model, the gas right inside the dead zone inner boundary will likely achieve a state that is MRI active in the midplane, while largely laminar in the disk surface.

Summary

In this study, we have developed a comprehensive chemical network that takes into account both thermal and non-thermal ionization mechanisms, and applied it to two disk models. Our findings reveal that the newly proposed chemical network predicts a significantly lower ionization fraction in the high layer, while almost maintaining the same level of ionization in the midplane, when compared to a simpler network. These results provide a solid microphysical foundation for future magnetohydrodynamic (MHD) simulations of the innermost regions of protoplanetary disks.

References

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