EVOLUTION OF SNOW LINE IN OPTICALLY THICK PROTOPLANETARY DISKS: EFFECTS OF WATER ICE OPACITY AND DUST GRAIN SIZE

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ABSTRACT

Evolution of a snow line in an optically thick protoplanetary disk is investigated with numerical simulations. The ice-condensing region in the disk is obtained by calculating the temperature and the density with the 1+1D approach. The snow line migrates as the mass accretion rate \( \dot{M} \) in the disk decreases with time. Calculations are carried out from an early phase with high disk accretion rates \( \dot{M} \sim 10^{-7} M_\odot \text{yr}^{-1} \) to a later phase with low disk accretion rates \( \dot{M} \sim 10^{-12} M_\odot \text{yr}^{-1} \) using the same numerical method. It is found that the snow line moves inward for \( \dot{M} \gtrsim 10^{-10} M_\odot \text{yr}^{-1} \), while it gradually moves outward in the later evolution phase with \( \dot{M} \lesssim 10^{-10} M_\odot \text{yr}^{-1} \).

In addition to the silicate opacity, the ice opacity is taken into consideration. In the inward migration phase, the additional ice opacity increases the distance of the snow line from the central star by a factor of 1.3 for dust grains \( \lesssim 10 \mu \text{m} \) in size and of 1.6 for \( \gtrsim 100 \mu \text{m} \). It is inevitable that the snow line comes inside Earth’s orbit in the course of the disk evolution if the viscosity parameter \( \alpha \) is in the range 0.001–0.1, the dust-to-gas mass ratio is higher than a tenth of the solar abundance value, and the dust grains are smaller than 1 mm. The formation of water-devoid planetesimals in the terrestrial planet region seems to be difficult throughout the disk evolution, which imposes a new challenge to planet formation theory.

Key words: accretion, accretion disks – planets and satellites: formation – protoplanetary disks – radiative transfer

Online-only material: color figures

1. INTRODUCTION

In a protoplanetary disk, a snow line, defined as the inner boundary of an ice-condensing region, is present. The snow line is considered to play an important role in planetary formation, since the solid mass density outside the snow line is high due to the condensation of water ice (water ice abundance is as large as silicate and iron in a protoplanetary disk with solar composition; Pollack et al. 1994). The snow line may also be related to the origin of the water distribution in our solar system. Water abundance in current solar system objects shows a clear variation; bodies in the inner part contain less, while bodies in the outer part have more. The terrestrial planets are significantly devoid of water. For example, Earth contains only 0.023 wt% water in its oceans, and Venus is considered to have contained an amount of water comparable with that of Earth (Lewis 2004). On the other hand, the outer planets and objects outside the asteroid belt contain a large amount of water. In the intermediate region, i.e., the asteroid belt, the radial distribution of asteroids also shows compositional zoning. From these facts, one may consider that the snow line might have been located in the asteroid belt when planetesimal formation occurred, since planetesimals that were formed outside the snow line would necessarily take in a large amount of icy materials.

The location of the snow line, which is used in many studies of planet formation, is the heliocentric distance where the temperature of the disk reaches about 170 K. In the solar nebula, the snow line location is estimated to be 2.7 AU, assuming that the solar nebula is optically thin (Hayashi 1981). Before planet formation takes place, however, protoplanetary disks are likely to be optically thick, since a large amount of fine dust particles is present. Thus, temperatures in optically thick disks should be obtained to determine the location of the snow line.

So far, the snow line location in an optically thick disk has been obtained theoretically from one-dimensional (1D) (radial) or 1+1D (radial and vertical) disk structure calculations (e.g., Cassen 1994; Stepiński 1998). The latest studies on the snow line location with a detailed disk structure calculation were made by Davis (2005) and Garaud & Lin (2007). They considered the stellar radiation flux and viscous dissipation of gas as the main heating sources in a disk, and obtained the disk temperature by solving the detailed radiative energy transfer. They revealed that the snow line migrates inward as the disk evolves and the mass accretion rate decreases, because viscous dissipation of gas, which is the main heating source in the disk, reduces as the disk evolves. Davis (2005) showed that the snow line reaches about 0.6 AU, which is the minimum radius in his calculations. Similarly, Garaud & Lin (2007) found that, in the later phase, the snow line migrates outward since stellar radiation penetrates deeper into the disk interior as the disk becomes optically thinner and its temperature rises.

One important point of their results is that the snow line comes inside the Earth’s orbit; the minimum heliocentric distance of the snow line is about 0.6 AU (Davis 2005; Garaud & Lin 2007). If sufficiently large bodies like planetesimals were formed when the snow line was located at such a small heliocentric distance, Earth would have been formed with icy planetesimals. Then, Earth should presently contain comparable amounts of water, silicate, and iron. This conflicts with the current water content on Earth.

In order to make clear the important inconsistency in planet formation, we investigate the detailed thermal evolution of protoplanetary disks using precise radiative transfer calculations, taking into account the dependence of opacity on frequency, the scattering process of dust particles, and the ice opacity that previous studies did not consider. According to Inoue et al. (2009) and Dullemond et al. (2002), disk midplane temperature varies by a factor of at most about two due to the first two effects. Ice opacity may change the optical properties of a disk or disk temperature structure significantly, since ice is as abundant as silicate in a protoplanetary disk of solar composition. The effect of the dust grain size, which changes the snow line location as
well, has not received enough consideration in previous studies. These effects are examined carefully in this work to see the location of the snow line.

In this study, the snow line location is simulated numerically with the 1+1D disk model, taking into account the water ice opacity, the variety of dust grain sizes, and the scattering process in the radiative transfer. Then we discuss whether the snow line location obtained theoretically is consistent with the water distribution in the current solar system.

2. MODEL

2.1. Disk Structure

A geometrically thin axisymmetric disk revolving around a central star is considered. A plane symmetry with respect to the midplane is assumed. Cylindrical coordinates \((R, \phi, Z)\) are adopted. The origin and the \(Z = 0\) plane are placed at the central star and the disk midplane.

The hydrodynamical and thermal structures of the disk are modeled in almost the same way as in Dullemond et al. (2002) and Inoue et al. (2009) except for the disk's gas surface density \(\Sigma(R)\). The radiative cooling and two heating sources, irradiation by the central star and viscous dissipation, are considered. The temperature is determined with the radiative equilibrium condition. To obtain the whole disk structure, the 1+1D approach is adopted. The direct irradiation from the central star at the disk inner edge is ignored, and the disk structure is assumed to change gradually in the radial direction. This approach is justified if the snow line location is sufficiently far from the inner edge. The 2D structure of the inner disk region (the puffed-up inner rim and the adjacent shadowed region) seems to be important only in the innermost part of the disk around a T Tauri star, judging from results for Herbig Ae/Be stars of Dullemond (2002). Although the shadowed region extends to slightly large heliocentric distances, it does not matter for the scope of this study because it only lowers the disk temperature and does not shift the snow line location outward. Details are given in the Appendix.

The radial distribution of the gas surface density is modeled assuming that the disk is in the steady accretion state, i.e., the mass accretion rate \(\dot{M}\) is constant along the radial direction \(R\). The gas surface density in a region where \(R \gg R_\ast\) (the stellar radius) is given as (e.g., Pringle 1981)

\[
\Sigma(R) = \frac{\dot{M}}{3\pi v_t(R)},
\]

where \(v_t(R)\) is the viscosity of the disk. The assumption of steady accretion is justified in the region around the snow line because the snow line is usually located within 10 AU, and the viscous diffusion timescale there is sufficiently smaller than the entire disk evolution timescale.

The viscosity \(v_t\) is modeled with the \(\alpha\)-prescription (Shakura & Sunyaev 1973) as \(v_t = \alpha c_s^2 / \Omega_K\), where \(\alpha\) is a non-dimensional parameter, \(c_s = \sqrt{\gamma P / \rho}\) is the isothermal sound velocity of gas, \(k\) is the Boltzmann constant, \(T\) is the gas temperature, \(\mu\) is the mean molecular weight, \(m_a\) is the atomic mass unit, \(\Omega_K = \sqrt{GM_\ast / R^3}\) is the Kepler angular velocity, \(G\) is the gravitational constant, and \(M_\ast\) is the stellar mass. The value of \(\alpha\) ranges from 0.001 to 0.1 according to ideal MHD simulations (Hawley et al. 1995, 1996). The value of \(\alpha = 0.01\) is adopted as a fiducial one throughout the disk in this study, except in Section 3.3. In the evaluation of \(v_t\), the sound velocity \(c_s\) at the midplane (\(Z = 0\)) is used. A value of \(\mu = 2.3\) is used for the mean molecular weight.

The frequency-dependent radiative transfer is solved numerically. Absorption and scattering by dust particles are taken into consideration as the opacity source in the disk. Isotropic scattering is assumed when the dust grain size is sufficiently smaller than the wavelength. When the dust grain size is larger than the wavelength, the scattering coefficient is set to zero because forward scattering dominates in that case.

The steady-state disk structure is solved self-consistently as a function of the mass accretion rate. Although density, viscosity, and temperature are related to one another, they are numerically obtained consistently by iterative calculations.

2.2. Dust Abundance and Opacity

Only dust particles suspended in the disk are considered to be the opacity source because the gas opacity is negligibly small. Two kinds of dust particles, silicate and pure water ice particles, are assumed to be present separately. Effects of icy mantles on silicate cores will be discussed in Section 5.2. It is assumed that dust particles are uniformly sized spheres and mass ratios of the silicate and ice particles to the gas are constant throughout the disk. Radial transport, vertical mixing, and sedimentation of dust particles are neglected. Also, complete thermal coupling between dust particles and gas is assumed; this is valid in the disk considered in this study (Kamp & Dullemond 2004).

Absorption and scattering coefficients of dust particles and mass ratios to the gas are taken from Miyake & Nakagawa (1993); silicate and (maximum) ice mass ratios to the gas are \(\xi_{\text{sil}} = 0.0043\) and \(\xi_{\text{ice}} = 0.0094\), respectively, which are consistent with the solar elemental abundance given by Anders & Grevesse (1989). With this water ice abundance and the mean molecular weight of 2.3, the H_2O mole fraction in the disk gas becomes \(1.2 \times 10^{-3}\). Figure 1 shows the absorption and scattering coefficients of a unit mass disk medium.

The ice abundance in the disk gas is determined with the thermal equilibrium condition under which the partial pressure...
The black and gray curves show the results with and without ice opacity. The solid circle and the solid square on each curve show the height of \(H_s\); the lower part shows the vertical profile of the ice-condensing ratio. The solid and dotted curves show the results with and without scattering by dust particles, respectively. The horizontal axis represents the height from the midplane normalized by the heliocentric distance. In each panel, the upper part shows the temperature profile and the disk gas, \(x\). Then, the mass ratio of ice to the total water molecules in the disk medium, \(\kappa\), is given by

\[
P_{\text{H}_2\text{O}} = X_{\text{H}_2\text{O}}P. \tag{3}
\]

The water vapor mole fraction \(X_{\text{H}_2\text{O}}\) is limited to \(1.2 \times 10^{-3}\), so excess water molecules condense as water ice. Thus, \(X_{\text{H}_2\text{O}}\) is given by

\[
X_{\text{H}_2\text{O}} = \begin{cases} 
1.2 \times 10^{-3} & \text{if } P \leq \text{P_{sat}(T)} \text{ or } \text{P}_{\text{sat}(T)} / P \leq 1, \\
\text{P}_{\text{sat}(T)} / P & \text{if } P > \text{P}_{\text{sat}(T)}. \end{cases} \tag{4}
\]

Then, the mass ratio of ice to the total water molecules in the disk gas, \(x_{\text{ice}}\), is given by

\[
x_{\text{ice}} = 1 - X_{\text{H}_2\text{O}}/(1.2 \times 10^{-3}). \tag{5}
\]

Using \(x_{\text{ice}}\), the absorption and scattering coefficients of the disk medium, \(\kappa_{\text{abs}}\) and \(\kappa_{\text{sca}}\), are given as

\[
\kappa_{\text{abs}} = \kappa_{\text{sil},\text{abs}} + x_{\text{ice}}\kappa_{\text{ice},\text{abs}}, \tag{6}
\]

\[
\kappa_{\text{sca}} = \kappa_{\text{sil},\text{sca}} + x_{\text{ice}}\kappa_{\text{ice},\text{sca}}, \tag{7}
\]

where \(\kappa_{\text{sil},\text{abs}}, \kappa_{\text{sil},\text{sca}}, \kappa_{\text{ice},\text{abs}},\) and \(\kappa_{\text{ice},\text{sca}}\) represent the absorption and scattering coefficients of the disk medium attributed to silicate and ice dust particles, respectively. Equations (6) and (7) are solved consistently by iterative calculations.

3. RESULTS

3.1. Effects of Water Ice Opacity

Numerical results shown in this subsection are obtained by calculations with the following input parameters: \(T_{\text{eff}} = 3000\ \text{K}, R_* = 2\ R_\odot,\) and \(M_* = 0.5\ M_\odot\). The dust grain size is \(0.1\ \mu\text{m}\).

3.1.1. Disk Structure

Figures 2 and 3 show vertical temperature profiles at various heliocentric distances. The mass accretion rate is fixed to be \(10^{-8} M_\odot\ \text{yr}^{-1}\). Other parameters are \(M_* = 0.5\ M_\odot, R_* = 2\ R_\odot, T_{\text{eff}} = 3000\ \text{K},\) and \(\alpha = 0.01;\) the dust grain size is \(0.1\ \mu\text{m}\). Panels (a)–(d) show the profiles at the heliocentric distances of 0.5, 1, 2, and 4 AU, respectively. The black and gray curves show the results with and without ice opacity. The solid circle and the solid square on each curve show the height of \(H_s\) and the pressure scale height, respectively.

of water vapor is limited by the saturated vapor pressure (Bauer et al. 1997):

\[
P_{\text{sat}}(T) = \exp(-6070\ \text{K}/T + 30.86)\ \text{dyn cm}^{-2}. \tag{2}
\]

The partial pressure of water vapor \(P_{\text{H}_2\text{O}}\) is given approximately by the product of the water vapor mole fraction \(X_{\text{H}_2\text{O}}\) and the total gas pressure:

\[
X_{\text{H}_2\text{O}} = 1 \left(1 - \frac{X_{\text{H}_2\text{O}}}{1.2 \times 10^{-3}}\right). \tag{5}
\]

Using \(x_{\text{ice}}\), the absorption and scattering coefficients of the disk medium, \(\kappa_{\text{abs}}\) and \(\kappa_{\text{sca}}\), are given as

\[
\kappa_{\text{abs}} = \kappa_{\text{sil},\text{abs}} + x_{\text{ice}}\kappa_{\text{ice},\text{abs}}, \tag{6}
\]

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\]

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height from the midplane where the incident stellar radiation energy flux is reduced by a factor of \(e\).

The disk temperature is altered only a little by considering dust scattering, because a single scattering albedo dust particles of size \(0.1\ \mu\text{m}\) is small. Though small, the midplane temperature is increased slightly when viscous heating is dominant (Figure 2); the scattering by dust particles enhances the optical depth in the disk and increases the blanket effect. On the other hand, the midplane temperature is lowered slightly when stellar irradiation is the dominant heating source (Figure 3), since a large fraction of incident radiation is reflected toward space (Dullemond & Natta 2003; Inoue et al. 2009).

3.1.2. Evolution of the Ice-Condensing Region

Figure 4 shows the ice-condensing region in the \((R, Z)\) sectional plane with various mass accretion rates.\(^1\) A decrease in the mass accretion rate can be regarded as the time evolution of the disk.

When \(\dot{M}\) is high \((\geq 10^{-9} \ M_\odot \ \text{yr}^{-1})\), the condensation front has a two-branched structure, as found by Cassen (1994) and Davis (2005). The condensation front in the upper layer extends closer to the central star than to the snow line (hereafter, the snow line is defined as the condensation front at the midplane) irrespective of the presence of ice. The lower branch of the condensation front is formed by a high temperature caused by viscous dissipation, while the upper branch is formed by a high temperature caused by direct stellar radiation and a low partial pressure of water vapor. The snow line shifts outward by a factor of 1.3 due to the ice opacity independent of the mass accretion rate.

On the other hand, when \(\dot{M}\) is low \((\leq 10^{-10} \ M_\odot \ \text{yr}^{-1})\), the condensation front is a smooth curve and the snow line location is not shifted significantly by the ice opacity. This can be attributed to two reasons: when the disk is mainly heated by stellar irradiation (1) the midplane temperature does not depend so much on the opacity of the disk medium and (2) icy dust particles do not condense in the upper layer above the snow line due to the temperature increasing with height.

3.1.3. Evolution of the Snow Line

Figure 5 shows the snow line locations obtained with and without ice opacity as a function of the mass accretion rate. In both cases, the snow line migrates inward when \(\dot{M}\) is high \((\geq 10^{-9} \ M_\odot \ \text{yr}^{-1})\) and outward when \(\dot{M}\) is low \((\leq 10^{-10} \ M_\odot \ \text{yr}^{-1})\). An inward migration is caused by the decrease of the midplane temperature due to the reduction of viscous heating and the decrease of the blanket effect. The inward migration ceases when stellar irradiation starts to dominate the heating around the midplane. Then, an outward migration is started by the decrease in the disk’s optical thickness, which results in a higher temperature due to a deeper penetration of the stellar radiation into the disk interior. The snow line in this study migrates outward more slowly than the results of Garaud & Lin (2007) (see Section 3.3).

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\(^1\) The flaring index \(\xi\) is chosen to be zero at small heliocentric distances \((R \lesssim 4\ \text{AU})\) for \(\dot{M} \geq 4 \times 10^{-9} \ M_\odot \ \text{yr}^{-1}\) because the grazing angle in an inner region becomes negative due to the high temperature caused by viscous heating, and the grazing angle recipe becomes invalid. Though this operation is artificial, the disk structure around the midplane is not affected significantly by the operation due to the fact that the dominant heating source around the midplane is viscous dissipation. This operation is also done if the grazing angle becomes negative in the other calculations in this study.
Figure 4. Ice-condensing region in the disk as a function of the mass accretion rate. Parameters are $M_\ast = 0.5 \, M_\odot$, $R_\ast = 2 \, R_\odot$, $T_{\text{eff}} = 3000$ K, and $\alpha = 0.01$; the dust grain size is 0.1 $\mu$m. Panels (a)–(f) show the ice-condensing regions with $\dot{M}$ labeled in each pane. The horizontal and vertical axes represent the distance from the central star on the midplane and the altitude from the midplane, respectively. The blue and light blue regions represent the ice-condensing regions with and without ice opacity. The black, red, and green curves represent the condensation front, the altitude of $H_s$, and the pressure scale height, respectively. The solid and dotted curves with each color represent the results with and without ice opacity, respectively. (A color version of this figure is available in the online journal.)

Figure 5. Heliocentric distance of the snow line as a function of the mass accretion rate. Parameters are $M_\ast = 0.5 \, M_\odot$, $R_\ast = 2 \, R_\odot$, $T_{\text{eff}} = 3000$ K, and $\alpha = 0.01$; the dust grain size is 0.1 $\mu$m. The horizontal and vertical axes represent the mass accretion rate and the snow line location, respectively. The solid and dashed curves represent the results with and without ice opacity, respectively.

When $\dot{M}$ is high ($\gtrsim 10^{-10} \, M_\odot$ yr$^{-1}$), the ratio of the snow line distance with ice opacity ($R_{\text{SL,sil+ice}}$) to that without ice opacity ($R_{\text{SL,sil}}$), $f_{\text{SL}} = R_{\text{SL,sil+ice}} / R_{\text{SL,sil}}$, is about 1.3 and almost constant. This constant ratio of the snow line shift factor $f_{\text{SL}}$ originates from the assumptions that the disk is the steady accretion disk and the mass fraction of ice dust particles to silicate dust particles is uniform throughout the disk (see Section 4.1). On the other hand, when $\dot{M}$ is low ($\lesssim 10^{-10} \, M_\odot$ yr$^{-1}$), the snow line location is not substantially affected by ice opacity (i.e., $f_{\text{SL}} \simeq 1$). This small difference in snow line location is caused by a small difference in the disk structure around the snow line.

3.2. Dependence of Snow Line Location on Dust Grain Size

The stellar parameters in this subsection are set as $L_\ast = 1 \, L_\odot$, $M_\ast = 1 \, M_\odot$, and $T_{\text{eff}} = 4000$ K for comparison with the solar system. Figure 6 shows the heliocentric distance of the snow line as a function of the mass accretion rate. The different curves correspond to the different dust grain sizes assumed in each calculation. Calculations are stopped when the optical depth for stellar radiation in the region around the snow line becomes less than unity. When the grain size is $\gtrsim 100$ $\mu$m, the scattering coefficient is set to zero.

During the inward migration of the snow line, the snow line location is almost independent of the dust grain size if the grain
size is smaller than 10 \( \mu m \). The wavelength of radiation from the disk interior at the condensation temperature \((T \approx 170 \, K)\) is longer than 10 \( \mu m \), so the opacity of the dust particle is in the Rayleigh regime, dependent only on the total mass of the dust particles, and dominated by absorption. On the other hand, when the size is larger than 10 \( \mu m \), i.e., in the geometrical optics regime, the opacity depends on the total cross section of the dust particles and decreases with the dust grain size; hence, the temperature enhancement by viscous heating becomes inefficient, although both absorption and scattering contribute in this case.

When the dust grain size is larger than 10 \( \mu m \), the evolutionary track of the snow line levels off at the minimum value, because the opacity of large grains is almost independent of the wavelength emitted from the disk. This implies that the snow line necessarily passes the heliocentric distance of 1 AU, unless the dust grain size exceeds a certain large value. This point will be considered in Section 4.4.

The shift ratio of the snow line \( f_{SL} \) is qualitatively the same as in Figure 5. The snow line shifts to a larger heliocentric distance in its inward migration phase, whereas it does not shift substantially in its outward migration and leveling-off phases.

The shift ratio of the snow line \( f_{SL} \) depends on the dust grain size: \( f_{SL} \simeq 1.3 \) for dust grain sizes \( \lesssim 10 \, \mu m \), and \( f_{SL} \simeq 1.6 \) for grain sizes \( \gtrsim 100 \, \mu m \). When the dust grain size is small, the total dust opacity increases in proportion to the total mass of the dust, while the total dust opacity increases in proportion to the total cross section of dust particles when the dust grain size is large. This different dependence of the opacity on the total amount of dust causes the different dependence of the shift ratio.

The critical mass accretion rate, that is the mass accretion rate with which the snow line starts to migrate outward, also depends on dust grain size. The snow line starts to migrate outward when the disk region around the snow line becomes transparent. When the dust grain size is sufficiently larger than the wavelength of the stellar radiation (~1 \( \mu m \)), the total opacity of the dust is inversely proportional to the grain size. Thus, the critical mass accretion rate is proportional to the dust grain size. Indeed, when the dust grain size is 10 \( \mu m \), 100 \( \mu m \), and 1 mm, the snow line starts to migrate outward at about \( 10^{-11} \, M_\odot \, yr^{-1} \), \( 10^{-10} \, M_\odot \, yr^{-1} \), and \( 10^{-9} \, M_\odot \, yr^{-1} \), respectively (Figure 6).

3.3. Comparison with Garaud & Lin (2007)

The snow line evolution obtained from our numerical simulations is compared with that obtained from the semi-analytical model of Garaud & Lin (2007). The stellar parameters are \( L_*=1 \, M_\odot \), \( R_*=1 \, R_\odot \), and \( \alpha=0.01 \). Other settings are almost the same as in Garaud & Lin (2007).

Garaud & Lin (2007) used the Planck mean opacity; thus, a new frequency-dependent opacity model of the mixture of disk gas and dust particles is developed so that its Planck mean agrees with that of Garaud & Lin (2007). The Planck mean opacity is proportional to temperature, so the absorption opacity is modeled as a linear function of frequency: \( \kappa_{abs} = C \nu \), where \( C \) is a constant determined by

\[
\frac{\int_0^\infty \kappa_{abs} \nu B_\nu(T_{eff}) \, d\nu}{\int_0^\infty B_\nu(T_{eff}) \, d\nu} = \kappa_V, \tag{8}
\]

where \( \kappa_V \) is the Planck mean opacity with the stellar effective temperature, and \( \kappa_V \) is set to be 2 cm\(^2\) g\(^{-1}\) according to Garaud & Lin (2007).

The snow line location calculated as a function of \( M \) is shown in Figure 7, as is the result of Garaud & Lin (2007). Our result agrees well with that of Garaud & Lin (2007) for higher \( M (>10^{-9} \, M_\odot \, yr^{-1}) \), though our result does not show an abrupt outward shift of the snow line at \( M \sim 10^{-9.5} \, M_\odot \, yr^{-1} \). Garaud & Lin (2007) adopted a semi-analytical method to solve the temperature in the optically thin region. Although semi-analytical methods are much easier to use than numerical models, they may not be accurate enough for the evaluation of the disk midplane temperature in optically thin regions. (They are accurate enough and useful in optically thick regions.) The discontinuous evolution found by Garaud & Lin (2007) may come from the simplified treatment of the radiative transfer. Hereafter, the discontinuity is ignored and the overall features of the snow line evolution are discussed.

In order to obtain the midplane temperature, the estimation of the height of the superheated layer \( H_s \) is a key factor, because its radial dependence determines the grazing angle of the disk.
for irradiation. When the midplane temperature in a region is increased, the surface density there is lowered according to the steady accretion assumption (Equation (1)). Then, the grazing angle decreases, the midplane temperature tends to fall, and the surface density tends to increase: a negative feedback takes place. Therefore, in our calculations, the disk does not become optically so thin and the snow line migrates outward more slowly than in the result of Garaud & Lin (2007), in which $\alpha$ is assumed to be proportional to the disk pressure scale height.

The minimum heliocentric distance of the snow line obtained from our calculations is slightly smaller than that of Garaud & Lin (2007). This may be attributed to the two-layer model (Chiang & Goldreich 1997) they adopted. Inoue et al. (2009) showed that the three-layer approach is necessary to obtain an accurate midplane temperature.

Figures 8 and 9 show the midplane temperature and the surface density profiles from our calculation and from Garaud & Lin (2007). These figures clearly show that the midplane temperatures of both models agree well in the inner optically thick region, whereas our result is lower than that of Garaud & Lin (2007) in the outer optically thin region. Similarly, the surface density distributions in both models agree in the inner region, whereas there is a difference in the outer region.

We conclude that if we are concerned with the detailed evolution of the snow line in the optically thin phases in which planet formation may proceed, we need to calculate the temperature numerically. (If we are concerned with optically thick phases or qualitative features of the snow line evolution in entire phases, semi-analytical calculations are sufficient.)

4. SEMI-ANALYTICAL ESTIMATES

4.1. Dependence on Water Ice Opacity

In the early phase in which the snow line migrates inward, the main heating source at the midplane around the snow line is viscous dissipation (Figure 2). Thus, the temperature is determined by viscous heating and radiative cooling. The diffusive radiative energy transfer gives the midplane temperature, $T_c$, as (e.g., Nakamoto & Nakagawa 1994)

$$T_c = \left[ \frac{3}{2} + \frac{9}{16} \frac{G M_* \dot{M}}{4 \pi \sigma R^3} \right]^{1/2},$$

(9)

where $\tau_c$ is the optical depth for the midplane and $\sigma$ is the Stefan–Boltzmann constant. Substituting $\tau_c = \kappa \Sigma/2$ ($\kappa$ is the Rosseland mean opacity of the disk medium) and noticing that $\tau_c$ is much larger than unity, we obtain

$$T_c \simeq \left[ \left( \frac{9 \kappa \Sigma}{32} \right) \left( \frac{G M_* \dot{M}}{4 \pi \sigma R^3} \right) \right]^{1/2} \propto \left( \frac{\kappa \Sigma}{R^3} \right)^{1/2}. \quad (10)$$

The surface density of the steady accretion disk is given by

$$\Sigma = M/(3 \pi a c_s^2/\Omega) \propto 1/(T_c R^3/2).$$

So, we have

$$T_c^2 \propto \kappa R^{-3/2}. \quad (11)$$

In the annulus located at the snow line, both silicate and ice particles contribute to the opacity $\kappa$ (see Figure 4). This Rosseland mean opacity is denoted as $\kappa_{\text{sil+ice}}$, whereas the Rosseland mean opacity due to silicate particles only is expressed as $\kappa_{\text{sil}}$. Since the ice condensation temperature at the midplane is almost independent of the heliocentric distance, the right-hand side of Equation (11) can be regarded as constant, and a relation between the snow line locations with and without water ice opacity, $R_{\text{SL,\,sil+ice}}$ and $R_{\text{SL,\,sil}}$, is obtained as

$$\kappa_{\text{sil+ice}} R_{\text{SL,\,sil+ice}}^{-3/2} = \kappa_{\text{sil}} R_{\text{SL,\,sil}}^{-3/2}. \quad (12)$$

The shift factor of the snow line location due to the additional ice is then written as

$$f_{\text{SL}} = \frac{R_{\text{SL,\,sil+ice}}}{R_{\text{SL,\,sil}}} = \left( \frac{\kappa_{\text{sil+ice}}}{\kappa_{\text{sil}}} \right)^{3/2}. \quad (13)$$

Adopting the dust opacity model of Miyake & Nakagawa (1993), we have $\kappa_{\text{sil+ice}}/\kappa_{\text{sil}} \simeq 3$ for the thermal radiation at 170 K (the midplane temperature at the snow line) when the dust grain size is 0.1 $\mu$m. Then, $f_{\text{SL}}$ is evaluated as $f_{\text{SL}} = 3^{3/2} = 1.28$, which is consistent with our numerical results. Equation (13) implies that the snow line location is shifted outward in accordance with the water abundance around the snow line.

4.2. Dependence on Viscosity Parameter

The snow line location is considerably affected by $\alpha$, because $\alpha$ relates to the disk’s optical thickness and energy generation.
rate by viscous dissipation. In the early phase of the disk evolution, the midplane temperature in the inner disk region is obtained in the same way as in Section 4.1. Then, we have $T^* \propto \alpha^{-1} R^{-9/2}$. We then find the dependence of the snow line location $R_{\text{snow}}$ on $\alpha$ as

$$R_{\text{snow}} \propto \alpha^{-\frac{1}{3}}. \quad (14)$$

Taking into account the range of $\alpha$ ($0.001 \lesssim \alpha \lesssim 0.1$), the snow line location shifts inward or outward by at most 67% from the results with $\alpha = 0.01$ in the inward migration phase. Note that the minimum heliocentric distance of the snow line hardly changes, because it is determined not by viscous heating but by stellar radiation heating.

In the later phase of the disk evolution, a change in $\alpha$ changes the correlation between $R_{\text{snow}}$ and $M$. In the outward migration phase, $R_{\text{snow}}$ is a function of $\zeta$, and $M$ is proportional to the product of $\nu_t$ and $\Sigma$. The viscosity $\nu_t$ is proportional to $\alpha$, so $M$ corresponding to each $R_{\text{snow}}$ varies in proportion to $\alpha$. Thus, $R_{\text{snow}}$ in the later phase is shifted in proportion to $\alpha$ (Figure 6). This means that the $M$ at which the disk becomes optically thin to the stellar radiation also decreases in proportion to $\alpha$.

4.3. Dependence on Dust-to-Gas Mass Ratio

The dust-to-gas mass ratio, $\zeta_{d}$, changes the opacity of the disk medium. Hence, it changes the disk temperature in the same way as ice opacity. In the inward migration phase, assuming that the opacity of the disk medium varies in proportion to $\zeta_{d}$, a proportional relation between $R_{\text{snow}}$ and $\zeta_{d}$ is obtained in the same way as in Sections 4.1 and 4.2:

$$R_{\text{snow}} \propto \zeta_{d}^{\frac{2}{5}}. \quad (15)$$

In the outward migration phase, the correlation between $R_{\text{snow}}$ and $M$ depends on $\zeta_{d}$. In this phase, $R_{\text{snow}}$ is a function of solid mass surface density ($\zeta_{d}\Sigma$), and $M$ is proportional to $\Sigma$, which is the product of solid mass surface density and the inverse of $\zeta_{d}$. Thus, $M$ corresponding to each $R_{\text{snow}}$ varies in inverse proportion to $\zeta_{d}$. Hence, $R_{\text{snow}}$ is shifted in inverse proportion to $\zeta_{d}$ (Figure 6). The mass accretion rate with which the disk becomes optically thin to the stellar radiation increases in inverse proportion to $\zeta_{d}$.

4.4. Possibility of the Snow Line Coming Inside Earth’s Orbit

According to the results shown in Section 3, the snow line comes inside the Earth’s current orbit in the course of the disk evolution. However, if planetesimals in the terrestrial planet region were icy, this is not consistent with current solar system bodies. Here, discussing the snow line evolution track on the $(M, R_{\text{snow}})$-plane in Figure 6, we examine to what extent that conclusion is certain.

From Figure 6, we can see that if $(\alpha/\zeta_{d})$ is increased by more than a factor of 100 and if the dust grain size is 1 mm, the snow line would not come inside Earth’s orbit. However, there are some caveats. Noticing that the range of $\alpha$ is from 0.001 to 0.1 and the fiducial value used in our calculations is $\alpha = 0.01$, we realize that $\zeta_{d}$ should be decreased by a factor of at least 10 from the value found by Miyake & Nakagawa (1993) to increase the value of $(\alpha/\zeta_{d})$ by more than a factor of 100. When $\alpha < 0.1$, $\zeta_{d}$ should be much smaller depending on the size of $\alpha$. On the other hand, as the dust grain size becomes small, $(\alpha/\zeta_{d})$ should be large (or $\zeta_{sil}$ should be small). Thus, it seems that the snow line necessarily comes inside Earth’s orbit if the dust grain size is smaller than 1 mm, $\zeta_{d}$ is higher than a tenth of that of the solar abundance, and $\alpha$ ranges from 0.001 to 0.1.

Another possibility is an increase in ice abundance; this can prevent the snow line from coming inside Earth’s orbit. An increase in ice abundance lowers the value of $M$ at which the snow line migration levels off at the minimum distance or starts to move outward. For example, if the ratio of water ice mass to disk gas, $\zeta_{\text{ice}}$, is increased by a factor of $10^4$, it is expected that the snow line would not come inside Earth’s orbit even in the case in which $\alpha = 0.01$, the dust grain size is 1 mm, and $\zeta_{sil} = 0.0043$ (the solar abundance). When the dominant dust grain size or $(\alpha/\zeta_{d})$ is small, a greater increase in ice abundance is needed.

5. DISCUSSION

5.1. Comparison with the Current Solar System

In our solar system, the water distribution shows a drastic change at the asteroid belt; this may be a clue to the snow line. Terrestrial planets are thought to form from planetesimals that have formed inside the snow line, otherwise a large amount of water is inevitably accumulated into planets. Then, the timing of planetesimal formation may be restricted by the snow line evolution.

First, we consider the possibility that planetesimals form after the snow line migrates outward from the terrestrial planet region. When we look at the solid mass, planetesimal formation with dust grains of large size is favored because the gas surface density at which the snow line changes its direction of motion and moves outward increases as the dust grain size increases (Figure 6). The most favorable case from our numerical results is for dust grains of size 1 mm. Our numerical simulation shows that the surface density of solid material at the heliocentric distance of 1 AU is $1.1 \times 10^{-2}$ g cm$^{-2}$ when the outwardly moving snow line reaches 1 AU. This is much smaller than that of the minimum mass solar nebula model (about 10 g cm$^{-2}$). To match the minimum mass solar nebula model, or to match the current terrestrial planet’s mass, the size of the dust particles would necessarily be larger than 1 m. This would be unrealistic, partly because complete depletion of fine dust particles smaller than 1 m would be difficult, and partly because dust particles of size 1 m are eliminated efficiently by accretion toward the central star due to gas drag. Thus, planetesimal formation during the snow line’s outward migration would be unrealistic.

Next, let us consider the possibility of planetesimal formation during the snow line’s inward migration. If planetesimal formation completes before the inwardly migrating snow line reaches the terrestrial planet region, planetesimals devoid of water can be formed. As for the solid mass, planetesimal formation in this phase is favorable. However, as the grain size grows, the snow line quickly migrates inward and eventually comes inside Earth’s orbit; in Figure 6, at a fixed $M$, we can see that $R_{\text{snow}}$ is small if the grain size is large. Hence, the dust grain growth and planetesimal formation should be completed in a short period of time compared to the timescale with which the snow line moves inward. If not, a large amount of ice would necessarily accumulate deep within planetesimals. We are not sure if planetesimal formation is completed in such a short period of time.

In conclusion, the snow line location during disk evolution does not seem to match the current solar system. This inconsistency may originate from the following assumptions adopted in this study: (1) the continuous boundary condition at the inner
disk edge, (2) uniform dust grain size and uniform dust-to-gas mass ratio throughout the disk, and (3) neglecting the evolution of solid material and water distribution.

Here, we consider possible scenarios by relaxing the above assumptions.

1. Continuous disk boundary. The presence of the inner disk edge, where the disk is heated by direct stellar radiation and becomes hot, is ignored in this assumption. If the dust grain grows at the inner edge and the inner edge moves outward after planetesimal formation, dust grain growth would always proceed in a hot environment. Then the resulting planetesimals would be devoid of water.

2. Uniform dust grain size and dust-to-gas mass ratio. In a real disk, the dust grain size and the dust-to-gas mass ratio would be non-uniform. Dust particles grow mainly by collisions. Growth tends to proceed from the inner disk region, so the dust grain size in the inner disk is likely to be larger than that in the outer disk. When the dust grain is large enough, the height of the disk surface is lowered. Consequently, a disk region that is located just outside the dust grain region developed when dust grain growth is about to start can receive more stellar radiation flux. Then, dust grain growth may proceed at a hot temperature and water-deficit planetesimals may form.

3. Solid material and water distribution evolution. According to Ciesla & Cuzzi (2006) and Garaud (2007), large amounts of water vapor and fine dust particles are transported from the outer to the inner part of the disk during disk evolution. If fine dust particles or water vapor are supplied to the terrestrial planet region, and the snow line location is kept farther from the terrestrial planet region until planetesimal formation is completed, dust grain growth may proceed in a water-ice-free environment; consequently, water-deficit planetesimals may be formed. Whether or not this mechanism works may depend on the initial condition of the disk.

Yet another possible scenario may be the elimination of water from icy planetesimals after the snow line migrates outward from the terrestrial planet region. Future work on these points is needed.

5.2. Effects of the Ice Mantle on Silicate Dust Particles

In this study, it is assumed that ice condenses as pure ice particles and that no ice mantle forms on silicate particles. It would be more realistic, however, if H$_2$O molecules condense as ice mantles on silicate cores. Here, we discuss how ice mantle formation affects the snow line location. We consider its effects only in the inward migration phase, since ice opacity does not change the snow line location in the outward migration phase.

To evaluate the effects of the ice mantle, we consider to what extent the dust opacity changes due to the ice mantle. Dust opacity properties change as the ratio between the dust grain size and the wavelength of the thermal radiation ($\lambda \sim 10$–$20\mu$m) changes. When the dust grain size is sufficiently smaller than $10$–$20\mu$m (the Rayleigh regime), the total dust opacity is hardly affected by the ice mantle. On the other hand, when the dust grain size is sufficiently larger than $10$–$20\mu$m (the geometrical optics regime), the ice mantle changes the total dust opacity.

When the ice condenses, the opacity of dust particles generally increases. However, the opacity enhancement factor $g_{\text{ice}}$ can be different between cases in which the ice condenses as independent ice particles and those in which the ice condenses as ice mantles on silicate cores, even though the amount of condensed ice is the same. In the geometrical optics regime, $g_{\text{ice}}$ for the mantle case becomes smaller than that for the independent case, since the cross section of ice mantles is smaller than that of the independent particles. According to Miyake & Nakagawa (1993), the material densities of silicate and ice are 3.3 and 0.92 g cm$^{-3}$, respectively, and the mass fractions of silicate and water ice in the disk medium are 0.0043 and 0.0094, respectively. This means that ice has a volume about six times larger than that of silicate per unit mass at disk medium. As a result, if only pure ice particles are formed, the total cross section of the dust particles is increased by a factor of 7.9, while if ice mantles are formed on silicate cores, the total cross section of dust particles is increased only by a factor of 3.7. Thus, ice mantle formation reduces the opacity enhancement factor by ice condensation. Consequently, the snow line’s shift ratio by ice condensation ($f_{\text{SL}}$) would be reduced from 1.54 to 1.33 due to ice mantle formation (see Equation (13)).

Finally, we consider the non-uniformity of the dust grain size. When independent ice particles are formed, the opacity enhancement depends on the size distribution of ice particles. If all the ice particles are sufficiently small compared to the wavelength of the thermal radiation (the Rayleigh regime), the opacity enhancement depends only on the total mass of ice and is largest. When the dominant size of ice particles is larger than $10$–$20\mu$m, and as the dominant size increases, the opacity enhancement decreases. On the other hand, if ice mantles are formed on silicate particles, the opacity enhancement would be limited to a certain range. The real situation should be somewhere between the Rayleigh regime and the geometrical optics regime, so the enhancement of the dust opacity by ice condensation would be around 30%.

In summary, it is likely that the enhancement of the dust opacity would be limited to a range around 30% when ice mantles are formed around silicate dust particles. If pure ice particles are formed, the size distribution of ice particles is needed to evaluate the enhancement accurately.

6. CONCLUSIONS

The evolution of the snow line in an optically thick disk is simulated numerically and examined to see if it is consistent with the water distribution in the solar system. The evolution is examined from the early phase, in which the mass accretion rate in the disk is large and the optical depth of the disk is considerably high, to the later phase, in which the accretion rate is small and the optical depth is low with a single numerical scheme.

The snow line migrates as the mass accretion rate in the disk decreases (which is considered to be the evolution). Generally, in the early phase (high mass accretion phase), it moves inward because of the reduction in viscous heating, while in the later phase (low mass accretion phase), it moves outward due to stellar radiation. If the dust grain size is large ($\gtrsim 10\mu$m), the snow line stays at its minimum heliocentric distance for a wide range of mass accretion rates.

When the opacity of the condensed ice is taken into consideration, we find that the snow line location is shifted outward for the disk in the inward migration phase ($M \gtrsim 10^{-10} M_\odot$ yr$^{-1}$). This is due to the additional blanket effect of the condensed ice particles in the upper layer of the disk. The shift ratio of the snow line ($f_{\text{SL}} = R_{\text{SL,ice+sil}}/R_{\text{SL,sil}}$) varies with dust grain size: $f_{\text{SL}} = 1.3$ for grains $\lesssim 10\mu$m and $f_{\text{SL}} = 1.6$ for grains...
the surface density $\Sigma$ is given as

$$\Sigma = \frac{\int_0^{\infty} \rho \, dZ}{\int_0^{\infty} 1 \, dZ} = \frac{M_\ast}{\int_0^{\infty} 1 \, dZ},$$

where $P$ is the gas pressure and $\rho$ is the mass density of the gas. The equation of the state of the gas is given as

$$P = \rho c_s^2 = \frac{\rho M}{\mu m_w},$$

where $\mu$ is the mean molecular weight, $m_w$ is the atomic mass unit, and $c_s$ is the sound velocity. Integrating the density over $Z$, the surface density $\Sigma$ is given as

$$\Sigma = \int_0^{\infty} \rho \, dZ.$$ 

### A.1. Hydrostatic Equilibrium

The hydrostatic equilibrium along the vertical direction is expressed as

$$\frac{\partial P(R, Z)}{\partial Z} = -\rho(R, Z) \frac{GM_\ast}{R^3} Z,$$  \hspace{1cm} (A1)

where $P$ is the gas pressure and $\rho$ is the mass density of the gas. The equation of the state of the gas is given as

$$P = \rho c_s^2 = \frac{\rho M}{\mu m_w},$$

where $\mu$ is the mean molecular weight, $m_w$ is the atomic mass unit, and $c_s$ is the sound velocity. Integrating the density over $Z$, the surface density $\Sigma$ is given as

$$\Sigma = \int_0^{\infty} \rho \, dZ.$$ 

### A.2. Radiative Transfer

Two heating sources are taken into consideration: viscous dissipation and irradiation of the central star. Balancing the heating sources and the radiative cooling, the following equilibrium temperature is obtained:

$$q_{visc} + q_{irr} + \int_0^{\infty} \rho k_\nu (1 - \sigma_\nu) \, d\nu \oint \mathcal{I}_\nu(\Omega) \, d\Omega = 4\pi \int_0^{\infty} \rho k_\nu (1 - \sigma_\nu) B_\nu(T) \, d\nu,$$  \hspace{1cm} (A2)

where $q_{visc}$ is the heating rate by viscous dissipation, $q_{irr}$ is the heating rate by irradiation of the central star, $k_\nu$ is the extinction coefficient, $\sigma_\nu$ is the single scattering albedo, $I_\nu(\Omega)$ is the diffuse radiation field in the disk (intensity without including the direct radiation from the central star), and $B_\nu(T)$ is the Planck function. Quantities with subscript $\nu$ are a function of frequency $\nu$. The integral $\int \mathcal{I}_\nu(\Omega)$ on the left-hand side of Equation (A2) represents the integral over the entire solid angle.

The viscous heating rate $q_{visc}$ is given by (e.g., D'Alessio et al. 1998)

$$q_{visc} = \frac{q}{L} \rho_{eq} \Sigma_k R^2.$$ 

The diffuse component of the intensity $I_{\mu,\nu}(\Omega)$ and $q_{irr}$ are obtained by solving the radiative transfer. Assuming a plane-parallel structure along the $Z$-direction, the radiative transfer equation is written as

$$\mu \frac{dI_{\mu,\nu}(Z)}{dZ} = \rho k_\nu (S_\nu(Z) - I_{\mu,\nu}(Z)),$$  \hspace{1cm} (A3)

where $\mu$ is the cosine of the propagation direction of radiation and $S_\nu$ is the source function. The source function $S_\nu$ is given by

$$S_\nu(Z) = (1 - \sigma_\nu(Z)) B_\nu(T) + \sigma_\nu(Z) \int_0^{\infty} I_{\mu,\nu}(\Omega) \, d\Omega,$$  \hspace{1cm} (A4)

where $F_{irr,\nu}(Z)$ is the radiation energy flux from the central star. Therefore, isotropic scattering is assumed. The energy flux $F_{irr,\nu}(Z)$ is evaluated using the so-called grazing angle recipe (e.g., Chiang & Goldreich 1997; Dullemen et al. 2002)

$$F_{irr,\nu}(Z) = \frac{L_\nu}{4\pi R^2} \exp \left(- \frac{\tau_\nu(R, Z)}{\beta} \right),$$  \hspace{1cm} (A5)

where $\beta$, $L_\nu$, and $\tau_\nu(R, Z)$ are the cosine of the penetrating angle of the radiation from the central star into the disk surface, the luminosity of the central star, and the optical depth between a point $(R, Z)$ and infinity along the vertical direction $(R, \infty)$, respectively. The optical depth $\tau_\nu$ is defined as

$$\tau_\nu(R, Z) = \int_Z^{\infty} k_\nu \rho(R, Z) dZ.$$ 

The central star is assumed to emit a blackbody radiation with effective temperature $T_{eff}$, so the luminosity is given by

$$L_\nu = 4\pi R^2 B_\nu(T_{eff}).$$ 

The boundary condition for Equation (A3) is

$$I_{\mu,\nu}(+\infty) = 0 \hspace{1cm} (\mu < 0),$$  \hspace{1cm} (A6)
\[ I_{\mu,\nu}(0) = I_{-\mu,\nu}(0) \quad (\mu \geq 0). \] (A9)

This condition represents the mirror boundary at the \( Z = 0 \) plane and no incident diffuse radiation at the disk surface.

Vertical profiles of the diffuse radiation \( I_{\mu,\nu}(\Omega) \) and the temperature \( T \) are obtained by solving Equations (A2)–(A4) iteratively. A straightforward way to solve these equations converges very slowly, so the variable Eddington factor (VEF) method, described in Dullemond et al. (2002) and Inoue et al. (2009), is employed. In this study, the VEF method is modified to deal with the heating by viscous dissipation.

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