Radiation Hydrodynamics Simulations of Photoevaporation of Protoplanetary Disks by Ultraviolet Radiation: Metallicity Dependence

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Abstract

Protoplanetary disks are thought to have lifetimes of several million yr in the solar neighborhood, but recent observations suggest that the disk lifetimes are shorter in a low-metallicity environment. We perform a suite of radiation hydrodynamics simulations of photoevaporating protoplanetary disks to study their long-term evolution of ~10,000 yr and the metallicity dependence of mass-loss rates. Our simulations follow hydrodynamics, extreme and far-ultraviolet (FUV) radiative transfer, and nonequilibrium chemistry in a self-consistent manner. Dust-grain temperatures are also calculated consistently by solving the radiative transfer of the stellar irradiation and grain (re-)emission. We vary the disk metallicity over a wide range of 10^{-4} Z_\odot \leq Z \leq 10 Z_\odot. The photoevaporation rate is lower with higher metallicity in the range of 10^{-1} Z_\odot \leq Z \leq 10 Z_\odot, because dust shielding effectively prevents FUV photons from penetrating and heating the dense regions of the disk. The photoevaporation rate sharply declines at even lower metallicities in 10^{-2} Z_\odot \leq Z \leq 10^{-1} Z_\odot, because FUV photoelectric heating becomes less effective than dust–gas collisional cooling. The temperature in the neutral region decreases, and photoevaporative flows are excited only in an outer region of the disk. At 10^{-3} Z_\odot \leq Z \leq 10^{-2} Z_\odot, H\alpha photoionization heating acts as a dominant gas heating process and drives photoevaporative flows with a roughly constant rate. The typical disk lifetime is shorter at Z = 0.3 Z_\odot than at Z = Z_\odot, being consistent with recent observations of the extreme outer galaxy.

Key words: infrared: planetary systems – protoplanetary disks – stars: formation – stars: pre-main sequence – ultraviolet: stars

1. Introduction

Protoplanetary disks are geometrically thin Keplerian disks surrounding pre-main-sequence stars (e.g., Shu et al. 1994). They are considered to be the birthplaces of planets, and thus studying the structure and evolution of a protoplanetary disk is crucial in understanding planet formation.

Observationally, a star surrounded by a circumstellar disk shows a larger H − K excess than a star without a circumstellar disk because of the dust infrared (IR) emission (Lada & Adams 1992). This IR excess is a robust indicator of the presence of a protoplanetary disk. Applying this diagnostic to the members of a cluster, one can estimate the disk fraction, which is the ratio of the member stars with disks to the total number of members. It is observationally known that the disk fraction of the nearby clusters exponentially decreases with increasing cluster age, and it typically falls below 10% for the cluster age of \sim 6 Myr (Haisch et al. 2001; Hernández et al. 2007; Meyer et al. 2007; Mamajek 2009; Fedele et al. 2010; Ribas et al. 2014). Hence, the typical disk lifetime is estimated to be \sim 3–6 Myr for the nearby clusters (Alexander et al. 2014; Gorti et al. 2016; Ercolano & Pascucci 2017).

Interestingly, recent observations of the extreme outer Galaxy, where the metallicity is significantly lower than in the solar neighborhood, suggest that the typical disk lifetime is short (Yasu et al. 2009, 2010, 2016a, 2016b). The disk fraction there declines steeply with increasing cluster age and becomes \leq 10% within the cluster age of \sim 1 Myr. It appears that a protoplanetary disk in low-metallicity environments disperses earlier and/or faster than that of solar metallicity.

Protoplanetary disks lose their mass mainly via stellar accretion associated with angular momentum transfer, especially at the early stage of disk evolution (Shakura & Sunyaev 1973; Lynden-Bell & Pringle 1974). The evolutionary timescale is estimated to be of the order of a million yr at several tens of au and can be even longer at further outside regions (Hollenbach et al. 2000; Armitage 2011). Thus, viscous evolution alone cannot explain the observationally inferred disk lifetimes. Furthermore, viscous evolution predicts that the surface density should decrease with time as \Sigma \propto r^{-\nu}. This would contradict the existence of observed transitional disks (Andrews & Williams 2005) and a much shorter transitional timescale than a lifetime (e.g., Skrutskie et al. 1990; Kenyon & Hartmann 1995; Alexander et al. 2014). Clearly, in order to explain the timescale of disk dispersal and transition, there must be some other important physical mechanism(s).

Several dynamical processes, such as photoevaporation (e.g., Hollenbach et al. 1994), magneto-hydrodynamic (MHD) wind (e.g., Suzuki & Inutsuka 2009), stellar wind (e.g., Elmegreen 1979), and giant planet formation (Rice et al. 2003) have been proposed so far. In particular, photoevaporation is proposed as a main driver of disk dispersal. Photoevaporation appears to produce transitional disks when the effect is included in simulations of viscous disk evolution (Clarke et al. 2001; Alexander et al. 2006; Owen et al. 2010).

Photoevaporation from a disk is thought to occur in the following manner. The circumstellar disk is irradiated by the central star and/or a nearby star. In optically thin regions, the gas temperature increases through thermalization of the...
electrons that are ejected from atoms and dust grains by absorption of high-energy photons such as far-ultraviolet (FUV; \(6 \text{ eV} < h\nu < 13.6 \text{ eV}\)), extreme ultraviolet (EUV; \(13.6 \text{ eV} < h\nu < 0.1 \text{ keV}\)), and X-rays (\(h\nu > 0.1 \text{ keV}\)). The “hot” gas escapes from the star–disk system and flows out of the disk. This causes considerable disk mass loss.

According to Hollenbach et al. (1994), who performed 1+1D radiative transfer calculations, the diffuse EUV component is dominant for exciting photoevaporation and drives mass loss at a rate of \(\dot{M}_\text{ph} \sim 10^{-10} M_\odot \text{ yr}^{-1}\). In contrast, the recent 2D radiative transfer calculations of Tanaka et al. (2013) suggest that the direct component of EUV is dominant. They derive \(\dot{M}_\text{ph} \sim 10^{-9} M_\odot \text{ yr}^{-1}\). FUV can effectively heat denser regions of a disk than EUV, because FUV is attenuated at a higher column density (\(\sim 10^{21} \text{ cm}^{-2}\)) than EUV in general. EUV photoevaporation rates are thus generally higher than EUV photoevaporation rates (Gorti & Hollenbach 2009; Owen et al. 2012). Gorti & Hollenbach (2009) concluded that FUV photoevaporation rates are of the order of \(\sim 10^{-8} M_\odot \text{ yr}^{-1}\) for typical young low-mass stars. Photoevaporation excited by X-ray irradiation from a young low-mass star has also been studied (Alexander et al. 2004; Ercolano et al. 2008, 2009; Gorti & Hollenbach 2008, 2009; Owen et al. 2010, 2012). X-rays are also attenuated at a larger column density comparable to FUV, and thus X-ray photoevaporation also gives \(\dot{M}_\text{ph} \sim 10^{-8} M_\odot \text{ yr}^{-1}\) (Ercolano et al. 2008, 2009; Owen et al. 2010, 2012).

Ercolano & Clarke (2010; hereafter EC10) derived the metallicity dependence of X-ray photoevaporation rates by hydrostatic calculations and an analytic formula to estimate a disk lifetime for a given \(M_\text{ph}\). By applying the formula to the hydrostatic disks, EC10 derived the metallicity dependence of protoplanetary disk lifetimes. The obtained lifetimes monotonically decrease with metallicity, which appears to be consistent with the observed trend that disk lifetimes decrease with metallicity.

Unfortunately, none of these previous studies have derived the metallicity dependence of photoevaporation rates by using hydrodynamical simulations. Simultaneous modeling of photoevaporation and dynamical disk evolution is necessary to study how photoevaporative flows change the density structure of a disk and from where and with which speed photoevaporative flows are launched. Moreover, previous studies that calculate the hydrodynamics of photoevaporating protoplanetary disks irradiated by a central low-mass star do not solve radiative transfer self-consistently. It is also important to incorporate nonequilibrium chemistry. It allows us to study chemical evolution coupled with hydrodynamics and to accurately estimate the relevant heating/cooling rates. Yorke & Welz (1996) and Richling & Yorke (2000) self-consistently solved hydrodynamics and radiative transfer, including nonequilibrium chemistry, to follow the evolution of a disk irradiated by a central B star and an external radiation source, respectively. In the present paper, we solve the hydrodynamics of photoevaporating protoplanetary disks with self-consistent EUV/FUV radiative transfer and nonequilibrium chemistry. Our chemistry solver includes molecular species such as H\(_2\) and CO, as well as atomic species. Dust temperatures are also calculated self-consistently. We run a set of simulations of a disk with different metallicities. We calculate the photoevaporation rates in order to derive, if any, the metallicity dependence of EUV/FUV photoevaporation rates and estimate disk lifetimes.

The paper is organized as follows. In Section 2, we present the methods and problem settings of our simulation. In Section 3, we discuss the simulation results and present an analytic model of the photoevaporation rates. A final discussion and a summary are given in Sections 4 and 5, respectively.

2. Numerical Simulations

In order to calculate the fluid dynamics of photoevaporating protoplanetary disks, we make use of a modified version of the publicly available code PLUTO (version 4.1; Mignone et al. 2007). We also summarize the following physical processes we implement in the code: radiative transfer, a nonequilibrium chemistry network, and relevant heating/cooling processes.

2.1. Method

We consider the photoevaporation of protoplanetary disks caused by the UV irradiation from a central star covering a broad range of different metallicities, \(10^{-4} Z_\odot < Z < 10 Z_\odot\). We assume a central \(M_\star = 0.5 M_\odot\) star with constant EUV photon number luminosity \(\phi_{\text{EUV}} = 6 \times 10^{41} \text{ cm}^{-2} \text{s}^{-1}\) and FUV luminosity \(L_{\text{FUV}} = 3 \times 10^{32} \text{ erg s}^{-1}\). Although the stellar UV emissivities will vary with different metallicities, we ignore such potential variation to concentrate on the roles of heavy elements contained within the disk. We keep the above parameters fixed throughout our simulations. X-rays can also drive photoevaporation (Alexander et al. 2004; Ercolano et al. 2008, 2009; Gorti & Hollenbach 2008, 2009; Owen et al. 2010, 2012), but we do not include X-rays in the present study. Here we focus on the metallicity dependence of UV-driven photoevaporation.

Our multispecies chemistry model is based on Omukai (2000) and Omukai et al. (2005, 2010). We assume that the medium consists of gas and dust grains. The gas contains seven chemical species: H I, H II, H\(_2\), CO, O I, C II, and electron (hereafter, we refer to H I, H II, and H\(_2\) as H-bearing species and CO, O I, and C II as metal species). We assume that the amount of gas-phase metal elements and grains is proportional to the relative metallicity \(Z/Z_\odot\). The dust-to-gas mass ratio and the gas-phase elemental abundances of carbon and oxygen are set to the values of local interstellar clouds in the case of \(Z = Z_\odot\). Hence, we give the dust-to-gas mass ratio \(\mathcal{D}/\mathcal{G}\) by

\[
\mathcal{D}/\mathcal{G} = 0.01 \times Z/Z_\odot.
\]

The gas-phase elemental abundances of carbon and oxygen are \(X_C = 0.927 \times 10^{-4} Z/Z_\odot\) and \(X_O = 3.568 \times 10^{-4} Z/Z_\odot\), respectively (Pollack et al. 1994; Omukai 2000).\(^6\)

The parameters used in our model are listed in Table 1.

2.2. Basic Equations

We use 2D spherical polar coordinates \((r, \theta)\), taking into account the time evolution of the gas density; all three components of velocity \(v = (v_r, v_\theta, v_z)\); gas energy, including relevant heating/cooling sources; and chemical abundances,

\(^6\) The abundance of species \(i\) is defined as the ratio of its number density to hydrogen nuclei number density; \(n_i/m_i\). We adopt chemical symbol notation for elemental abundances and Romanian notation for chemical abundances. For example, \(X_C\) and \(X_O\) denote the elemental abundance of carbon and the chemical abundance of neutral carbon atoms, respectively. This is also the case with density and column density.
including advection and chemical reactions. The basic equations are

\[ \frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \mathbf{v}) = 0, \]

\[ \frac{\partial \rho \mathbf{v}}{\partial t} + \nabla \cdot (\rho \mathbf{v} \mathbf{v}) = -\frac{\partial P}{\partial r} - \rho \frac{GM_*}{r^2} + \rho \frac{v_r^2 + v_\theta^2}{r}, \]

\[ \frac{\partial \rho \mathbf{v}_\theta}{\partial t} + \nabla \cdot (\rho \mathbf{v}_\theta) = -\frac{1}{r} \frac{\partial P}{\partial \theta} - \rho \frac{v_r v_\theta}{r} + \frac{\rho v_\theta^2}{r} \cot \theta, \]

\[ \frac{\partial \rho v_r}{\partial t} + \nabla \cdot (\rho v_r) = 0, \]

\[ \frac{\partial E}{\partial t} + \nabla \cdot (H \mathbf{v}) = -\rho v_r \frac{GM_*}{r^2} + \rho (\Gamma - \Lambda), \]

and

\[ \frac{\partial n_H y_i}{\partial t} + \nabla \cdot (n_H y_i \mathbf{v}) = n_H R_i. \]  

In the above equations, \( \rho, v, P \) are the gas density, velocity, and pressure, respectively, and \( G \) is the gravitational constant. We do not include the gas self-gravity, which is currently negligible with the typical mass ratio between the star and disk, \( M_{\text{disk}} / M_* \sim 0.01 \). We denote the total energy and enthalpy per unit volume as \( E \) and \( H \), respectively; \( \Gamma \) is a heating rate per unit mass (specific heating rate); and \( \Lambda \) is a cooling rate per unit mass (specific cooling rate). We denote the fractional abundance of each of the seven chemical species as \( y_{\text{HI}}, y_{\text{HII}}, y_{\text{H}_2}, y_{\text{C}^+}, y_{\text{C}_2}, y_{\text{O}^+} \), and \( y_e \). Chemical reaction rates \( R_i \) include all relevant reactions (cf. Table 3).

PLUTO discretizes the azimuthal component of Euler equations in an angular momentum conserving form. The divergence operator of Equation (5) is represented by a different form compared to those of the other equations, and these divergence operators are defined as

\[ \nabla \cdot \mathbf{F} = \frac{1}{r^2} \frac{\partial}{\partial r} (r^2 F_r) + \frac{1}{r \sin \theta} \frac{\partial}{\partial \theta} (\sin \theta F_\theta), \]

\[ \nabla^I \cdot \mathbf{F} = \frac{1}{r^3} \frac{\partial}{\partial r} (r^3 F_r) + \frac{1}{r^2 \sin \theta} \frac{\partial}{\partial \theta} (\sin^2 \theta F_\theta), \]  

where \( \mathbf{F} \) is an arbitrary vector. Also, we do not consider angular momentum transfer due to viscous friction. We solve time evolution within the dynamical timescale of a disk, which is much smaller than the viscous timescale.

We use the equation of state for an ideal gas,

\[ e = \frac{kT}{\mu m_u (\gamma - 1)}, \]

\[ p = \frac{\rho kT}{\mu m_u}, \]

where \( e \) is the specific energy of the gas, \( \gamma \) is the adiabatic index, \( k \) is the Boltzmann constant, \( T \) is the gas temperature, \( \mu \) is the mean molecular weight, and \( m_u \) is the atomic mass unit. The ratio of specific heat \( \gamma \) is defined as

\[ \gamma = 1 + \frac{y_{\text{HI}} + y_{\text{HII}} + y_{\text{H}_2} + y_e}{\frac{1}{2} y_{\text{HI}} + \frac{2}{3} y_{\text{HII}} + \frac{5}{6} y_{\text{H}_2} + \frac{3}{2} y_e}. \]

where the contributions of the small abundances of the metal species are neglected. With the equation of state, the total energy and enthalpy per unit volume are explicitly written as

\[ E = \frac{1}{2} \rho \mathbf{v}^2 + \rho e = \frac{1}{2} \rho v_r^2 + \frac{P}{\gamma - 1}, \]

\[ H = E + P = \frac{1}{2} \rho v_r^2 + \frac{\gamma P}{\gamma - 1}. \]

The computational domain is set to be on \( r = [1, 400] \) au and \( \theta = [0, \pi/2] \) rad. We need to use a sufficiently large radial outer boundary so that the computational domain contains transonic points of photoevaporative flows at the metallicities of interest (see the discussion in Section 4.5). The sink region \( (\leq 1 \) au) is out of the computational domain, but disk materials exist there in reality and shield stellar photons. We take this effect into account approximately by assuming that the sink density distributions are radially uniform and the densities are given by those of the innermost cells in the computational domain. Thus, the sink column densities are calculated as

\[ N_i^{\text{sink}} = sn_i m_i, \]

where \( i \) is a label of the chemical species, \( s \) is the sink size (1 au), and \( n_i m_i \) is the density of the chemical species in the innermost cell. The stellar photon fluxes are reduced by the sink column densities in our simulations. We assume axisymmetry around the rotational axis \( (\theta = 0) \) and midplane symmetry \( (\theta = \pi/2) \) of a disk. We use 128 grid cells logarithmically spaced in the radial direction. In the meridional direction, we use different resolutions in two domains divided by \( \theta = 1 \). In each domain, we use 80 uniform grid cells. The high resolution in \( 1 \leq \theta \leq \pi/2 \) allows us to resolve the scale height of a disk and the launch points of photoevaporation flows, which are called photoevaporation bases.

The effective gravitational radius for an ionized gas \( (T = 10^4 \text{ K}) \) is \( \approx 1.4(M_*/M_\odot) \) au (Liffman 2003). Our inner extent of the computational domain is larger than the effective gravitational radius for a 0.5 \( M_\odot \) star. Therefore, our calculations might miss the contribution of mass loss from the region near the effective radius. However, the resulting base density profile of an ionized gas is expected to show, and actually has, a scaling of \( \propto R^{-1.5} \), where \( R \) is the cylindrical radius (Tanaka et al. 2013). In this case, the mass loss is dominated by the contribution from the outer regions of a disk, and the contribution from the region near the effective gravitational radius is sufficiently small. We have run simulations with small inner boundaries of \( r_{\text{inner}} = 0.1, 0.35, 0.5 \) au to confirm that the resulting photoevaporation rate is almost the same as that of a simulation with \( r_{\text{inner}} = 1 \) au. The contributions from \( R \leq 10 \) au are only about a few percent of the total. Hence,
we use $r_{\text{inner}} = 1$ au for the inner boundary of our computational domain.

We note that the absorption of direct EUV photons by the inner (<1 au) disk could be important. If all of the direct stellar photons are absorbed by the inner disk and its atmosphere, only diffuse photons emitted through recombination can reach the outer region. In the simulations with small inner boundaries of $r_{\text{inner}} = 0.1, 0.35, 0.5$ au, we find that the density of the ionized atmosphere is sufficiently small not to shield the EUV photons, and that the direct photons actually reach $r > 1$ au. In the outer region, the heating and ionization rates are almost the same as in the simulation with a boundary of $r_{\text{inner}} = 1$ au. We thus obtain essentially the same photoevaporation rate from the two simulations. Therefore, we justify using the computational domain of $r = [1, 400]$ au.

### Table 2

| Species | $j \rightarrow i$ | $\nu_j$ (Hz) | $A_j$ (s$^{-1}$) | $\gamma_j^\text{e}$ (cm$^3$ s$^{-1}$) | $\gamma_j^\text{H}$ (cm$^3$ s$^{-1}$) | Reference |
|---------|-----------------|--------------|-----------------|-----------------|-----------------|-----------|
| C II    | 2 $\rightarrow$ 1 | $2.4 \times 10^{-6}$ | $2.8 \times 10^{-3}(T/100 \text{ K})^{-0.5}$ | $8.0 \times 10^{-10}(T/100 \text{ K})^{0.07}$ | 1, 2 |
| O I     | 2 $\rightarrow$ 1 | $4.7 \times 10^{12}$ | $8.9 \times 10^{-5}$ | $1.4 \times 10^{-8}$ | $9.2 \times 10^{-11}(T/100 \text{ K})^{0.67}$ | 1, 3 |
| O I     | 3 $\rightarrow$ 1 | ... | $1.0 \times 10^{-10}$ | $1.4 \times 10^{-8}$ | $4.3 \times 10^{-11}(T/100 \text{ K})^{0.80}$ | 1, 3 |
| O I     | 4 $\rightarrow$ 1 | ... | $6.3 \times 10^{-3}$ | $1.0 \times 10^{-10}$ | $1.0 \times 10^{-12}$ | 1, 3 |
| O I     | 5 $\rightarrow$ 1 | ... | $2.9 \times 10^{-4}$ | $1.0 \times 10^{-10}$ | $1.0 \times 10^{-12}$ | 1, 3 |
| O I     | 3 $\rightarrow$ 2 | $2.1 \times 10^{12}$ | $1.7 \times 10^{-5}$ | $5.0 \times 10^{-9}$ | $1.1 \times 10^{-10}(T/100 \text{ K})^{0.44}$ | 1, 3 |
| O I     | 4 $\rightarrow$ 2 | ... | $2.1 \times 10^{-3}$ | $1.0 \times 10^{-10}$ | $1.0 \times 10^{-12}$ | 1, 3 |
| O I     | 5 $\rightarrow$ 2 | ... | $7.3 \times 10^{-2}$ | $1.0 \times 10^{-10}$ | $1.0 \times 10^{-12}$ | 1, 3 |
| O I     | 4 $\rightarrow$ 3 | $4.7 \times 10^{14}$ | $7.3 \times 10^{-7}$ | $1.0 \times 10^{-10}$ | $1.0 \times 10^{-12}$ | 1, 3 |
| O I     | 5 $\rightarrow$ 3 | ... | $0$ | $1.0 \times 10^{-10}$ | $1.0 \times 10^{-12}$ | 1, 3 |
| O I     | 5 $\rightarrow$ 4 | $5.4 \times 10^{14}$ | $1.2$ | 0 | 0 | 1, 3 |

Note. In the columns, $i, j$ are the labels of energy levels; $\nu_j$ is the corresponding frequency of the energy difference between level $i$ and level $j$; $A_j$ is an Einstein A coefficient; and $\gamma_j^\text{e}$ is the collisional rate with a species $\lambda$. The labels of energy levels are defined as follows: $^2P_{1/2}$ of C II (label 1) and $^2P_{3/2}$ of C II (label 2), respectively. $^3P_2$ of O I (label 1), $^3P_1$ of O I (label 2), $^3P_0$ of O I (label 3), $^3D_2$ of O I (label 4), and $^3S_0$ of O I (label 5), respectively.

References. (1) Osterbrock (1989), (2) Santoro & Shull (2006), (3) Hollenbach & McKee (1989).

We incorporate the relevant chemical reactions of the seven chemical species tabulated in Table 3. As well as collisional chemical reactions, we implement the photochemical reactions: photoionization of H I, photodissociation of H$_2$ (Draine & Bertoldi 1996), and photodissociation of CO (Lee et al. 1996).

We follow Richling & Yorke (2000) and assume that C I, whose ionization energy is close to the dissociation energy of CO, is quickly converted to C II following CO photodissociation. In practice, we assume that the CO dissociation front is located at the same position as the C II ionization front. As the reverse reaction of CO photodissociation, we adopt the simplified chemistry model of Nelson & Langer (1997). This model can treat the formation of CO molecules from C II via the reactions of hydrocarbon radicals without explicitly including C I as a chemical species. These approximations greatly save computational costs. We have checked the validity of this approximation by performing postprocess calculations with solving C I photoionization consistently. The results show that the C I region is geometrically thin, with at most an $\sim 10$% thickness of the C II and CO regions; otherwise, the structures of the C II/CO regions are hardly affected after the postprocessing. The details of the chemical reactions are described in Appendix B.

### 2.4. Chemical Reactions

2.3. Cooling/Heating

We implement photoionization heating caused by EUV and photoelectric heating caused by FUV. We use the analytic formula presented by Bakes & Tielens (1994) to calculate photoelectric heating. Bakes & Tielens (1994) assumed the Mathis-Rumpl-Nordsieck (MRN) distribution (Mathis et al. 1977) for the dust model to derive the formula. The same size distribution is assumed for small carbon grains, polycyclic aromatic hydrocarbons (PAHs). Note that the observed PAH abundances around T Tauri stars are typically several tens of times smaller than the interstellar medium (ISM) value (Gorti & Hollenbach 2008, 2009). We examine the effect of the PAH abundance on disk photoevaporation rates in Section 4.3.

We also implement radiative recombination cooling of H II (Spitzer 1978), dust–gas collisional cooling (Yorke & Welz 1996), Ly$\alpha$ cooling of H I (Aminos et al. 1997), fine-structure line cooling of O I and C II (Hollenbach & McKee 1989; Osterbrock 1989; Santoro & Shull 2006), and molecular line cooling of H$_2$ and CO (Galili & Palla 1998; Omukai et al. 2010). Other collisional excited lines (CELS) can be important cooling in H II regions, but they are neglected in this study for simplicity. We discuss the validity of this simplification in Section 4.7.

We do not include O I photoionization explicitly in our calculations. To treat O I cooling in the H II region approximately, while saving computational time, we set the O I abundance as $\gamma_{\text{O I}}(1 - \gamma_{\text{H II}})$. This approximation is based on the fact that the O I ionization energy is close to the H I ionization energy. Although a more detailed treatment of O I photoionization would be necessary to model the fine structure of the O I and O II regions, we simplify the O I chemistry because O I cooling remains subdominant in the H II region, compared with adiabatic cooling (see also our discussion above). The heating/cooling rates are described in detail in Appendix A.

2.5. Radiative Transfer

We solve radiative transfer to calculate photochemical reaction rates, photoheating rates, and dust temperatures consistently. Gas and dust column densities are updated at each timestep. EUV radiative transfer is solved by ray tracing. The diffusion component is neglected in our simulation, and we
use case B recombination. Compared with the diffusion component, the direct component plays a dominant role in EUV photoevaporation (Tanaka et al. 2013), as discussed in Section 3.3. Although EUV photons are absorbed by H1 and dust in general, we ignore the absorption by dust. The dust absorption of EUV photons is not dominant in our computational domain with the assumed EUV luminosity.7

FUV radiative transfer is also solved by ray tracing in order to calculate photoelectric heating rates, H2 photodissociation rates, and CO photodissociation rates. We include the absorption of FUV photons by H2 and CO molecules. The details of EUV/FUV radiative transfer are described in Appendices A and B.

We calculate the grain temperatures by solving the radiation transfer of both direct and diffusion components. We use a hybrid scheme: the direct component (stellar irradiation) is solved by ray tracing, while the diffusion component due to thermal (re-)emission is solved by a flux-limited-diffusion (FLD) approximation. For these processes, we use the radiation transport module presented in Kuiper et al. (2010b). The hybrid scheme allows us to accurately model shadows caused by an optically thick disk (Kuiper & Klessen 2013). Although the FLD approximation does not strictly hold in disk wind regions (\(A_V < 1\)), the region is directly illuminated by the stellar irradiation; hence, the local radiation field is dominated by the

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### Table 3

The List of the Chemical Reactions Incorporated in Our Simulations

| Label | Reaction | Rate Coefficient | Reference |
|-------|----------|------------------|-----------|
| k1    | H + e → H+ + 2e | \( \exp(-32.71396786 + 13.536556 \ln T_{\text{eV}} - 5.73932875 (\ln T_{\text{eV}})^2 + 1.56315498 (\ln T_{\text{eV}})^3 - 0.287056 (\ln T_{\text{eV}})^4 + 3.48255977 \times 10^{-2} (\ln T_{\text{eV}})^5 - 2.63197617 \times 10^{-3} (\ln T_{\text{eV}})^6 + 1.11954395 \times 10^{-4} (\ln T_{\text{eV}})^7 - 2.03914985 \times 10^{-6} (\ln T_{\text{eV}})^8) \) | 1 |
| k2    | H+ + e → H + γ | \( \exp(-28.6130338 - 0.72411256 \ln T_{\text{eV}} - 2.02604478 \times 10^{-2} (\ln T_{\text{eV}})^2 - 2.38086188 \times 10^{-3} (\ln T_{\text{eV}})^3 - 3.21260521 \times 10^{-4} (\ln T_{\text{eV}})^4 - 1.42150291 \times 10^{-5} (\ln T_{\text{eV}})^5 + 4.98910982 \times 10^{-6} (\ln T_{\text{eV}})^6 + 5.75561414 \times 10^{-7} (\ln T_{\text{eV}})^7 - 1.85676704 \times 10^{-8} (\ln T_{\text{eV}})^8 - 3.07113524 \times 10^{-9} (\ln T_{\text{eV}})^9) \) | 1 |
| k12   | H2 + e → 2H + e | \( 4.4 \times 10^{-10} \exp(-1.02 \times 10^{3}/T) \) | 1 |
| k13   | H2 + H → 3H | \( k_{\text{dis}}(k_{\text{dis}}/k_{\text{H}}) a, k_{\text{H}} \equiv 1.12 \times 10^{-10} \exp(-7.035 \times 10^{4}/T), k_{\text{dis}} \equiv 6.5 \times 10^{-7} /T \exp(-5.2 \times 10^{4}/T)(1 - \exp(-6000/T)) \), \( \log n_{\text{eH}} \equiv 4 - 0.416 \log (T/1.0 \times 10^{4}) - 0.327 \log (T/1.0 \times 10^{4})^2 \), \( a \equiv (1 + n_{\text{eH}}/n_{\text{H}})^{-1} \) | 1 |
| k19   | 3H → H2 + H | \( 5.5 \times 10^{-29}/T \) | 1 |
| k20   | 2H + H2 → 2H2 | \( k_{\text{dis}}(k_{\text{dis}}/k_{\text{H}}) a, k_{\text{H}} \equiv 1.18 \times 10^{-9} \exp(-6.95 \times 10^{4}/T), k_{\text{dis}} \equiv 8.125 \times 10^{-7} /T \exp(-5.2 \times 10^{4}/T)(1 - \exp(-6000/T)) \), \( \log n_{\text{eH}} \equiv 4.845 - 1.3 \log (T/1.0 \times 10^{4}) + 1.62 \log (T/1.0 \times 10^{4})^2 \), \( a \equiv (1 + n_{\text{eH}}/n_{\text{H}})^{-1} \) | 1 |
| k22   | 2H → H+ + e + H | \( 1.7 \times 10^{-4} \) | 1 |
| k23   | 2H → H2 | \( 6.0 \times 10^{-17} \sqrt{T/300} f_{\text{d}} (Z/Z_{\odot}) \times[1.0 + 4.0 \times 10^{-2} \sqrt{T} + T_{\text{dust}} + 2.0 \times 10^{-3} T + 8.0 \times 10^{-6} T^2]^{-1}, f_{\text{d}} \equiv [1.0 + \exp(7.5 \times 10^{2}/(175 - T_{\text{dust}}))]^{-1} \) | 1 |
| p1    | H + γ → H+ + e | \( R_{\text{H+}}(\text{cf. Equation (38)}) \) | ... |
| p2    | H2 + γ → 2H | \( R_{\text{H2,dis}}(\text{cf. Appendix B.1}) \) | 2 |
| p3    | CO + γ → C+ + O | \( R_{\text{CO,dis}}(\text{cf. Appendix B.2}) \) | 3 |
| k24   | C+ + O → CO | \( R_{\text{CO,form}}(\text{cf. Appendix B.3}) \) | 4 |

Note. Here, \( T_{\text{eV}} \) is the gas temperature in eV, \( T \) is the gas temperature in K, and \( T_{\text{dust}} \) is the dust temperature in K.

References. (1) Omukai (2000), (2) Draine & Bertoldi (1996), (3) Lee et al. (1996), (4) Nelson & Langer (1997).

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7 The EUV luminosity yields the maximum density of the ionization front to be \( n_{\text{HI}} \sim 10^{10} \text{ cm}^{-3} \) in the innermost region of the computational domain. With this density, H1 becomes optically thick against EUV within the length of \( \sim 0.1 \text{ au} \) near the ionization front. The corresponding H1 column density is \( N_{\text{HI}} \sim 10^{24} \text{ cm}^{-2} \). EUV absorption by dust grains is effective at much higher column densities (\( N_{\text{HI}} \sim 10^{21} \text{ cm}^{-2} \)). Hence, the assumption of effectively optically thin dust is valid for \( N_{\text{HI}} \sim 10^{18} \text{ cm}^{-2} \).
stellar irradiation component, rather than the diffuse radiation component. In the region near the photoevaporation base ($A_V \sim 1$), the direct field is attenuated to some extent, but the region is optically thin for the diffusion component. As well as the wind region ($A_V < 1$), the dust temperatures in the $A_V \sim 1$ region are largely determined by the balance between the direct stellar irradiation and thermal re-emission of the dust. We have explicitly checked that the dust temperatures derived with and without including the diffusion component agree with each other well. The difference is $\sim 2\%$, on average, and at most $6\%$. Thus, we conclude that our calculations provide accurate dust temperatures in wind regions. We note that our radiation transfer model has been applied in many studies of massive star formation and feedback effects (Kuiper et al. 2010a, 2012; Kuiper & Yorke 2013a; Kuiper et al. 2015, 2016), massive accretion disks (Kuiper et al. 2011; Meyer et al. 2017a, 2017b), stellar evolution (Kuiper & Yorke 2013b), formation of primordial stars (Hosokawa et al. 2016), and planet formation (Marleau et al. 2017). In our simulation, we use the opacity table taken from Draine & Lee (1984).

2.6. Initial Conditions

The disk is assumed to consist of an initially neutral gas. There, all of the hydrogen nuclei are assumed to be in molecular ($H_2$) form, and all of the carbon nuclei are in CO at $t = 0$.

The initial grain and gas temperatures are set to be $T = T_{dust} = 100$ K ($R/1$ au)$^{-1/2}$ (e.g., Kenyon & Hartmann 1987), except the case of $Z = 10^{-4} Z_\odot$. In the case of $Z = 10^{-4} Z_\odot$, we first calculate the thermochemical structure without updating the density structure for $\sim 1$ Myr and start the simulation after that, otherwise the gas temperature does not couple with the dust temperature within the timescale of interest in the region near the midplane, which might be unrealistic.

The initial density structure is set to be hydrostatic equilibrium,

$$n_H = n_0 \left( \frac{R}{1 \text{ au}} \right)^{-9/4} \exp \left[ -\frac{z^2}{2h^2} \right],$$

where $R$ and $z$ are positions in the 2D cylindrical polar coordinates $(R, z) = (r \sin \theta, r \cos \theta)$ and $h$ is the scale height of a disk defined as $h = c_s / \Omega_K$, where $c_s$ is the isothermal sound speed and $\Omega_K$ is the Keplerian angular velocity. We denote $n_0$ as the midplane density of a disk at 1 au, and we set $n_0 = 10^{14} \text{ cm}^{-3}$. In Equation (15), the surface density $\Sigma(\approx \sqrt{2 \pi} h_m; \rho_m$ is the midplane density structure) is assumed to have the profile of $\Sigma \propto R^{-1}$. The initial density distribution is shown in the top panel of Figure 1.

3. Results

Photoionization heating (hereafter EUV heating) plays a dominant role in H II regions, while photoelectric heating (hereafter FUV heating) is important in neutral (H I, H$_2$) regions. These two processes drive disk photoevaporation in our simulations. In this section, we first discuss physical quantities such as density, velocity field, temperature, and chemical structure of a photoevaporating disk with solar metallicity, and then we show their metallicity dependence (Sections 3.1 and 3.2). Next, we study how the resulting photoevaporation rates vary with different metallicities (Section 3.3). Finally, we develop a semi-analytic model to interpret our numerical results (Section 3.4).

3.1. Structure of a Solar-metallicity Disk

3.1.1. Density, Velocity, and Temperature Structures

Figure 1 shows photoevaporative flows from both H II regions and neutral regions. Gas flows from neutral regions are excited by FUV heating. We perform a test simulation in which the FUV heating is initially included but is switched off at the time $t = t_c \equiv 100$ au/$1$ km s$^{-1}$ $\approx 4.74 \times 10^2$ yr is the typical crossing time of the neutral flow over the computational domain. In each panel, the left half shows the chemical structure regarding the H-bearing species. With the color scales presented in the lowest part, layers dominated by H II, H I, and H$_2$ are marked by green, white, and blue. The right half of each panel shows the density and velocity structure of the disk. The arrows represent the poloidal velocity field $v_p = (v_r, v_z)$ only for $|v_p| > 0.25$ km s$^{-1}$. We also plot the density contours with the dotted lines: $n_H = 10^4$ cm$^{-3}$ (red), $10^5$ cm$^{-3}$ (black), $10^6$ cm$^{-3}$ (blue), and $10^7$ cm$^{-3}$ (purple).
FUV radiation is attenuated by dust once the hydrogen column density \( N_H \gtrsim 10^{21} \text{cm}^{-2} \) in the case of \( Z = Z_\odot \), while EUV radiation is strongly attenuated once the H I column density becomes \( N_{\text{HI}} \gtrsim 10^{17} \text{cm}^{-2} \). Therefore, FUV photons typically reach and heat the denser regions of a disk than EUV photons. The typical density of the neutral flows, \( n_{\text{HI}} \approx 10^{-3} - 10^{-1} \text{cm}^{-3} \), is much larger than the typical density of the H II region flow, \( n_{\text{HII}} \approx 10^{-3} - 10^{-4} \text{cm}^{-3} \), as visualized in Figure 1.

As shown in Figure 2, in the H II region, the main heating source is EUV heating, and the main cooling source is adiabatic cooling due to gas expansion rather than radiative recombination cooling. The recombination timescale, \( t_{\text{rec}} \approx 10^2 \text{yr} (n_{\text{HI}}/10^4 \text{cm}^{-3})^{-3} \), is longer than the sound-crossing time in the ionized gas, \( t_s \approx (100 \text{au}/30 \text{km s}^{-1}) \approx 16 \text{yr} \). Hence, the gas flows out of the disk system before recombining.

The heating/cooling processes bring the gas temperature to \( \approx 10^4 \text{K} \) in this region. The corresponding sound speed is \( c_s \approx 10 \text{ km s}^{-1} \). The gas is accelerated outward by the local pressure gradient. The poloidal velocity \( v_p = \sqrt{v_r^2 + v_\phi^2} \) reaches a few times the sound speed (\( \approx 30 \text{ km s}^{-1} \)) in the H II region of Figure 1, as is also presented by the previous hydrodynamical simulation of EUV photoevaporation (Font et al. 2004).

In the neutral region, FUV heating balances O I cooling, H2 cooling, and dust–gas collisional cooling. The most effective cooling source is O I line cooling in the region between the H II ionization front and the H2 photodissociation front, while the dominant process is H2 line cooling in the H2 region. Dust–gas collisional cooling becomes dominant among the three coolants in regions with much larger densities. Similar features are observed in previous studies (e.g., Nomura & Millar 2005; Nomura et al. 2007), but H2 cooling is not included in these studies. Our simulations show that H2 line cooling can be an effective cooling source, as well as O I cooling and dust–gas collisional cooling in the neutral region of disks.

Adiabatic heating/cooling is subdominant in the region where FUV heating is dominant, in contrast to the H II region. The resulting temperature is \( \approx 10^2 - 10^3 \text{K} \) (\( c_s \approx 1 - 3 \text{ km s}^{-1} \)). The gas is accelerated by the pressure gradient and achieves \( \approx 1 - 5 \text{ km s}^{-1} \) in the neutral region while it expands.

### 3.1.2. Distribution of Hydrogen-bearing Species

The H2 photoevaporative flows are excited through the following processes (Figure 1). Advection of H2 associated with photoevaporation replenishes H2 molecules into the neutral gas. It makes the height of the H/H2 boundary large. Heinzeller et al. (2011) argued that the H/H2 boundary above a protoplanetary disk can move upward owing to advection with winds, but hydrodynamics are not directly incorporated in their study. Our hydrodynamical simulations confirm that the H/H2 boundary is actually raised by FUV photoevaporative advection from the dense region, where H2 molecules are abundant.

In order to excite H2 flow in the atmosphere, FUV photons should be sufficiently attenuated by dust shielding and/or H2 self-shielding so that the H2 photodissociation rate is lower than the replenishing rate of H2. The self-shielding becomes...
effective when the H$_2$ column density is $N_{H_2} \gtrsim 10^{14}$ cm$^{-2}$. We give the self-shielding function of H$_2$ as $f_{\text{shield}} = \min[1, (N_{H_2}/10^{14}$ cm$^{-2})^{-0.77}]$ (Draine & Bertoldi 1996; cf. Appendix B). As shown in Figure 3, the photodissociation front coincides with the boundary where the H$_2$ self-shielding factor (the blue line in the bottom panel) sharply declines, i.e., self-shielding becomes strongly effective. Thus, H$_2$ molecules replenished by photoevaporation protect themselves against photodissociation by self-shielding rather than dust shielding.

It has been proposed, in the study of the protoplanetary disk chemistry, that self-shielding protects H$_2$ molecules against photodissociation, especially in outer region of the disk (e.g., Woitke et al. 2009; Walsh et al. 2012). The height of the H/H$_2$ boundary is much larger than those of the previous studies. For example, the height of the H/H$_2$ boundary in our study is $z \approx 70$ au at $R = 50$ au (see Figure 1), while Woitke et al. (2009) showed that it is $z \approx 15$–20 au at $R \approx 50$ au. Thus, hydrodynamics significantly affects the chemical structure of protoplanetary disks, and the actual chemical structure is different from the results of a hydrostatic calculation.

In the upper regions above the H/H$_2$ boundary in Figure 1, FUV photons are unshielded, and the H$_2$ abundance is determined by the balance between the strong (unshielded) photodissociation and the H$_2$ formation on dust grains. In the lower regions below the H/H$_2$ boundary, gas advection effectively replenishes H$_2$ molecules in addition to the H$_2$ formation on grains. In the H I region, weak (shielded) photodissociation and H$_2$ formation on dust grains determine 

3.1.3. Distribution of Metal Species

Molecules of CO are protected from photodissociation by self-shielding, H$_2$ shielding, and dust shielding of FUV photons (see Appendix B.2 for details). Figure 4 shows that CO molecules are photodissociated where the dust shielding factor $f_2(N_{CO})$ is large. This indicates that dust is the most important shielding source for FUV photons among the three kinds of shielding sources. Therefore, the position of the CO photodissociation front is determined by dust shielding. This is why the CO photodissociation front is almost identical to the boundary where FUV heating is effective, in contrast to the H$_2$ photodissociation front, which is determined by the self-shielding of H$_2$ (Figure 2).

The C II ionization front is assumed to be identical to the CO photodissociation front, which is caused by FUV in our model. Therefore, in Figure 2, the position of the C II ionization front is not identical to that of the H II ionization front but is embedded in a higher-density region (i.e., the larger $\theta$ region) than the H II ionization front.

The CO photodissociation front is almost identical to the boundary above which FUV heating is effective. Therefore, the difference in the height of the C$^+$/CO boundary between our study and previous hydrostatic studies is smaller than that of the H/H$_2$ boundary. For example, our study shows that the height of the C$^+$/CO boundary is $z \approx 20$ au at $R = 50$ au, while Woitke et al. (2009) showed $z \approx 15$ au at $R \approx 50$ au. Hence, the chemical structure of CO molecules is not significantly affected by photoevaporation, in contrast to that of H$_2$ molecules in our model.
3.2. Variations with Different Metallicities

3.2.1. Structure of Photoevaporative Flow

Figure 5 presents the structure of the photoevaporative flow with different metallicities, $Z = 10^{-0.5} Z_\odot$, $Z = 10^{-0.5} Z_\odot$, and $Z = 10^{-4} Z_\odot$ (top to bottom). Although the photoevaporative flow is excited for all of these cases, the dense neutral flow only appears with $Z = 10^{-0.5} Z_\odot$ and $Z = 10^{-4} Z_\odot$. Remarkably, we also see that the neutral flow for $Z = 10^{-0.5} Z_\odot$ is denser than that for $Z = 10^{-4} Z_\odot$. In fact, the typical density of the neutral flow is $n_{H} \sim 10^5$–$10^6$ cm$^{-3}$ for $Z = 10^{-0.5} Z_\odot$ and $n_{H} \sim 10^5$–$10^7$ cm$^{-3}$ for $Z = 10^{-4} Z_\odot$. We have confirmed that the density at the base of the neutral flow is almost proportional to $Z^{-1}$ in our simulations. The figure suggests that the metallicity of $Z \gtrsim 10^{-0.5} Z_\odot$ is required to excite the FUV-driven neutral photoevaporative flow but that its density is higher with lower metallicity once launched.

Since the visual extinction is proportional to the column density of grains along a line of sight $A_V \propto N_H Z$, FUV photons can reach the denser part of the disk with the lower metallicity. This explains why the density of the neutral flow in the $Z = 10^{-0.5} Z_\odot$ disk is much higher than that in the $Z = 10^{0.5} Z_\odot$ disk (Figure 5). We conclude that, for $Z \gtrsim 10^{-0.5} Z_\odot$, the neutral flow has a higher density with a lower metallicity because the FUV radiation can reach and heat the dense part of the disk.

Next, we consider why the neutral photoevaporative flow turns to become weak for $Z \lesssim 10^{-0.5} Z_\odot$ and almost ceases at $Z = 10^{-4} Z_\odot$. With our assumed dust-to-gas mass ratio in proportion to the metallicity, the relative amount of grains to gas decreases with metallicity. Therefore, the specific FUV heating rate becomes small as the metallicity decreases. In addition, under our chemistry model, the electron abundance is set to be equal to the abundance of the ionized carbon generated by CO photodissociation in the neutral region. The recombination timescale of charged grains becomes long at a fixed gas density as metallicity decreases, and dust grains are easy to charge positively. Because of the deep coulomb potential of the positively charged grains, electrons become hard to eject from dust grains by the photoelectric effect. This yields a low efficiency of the photoelectric effect (cf. Equation (40)) and reduces the resulting heating rate in the low-density part of the neutral region (the region close to the H$^+$/H boundary).

Likewise, the specific cooling rates also become generally small with decreasing metallicity. This behavior is clearly shown in the second row of Figure 6, which summarizes the specific heating and cooling rates within the $Z = 10^{0.5} Z_\odot$, $Z = 10^{-0.5} Z_\odot$, and $Z = 10^{-4} Z_\odot$ disks (left to right). Whereas the main cooling source is adiabatic cooling in the H II region, O I cooling, H$_2$ cooling, and dust--gas collisional cooling dominate in the neutral region for $Z \gtrsim 10^{-0.5} Z_\odot$. These cooling rates decrease with metallicity and become so small that adiabatic cooling dominates in both the H II and H I regions at the lowest metallicity $Z = 10^{-4} Z_\odot$.

The specific FUV heating rate, O I cooling rate, and dust--gas collisional cooling rate all decrease with metallicity owing to the decreasing amount of grains and metal species. However, the temperature of the neutral region also falls with metallicity, as Figure 6 shows. This implies that FUV heating becomes less effective than cooling in the region as metallicity decreases.

In the low-density part of the neutral region where O I cooling and H$_2$ cooling are dominant, the FUV heating rate is reduced by the low photoelectric efficiency, in addition to the small amount of grains, as metallicity decreases. The O I cooling rate is reduced only by the small amount of O I, and the H$_2$ cooling rate does not explicitly depend on metallicity. Therefore, compared with these cooling sources, FUV heating becomes relatively ineffective as metallicity decreases. In the high-density part of the neutral region, the temperature is determined by the balance between the FUV heating and dust--gas collisional cooling. The photoelectric efficiency, which depends on the electron density, does not strongly depend on metallicity in the region, because the hydrogen nuclei density and the electron abundance in this region are basically...
proportional to $Z^{-1}$ and $Z$, respectively. Therefore, the specific FUV heating rate is basically proportional to metallicity (the amount of grains). In contrast, the specific dust–gas collisional cooling rate depends on dust temperature and is proportional to metallicity and hydrogen nuclei density. Dust temperature is determined by the balance between absorption and (re-) emission, whose opacities are proportional to metallicity, and thus dust temperature does not strongly depend on metallicity. The density is proportional to $Z^{-1}$ in the region, so the specific dust–gas collisional cooling does not have explicit metallicity dependence in this region. As a result, similar to the low-density part of the neutral region, FUV heating becomes relatively less effective than dust–gas collisional cooling in the high-density part of the neutral region. Hence, as metallicity decreases, FUV heating is reduced more strongly than O I cooling, H$_2$ cooling, or dust–gas collisional cooling in the neutral region, so that the temperature of the neutral region falls with metallicity.

As metallicity decreases, FUV heating becomes unable to give neutral gas sufficient energy to escape from the gravitational binding of the central star. In the lowest-metallicity range
of $Z \lesssim 10^{-2} Z_{\odot}$, FUV heating does not even excite neutral photoevaporation.

### 3.2.2. Distribution of Hydrogen-bearing Species

As discussed in Section 3.1, the chemical structures of $H_2$ and $H$ are determined by the balance of photodissociation, the photoevaporative advection of $H_2$, and $H_2$ formation on grains. As the solar-metallicity disk, $H_2$ molecules are protected against photodissociation by self-shielding with any metallicity, as shown by Figure 7.

The $H/H_2$ boundary is determined by the balance of $H_2$ advection and unshielded photodissociation, and it depends on the radius where sufficient $H_2$ flow occurs. The resulting gas temperature of the neutral region becomes high with high metallicity due to the efficient FUV heating. This allows $H_2$ molecules to evaporate even from the inner regions of a disk where the central star’s gravitational binding is strong. The $H_2$ flow density is small with high metallicity due to a large attenuation of dust. (See also Section 3.4 for more quantitative discussions.) Thus, with high metallicity, low-density $H_2$ flow is excited even from the inner region of a disk, and the small-density $H/H_2$ boundary is formed.

The density of the $H^+/H$ boundary is determined by the balance of photoionization and recombination of ionized hydrogen, and therefore it is independent of metallicity. The density of the $H/H_2$ boundary is small with high metallicity. Hence, the density of the $H_2/H$ boundary becomes close to that of the $H^+/H$ boundary with high metallicity, and this leads to a geometrically thin $H$ region with high metallicity, as Figure 5 shows.

### 3.2.3. Distribution of Metal Species

The amount of dust is small at small metallicity, and the dust shielding factor becomes subdominant among the three shielding factors of CO photodissociation as metallicity decreases. As Figure 8 shows, the most dominant shielding factor is the dust extinction factor $\Theta_3(A_V)$ with $Z = 10^{0.5} Z_{\odot}$ and $Z = 10^{-0.5} Z_{\odot}$, while it is the $H_2$ shielding factor $\Theta_2(N_{H_2})$ with $Z = 10^{-4} Z_{\odot}$. Thus, as metallicity becomes low, the most dominant attenuation source turns from dust to $H_2$, whose abundance does not depend on metallicity. In contrast, it is similar to the solar-metallicity disk from Section 3.1 that the CO photodissociation front is embedded in the dense regions of the disks at all metallicities, as shown in Figure 6.

### 3.3. Metallicity Dependence of Photoevaporation Rate

We calculate photoevaporation rates $M_{\text{ph}}$ by integrating the mass flux component normal to a spherical surface $S$,

$$M_{\text{ph}} = \int_S dS \cdot \rho v = r_S^2 \int S d\rho d\phi \sin \theta \rho \nu,$$

(16)

where $dS$ is an infinitesimal surface element vector orthogonal to the spherical surface and $r_S$ is the radius of $S$. If the specific enthalpy

$$\eta = \frac{1}{2} \nu^2 + \frac{\gamma}{\gamma - 1} c_s^2 - \frac{GM}{r},$$

(17)

is negative at the boundary $S$, we regard that the gas remains bound in the disk. Therefore, we sum up only the gas with $\eta > 0$ in Equation (16). Without this condition, the bound disk,
which has a very high density, can give a large contribution to Equation (16) even with very small velocity.

Figure 9 shows the resulting \( \dot{M}_{\text{ph}} \) of the different metallicity disks estimated by Equation (16) with \( r_S = 100, 150, 200, \) and 250 au. We give each of the dots as the time-averaged value of \( \dot{M}_{\text{ph}} \) from \( t = 0 \) to 16 \( t_c \approx 7.58 \times 10^3 \) yr. The figure shows that the photoevaporation rates increase with the measuring radius \( r_S \). This trend indicates that \( \eta > 0 \) is satisfied in the outer region rather than the gravitational radius, where \( \eta = 0 \) (Liffman 2003).

The gravitational radius is inversely proportional to the gas temperature (Hollenbach et al. 1994; Liffman 2003). In other words, the gas temperature \( T_{\text{esc}} \) necessary for escape is inversely proportional to the radius. If the base temperature \( T_{\text{base}} \) decreases more smoothly than \( T_{\text{esc}}(\propto r^{-1}) \), there is a radius where \( T_{\text{base}} = T_{\text{esc}} \). In the further region than the radius where \( T_{\text{base}} = T_{\text{esc}} \), photoevaporative flows are excited from anywhere because \( T_{\text{base}} > T_{\text{esc}} \) is always satisfied in the region. In this case, \( \dot{M}_{\text{ph}} \) calculated by Equation (16) increases with \( r_S \) and does not converge. In our simulation, the base temperatures decrease as \( T_{\text{base}} \propto r^{-\alpha} (\alpha < 0.5) \), while \( T_{\text{esc}} \) decreases more rapidly following \( r^{-1} \). Thus, \( \dot{M}_{\text{ph}} \) generally increases with \( r_S \), as Figure 9 shows, at least for \( r_c \lesssim 250 \) au. We do not consider the further large \( r_S \) because other effects, such as external photoevaporation (e.g., Adams et al. 2004; Facchini et al. 2016), dominate the evolution in such an outer part in typical environments. Including such effects is beyond the scope of the current work.

In the metallicity range of \( 10^{-4} Z_\odot \lesssim Z \lesssim 10^{-2} Z_\odot \), \( \dot{M}_{\text{ph}} \) is roughly independent of metallicity, as shown in Figure 9. As discussed in Section 3.2, FUV heating is less efficient than dust cooling in this metallicity range, and neutral flows are not driven.

The resulting EUV photoevaporation rate is \( \dot{M}_{\text{ph,EUV}} \approx 1.0 \times 10^{-9} M_\odot \) yr\(^{-1} \), as shown by Figure 9. In previous studies, such as Hollenbach et al. (1994) and Font et al. (2004), the typical EUV photoevaporation rate is given by \((2.7-7.3) \times 10^{-10} M_\odot \) yr\(^{-1} \) for \( \Phi_{\text{EUV}} = 6 \times 10^{41} \) s\(^{-1} \) and \( M = 0.5 M_\odot \), which is smaller than our \( \dot{M}_{\text{ph,EUV}} \). The photoevaporation rates of the previous studies are derived on the basis of the idea that the diffusion component of EUV dominates the direct component of EUV in a disk system. However, Tanaka et al.
(2013) recently showed that the direct component is more dominant than the diffuse component by solving 2D radiative transfer, which is clearly more adequate than the approximated 1+1D radiative transfer. The estimated photoevaporation rate is typically five times larger than those estimated by the 1+1D radiative transfer. The EUV photoevaporation rates seem to be underestimated in previous studies, such as Hollenbach et al. (1994) and Font et al. (2004), and this is the reason why the photoevaporation rates are smaller than those of our study, where the diffusion component of EUV is not incorporated. We note that the geometrical structure of a disk is also crucial to determine which of the EUV components is dominant and affects a resulting photoevaporation rate. These differences in the photoevaporation rates of previous studies and our model might also reflect the differences in the geometrical structures of the disks. Hence, it is important to solve radiative transfer by including self-consistent flow structure and scale height in order to estimate a photoevaporation rate.

In the range of \(10^{-1} Z_\odot \leq Z \leq 10 Z_\odot\), both neutral flows and ionized flows are constantly excited, as shown in Figure 5. As discussed in Section 3.2, FUV photons can reach and heat dense parts of the disk when the dust opacity is small. The density of the excited neutral photoevaporative flow is higher for lower metallicity, and the resulting density of the excited neutral photoevaporative flow is lower for higher metallicity, while that of our study is smaller. The metallicity dependence effect to regulate the EUV photoevaporation rates is reported in context of massive star formation, a similar dust attenuation might also re...

3.4. Semi-analytic Model

In this section, we develop a semi-analytic model to interpret our numerical results. As discussed in Sections 3.2 and 3.3, \(M_{\text{ph}} \) is largely determined by FUV-driven neutral flows with a strong metallicity dependence. We focus on modeling the FUV-driven photoevaporation rate \(M_{\text{ph}}^{\text{FUV}} \) with different metallicitics of \(10^{-2} Z_\odot \leq Z \leq 10 Z_\odot\). Regarding the photoevaporation via the EUV irradiation, we simply assume a constant rate \(M_{\text{ph}}^{\text{EUV}} = 1.0 \times 10^{-9} M_\odot \text{ yr}^{-1}\). The EUV photoevaporation rate is taken from our calculation in Section 3.3.

We consider a situation shown in the schematic picture in Figure 10. We further adopt the following assumptions to construct our model:

1. The disk system is in a steady state.
2. Evaporative flows are launched from the regions where \(A_V \sim 1/2\).
3. All hydrogen is in the molecular form, but CO molecules are completely photodissociated at the base.
4. Evaporative flows are launched at the speed \(v_0\), where \(\dot{M}(R, Z)\) is the Mach number and \(R\) is the distance in cylindrical coordinates.
5. The azimuthal velocity is given by \(v_0 \sim \sqrt{GM_\odot/r}\) at the base.
6. The gas temperature at the base is determined by the thermal balance between the dominant heating and cooling processes, i.e., photoelectric heating, \(H_2\) cooling, dust–gas collisional cooling, and \(O1\) cooling.
7. The evaporative flow is launched only from the base, where the gas has the positive specific enthality \(\eta\) (Liffman 2003).
8. The profile of the base is approximated by a quadratic function,

\[ z = f(R, Z) = a(Z)R^2 + b(Z)R, \]

where the coefficients \(a(Z)\) and \(b(Z)\) are provided later.

We use \(\sim 2A_V\) as the exponent of the dust shielding factor for FUV heating. Therefore, the points where \(A_V \sim 1/2\) approximately correspond to the boundary that FUV can reach in the disk. The visual extinction is defined as

\[ A_V = \Sigma_d N_H = \Sigma_d \int_{R_\ast}^R dr' n_H, \]

where \(N_H\) is hydrogen nuclei column density and \(\Sigma_d = 5.34 \times 10^{-22} \text{ mag cm}^2\) is the visual extinction per hydrogen nucleon. We expect, from Figures 1 and 5, that the density does not significantly vary along the line of sight from the central star, so the integral part of Equation (19) can be approximately rewritten to \(N_H \sim n_H r\). Hence, in our semi-analytical model, we approximate the visual extinction as \(A_V \sim \Sigma_d (Z/Z_\odot) n_H r\).

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**Figure 10.** Schematic picture of the situation considered in our semi-analytic modeling. The blue curve represents the base of the neutral photoevaporative flow, to which the visual extinction measured from the star reaches \(A_V = 1/2\). We assume that the profile of the base is simply described as an analytic function \(z = f(R)\). At a given point on the base, the flow is launched at a speed of \(\dot{M}_{\ast}\), in the direction of the angle \(\beta\), for which we use the values taken from the numerical simulations.
and the base number density is given by
\[ n_b = \frac{1}{2\Sigma_d(Z/Z_\odot)r}. \]

(20)

Hydrogen dominates the gas mass in our chemistry model, and thus the base density is approximately given by
\[ \rho_b = m_H/(2\Sigma_d(Z/Z_\odot)r). \]

The FUV flux is analytically given at each point of the base. The density of each chemical species is derived by the third assumption and Equation (20). The dust temperature is determined by the balance between the absorption of stellar irradiation and (re-)emission at the base, so that it is basically independent of metallicity. We use \( T_{f_{\text{fit}}} = 120 \, \text{K} \) as the base dust temperature in our analytical model, which we have derived from our simulation results. Under the assumptions above, we can calculate the base gas temperature by solving a single nonlinear equation of thermal equilibrium (the sixth assumption) at any metallicity. The resulting temperature is well described by a fit
\[ T_{\text{fit}} = T_0(Z) \left( \frac{r}{r_0} \right)^{\alpha(Z)}, \]

(21)

\[ T_0(Z) = 5.20 \times 10^2 (Z/Z_\odot)^{0.378} \, \text{K}, \]

(22)

\[ \alpha(Z) = -6.05 \times 10^{-2} (\log(Z/Z_\odot))^3 \]
\[ + 2.64 \times 10^{-2} (\log(Z/Z_\odot))^2 \]
\[ + 5.90 \times 10^{-3} \log(Z/Z_\odot) \]
\[ + 3.19 \times 10^{-1}. \]

(23)

where \( r_0 = 100 \, \text{au} \). Note that \( \alpha \) takes a value in the range of \( 0.28 < \alpha < 0.40 \) with \( 10^{-2} \, Z_\odot \lesssim Z \lesssim 10 \, Z_\odot \).

Under the above assumptions, the specific enthalpy at the base can be written as
\[ \eta = \frac{1}{2} \frac{r^2}{r_b^2} + \frac{\gamma}{\gamma - 1} \frac{c_s^2}{\gamma - 1} - \frac{GM_b}{r} - \frac{1}{2} \frac{c_s^2}{c_s^0}. \]

(24)

Thus, the condition \( \eta > 0 \) (the seventh assumption) corresponds to
\[ r > r_{\text{min}} \equiv r_0 \left[ \frac{1}{1 + \alpha} \frac{1 - \gamma}{\gamma} - \frac{GM_b}{r_0^2 r_b^2} \right]. \]

(26)

Therefore, the seventh assumption is equivalent to the assumption that photoevaporation is excited from the region where \( r > r_{\text{min}} \). The quadratic coefficients in Equation (18) are obtained by fitting our simulations as
\[ a = [-0.303(\log(Z/Z_\odot) + 7.92 \times 10^{-2})^2 + 0.534] \times (100 \, \text{au})^{-1}, \]

(27)

\[ b = [1.34 \times 10^{-2}(\log(Z/Z_\odot))^3 \]
\[ + 3.26 \times 10^{-2}(\log(Z/Z_\odot))^2 \]
\[ + 4.46 \times 10^{-3}\log(Z/Z_\odot) + 0.421]. \]

(28)

By using all of the elements above, we can finally derive \( M_{\text{FUV}}^{\text{ana}} \). Note that our model is based on 1D distributions of the relevant physical quantities along the base. The FUV photoevaporation rate is given by
\[ \dot{M}_{\text{FUV}}^{\text{ana}} = \int_{\eta>0} ds \ 2\pi R \rho_b \sin \beta, \]

(29)

where \( ds \) is a line element of the base and given by
\[ ds = dR \sqrt{1 + f^2}, \]
\[ \text{and} \quad \beta = \beta(R, Z) \]
\[ \text{is the angle of the poloidal velocity} \ v_p \ \text{relative to the line element} \ ds. \]

In our model, Equation (29) is rewritten to
\[ \dot{M}_{\text{FUV}}^{\text{ana}} = 2 \int_{\eta>0} dR \sqrt{1 + f^2} \ 2\pi R \rho \mu c_s \sin \beta \]
\[ \times \int_{R_{\text{min}}}^{R_{\text{max}}} dR \sqrt{1 + f^2} \frac{R \mu c_s}{r_\perp + \alpha/2} \sin \beta, \]

(30)

where \( R_{\text{max}} \) is the upper limit of the integration, and it is set to be the real root of \( R_{\text{max}}^2 + f(R_{\text{max}})^2 = R_{\text{min}}^2 \). We set \( \mu = 0.6 \) and \( \alpha = \pi/6 \) rad. These values are determined from the simulation results in the regions where \( \eta > 0 \). We approximate the gradient of the base as \( \dot{f} = [f(R_{\text{max}}) - f(R_{\text{min}})]/(R_{\text{max}} - R_{\text{min}}) \). Then, Equation (30) is rewritten as
\[ \dot{M}_{\text{FUV}}^{\text{ana}} \approx \frac{4\pi}{\Sigma_d(Z/Z_\odot)} \frac{m_H k T_X}{\mu c_s} \frac{2}{2 + \dot{f}^2(\dot{f}^2 + b)} \]
\[ \times \frac{r_{\text{max}}}{1 - \alpha/2} \left[ 1 - \left( \frac{r_{\text{min}}}{r_{\text{max}}} \right)^{1-\alpha/2} \right], \]

(31)

where \( T_X \equiv T_{\text{fit}}(r_{\text{max}}) \).

The model photoevaporation rate \( M_{\text{model}} = \dot{M}_{\text{FUV}}^{\text{ana}} + \dot{M}_{\text{FUV}}^{\text{ana}} \) is shown by the red line in Figure 11. It is clear that our model explains well the metallicity dependence of the photoevaporation rate derived from our simulations. The discrepancy between the photoevaporation rates of the model and simulations is relatively large in \( Z \lesssim 10^{-2} \, Z_\odot \). In this metallicity range, adiabatic cooling is comparable to or dominates the other cooling/heating processes and thus primarily determines the temperature in the neutral region. The base temperature is calculated to be higher in our model than in the simulations owing to the absence of adiabatic cooling. This suggests that hydrodynamical simulations are necessary to derive photoevaporation rates when the characteristic dynamical time is comparable to or shorter than the characteristic cooling time.
Equation (31) also gives the $r$-dependence of $\dot{M}_{\text{FUV}}^{\text{ana}}$ by replacing $r_{\text{max}}$ with $r_{\text{min}}$. In order to compare the $r$-dependence of the model photoevaporation rates with that of the simulation results, we use Equation (16) with a small modification:

$$M_{\text{FUV}}^{\text{sim}}(r) = r^2 \int_{S(r)} d\theta d\phi \sin \theta \rho \nu_r.$$  (32)

In the equation, $S(r)$ is the region where $\gamma_{\text{H II}} < 0.5$ in the spherical surface at $r$. We use the condition $\gamma_{\text{H II}} < 0.5$ to calculate the contribution of the neutral photoevaporative flow to the photoevaporation rates. Figure 12 compares the $r$-dependence of the analytic photoevaporation rate with that of the simulation results. The model photoevaporation rate of Equation (31) can explain not only the metallicity dependence but also the $r$-dependence of the photoevaporation rates.

In Equation (31), we can give the approximate forms of $r_{\text{min}}$ as functions of metallicity $r_{\text{min}} \simeq 12.4 (Z/Z_\odot)^{-0.55}$ au. Also, we can approximate the last factor of Equation (31) to $\sim 0.5$ with an error of less than 4%. With these quantities, Equation (31) can be further approximated to the form that explicitly depends on $r$ and $Z$,

$$M_{\text{FUV}}^{\text{ana,fit}} \simeq 2.1 \times 10^{-8} M_\odot/\text{yr} \tilde{Z}^{-0.81} \times [\tilde{r}_2^{-1/2} - (0.12 \tilde{Z}^{-0.55})^{1-\alpha/2}],$$  (33)

where $r_2 \equiv r/(10^2 \text{ au})$ and $\tilde{Z} \equiv (Z/Z_\odot)$. In Figure 12, $M_{\text{FUV}}^{\text{ana,fit}}$ (Equation (33)) is shown by the green solid line and compared with $M_{\text{FUV}}^{\text{ana}}$ (Equation (31)), denoted by the red solid line.

4. Discussion

4.1. Comparison with X-Ray Photoevaporation

In the present study, $\dot{M}_{\text{ph}}$ increases with decreasing metallicity in the range of $10^{-1} Z_\odot \leq Z \leq 10 Z_\odot$, which is similar to that of EC10, while $\dot{M}_{\text{ph}}$ decreases with metallicity in the range of $10^{-2} Z_\odot \leq Z \leq 10^{-1} Z_\odot$, which is different from that of EC10, who derived EUV/X-ray photoevaporation rates. Evidently, it is worth investigating the metallicity dependence obtained from the numerical results and that provided by our semi-analytic modeling. The top, middle, and bottom panels show the cases with different metallicities of $Z = 10^{0.5} Z_\odot$, $Z = Z_\odot$, and $Z = 10^{-0.5} Z_\odot$. In each panel, the thin dashed lines show the snapshots taken every 0.1 yr in the simulation, and the blue line represents their averaged profile. The red and green lines represent the rates given by our semi-analytic models, i.e., Equations (31) and (33), respectively. Note that the plotted range of the vertical axis differs between the top and bottom panels.
of FUV/EUV/X-ray photoevaporation. In future work, we plan to incorporate X-ray radiative transfer in our photoevaporation model and derive the metallicity dependence of photoevaporation excited by FUV/EUV/X-ray.

4.2. Disk Lifetime

The crossing time of the photoevaporative flow is much shorter than the timescale of the lifetime. This implies that it is computationally expensive to simulate the photoevaporation of a protoplanetary disk until the disk disperses completely. Instead of calculating the global evolution, we can use the analytic formula presented by EC10 to estimate a lifetime by giving a photoevaporation rate. When we set the exponent of the initial surface density profile $\Sigma \propto R^{-p}$ to $p = 1$, the formula is given by $t_{\text{life}} \propto M_{\text{ph}}^{-2/3}$. By assuming that the initial mass and radius of protoplanetary disks are independent of metallicity, we can evaluate the metallicity dependence of lifetimes from the metallicity-dependent photoevaporation rates of our simulations. Figure 13 compares the estimated lifetimes from the photoevaporation rates of our study with the metallicity dependence of the observational lifetimes. We choose 3 Myr at $Z = Z_\odot$ (Haisch et al. 2001) and 1 Myr at $Z = 0.2 Z_\odot$ (Yasui et al. 2009, 2010) as the observational lifetimes. The formula merely gives the simple relation between the lifetime and the photoevaporation rate. Therefore, it needs to be normalized to give a specific lifetime from a photoevaporation rate. In order to enable the comparison between the observational lifetimes and the estimated lifetimes, we normalize the formula so that it gives the same lifetime as the observational lifetime at $Z = Z_\odot$. The estimated lifetime is $\sim 2$ Myr with $Z = 0.2 Z_\odot$ in Figure 13, while the observational lifetime is 1 Myr. Thus, the metallicity dependence of the estimated lifetimes is less steep than that of the observational lifetimes in the range $0.2 Z_\odot \lesssim Z \lesssim Z_\odot$.

We have only two data points from observations in Figure 13. A reasonable and meaningful comparison with our model requires more observational data. In addition, disk lifetimes are influenced by the accretion process, which has not been fully understood yet. However, at least we can report here that the slope of the estimated lifetimes in the range $10^{-0.5} Z_\odot \lesssim Z \lesssim 10 Z_\odot$, $(-0.85) \times (-2/3) = 0.57$, is quite consistent with that of the observational lifetimes, 0.68. Hence, it is suggested that FUV photoevaporation also has the potential to explain the short lifetimes of the protoplanetary disks in low-metallicity environments as X-ray photoevaporation.

It has been observationally shown that the gas-giant occurrence decreases with the host star’s metallicity at $Z \gtrsim 10^{-0.5} Z_\odot$, which is called “planet–metallicity correlation” (e.g., Gonzalez 1997; Johnson et al. 2010; Mortier et al. 2013). The apparent correlation is thought to reflect the fact that planet formation is inefficient in a low-metallicity disk. Interestingly, EC10 showed that in the context of the core accretion scenario, the higher planet occurrence is attributed mainly to the faster core growth due to a larger amount of solids in a higher-metallicity disk rather than the reduced lifetimes due to X-ray photoevaporation. On the other hand, Wang & Fischer (2015) concluded that the terrestrial planet occurrence is not as strongly dependent on metallicity as the gas-giant occurrence. This observational result would suggest that the core growth of planets is not so strongly dependent on metallicity. In that case, the metallicity dependence of FUV and/or X-ray photoevaporation could have effects on the metallicity dependence of the gas-giant occurrence.

4.3. Grain Effects on FUV Photoevaporation

Photoelectric heating generally depends on both the local dust-to-gas mass ratio and the local size distribution of dust/PAH grains. Though we assume a constant dust-to-gas mass ratio and a constant size distribution in the whole computational domain, they are, in general, variable because of settling, grain growth, and entrainment into the disk wind (Takeuchi et al. 2005; Owen et al. 2011; Hutchison et al. 2016a, 2016b). In fact, a variable dust-to-gas mass ratio and grain size distribution are observationally proposed in both the radial and vertical directions (e.g., Pinte et al. 2016). Therefore, for the metallicity dependence derived in this study, the photoevaporation rate is further affected by spatial grain distribution, grain size distribution, and grain aerodynamics.

The PAH abundance significantly affects the gas–grain photoelectric heating rate and hence the resulting FUV photoevaporation rate (Gorti & Hollenbach 2008, 2009). In our fiducial model, we adopt the ISM value, which may be larger than the PAH abundances around T Tauri stars (Geers et al. 2007; Oliveira et al. 2010; Vicente et al. 2013). Although there remain large uncertainties in the observationally determined PAH abundances, it is worth examining the overall impact of the assumed PAH abundance on our results.

According to Bakes & Tielens (1994), about half of the total photoelectric heating rate is contributed by the grain species with sizes smaller than $15 \mu m$ $(N_C \lesssim 1500)$. By reducing the FUV heating rate to half of that given by Equation (40), we can approximate an effective photoelectric heating rate without PAH contribution.

We perform additional simulations using the reduced FUV heating rate. The resulting photoevaporation rates are shown in Figure 14. Clearly, the FUV-driven flows contribute to $M_{\text{ph}}$ in...
the range of $Z \gtrsim 0.1 Z_\odot$, even in the case where there is no PAH contribution.

The halved FUV heating makes base temperatures lower. The lower base temperatures yield the result that photoevaporative flows are excited in the outer region of the disks. In $Z \gtrsim Z_\odot$, the base temperatures are still high to excite photoevaporative flows in the large part of the disk even if PAHs do not contribute to the FUV heating. Consequently, the abundance and size of PAHs do not significantly change the photoevaporation rates. In $0.1 Z_\odot \lesssim Z \lesssim Z_\odot$, the dust–gas collisional cooling is effective enough to suppress the excitation of photoevaporative flows even at $Z \simeq 10^{-0.3} Z_\odot$. As a result, $M_{\text{ph}}^{\text{f}}$ drops at higher metallicity in the case where PAHs are absent than in the case where PAHs exist.

Although the small PAH abundances result in smaller FUV photoevaporation rates, as we demonstrate, other grain effects could also affect FUV photoevaporation rates (Gorti et al. 2015). For example, if dust growth and settling are incorporated, disk opacity for UV photons would be reduced. In this case, photoevaporation rates are increased because UV photons reach the higher-density interior of the disk. Actually, a low visual extinction $A_V \sim 0.1–0.2$ is observed for high column density regions with $N_H \sim 10^{22} \text{ cm}^{-2}$ (Vicente et al. 2013). This suggests that the effects of grain growth/settling might deplete dust grains with a size of $\sim 0.1 \mu$m in the neutral region, and the effects would reduce the disk opacities for UV photons. Hence, for a comprehensive modeling of FUV photoevaporation, we need to take into account not only the reduced PAH abundance but also other effects, such as grain growth, destruction/fragmentation, and settling.

4.4. MHD Wind

An MHD-driven disk wind has been proposed as another important mechanism for disk evolution (Suzuki & Inutsuka 2009; Suzuki et al. 2010; Armitage et al. 2013; Bai & Stone 2013a, 2013b, 2017; Fromang et al. 2013; Lesur et al. 2013; Simon et al. 2013a, 2013b; Gressel et al. 2015; Bai 2016; Suzuki et al. 2016). Magnetorotational instability (MRI) excites turbulence that can drive a wind from disk surfaces (Suzuki & Inutsuka 2009; Suzuki et al. 2010). Recent nonideal MHD studies show that MRI is mostly suppressed because of a low ionization degree in the interior of a disk, but magnetocentrifugal winds can be launched from disk surfaces (Bai & Stone 2013b; Gressel et al. 2015). The winds extract the disk angular momentum and can promote accretion onto the central star.

The MHD effects on disk evolution and photoevaporation have been studied independently, but the interplay between them is an important question for realistic modeling of the dispersal. Bai (2016) and Bai et al. (2016) examine evolution of protoplanetary disks by incorporating MHD and external thermal heating (irradiation). They show that the wind mass-loss rate is actually affected by both the strength of the magnetic field and thermal heating, and that it is characterized by the ratio of sound speed and Alfvén speed at the base.

The base position and density and the ionization degree there depend critically on metallicity. Therefore, for a complete picture of the metallicity dependence of disk dispersal, it would be necessary to study the global evolution of protoplanetary disks with both MHD and photoevaporation with a detailed treatment of the relevant thermal processes.

4.5. Outer Boundary Effect

In general, the profiles of photoevaporation and the derived photoevaporation rate can be affected by the bogus reflection at the boundary of the computational domain to some extent, especially when outgoing flow is subsonic. In this study, the reflection possibly happens in the region close to both the launching points of the photoevaporative flow and the outer boundary of the computational domain, where the flow is not yet accelerated up to $a_\text{c} > 1$. The bogus reflection leads to smoothing the pressure gradient owing to the accumulation of the gas near the outer boundary. In this case, gravitational force dominates over the pressure gradient, so that the gas is artificially decelerated in the region.

The bogus reflection propagates at the sound speed. It can make photoevaporation profiles and rates have some features that vary with the timescale of the order of the crossing time. The effects will be significant when the outer boundary is so small that the computational domain does not contain transonic points of photoevaporative flows. In order to examine the effect of the bogus reflection, we carry out simulations with a smaller outer boundary $L = 100$ au, keeping the numbers of the cells the same as the settings described in Section 2.1. Figure 15 shows the time evolution of $M_{\text{ph}}$ derived by Equation (16) with $r_5 = 80$ au. We find that $M_{\text{ph}}$ varies periodically in runs with $Z \gtrsim 10^{-1.5} Z_\odot$. Evaporative flows are driven by FUV in this metallicity range, but they are not yet accelerated to $a_\text{c} > 1$ at the outer boundary. The flows are spuriously reflected, causing oscillational trends in the photoevaporation rates. With $10^{-4} Z_\odot \lesssim Z \lesssim 10^{-1.5} Z_\odot$, the time evolution of $M_{\text{ph}}$ is almost independent of metallicity and always similar to that of $Z = 10^{-2} Z_\odot$, indicated by the magenta line in Figure 15. Only the ionized flows contribute to $M_{\text{ph}}$ in this metallicity range. The flow velocity usually exceeds the sound speed soon after they are launched at the base, and thus the oscillation does not appear in $M_{\text{ph}}$.

We have also performed simulations with $L = 200$ au and confirmed that the oscillation is actually caused by the bogus reflection. The top panel of Figure 16 shows the time-dependent $M_{\text{ph}}$ of the $Z = Z_\odot$ and $Z = 0.1 Z_\odot$ disks, where $r_5 = 80$ au again. The oscillation of $M_{\text{ph}}$ for $Z = Z_\odot$ is damped with time in the case of $L = 200$ au. This can be interpreted as...
that expanding the computational domain prevents the bogus reflection in the region close to both the launching point and \( r \sim 100 \) au, where the neutral gas has a subsonic velocity and contributes significantly to \( \dot{M}_\text{ph} \). In the case of \( Z = 0.1 Z_\odot \), the oscillation is still found with \( L = 200 \) au. We run simulations with outer boundaries of \( L = 300 \) and \( 400 \) au. In these cases, the numerical oscillations disappear, and the photoevaporation rates converge after \( \sim 1000 \) yr of calculation (bottom panel of Figure 16). With the enlarged outer boundaries, the transonic point of the photoevaporative flow lies inside the computational domain. The outgoing gas has a supersonic velocity at the boundary, and so the artificial reflection does not occur. Clearly, in order to eliminate or mitigate the outer boundary effect and obtain converged photoevaporation rates, the transonic points of streamlines in photoevaporative flow should be included in the computational domain.

We perform simulations with \( L = 100, 200, 300, \) and \( 400 \) au with all of the metallicities we consider here. Figure 17 shows the resulting time-averaged photoevaporation rates. The bogus reflection affects the resulting photoevaporation rates, especially in the subsolar metallicity range, where inefficient photoelectric heating reduces gas temperature and yields slower flow velocity. The photoevaporation rates converge if sufficiently large outer boundaries are set, as the red and green lines show in Figure 17. Note that the photoevaporation rates are in a better agreement with the analytical one. This result just reflects the fact that excluding the bogus reflection by using large outer boundaries allows the simulations to reach a steady state, as assumed in the analytical model.

4.6. Photoevaporation Estimate

As discussed in Section 3.3, \( \dot{M}_\text{ph} \) increases with \( r_5 \). In order for \( \dot{M}_\text{ph} \) to converge, the mass flux should have a dependence \( \rho_{\text{base}} v_{\text{base}} \propto R^p \) with \( p < -2 \) because \( d\dot{M}_\text{ph} \propto \rho_{\text{base}}^p v_{\text{base}} R^2 d(\log R) \). The radius dependence of the base velocity \( v_{\text{base}} \) is generally not so strong as \( \rho_{\text{base}} \), so \( \rho_{\text{base}} \) needs to be \( \rho_{\text{base}} \propto R^p \) with \( p' \lesssim 2 \). In our simulations, the base density has \( p' \gtrsim -(1.2-1.5) \). Therefore, \( \dot{M}_\text{ph} \) does not converge.

Figure 15. Time evolution of the photoevaporation rates with various metallicities in the simulations with \( L = 100 \) au, \( Z = 10^{0.5} Z_\odot \) (red), \( Z_\odot \) (orange), \( 10^{-1} Z_\odot \) (green), \( 10^{-0.5} Z_\odot \) (blue), and \( 10^{-2} Z_\odot \) (magenta). We do not plot any cases with \( Z \lesssim 10^{-2} Z_\odot \), where the time evolution is almost the same as for \( Z = 10^{-2} Z_\odot \).

Figure 16. Top: time dependence of the photoevaporation rates. The orange and blue lines represent the cases with \( Z = Z_\odot \) and \( Z = 0.1 Z_\odot \). The solid and dashed lines indicate different sizes of the computational domain: \( L = 100 \) and \( 200 \) au, respectively. Bottom: time dependence of the photoevaporation rates of \( Z = 0.1 Z_\odot \) disks with different outer boundaries. The solid and dashed lines are the same as in the top panel, and the red and orange lines indicate the photoevaporation rates with different sizes of outer boundaries of \( L = 300 \) and \( 400 \) au, respectively. These two lines are almost overlapped.

Figure 17. Time-averaged photoevaporation rates measured at \( r_5 = 80 \) au in the simulations with different sizes of outer boundaries. The blue, orange, green, and red lines show the metallicity dependences with outer boundaries of \( L = 100, 200, 300, \) and \( 400 \) au, respectively. The black dotted line shows the analytical photoevaporation rate, which is presented in Section 3.4.
until $r_S$ reaches the disk edge. Similar results are reported by Tanaka et al. (2013) for EUV photoevaporation and can be inferred from the figures of Gorti & Hollenbach (2009) and Figure 4 of Owen et al. (2010), where the cumulative X-ray photoevaporation rate does not converge with radius up to 70 au. In summary, in order to obtain the total photoevaporation rate, the computational domain should contain the whole disk.

4.7. CELs in HII Regions

CELs such as O II (3730 Å, 3727 Å), N II (6585 Å, 6550 Å), O III (88.36 μm, 51.81 μm, 5008 Å, 4960 Å), Ne II (12.81 μm), S II (6733 Å, 6718 Å), and S III (33.48 μm, 18.71 μm, 9071 Å, 9533 Å) can be important cooling sources in an H II region, especially when the gas metallicity is higher than the solar metallicity (Draine 2011). The total CEL cooling rate is estimated to be $\sim 10^3 (n_H/10^3 \text{ cm}^{-3})(Z/Z_{\odot})$ erg g$^{-1}$ s$^{-1}$ in a typical H II region (Draine 2011). The rate of adiabatic cooling, which is shown to be an important cooling in the photoevaporative winds that we study here, is given as $P(d/dt)(1/\rho) = (P/\rho) \nabla \cdot \mathbf{v} \sim c^2/r \sim 10^6 \left( c_s/30 \text{ km s}^{-1}\right)^2 (r/1 \text{ au})^{-1}$ erg g$^{-1}$ s$^{-1}$. Thus, the CEL cooling can dominate over the adiabatic cooling in the inner, high-density part of an H II region. If we choose $n_H \sim 10^8 \text{ cm}^{-3}(r/1 \text{ au})^{-1.5}$ as a typical base density (Hollenbach et al. 1994; Tanaka et al. 2013), the CEL cooling dominates over the adiabatic cooling in $r \lesssim 1$ au, where the base temperature can be lowered by a few to several tens of percent. Note that this is outside our computational domain. The ionized gas will then be more strongly bound there, and the contribution from $r \lesssim 1$ au to the photoevaporation rate is sufficiently small, as discussed already. In the wind region (atmosphere), the density is much smaller than the base density, and thus the CELs are less important. Overall, the impact of the CELs on the net photoevaporation rate is unimportant in our simulations.

5. Summary

We have performed radiation-hydrodynamical simulations of the photoevaporation of protoplanetary disks with self-consistent modeling of multispecies chemistry. In particular, we have considered a broad range of metallicities from $10^{-4} Z_{\odot}$ to 10 $Z_{\odot}$, to examine the metallicity dependence, if any, of the disk lifetime. Our findings are summarized as follows:

1. As the metallicity decreases, the dust shielding effect is reduced, and FUV photons reach and heat denser regions of the disk. Thus, $M_{\text{ph}}$ increases with decreasing metallicity in the range of $10^{-1} Z_{\odot} \lesssim Z \lesssim 10 Z_{\odot}$.

2. As the metallicity decreases, FUV photoelectric heating becomes less efficient than cooling in neutral regions. The temperature decreases so that a large portion of the disk gas is gravitationally bound. This reduces the contribution of the FUV-driven neutral flow to photoevaporation at $10^{-2} Z_{\odot} \lesssim Z \lesssim 10^{-1} Z_{\odot}$.

3. The photoevaporation rate shows a peak as a result of the combination of the above two effects.

4. In the metallicity range of $10^{-4} Z_{\odot} \lesssim Z \lesssim 10^{-2} Z_{\odot}$, EUV photons primarily drive photoevaporative flows if the X-ray is not considered. Hence, $M_{\text{ph}}$ is nearly independent of metallicity in this extremely low-metallicity environment.

5. We develop a semi-analytical model of disk photoevaporation that accurately describes both the metallicity dependence of $M_{\text{ph}}$ (see Figure 9) and the outflow profile $M_{\text{ph}}^\text{outflow}(r)$ (see Figure 12).

6. Generally, $M_{\text{ph}}$ cumulatively increases with radius where it is measured. Hence, $M_{\text{ph}}$ depends on the disk radius. Global simulations are necessary to derive total photoevaporation rates.

7. In numerical simulations, the bogsus reflection at the outer boundary affects the photoevaporative flow profiles. It can even lead to a wrong conclusion regarding photoevaporation rates. A sufficiently large outer boundary should be used so that it can contain the transonic points of the photoevaporative flows, or one would need to use a nonreflecting boundary condition.

Ercolano & Clarke (2010) argued that X-ray photoevaporation also causes a metallicity dependence of the photoevaporation rates, and that the result is roughly consistent with that of the observational disk lifetimes. Their photoevaporation rates are derived by hydrostatic calculations and thus are subjected to several critical assumptions on the dynamical process. Based on the findings in this paper, we argue that it is necessary to examine the metallicity dependence of X-ray photoevaporation by using hydrodynamical simulations. We will address this issue in our forthcoming paper (R. Nakatani et al. 2018, in preparation).

Our analytic model in Section 4.2 suggests that the FUV-driven photoevaporation can explain the short lifetimes of the disks in low-metallicity environments. A complete model of the protoplanetary disk dispersal would need to incorporate FUV/EUV/X-ray radiative transfer and possibly the effect of magnetic fields. We aim to extend our work to simulate the long-term evolution of protoplanetary disks to derive their lifetimes and metallicity dependence.

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Appendix A

Cooling/Heating

In this section, we summarize the heating/cooling processes included in our simulations.
A.1. Photoheating

We implement the photoheating processes by stellar EUV/FUV irradiation. We directly solve radiative transfer to calculate the photoionization heating (EUV heating) rate, while we simply use an analytic formula presented in Bakes & Tielens (1994; hereafter BT94) to obtain the photoelectric heating (FUV heating) rate.

We consider the absorption of the direct EUV photons from the central star. We solve

\[ \frac{1}{r^2} \frac{\partial}{\partial r} (r^2 F_\nu) = -n_{\text{H}_1} \sigma_\nu F_\nu, \]  

(34)

where \( \nu \) is a frequency of EUV photons, \( F_\nu \) is the specific number flux of the direct EUV field, \( n_{\text{H}_1} \) is the number density of H I, and \( \sigma_\nu \) is the absorption cross section of H I. We use the approximate absorption cross section

\[ \sigma_\nu = 6.3 \times 10^{-18} \left( \frac{h\nu}{h\nu_\text{Ly}} \right)^{-3} \text{cm}^2 \]  

(35)

(e.g., Osterbrock & Ferland 2006). In Equation (35), \( \nu_\text{Ly} \) is the frequency at the Lyman limit (\( h\nu_\text{Ly} \approx 13.6 \text{ eV; } \lambda_\text{Ly} \equiv c/\nu_\text{Ly} \approx 91.2 \text{ nm, where } c \) is the light speed). Equation (34) can be solved analytically,

\[ F_\nu(r, \theta, t) = \frac{\Phi_\nu(R_\odot)}{4\pi r^2} \exp\left[-\sigma_\nu n_{\text{H}_1}\right], \]  

(36)

where \( \Phi_\nu(R_\odot) \) is the specific photon number luminosity of the EUV emitted from the stellar surface, and \( n_{\text{H}_1} = N_{\text{H}_1}(r, \theta, t) \) is the column density of hydrogen atoms between the stellar surface and a certain point in the computational domain:

\[ N_{\text{H}_1}(r, \theta, t) = \int dr' n_{\text{H}_1}(r', \theta, t). \]  

(37)

With Equation (36), the photoionization rate and specific photoionization heating rate are given as

\[ R_{\text{ionize}} = \gamma_{\text{H}_1} \int_{\nu_1}^{\infty} d\nu \sigma_\nu F_\nu, \]  

(38)

\[ \Gamma_{\text{EUV}} = \frac{1}{\rho} n_{\text{H}_1} \int_{\nu_1}^{\infty} d\nu \sigma_\nu h(\nu - \nu_1) F_\nu, \]  

(39)

respectively. We assume that the spectral energy distribution of the EUV photons is given by a blackbody spectrum with an effective temperature \( T_{\text{eff}} = 10^4 \text{ K} \). The corresponding total stellar EUV luminosity is then \( \Phi_{\text{EUV}} \approx 1.5 \times 10^{41}(R_\odot/R_\star)^2 \text{ s}^{-1} \). We use 81 frequency bins for the numerical integrations.

For the photoelectric heating rate, we use the analytic formula presented in BT94. BT94 derived the photoelectric heating rate theoretically by using the dust size distribution of the MRN dust model (Mathis et al. 1977). The analytic formula is

\[ \Gamma_{\text{pe}} = 10^{-24} \epsilon_{\text{pe}} G_{\text{FUV}} n_{\text{H}} \times (Z/Z_\odot), \]  

(40)

where \( \epsilon_{\text{pe}} \) is the photoelectric effect efficiency of the grains, which corresponds to the ratio of the gas heating rate to FUV absorption rate of the grains, and \( \gamma_{\text{pe}} \) is the ratio of the dust/PAH photoionization rate to the dust/PAH recombination rate with electrons, which is given by \( \gamma_{\text{pe}} \equiv G_{\text{FUV}} \sqrt{T}/n_e \). Here \( G_{\text{FUV}} \) is the FUV flux \( (6 \text{ eV} < h\nu < 13.6 \text{ eV}) \) at the local point in the unit of the averaged interstellar flux \( F_{\text{ISRF}} = 1.6 \times 10^{-3} \text{ erg cm}^{-2} \text{ s}^{-1} \) and given by \( G_{\text{FUV}} = L_{\text{FUV}} e^{-1.86h\nu} / (4\pi r^2 F_{\text{ISRF}}) \). The last factor \( Z/Z_\odot \) of Equation (40) is multiplied to take into account the effect of the grain amount on the heating rate.

A.2. Dust–gas Collisional Cooling

Dust grains act as a cooling/heating agent for a gas via collisional heat transfer between gas and dust. We adopt the dust–gas collisional cooling function of Yorke & Welz (1996), which is given by

\[ \Lambda_{\text{dust}} = -4 \pi a_{\text{dust}}^2 c_s \rho_{\text{dust}} \frac{m_{\text{dust}}}{m_{\text{H}_1}} k(T - T_{\text{dust}}) (Z/Z_\odot), \]  

(42)

where \( a_{\text{dust}}, \rho_{\text{dust}}, m_{\text{dust}}, \) and \( T_{\text{dust}} \) are the mean dust size, dust mass density, mean dust mass, and dust temperature, respectively. We use the dust parameters of Yorke & Welz (1996): \( a_{\text{dust}} = 5 \times 10^{-6} \text{ cm} \) and \( m_{\text{dust}} = 1.3 \times 10^{-15} \text{ g} \).

A.3. Atomic/Molecular Line Cooling

We implement radiative recombination cooling of H II, Ly α cooling of H I, C II line cooling, O I line cooling, H_2 line cooling, and CO line cooling as line-cooling sources of gas.

When a hydrogen ion recombines with a free electron in the H II region, approximately two-thirds of the electron energy \( \sim kT \) is lost by radiative recombination (e.g., Spitzer 1978). We adopt the radiative recombination cooling rate

\[ \Lambda_{\text{rec}} = 0.67 kT R_{k2} n_e n_{\text{H}_1}, \]  

(43)

where \( R_{k2} \) is the reaction coefficient of H II recombination (the reaction labeled “k2” in Table 3).

A neutral hydrogen atom is excited by collision and then de-excited by emitting a Lyα photon. We simply refer to this cooling process as Lyα cooling. We use the Lyα cooling function presented in Anninos et al. (1997),

\[ \Lambda_{\text{Lyα}} = \xi_{\text{Lyα}} n_e n_{\text{H}_1}, \]  

(44)

\[ \xi_{\text{Lyα}} = \frac{7.5 \times 10^{-19} e^{-118348/T_K}}{1 + \sqrt{T_K/10^5}} \text{ erg cm}^3 \text{ s}^{-1}, \]  

(45)

where \( T_K \) is the gas temperature in K.

Here C II and O I have fine-structure transitions, and they work as line-cooling sources by spontaneous emissions. The total line-cooling rate of each atom is given by the equation

\[ \Lambda_X = \sum_j \chi_j \sum_{j>i} A_{ji} \Delta E_{ji}, \]  

(46)

The label X indicates C II or O I. The indexes \( i, j (=1, 2, 3, \ldots) \) are the label of an energy level, \( \chi_j \) is the population of level \( j, A_{ji} \) is the Einstein A coefficient of the transition \( j \rightarrow i \), and \( \Delta E_{ji} \) is its corresponding energy difference, respectively. Each of the level populations is derived by solving the equations of
statistical equilibrium simultaneously,
\[ x_i \sum_{j \neq i} c_{ij} = \sum_{i \neq j} x_j c_{ji}, \]  \hspace{1cm} (47)

where
\[ c_{ij} \equiv \begin{cases} A_{ij} + \sum \gamma_{ij}^\lambda n_\lambda & \text{for } (i > j), \\ \sum \gamma_{ij}^\lambda n_\lambda & \text{for } (i < j). \end{cases} \]  \hspace{1cm} (48)

The collisional excitation (de-excitation) rate of the transition \( i \rightarrow j \) with a collisional counterpart \( \lambda \) is represented as \( \gamma_{ij}^\lambda \). In this study, we treat these line emissions as optically thin for simplicity. Therefore, an escaping probability, absorption of external radiation, or induced radiation is ignored in Equation (48). The fine-structure line parameters for C II and O I are listed in Table 2.

The H2 and CO molecules have rovibrational transitions, and they also work as line-cooling sources. These cooling rates could also be directly calculated by Equation (46), but we use the analytic formula presented in Galli & Palla (1998) for H2 line cooling and the tabulated values presented in Omukai et al. (2010) for CO line cooling.

Appendix B
Chemical Reactions

We take into account all of the chemical reactions listed in Table 3. We include photochemical reactions, such as H I photoionization, H2 photodissociation, and CO photodissociation, as well as collisional reactions. We summarize these chemical reactions in this section.

B.1. Photodissociation of H2

The H2 is photodissociated by FUV photons in the energy range of 11.2 eV \( \lesssim h\nu \lesssim 13.6 \) eV as follows. The H2 is pumped up to an upper electronic bound state by absorbing an FUV photon, then it goes back to an excited vibrational state of the ground electronic state with fluorescence emission or to a continuum vibrational state of the ground electronic state; then it is photodissociated with fluorescence emission. Photodissociation occurs in \( \sim 10^-9\%\sim15\% \) of pumped-up H2 molecules.

FUV photons are shielded by dust and H2 molecules themselves. We adopt the photodissociation rate function and self-shielding function presented in Draine & Bertoldi (1996). The photodissociation rate per unit volume is given by
\[ R_{\text{H2, diss}} = f_{\text{shield}}(N_{\text{H2}}) e^{-\tau_{\text{H2}} L_{\text{FUV}}} n_{\text{H2}}, \]  \hspace{1cm} (49)

where \( \tau_{\text{H2,1000}} \) is the optical depth of the dust at the wavelength of 1000 Å, and \( L_{\text{FUV}} \approx 4 \times 10^{-11} G_{\text{FUV2}} \) s\(^-1\) is the unshielded photodissociation rate. The definition of \( G_{\text{FUV2}} \) is similar to that in Appendix A and given by \( G_{\text{FUV2}} = L_{\text{FUV}}/(4\pi r^2 F_{\text{ISRF}}) \). The self-shielding function (Equation 49) is
\[ f_{\text{shield}} = \begin{cases} 1 & \text{for } N_{\text{H2}} \leq N_0, \\ (N_0/N_0)^{-0.75} & \text{for } N_0 \leq N_{\text{H2}}, \end{cases} \]  \hspace{1cm} (50)

where \( N_0 \approx 10^{14} \) cm\(^2\).

B.2. Photodissociation of CO

The CO is also photodissociated by processes similar to H2 photodissociation, and its photodissociation is also a line process like H2 photodissociation. FUV photons are shielded by CO once the column density of CO becomes large. In addition, CO is shielded by H2 molecules owing to line overlap. Note that H2 is a more abundant species than CO.

We adopt the CO photodissociation function and shielding functions presented in Lee et al. (1996):
\[ R_{\text{CO, diss}} = G_{\text{FUV2}} n_{\text{CO}} 	imes \Theta_1(N_{\text{CO}}) \Theta_2(N_{\text{H2}}) \Theta_3(A_V), \]  \hspace{1cm} (51)

where \( \Theta_1 = 1.03 \times 10^{-10} \text{s}^{-1} \) is the unsheilded photodissociation rate of CO. The factors \( \Theta_1, \Theta_2, \) and \( \Theta_3 \) are the self-shielding factor, H2 shielding factor, and dust shielding factor, respectively. These quantities are tabulated in the table of Lee et al. (1996).

B.3. Carbon Chemistry

We assume that C I is converted to C II as soon as it is produced by the photodissociation of CO, as presented in Richling & Yorke (2000). In other words, we assume that the CO dissociation front coincides with the C II ionization front. As the reverse process of CO photodissociation, we use the simplified chemistry model for CO formation described in Nelson & Langer (1997). In the model, CO formation is initiated by the reaction C\(^+\) + H2 \rightarrow CH\(^+\) + \gamma (reaction rate; \( k_5 = 5 \times 10^{-16} \text{cm}^3 \text{s}^{-1} \)). The CH\(^+\) ions rapidly convert to CH and H2 by dissociative recombinaction with electrons and ion-molecule reactions with H2 molecules. These hydrocarbon radicals react with oxygen atoms to form CO (reaction rate; \( k_5 = 5 \times 10^{-10} \text{cm}^3 \text{s}^{-1} \)) or are photodissociated to form ions (dissociation rate; \( \Gamma_{\text{CH}} \)). As a result, the effective CO formation rate per unit volume is given by
\[ R_{\text{CO, form}} = k_0 n_{\text{H2}} n_{\text{H2}} k_{n_{\text{OL}}} \Gamma_{\text{CH}} \]  \hspace{1cm} (52)

(for the detailed derivation of this formula, see, e.g., Nomura & Millar 2005). We set the dissociation rate of the hydrocarbons \( \Gamma_{\text{CH}} \) to five times that of the CO dissociation rate for simplicity.

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