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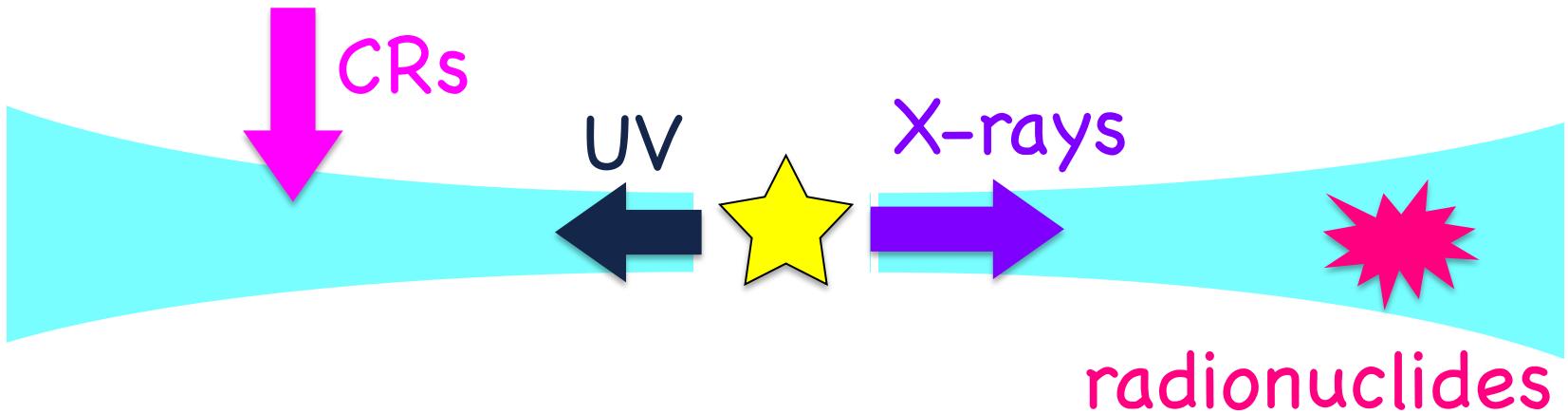
# MHD Simulations of Protoplanetary Disks with Non-equilibrium Ionization Chemistry

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# Weak Ionization of PPDs

protoplanetary disks

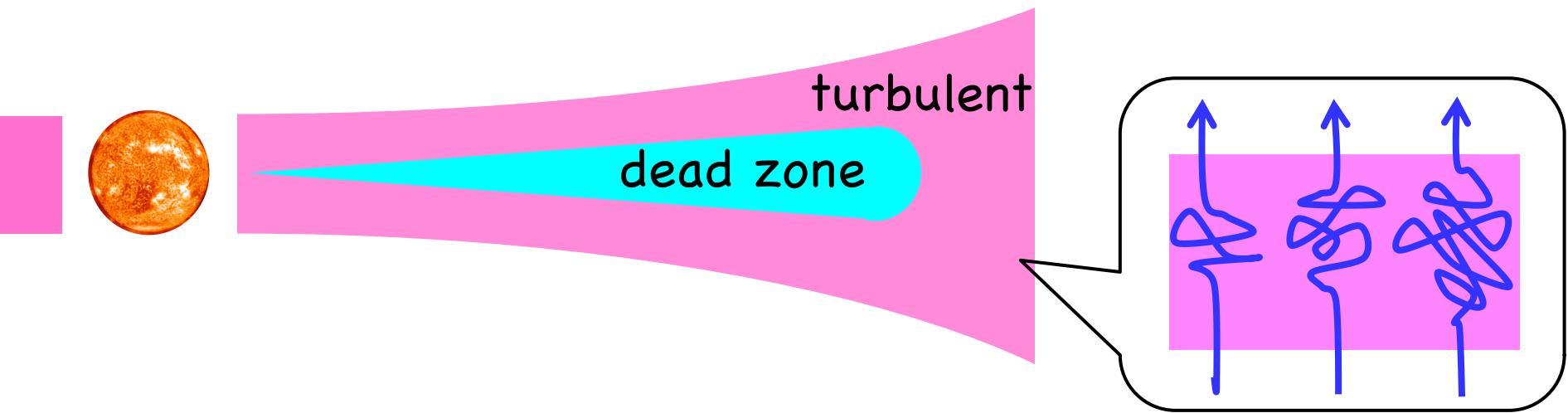


PPDs are cool and dense

- ⇒ not coupled to magnetic fields everywhere
- ⇒ need to consider non-ideal MHD effects

# Are PPDs Turbulent?

Strength of turbulence is important for planet formation



Disk dynamics depends on MRI\*

- active layer: high accretion rate
- dead zone: low accretion rate

disk gas must be  
sufficiently ionized

\*MRI: magnetorotational instability (Balbus & Hawley (1991))

# Disk Dynamics due to MRI



disk wind: mass loss from disk surface

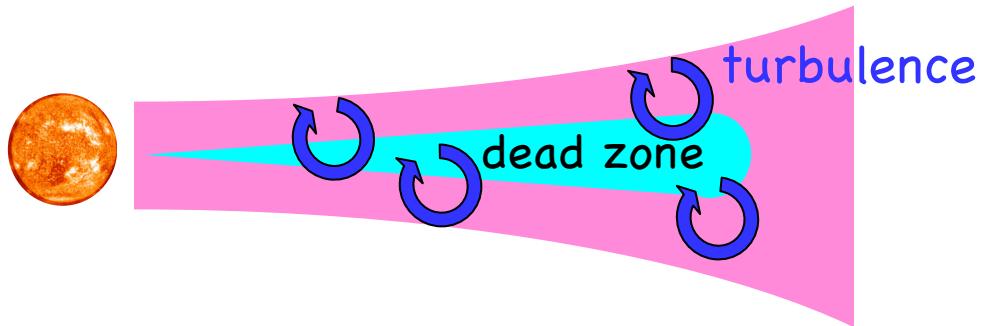
Suzuki & Inutsuka (2009), Suzuki et al. (2010), Bai & Stone (2013)

turbulence affects dead-zone boundary

Turbulent mixing may change dead-zone size (dust-free case).

Inutsuka & Sano (2005), Turner et al. (2007), Ilgner & Nelson (2008)

# Disk Dynamics due to MRI



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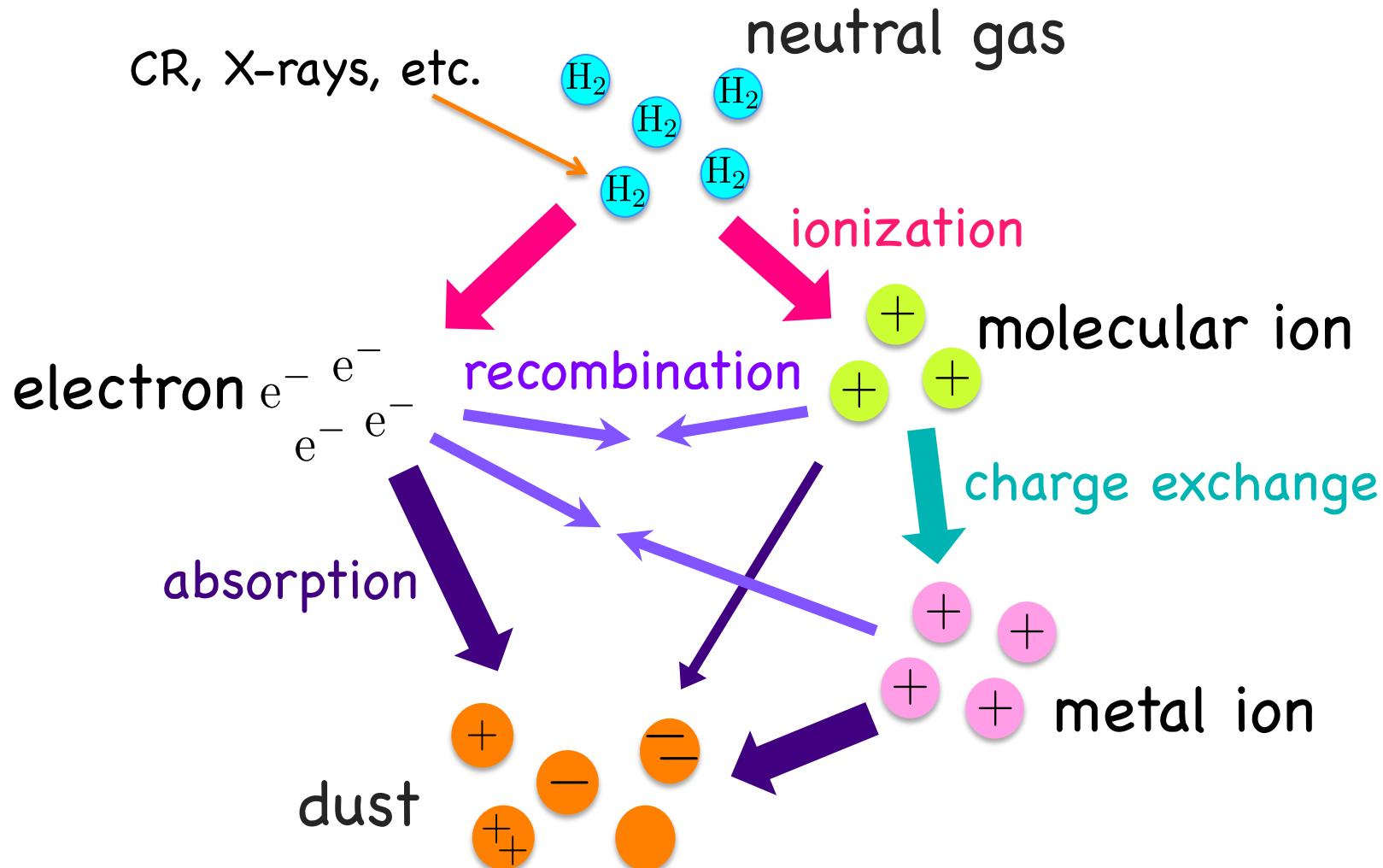
turbulence affects dead-zone boundary

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What about with dust grains?

# Simplified Chemical Network



# Reaction Equations

$m^+$  : mol. ion  
 $M^+$  : metal ion  
 $e$  : electron  
 $d$  : dust grains  
 $Z$  : dust charge

molecular ion's number density

$$\frac{dn_{m^+}}{dt} = \zeta n_n - \alpha_{m^+} n_{m^+} n_e - \beta n_{m^+} n_M - \sum_Z k_{m^+d}(Z) n_d(Z) n_{m^+}$$

ionization    recombination    charge exchange    absorption by grains

metal ion's number density

$$\frac{dn_{M^+}}{dt} = -\alpha_{M^+} n_{M^+} n_e + \beta n_{m^+} n_M - \sum_Z k_{M^+d}(Z) n_d(Z) n_{M^+}$$

recombination    charge exchange    absorption by grains

electron's number density

$$\frac{dn_e}{dt} = \zeta n_n - \alpha_{m^+} n_{m^+} n_e - \alpha_{M^+} n_{M^+} n_e - \sum_Z k_{ed}(Z) n_d(Z) n_e$$

ionization    recombination    absorption by grains

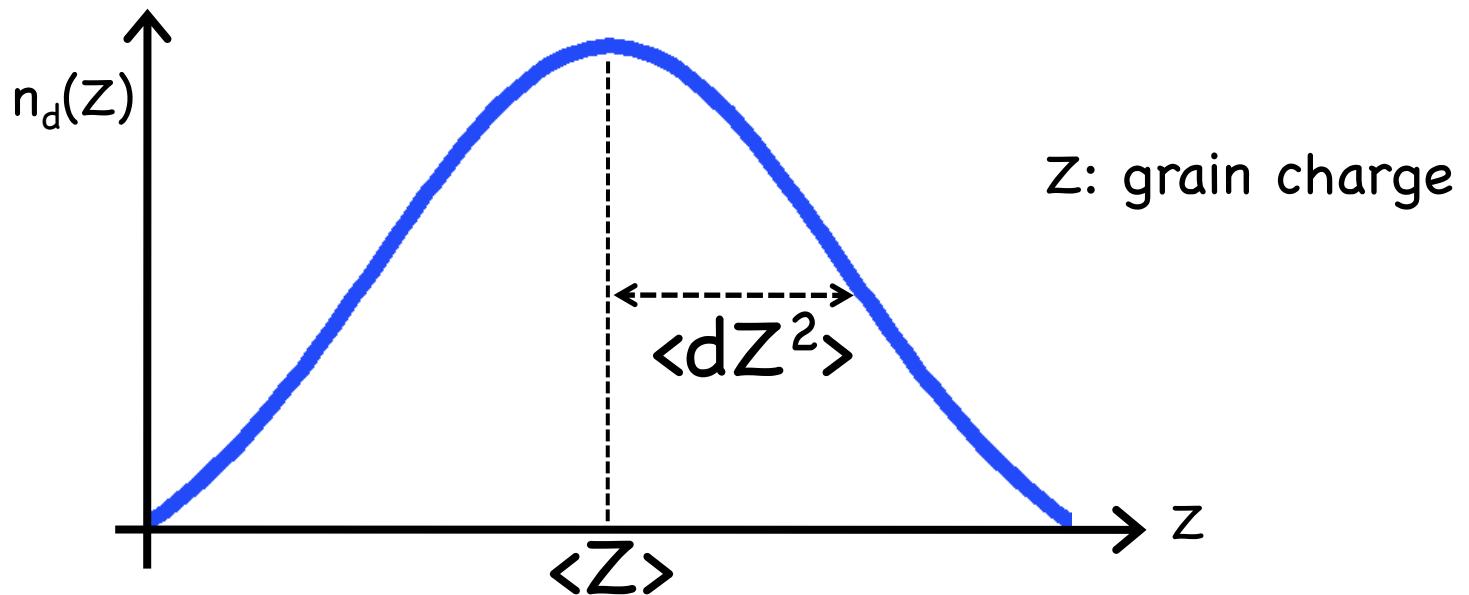
number density of grains with charge "Z"

$$\begin{aligned} \frac{dn_d(Z)}{dt} &= -k_{m^+d}(Z) n_d(Z) n_{m^+} - k_{M^+d}(Z) n_d(Z) n_{M^+} \\ &\quad - k_{ed}(Z) n_d(Z) n_e + k_{m^+d}(Z-1) n_d(Z-1) n_{m^+} \\ &\quad + k_{M^+d}(Z-1) n_d(Z-1) n_{M^+} + k_{ed}(Z+1) n_d(Z+1) n_e \end{aligned}$$

e.g. Oppenheimer & Dalgarno (1974)  
 Sano et al. (2000)  
 Ilgner & Nelson (2009)  
 Okuzumi (2009)  
 Fujii et al. (2011)

# Dust Charge Distribution

- approximated by Gaussian distribution  
(Okuzumi, 2009)
- solve  $\langle Z \rangle$  and  $\langle dZ^2 \rangle$  instead of  $n_d(Z)$



⇒ number of equations can be reduced

# 3D Non-ideal MHD Simulations

- Setup (local box @2AU)

- Athena MHD code with time-dependent ionization  
(Stone et al., 2008) (Fujii et al. 2011 + $\alpha$ )

- box size

- $(x, y, z) = (\pm 0.5h, \pm 2h, \pm 4h)$

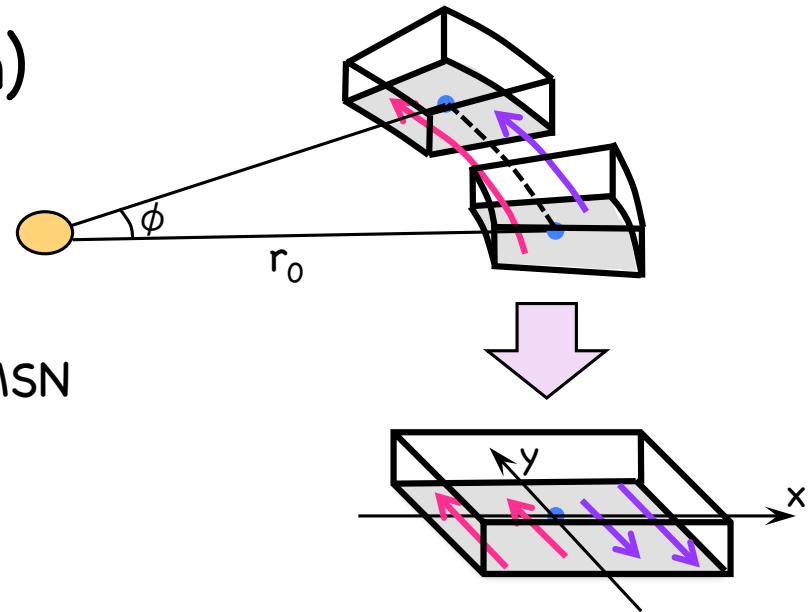
- $16 \times 32 \times 192$  grids

- surface density:  $\Sigma = 0.01\Sigma_{\text{MMSN}}$

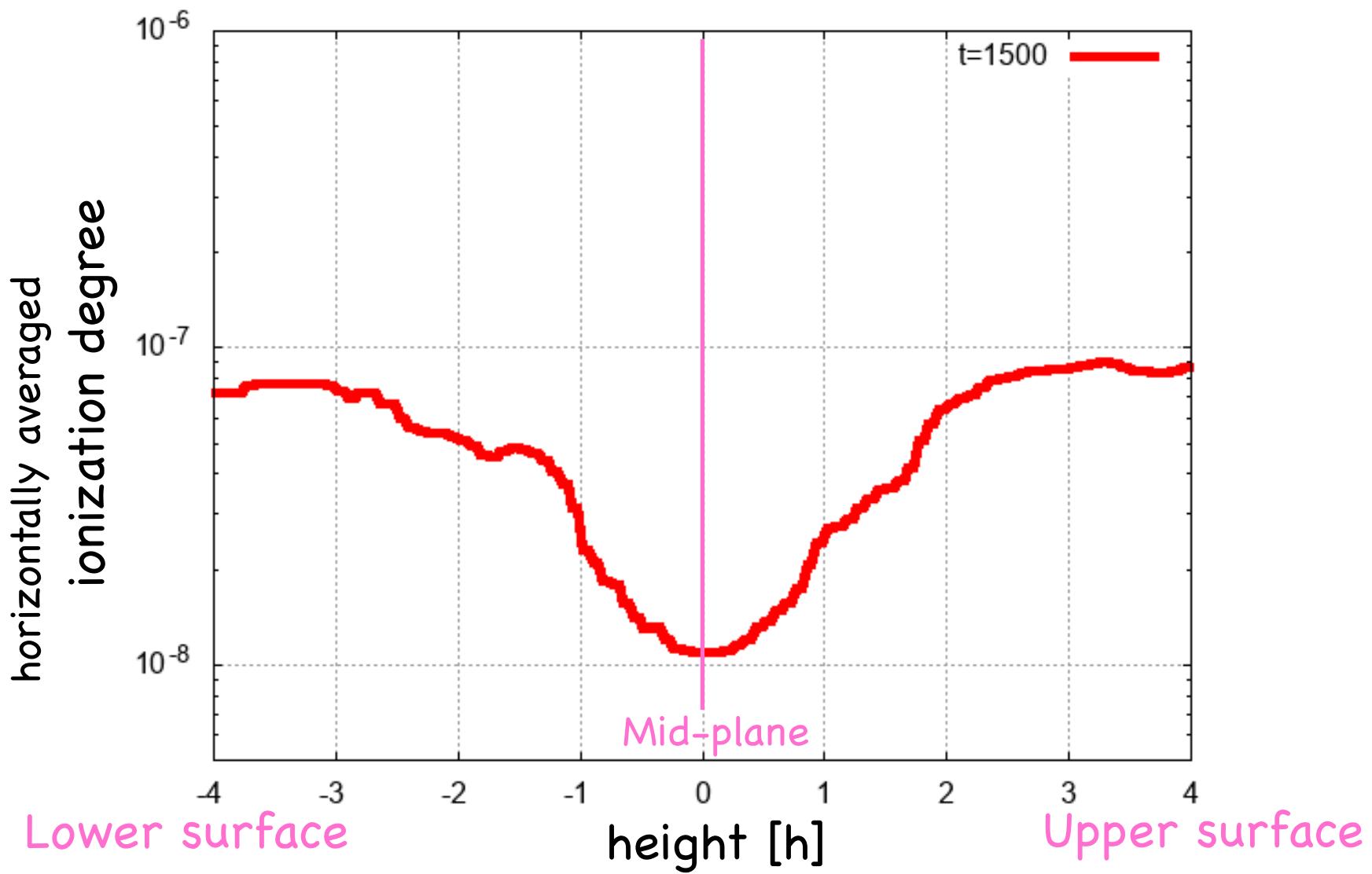
- dust-to-gas ratio:  $f_{dg} = 10^{-4}$

- dust radius:  $a = 1\mu\text{m}$

$$h = \sqrt{2c_s/\Omega}$$



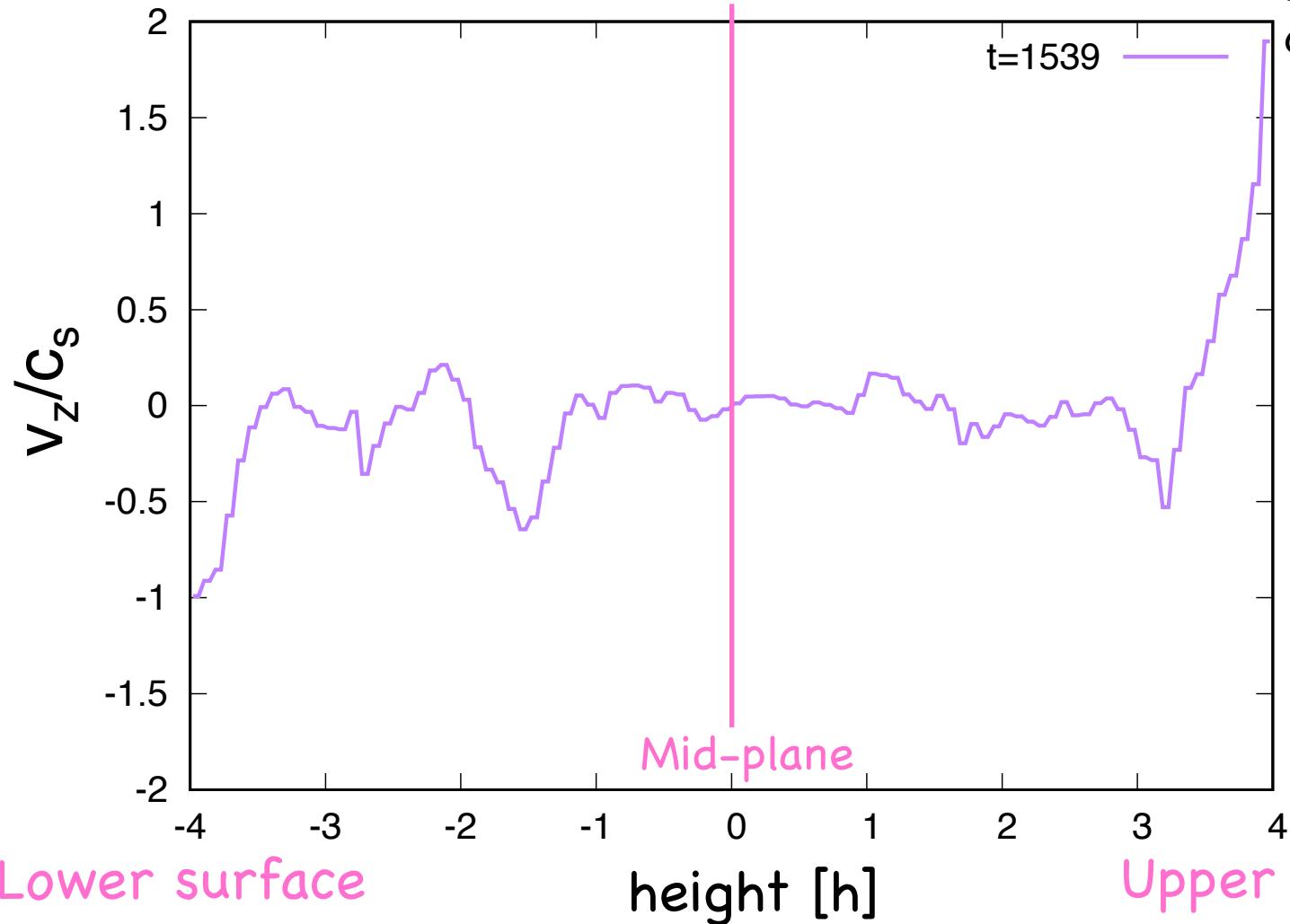
# Propagation of Ionization Degree



# Wind Velocity



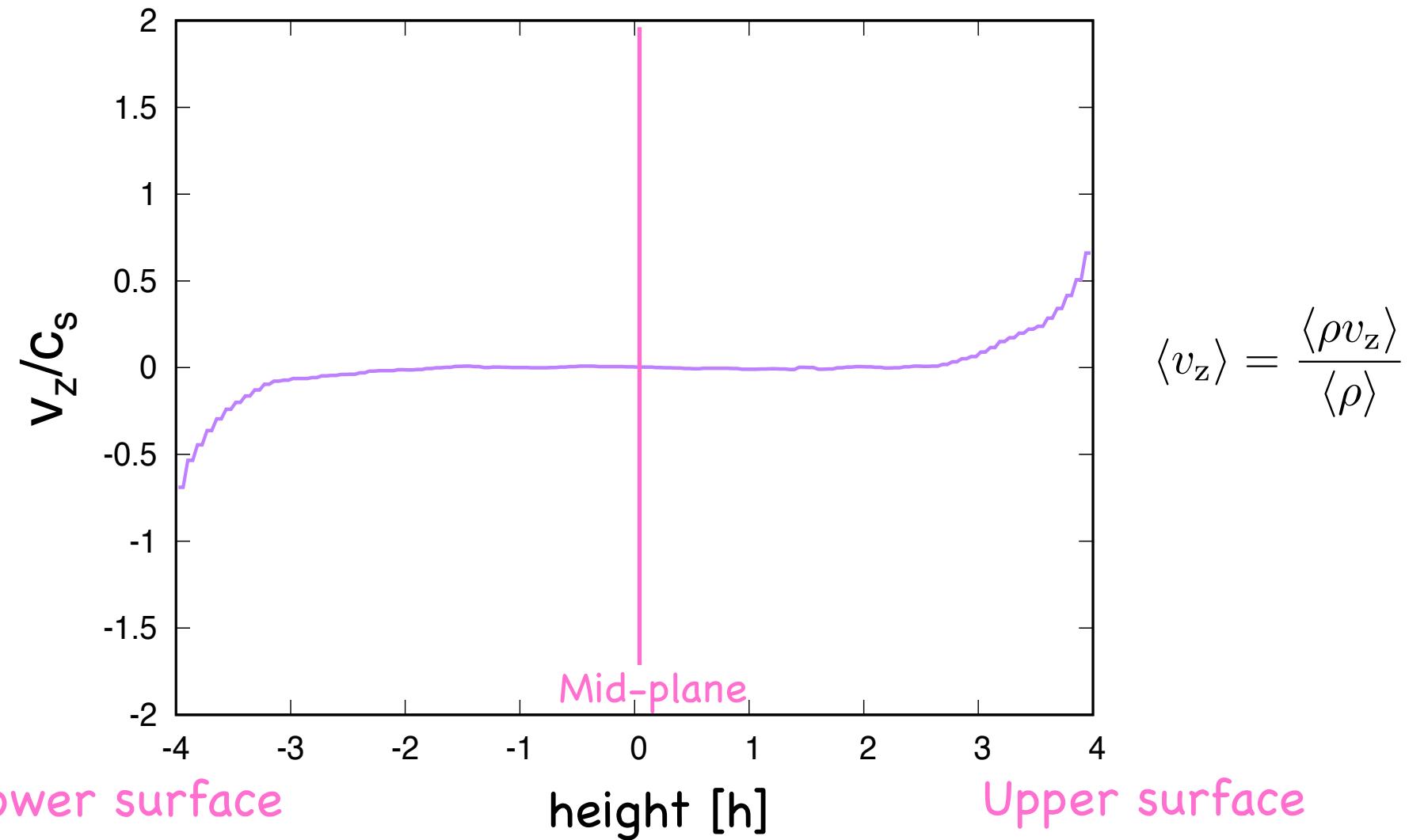
Lunched every 5-10  
orbital periods



$$\langle v_z \rangle = \frac{\langle \rho v_z \rangle}{\langle \rho \rangle}$$

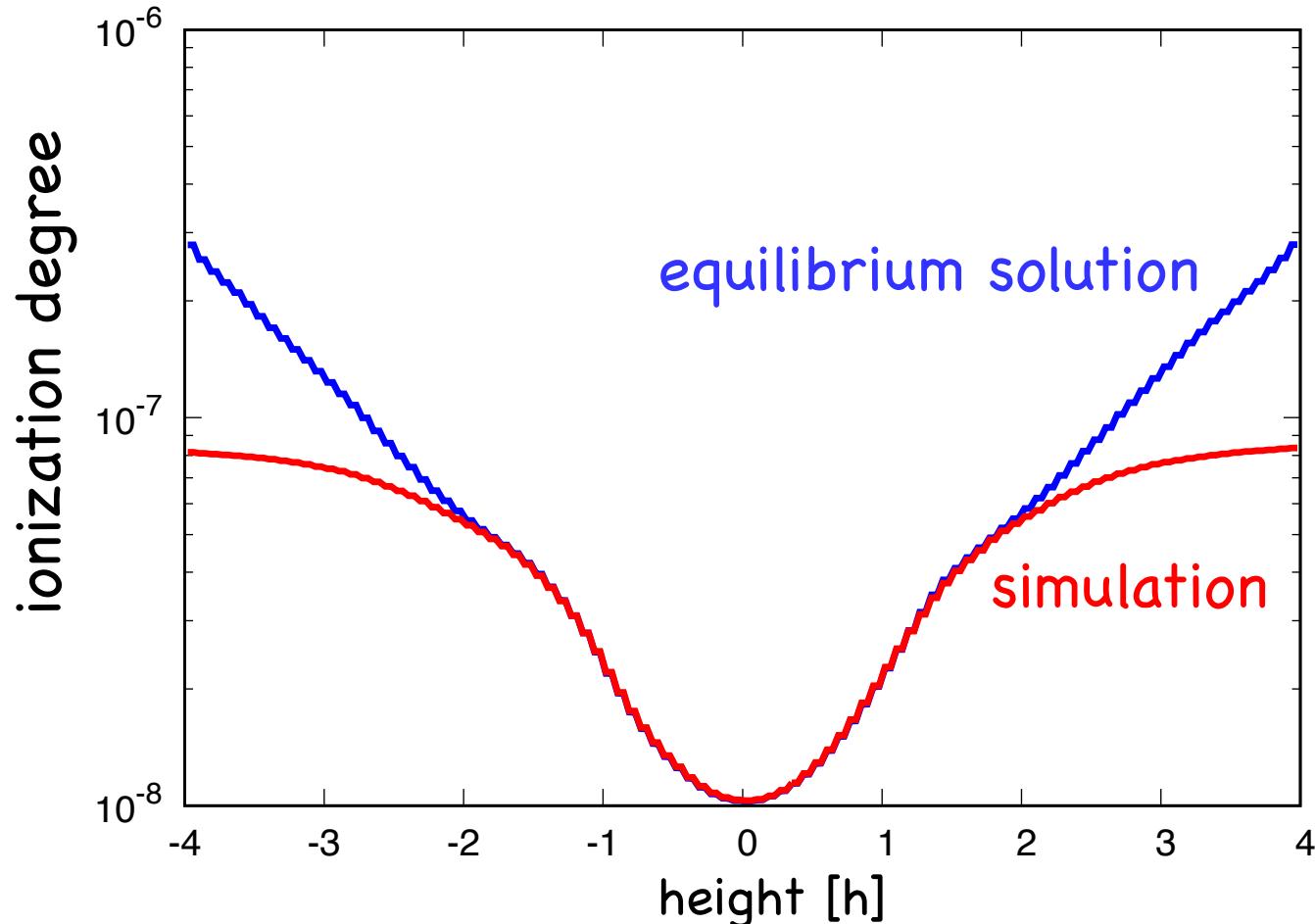
horizontally  
averaged

# Time-averaged Wind Velocity



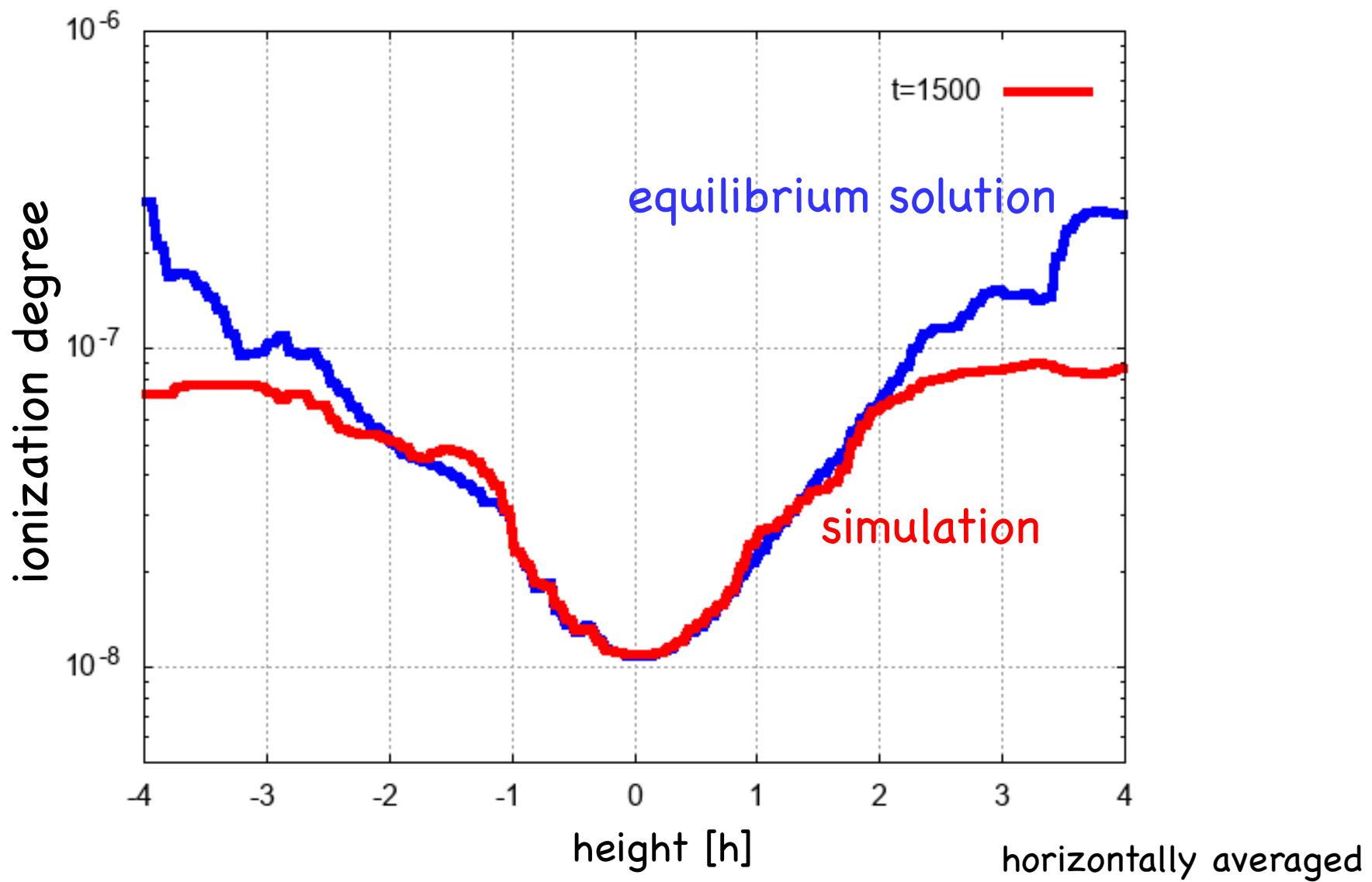
# Time-Averaged Ionization Degree

over 200 orbits

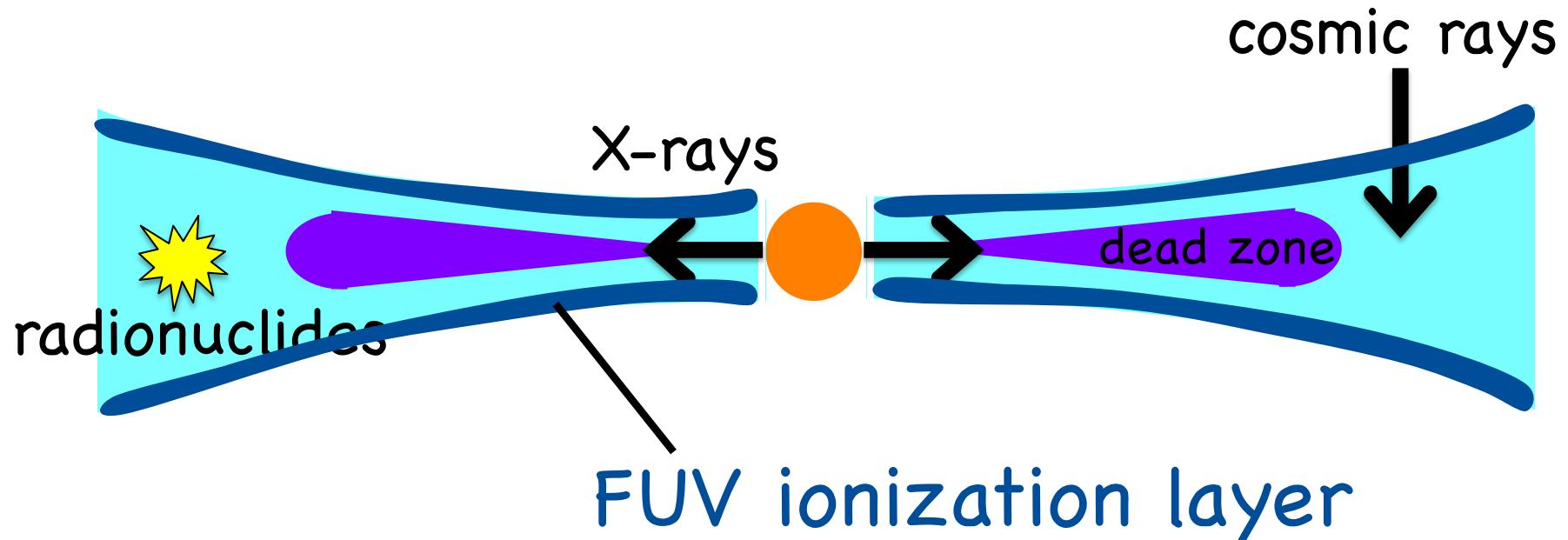


Lower than equilibrium ionization at high altitude

# Comparison with Equilibrium $x_e$



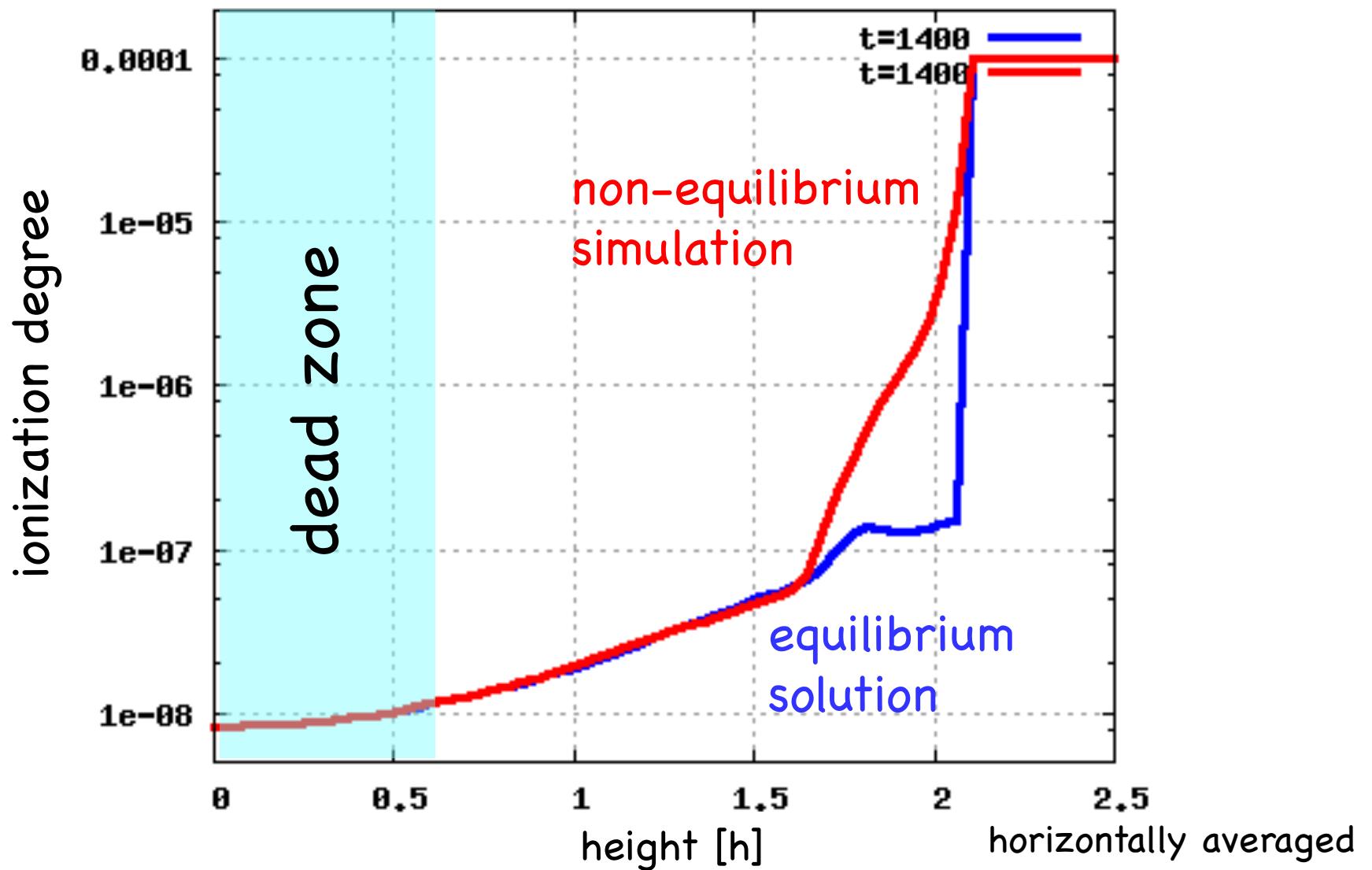
# Photoionization



$$\Sigma < 0.01 \text{ g/cm}^2 \Rightarrow x_e = 10^{-4}$$

Ambipolar diffusion is also considered  
Molecular ions are omitted

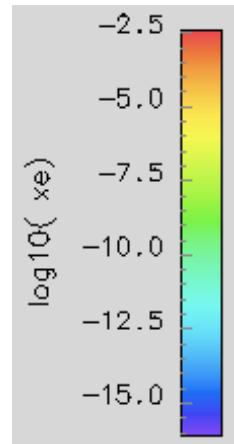
# Comparison with Equilibrium $x_e$



# Global MHD simulations

with advection of chemical species

without advection



preliminary

The difference becomes larger in later evolution stage of disk

# Summary

- Presence of dust grains makes turbulent mixing less/not effective
- Ionization degree has time variation  
⇒ indirect evidence of disk wind?

Without FUV layer:

- Poorly ionized gas is brought upward by disk wind

With FUV layer:

- Boundary of FUV layer is smoothed
- Affected layers are MRI-active region
  - Dead zone size is not likely to be modified
  - Chemical evolution may be affected