Many planets orbit within 1 au of their stars, raising questions about their origins. Particularly puzzling are the planets found near the silicate sublimation front. We investigate conditions near the front in the protostellar disk around a young intermediate-mass star, using the first global 3D radiation nonideal MHD simulations in this context. We treat the starlight heating; the silicate grains’ sublimation and deposition at the local, time-varying temperature and density; temperature-dependent ohmic dissipation; and various initial magnetic fields. The results show magnetorotational turbulence around the sublimation front at 0.5 au. The disk interior to 0.8 au is turbulent, with velocities exceeding 10% of the sound speed. Beyond 0.8 au is the dead zone, cooler than 1000 K and with turbulence orders of magnitude weaker. A local pressure maximum just inside the dead zone concentrates solid particles, favoring their growth. Over many orbits, a vortex develops at the dead zone’s inner edge, increasing the disk’s thickness locally by around 10%. We synthetically observe the results using Monte Carlo transfer calculations, finding that the sublimation front is near-infrared bright. The models with net vertical magnetic fields develop extended, magnetically supported atmospheres that reprocess extra starlight, raising the near-infrared flux 20%. The vortex throws a nonaxisymmetric shadow on the outer disk. At wavelengths $>2 \mu m$, the flux varies several percent on monthly timescales. The variations are more regular when the vortex is present. The vortex is directly visible as an arc at ultraviolet through near-infrared wavelengths, given sub-au spatial resolution.

**Key words:** accretion, accretion disks – magnetohydrodynamics (MHD) – protoplanetary disks – radiative transfer

1. Introduction and Motivation

Our grasp of planetary systems’ origins relies on our understanding of the disks of gas and dust found orbiting young stars. Here we focus on the environment for planet formation in the disks’ hot central region, where temperatures exceed 1000 K. Among the main processes governing the temperatures in this region are the sublimation and deposition of silicate grains, which change the opacity by orders of magnitude (Pollack et al. 1994). Since the starlight is a major source of heating, the opacity has a major impact on temperatures.

A key process governing the turbulent stirring of the planet-forming materials is magnetorotational instability (Balbus & Hawley 1991). Magnetic fields are coupled to the plasma, and the instability converts gravitational potential energy into the kinetic and magnetic energy of turbulence (Gammie 1996; Jin 1996; Miller & Stone 2000; Hirose & Turner 2011), when temperatures are high enough for thermal ionization (Umebayashi & Nakano 1988; Desch & Turner 2015). The decline in temperature with distance from the star thus leads to a decline in the magnetic stresses across the thermal ionization threshold. This means that the surface density increases across the threshold if the inflow is in steady state, so that the mass flow rate is independent of distance. The resulting local pressure maximum can concentrate solid particles in the size range where their stopping time due to gas drag is comparable to the orbital period (Haghighipour & Boss 2003; Lyra et al. 2008; Kretke et al. 2009; Dzyurkevich et al. 2010; Lyra & Mac Low 2012; Faure et al. 2015), possibly allowing for in situ planet formation (Chatterjee & Tan 2014).

In addition, the pressure maximum can act as a planet trap: young planets’ inward migration under their tidal interaction with the disk comes to a halt near the pressure peak (Masset et al. 2006; Matsumura et al. 2009; Kretke & Lin 2012; Bitsch et al. 2014; Hu et al. 2016). Concentrating both pebbles and protoplanets in a region where dynamical timescales are short has the potential to lead quickly to the growth of planets.

Of all young stars, perhaps the best suited for measuring the disks’ hot central regions are the Herbig stars, which have masses a few times the Sun’s. Nearby examples are bright enough to be observed with near-infrared (NIR) interferometry down to the angular scale of the disk’s inner rim (Dullemond & Monnier 2010; Kraus 2015), yielding maps of the silicate sublimation front (Benisty et al. 2011). However, these objects’ spectra show puzzlingly large NIR fluxes (Hillenbrand et al. 1992; Chiang et al. 2001; Meeus et al. 2001; Millan-Gabet et al. 2001; Vinković et al. 2006). Radiation hydrostatic (Mulders & Dominik 2012) and radiation hydrodynamic models (Flock et al. 2016) produce too little flux at wavelengths 2–4 $\mu m$ by factors up to several. Ingredients modelers must consider include the transfer of the starlight into the disk and the escape of the reradiated infrared emission, the sublimation and deposition of the dust grains that provide most of the opacity, and the forces supporting the disk material against the star’s gravity (Kama et al. 2009). Models can yield NIR excesses closer to the observed range if some disk material near the sublimation front is either launched into a wind (Bans & Königl 2012) or supported on the magnetic fields escaping from magnetorotational instability (MRI) turbulence within the disk (Turner et al. 2014a). In both pictures, the magnetic forces lift some material above its hydrostatic position, increasing the height where the starlight is absorbed, so that a bigger fraction...
of the stellar luminosity is reprocessed into thermal emission at distances where the emission comes out at NIR wavelengths. Until now, there was no global modeling of magnetorotational turbulence at the inner rim, treating the dust sublimation and radiation transfer together with the MHD.

In this work we present the first 3D radiation nonideal MHD simulations of protostellar disks to include starlight heating, silicate grains’ sublimation and deposition at the local temperature and density, and ohmic dissipation depending on the thermal ionization. We test the results against various observational constraints, comparing the spectral energy distributions (SEDs), images, and light curves at different wavelengths. The models let us address several important questions: How does the MHD turbulence affect the sublimation front? What are the consequences for the starlight-absorbing surface, the system’s NIR emission, and its time variability? And what controls the dynamics at the location where the solids are concentrated?

We describe in Section 2 the radiation MHD methods and the treatment of the dust sublimation and deposition. Section 3 deals with the results of the calculations, and Section 4 with the comparison against observations. We discuss the implications in Section 5 and summarize our conclusions in Section 6.

2. Methods and Setup

In this section we briefly summarize the method and the setup of the 3D radiation nonideal MHD simulations. The relevant equations are given in Section 2.1. The resistivity module that determines the magnetic field coupling parameter is presented in Section 2.2. The initial and boundary conditions are presented in Sections 2.3 and 2.4. For full details of the radiation transfer and the dust evaporation modules, we refer the reader to our previous works (Flock et al. 2013, 2016).

2.1. Radiation Nonideal MHD Equations

In this paper, we solve the following radiation nonideal MHD equations in a spherical coordinate system (r, \( \theta \), \( \phi \)):

\[
\frac{\partial \rho}{\partial t} + \nabla \cdot [\rho \mathbf{v}] = 0, \tag{1}
\]

\[
\frac{\partial \rho \mathbf{v}}{\partial t} + \nabla \cdot [\rho \mathbf{v} \mathbf{v} + \mathbf{B} \mathbf{B}^T] + \nabla P_g = -\rho \nabla \Phi, \tag{2}
\]

\[
\frac{\partial E}{\partial t} + \nabla \cdot [(E + P) \mathbf{v} - (\mathbf{v} \times \mathbf{B}) \mathbf{B}] = -\rho \nabla \Phi \mathbf{v} - \nabla \cdot F_g - \kappa_T \rho c(a_T T^4 - E_R) - \nabla \cdot [(\eta \times \mathbf{J}) \times \mathbf{B}], \tag{3}
\]

\[
\frac{\partial E_R}{\partial t} - \nabla \cdot \frac{c \lambda}{\kappa_T \rho} E_R = \kappa_T \rho c(a_T T^4 - E_R), \tag{4}
\]

\[
\frac{\partial \mathbf{B}}{\partial t} - \nabla \times (\mathbf{v} \times \mathbf{B}) = -\nabla \times (\eta \times \mathbf{J}), \tag{5}
\]

where \( \rho \) is the density, \( \mathbf{v} \) is the velocity, and \( \mathbf{B} \) is the magnetic field.\(^4\) \( \mathbf{J} = \nabla \times \mathbf{B} \) is the current density, and \( \eta \) is the tensor magnetic resistivity. The total pressure is given by \( P = P + B^2/2 \), where the gas pressure relates to the temperature \( T \) through

\[
P = \frac{\rho k_B T}{\mu_s u}, \tag{6}
\]

where \( \mu_s \) is the mean molecular weight, \( k_B \) is the Boltzmann constant, and \( u \) is the atomic mass unit. \( T \) stands for the temperatures of the gas and dust, which are assumed to be equal thanks to collisional exchange of thermal energy at these high gas densities.

Introducing the gravitational constant \( G \), the gravitational potential is calculated according to

\[
\Phi = G M_* / r, \tag{7}
\]

where \( M_* \) is the stellar mass. \( E \) denotes the total energy and is given by the relation \( E = \rho c + 0.5 \rho \mathbf{v}^2 + 0.5B^2 \), where \( \rho c = P/(\Gamma - 1) \) is the gas internal energy, \( \Gamma \) being the adiabatic index. The radiation energy is denoted \( E_R \), while \( F_g \) stands for the frequency-integrated irradiation flux. \( F_g \) is calculated as

\[
F_g(r) = \left( \frac{R_*}{r} \right)^2 \sigma B T_*^4 e^{-\tau_B}, \tag{8}
\]

with the Stefan–Boltzmann constant \( \sigma \), the stellar surface temperature \( T_* \), and the radius \( R_* \) of the star. The radial optical depth of the irradiation flux \( \tau_B \) is calculated using the opacity at the stellar temperature \( \kappa_T(T_*) = 2100 \text{ cm}^2 \text{ g}^{-1} \); see also Section 2.1 in Flock et al. (2016). \( \kappa_T \) and \( \kappa_p \) are the Rosseland and Planck mean opacities, respectively. Both opacities include gas and dust contributions. The dust opacity is set to \( \kappa_T(T_*) = 700 \text{ cm}^2 \text{ g}^{-1} \), which represents the opacity at the dust sublimation temperature per gram of dust. The gas opacity is set constant to \( 10^{-4} \text{ cm}^2 \text{ g}^{-1} \), which represents the opacity per gram of gas. For more details on the opacities we refer to our previous work (Flock et al. 2016). Finally, \( a_R \) is the radiation constant, and \( c \) stands for the speed of light.

The gas is a mixture of hydrogen and helium with solar abundance (Decampli et al. 1978) so that \( \mu_g = 2.35 \) and \( \Gamma = 1.42 \). For the typical density and temperature we considered, most of the hydrogen is bound in molecular hydrogen.\(^5\) Silicate dust grains are present when the temperature is smaller than a critical temperature noted \( T_{\text{ev}} \), and sublimes otherwise. As in our previous paper (Flock et al. 2016), we follow Pollack et al. (1994) and Isella & Natta (2005) and determine \( T_{\text{ev}} \) according to

\[
T_{\text{ev}} = 2000 K \left( \frac{\rho}{1 \text{ g cm}^{-3}} \right)^{0.0195}. \tag{9}
\]

\( T_{\text{ev}} \) is then used to calculate the local dust density \( \rho_{\text{dust}} \), assuming perfect mixing of dust and gas (see Equation (10) in Flock et al. 2016).

2.2. Resistivity

We implemented a simple treatment of the resistivity in order to model the ionization transition at 1000 K (Umeyayashi

\(^4\) The magnetic field already includes the normalization factor \( 1/\sqrt{4\pi} \).

\(^5\) We have checked that for \( \rho < 10^{-14} \text{ g cm}^{-3} \) and \( T < 1500 \text{ K} \) over 50% of the hydrogen is bound in H$_2$.\)
& Nakano 1988; Desch & Turner 2015). To do so, we set

$$\eta = \frac{c_s^2}{\Omega \text{Re}_m},$$

where the magnetic Reynolds number ($\text{Re}_m$) dependence on the temperature is given by

$$\text{Re}_m = 5 \times 10^4 \left[1 - \tanh \left(\frac{1000 - T}{25}\right)\right].$$

The asymptotic value of the magnetic Reynolds number $\text{Re}_m = 10^5$ is used for temperatures above 1000 K. This upper limit is high enough to obtain sustained MRI turbulence closely resembling the ideal MHD limit (Flock et al. 2012b). For temperatures below 1000 K the Reynolds number decreases and we set the lower limit of the magnetic Reynolds number to $\text{Re}_m^z = 1$. Such a value is low enough to ensure the damping of the MRI inside the dead zone (Elsässer number $\ll 1$).

### 2.3. Initial Conditions

In order to initialize the simulations presented here, we used the final snapshot of the axisymmetric radiation viscous 2.5D$^6$ hydrodynamical simulation RMHD$_1 e^{-8}$ of Flock et al. (2016), for which the flow has reached a steady state characterized by a uniform accretion rate of $M = 10^{-8}$. We refer the reader to Flock et al. (2016) for more details on that particular simulation and only show here the resulting 2D distribution of $\rho$, $\beta_f$, and $T$ in the disk meridional plane (Figure 1). These 2D fields are extended in the azimuthal direction to cover the range [0, 0.4] rad and [0, 1.6] rad for the models RMHD$_{P-4}$ and RMHD$_{P-1, 6}$, respectively.

To trigger the MRI, we investigate two different configurations for the magnetic field geometry at the beginning of the simulations. First, a random zero-net-flux magnetic field is used for the models RMHD$_{P-4}$ and RMHD$_{P-1, 6}$. A snapshot of the initial magnetic field is shown in Figure 1 (bottom panel). For model RMHD$_{P-4, BZ}$, we also added a vertical net-flux magnetic field. In Appendix B, we detail the procedure we used to generate the magnetic vector potential in both cases. The naming convention of the radiation MHD (RMHD) models includes the size of the azimuthal domain given in radians (e.g., $P-4$ for $\Phi_{\text{max}} = 0.4$) and if a vertical magnetic field is included, $BZ$. The model parameters are summarized in Table 1.

### 2.4. Boundary Conditions and Buffer Zones

In the radial direction we use zero-gradient conditions for all variables, while $v_r$ is set to enforce vanishing mass inflow. In the meridional direction we extrapolate the logarithmic density and the temperature in the ghost cells. The ghost cells are a set of additional cells at the domain boundary that provide the boundary values for the integration. For the velocity $v_\theta$ we set a zero-mass-inflow condition. The azimuthal boundaries are periodic. In addition, we use a buffer zone at the radial inner boundary over the radial range [0.3, 0.35] au to avoid effects arising from the presence of the boundary. In this zone we damp the radial and vertical velocities and increase linearly the magnetic resistivity in order to reach a magnetic Reynolds number of 10 at the location of the inner radial boundary. In addition, we used the same modified gravitational potential inside the buffer zone as used in the 2D radiation

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**Table 1**

| Parameter | Value |
|-----------|-------|
| $M$ | $10^{-8} M_\odot \text{ yr}^{-1}$ |
| Stellar parameter | $T_s = 10000 \text{ K}, R_s = 2.5 R_\odot, M_s = 2.5 M_\odot$ |
| Opacity | $\kappa_p(T_s) = 2100 \text{ cm}^2\text{ g}^{-1}$, $\kappa_r(T_s) = 700 \text{ cm}^2\text{ g}^{-1}$ |
| Dust-to-gas mass ratio | $f_0 = 0.01$ |
| Cell aspect ratio | $R \Delta \theta / \Delta R : R \Delta \phi / \Delta R \sim 1.1 : 1.2$ |
| $R_{\text{in}} - R_{\text{out}} : Z / R$ | $0.3 - 3 \text{ au} : \pm 0.36$ |
| $N_x \times N_y$ | $896 \times 128$ |
| RMHD$_{P-4}$ | $\Phi_{\text{max}} = 0.4, N_x = 128, \text{ runtime 300 orbits}$ |
| RMHD$_{P-1, 6}$ | $\Phi_{\text{max}} = 1.6, N_x = 512, \text{ runtime 150 orbits}$ |
| RMHD$_{P-4, BZ}$ | $\Phi_{\text{max}} = 0.4, N_x = 128, \text{ runtime 70 orbits}$ |

---

$^6$ 2.5D represents the use of two dimensions ($r, \theta$) and three components ($r, \theta, \phi$) for the velocity and magnetic field vectors.
hydodynamical simulations (see Appendix E in Flock et al. 2016). This last modification affects the region with $|Z/R| > 0.1$ and $R < 0.35$ au and manifests itself as a layer with temperatures slightly larger than expected (see white zone in Figure 1, third panel). $R$ and $Z$ represent here the cylindrical coordinates. This buffer zone is excluded from the analyses presented below.

### 2.5. Diagnostics

We determine the strength of the turbulence by calculating the stress-to-pressure ratio $\alpha$:

$$\alpha = \frac{\int \rho \left( \frac{T_0}{P} + \frac{M_0}{T} \right) dV}{\int \rho dV} = \frac{\int \rho \left( \frac{\rho \frac{v_\phi}{r}}{P} - \frac{B_0 R}{P} \right) dV}{\int \rho dV},$$

(12)

which is the sum of the Reynolds stress $T_0$ and Maxwell stress $M_0$. Radial profiles of $\alpha$ are obtained by integration along $\theta$ and $\phi$. 2D profiles are obtained by integration along $\phi$.

We note that the time units are inner orbits, which always refer to the orbital time at 0.3 au.

### 3. Results

We focus our analysis on the dynamics of three distinct regions of the disk. The first is the inner rim, which we define as the irradiation $\tau_\alpha = 1$ line. The second is the inner edge of the dead zone, defined as the region where the Elsässer number $\Lambda = v_a^2/(\eta \Omega)$ ($v_a$ being the Alfvén velocity) is smaller than unity. MRI turbulence is damped when $\Lambda$ is less than unity (Sano & Stone 2002). The third is the dust concentration radius and is defined as the location when pressure reaches a maximum and where the gas azimuthal velocity is exactly Keplerian. The gas is rotating with super(sub)-Keplerian velocities inward (outward) of that location. We will focus on those three regions in the following analysis, and we mark their positions in Figures 2–7.

We first investigate the detailed disk dynamics using the results of model RMHD_P0_4 in Sections 3.1 and 3.2. The results of model RMHD_P0_4_B2 are presented in Section 3.3. The question of whether large-scale and long-term nonaxisymmetric perturbations arise in the simulations is investigated using model RMHD_P1_6 in Section 3.4.

#### 3.1. Time Evolution

Figure 2 shows the time evolution of the stress-to-pressure ratio $\alpha$ over radius for model RMHD_P0_4. Midplane positions are shown for (from left to right) the inner rim (green dashed line), the 900 K temperature contour (yellow dashed line), the inner dead-zone edge with $\Lambda = 1.0$ (yellow solid line), and the dust concentration radius (blue dashed line).

Figure 3 shows the time evolution of the disk structure. Figure 3 shows the time evolution of the surface density and three selected temperature contours. For the simulation runtime the disk remains stable. Overplotted temperature contours in steps of 400 K show the temperature variations over time at different disk locations. Close to the inner rim, the 1200 K contour shows only small radial fluctuations. The 800 and 400 K contours behind the inner rim move slightly radially inward by around 0.1 au in the first 40 local orbits, due to the extended height of the dust rim by magnetic fields, which causes a steeper temperature drop in the shadow behind the rim. Figure 4 shows the time-averaged radial temperature profile of model RMHD_P0_4, overplotting the standard deviations. The temperature fluctuations remain small. The maximal deviations are around 10–30 K and appear to be due to variations of the rim surface and hence grazing angle variations of the irradiation.

To summarize, the disk structure for model RMHD_P0_4 remains stable over the simulation time. The model shows a quasi-steady state on dynamical timescales. However, we emphasize that this model is not in inflow equilibrium on the longer accretion flow timescale. The initial surface density profile was calculated assuming $\alpha_{DZ} = 10^{-3}$ for temperatures above a large number of uncorrelated turbulent density fluctuations. The dead-zone inner edge is located at around 0.8 au (yellow solid line). At this position, the Elsässer number $\Lambda$ drops below unity. In our model, the dead-zone inner edge is also close to the temperature contour $T \sim$ 900 K (yellow dashed line) and corresponds to the location where the magnetic Reynolds number drops below $\sim 100$. At this position, the value of $\alpha$ drops by several orders of magnitude. We note that the exact radial position of the dead-zone inner edge shows variations of around 2–3 disk scale heights in the radial direction with time (with typical displacement of the order of $\Delta R \sim 0.1$ au). This is due to temperature variations associated with the turbulence. Finally, the dust concentration radius is located inside the dead zone at around 1 au (blue dashed line) and displays little sign of radial variations.
below 1000 K. In our 3D models we find values of $\alpha$ that are orders of magnitude smaller. In such a case the surface density should be much higher to balance the drop in accretion stress. In the discussion section we explore this point further.

### 3.2. Time-averaged Results: Zero-net-flux Model

The time-averaged meridional distribution of the stress-to-pressure ratio for model RMHD\,P\,⊙\,4 is plotted in Figure 5, along with the positions of the inner rim and the dead-zone inner edge (green and yellow dashed lines, respectively). The plot shows that the entire inner rim surface is embedded in the turbulent region of the disk. The dead-zone edge is located at $R \sim 0.8$ au. Its shape is roughly vertical around the disk midplane ($|Z/R| < 0.12$), while in the upper disk layers it curves radially outward, consistent with the fact that the disk surface is radiatively heated by the central star. In agreement with the results described above, turbulent activity quickly drops to a very small value inside the dead zone.

The time-averaged and meridionally integrated 1D profile of the stress-to-pressure ratio $\alpha$ is shown in Figure 6 (top panel). The plot features a plateau with a constant value of $\alpha = 0.03$ over the entire inner disk, without any noticeable change across the dust rim. In agreement with previously published simulations performed in the ideal MHD limit (Brandenburg et al. 1995; Miller & Stone 2000; Simon et al. 2009; Davis et al. 2010), the Maxwell stress is around 3 times larger than the Reynolds stress. At the dead-zone inner edge, the Maxwell stress drops sharply by roughly four orders of magnitude. By
contrast, the Reynolds stress decrease is more shallow, so that it dominates the total stress in a small region between 0.8 and 1.1 au, which corresponds to roughly 10 disk scale heights. Over that region, the total stress takes values that range between $\alpha = 10^{-4}$ and $10^{-6}$ times the pressure. The Maxwell stress amounts to about $10^{-6}$ and is governed by mean magnetic fields that diffuse into the dead zone. The mean Maxwell stress is computed from the volume-averaged fields (see the red dashed curve in the top panel). The relatively large Reynolds stress is mainly due to density waves that are excited in the inner disk turbulence (Heinemann & Papaloizou 2009a). Previous global MHD simulations of the inner dead-zone edge have found similar amounts of Reynolds stress close to the dead-zone inner edge (Dzyurkevich et al. 2010; Faure et al. 2014). These density waves propagate into the dead zone and are quickly damped after around 10 scale heights. In Appendix C we review and discuss in more detail the damping mechanism. Finally, outside of 1.1 au, $\alpha$ drops further to values of about $10^{-7}$.

The radial profile of the (mass-weighted) turbulent velocity fluctuations shown in Figure 6 (middle panel) displays similarities with the radial profile of $\alpha$. It plateaus inside 0.8 au, with values between 300 and 400 m per second that correspond to several tens of percent of the sound speed. At the rim position, there is a small decrease that we trace to the sudden temperature decrease and the associated drop in the sound speed (see red dotted line in Figure 6, middle panel). This is not surprising since the value of $\alpha$ remains roughly constant across the inner rim. At the dead-zone inner edge ($r \sim 0.8$ au), the turbulent velocities quickly drop by several orders of magnitude so that, at the position of the dust concentration radius ($r \sim 1$ au), the turbulent velocity fluctuations are reduced to values around 10 m s$^{-1}$.

The radial profiles of the turbulent and mean magnetic field given in Figure 6 (bottom panel) were calculated by performing a simple average over one scale height above and below the midplane. Inside the MRI active region, the turbulent magnetic fields show a power-law radial profile with a slope of about $-3/2$ and a strength of 1 G at 0.6 au. This profile is slightly steeper than the $r^{-1}$ radial profile found in toroidal net-flux global 3D isothermal simulations (Flock et al. 2011) and also recently again by Suzuki & Inutsuka (2014) in global simulations with a vertical net-flux field. The radial profiles of the turbulent and mean magnetic field (the latter being dominated by the toroidal component) both follow the profile that would be expected in a gas characterized by a constant $\beta$ value, where $\beta = 2P/B^2$ is the ratio between gas and magnetic pressure (see red dotted line, which corresponds to $\beta = 100$). At the dead-zone inner edge, the turbulent field strength quickly drops, leaving a dominant mean magnetic field inside the dead zone. The plot shows that the mean magnetic field diffuses outward in the dead zone from its inner edge at 0.8 au.

### 3.3. Stronger Turbulence: The Net-flux Model

In this section we present the results of model RMHD_P0_4_BZ. It is intended to simulate the conditions in a protoplanetary disk that is under the influence of a vertical magnetic field. Model RMHD_P0_4_BZ was computed by restarting model RMHD_P0_4 after 210 inner orbits, adding a uniform vertical magnetic field (see Appendix B for details) whose strength is such that $\beta = 3.5 \times 10^4$ at 1 au in the disk midplane. We find that the radial locations of the inner rim, the dead-zone edge, and the dust concentration are only weakly modified compared to model RMHD_P0_4.

Figure 7 (top panel) plots the time-averaged and meridionally integrated radial profile of the stress-to-pressure ratio. Time averaging is done between 20 and 70 inner orbits. The model RMHD_P0_4_BZ shows a substantially increased turbulent activity compared to model RMHD_P0_4, with a high plateau of $\alpha \sim 0.1$ in the inner disk. Such high $\alpha$ values are expected in the ideal MHD limit when the disk is threaded by a vertical net-flux magnetic field (Bai & Stone 2013). The mean Maxwell stress is large even in the MRI active region and accounts for about half of the angular momentum transport. It drops by one order of magnitude only at the dead-zone inner edge (see red dot-dashed line) and dominates the total stress in the bulk of the dead zone, with a typical $\alpha$ of order $10^{-3}$. Such large values generated by axisymmetric magnetic fields have also been found in local box simulations that include an ohmic dead zone only (see model V1 by Turner et al. 2007, model X1d by Okuzumi & Hirose 2011, or model D1-NVFb by Gressel et al. 2012).
The middle panel of Figure 7 shows the radial profile of the time-averaged and mass-weighted turbulent velocity fluctuations. Compared to RMHD_P0_4, \( v_{\text{rms}} \) is increased by a factor of two to three in the inner disk. Finally, the time-averaged turbulent and mean magnetic fields are shown in Figure 7 (bottom panel). Again, in the MRI active region, we find an increase by a factor of two to three compared to model RMHD_P0_4. Their radial slopes, however, remain similar in this region. The biggest difference is the presence of a large mean field in the whole domain (compare black dashed lines in the bottom panel of Figures 6 and 7). This is particularly true in the dead zone, where the mean field in model RMHD_P0_4_B2 is almost two orders of magnitudes larger than the typical value we found in model RMHD_P0_4. Finally, we caution that the total duration of the simulation for model RMHD_P0_4_B2 remains fairly small. We refer the reader to the discussion section for more details.

3.4. Long-lasting Nonaxisymmetric Perturbations

In this section, we investigate the potential growth of nonaxisymmetric structures. This is done by using model RMHD_P1_6, which is similar to model RMHD_P0_4 but features a larger azimuthal extent. The initial conditions for this simulation are generated using a snapshot of the flow in model RMHD_P0_4 after 150 inner orbits and periodically repeating the azimuthal domain four times. Velocity perturbations of the order \( 10^{-4} \) are applied cellwise to each component to break the symmetry. Model RMHD_P1_6 quickly reaches a new turbulent state, albeit with statistical properties similar to model RMHD_P0_4 (see Appendix A). The 3D rendering of the dust density after 50 inner orbits is shown in Figure 8 (left panel). The plot confirms that dust particles are found between the rim and the dead-zone inner edge in a highly turbulent environment. As discussed in the previous sections, the dust density increases sharply at the dead-zone inner edge, following a similar increase in the gas surface density that is due to the drop of the accretion stress (Flock et al. 2016). The right panel shows the tangled structure of the turbulent magnetic field. It is dominated by the toroidal component, which reaches amplitudes of several gauss.

We next compute discrete Fourier transforms of the density along azimuth. We focus on three different locations: (1) the midplane at 0.5 au, which is fully turbulent; (2) the upper layer close to the inner rim surface and the dead-zone edge \((R = 0.83 \text{ au} \text{ and } Z/R = 0.13)\); and (3) the midplane at 0.83 au. The results are summarized in Figure 9. Initially, the large-scale density variations are weak. They amount to a few percent in both the turbulent midplane at \( R = 0.5 \text{ au} \) and the disk upper layers at \( R = 0.83 \text{ au} \) (see black solid and red dashed lines). They are even smaller in the disk midplane at \( R = 0.83 \text{ au} \) (i.e., at the dead-zone edge), where they only reach values of \( \sim 10^{-3} \) (red dotted line). In the MRI active region, these density perturbations do not grow for 60 local orbital periods (\( \sim 129 \) inner orbits). However, there is a clear increase by about two orders of magnitude at the location of the dead-zone edge (both red lines). In particular, the relative perturbations reach order unity in the disk upper layers at \( R = 0.83 \text{ au} \). The presence of a sharp surface density change at that location and the growth timescale of \( \sim 20 \) local orbits both suggest the Rossby wave instability (RWI; Lovelace et al. 1999; Meheut et al. 2013). This is confirmed by the appearance of a localized vortex (not shown) characterized by a midplane relative vorticity of about \( \langle \nabla \times \vec{v} \rangle / \Omega \approx -0.3 \) in the vortex core. Similar values have been reported in the literature for vortices produced by the RWI (Lyra & Mac Low 2012; Meheut et al. 2013; Flock et al. 2015). Figure 9 indicates that the vortex is not growing anymore after 20 local orbits. Regarding the expected lifetime of the vortex, we can only make predictions based on its shape. The vortex has an extent of \( \sim 2H \) in radius and \( \sim 22H \) in azimuth \((H/R \approx 0.04 \text{ at the vortex location})\). Such an elongated vortex is known to be vulnerable to elliptical instabilities (Lesur & Papaloizou 2009), which will limit its subsequent growth. An alternating vortex growth and destruction, as was found in Flock et al. (2015), could be also possible.

The vortex appears in Figure 10 (top panel) in the snapshot of the dust density after 150 inner orbits as a clear nonaxisymmetric density maximum. The middle and bottom panels of Figure 10 show the dust density in the \( R-Z/R \) plane inside and outside the vortex (along the lines labeled “A” and “B” on the top panel, respectively). Inside the overdensity, the irradiation optical depth unity line (or, equivalently, the height of the rim) is increased vertically (see the dotted lines on the middle and bottom panels of Figure 10): at \( R = 0.85 \text{ au} \), we measured \( (Z/R)_{\text{max}} = 0.17 \) for cut “A” and \( (Z/R)_{\text{max}} = 0.14 \) for cut “B.” As will be further discussed in Section 4.3, such a
The difference in height is enough to create an extended shadow on the disk beyond.

4. Observational Constraints

In this section we post-process our models with Monte Carlo radiation transfer tools in order to translate the results described in the previous sections into observational constraints. This is done using the Monte Carlo radiative transfer code RADMC3D (Dullemond 2012), for which we use the same parameters as in Flock et al. (2016). For more details on the post-processing and the RADMC configuration we use, we refer the reader to Appendix D. We first focus on the disk SED in Section 4.1 and next compute synthetic images in Section 4.2. Then, we discuss the time variability associated with the disk dynamics in Section 4.3.

4.1. SED

First, we determine the SED of the models RMHD_P1_6 and RMHD_P0_4_BZ and compare them with the initial radiation HD models. The system is seen inclined 45° from face-on, and the azimuthal domain is repeated to cover the entire 2\pi azimuthal range. We calculate the flux at seven individual wavelengths between 1 and 7 \( \mu \)m, as it is the relevant wavelength range for our domain size and temperature range. The results are plotted in Figure 11. The 3D radiation nonideal MHD model RMHD_P1_6 is very close to the 2D radiation hydrodynamical model, with a modest increase of the emission around 2 \( \mu \)m of 5\% due to the weak magnetized corona. By contrast, model RMHD_P0_4_BZ, for which the magnetic activity is much stronger, shows a significant increase of about 20\% compared to the hydrodynamical model.

A discussion of the origin of the emission arising at different wavelengths is enlightening to understand this difference. Most of the NIR emission is thermal in origin and comes from the surface located where \( Z/R < 0.05 \) and \( R < 0.6 \)au. At these locations, the magnetic field is weak and does not alter the density distribution: the area of the emitting region is unchanged. This can be illustrated with the help of the quantity \( \beta \), which indicates the importance of gas relative to magnetic pressure. Figure 12 shows the distribution of \( \beta \) in the \( R-Z/R \) plane for model RMHD_P0_4_BZ, averaged in time and in azimuth. The upper layers are magnetically dominated (\( \beta \geq 1 \)), while the midplane region remains gas pressure dominated (\( \beta < 1 \)). The equipartition line (\( \beta = 1 \)) stays above the rim surface (\( t_e = 1 \)) for \( R > 0.6 \)au. Most of the J- and K-band NIR emission is coming from a narrow region: the solid yellow line in Figure 12 marks the location of the peak emission (solid), and the area between the dashed yellow lines corresponds to the location where 50\% of total flux at 2.2 \( \mu \)m is emitted (at face-on orientation). Although it is shown here for model RMHD_P0_4_BZ, this result is similar for model RMHD_P1_6. Figure 13 helps to understand the increased NIR emission in model RMHD_P0_4_BZ: it shows a radial cut from the synthetic image at 2.2 \( \mu \)m for both models.
hydrodynamical calculations indicate unity from the initial 2D radiation HD model. RMHD models coming from.

Figure 12. The magnetic pressure is stronger than the gas increased emission in model RMHD Figure 13. 

Figure 11. SED calculated for the 3D radiative MHD models RMHD_P1_6 (black dotted line) and RMHD_P0_4_BZ (red dashed line), normalized over the SED from the initial 2D radiation HD model.

Figure 12. Space (azimuthally) and time (50 inner orbits) averaged plasma β profile in the R-Z/R plane for model RMHD_P0_4_BZ. The line of plasma β unity (red solid line) and the τ_b = 1 line (green dashed line) are overplotted. The solid yellow line shows the position of the peak emission at 2.2 μm assuming a face-on orientation. The yellow dotted lines and the shading demonstrate the spatial extent where 50% of the total emission at 2.2 μm is coming from.

Figure 13. Radial cut from a face-on synthetic image calculated at 2.2 μm for models RMHD_P1_6 and RMHD_P0_4_BZ.

The regions outward from 0.6 au mainly contribute to the increased emission in model RMHD_P0_4_BZ. As seen in Figure 12, the magnetic pressure is stronger than the gas pressure at the position of τ_b = 1, which results in increased magnetic support and thereby a shallower density profile in the disk upper layers. By contrast, model RMHD_P1_6 presents weaker magnetic activity and a thinner magnetically supported corona, which leads to the SED profile being closer to the hydrodynamical model. Overall, these results suggest that magnetic fields are able to increase the emission between 2 and 3 μm by 5%–20%. We discuss the possibility of obtaining an even higher NIR excess in Section 5.

4.2. Synthetic Images

Synthetic images are shown in Figure 14 corresponding to the radiation hydrodynamical model (top panel) and the global 3D radiation nonideal MHD models (bottom three panels). For all cases, the images cover a region that is approximately 2 au wide. The fluxes are calculated at 1.25, 2.2, and 4.8 μm and mapped to the blue, green, and red channels using a shared linear color scale and normalized over the maximum intensity at 4.8 μm. In the synthetic images of the 3D models computed at early times during the simulations (second and third panels), small turbulent structures can be identified, especially in the uppermost layers of the NIR-emitting region. Model RMHD_P0_4_BZ (second panel) shows a slightly narrower and brighter ring compared to model RMHD_P1_6 (third panel). This is because the rim surface is slightly steeper compared to the other models (see also the τ_b = 1 line in Figure 12) owing to the magnetic support. At a later time during the evolution of model RMHD_P1_6, the effect of the vortex becomes visible in the synthetic image of the NIR emission (bottom panel in Figure 14) as a spiral pattern visible in the M-band emission. We note that the m = 4 pattern comes from duplicating the simulation domain in the azimuthal direction before viewing the snapshot. Global 2π hydrodynamical calculations indicate that such multiple RWI vortices merge, leaving a single m = 1 pattern (Lyra & Mac Low 2012; Meheut et al. 2012).

Using the final snapshot of model RMHD_P1_6, we also computed the synthetic image at 0.3 μm in Figure 15. At this wavelength, most of the surface brightness is due to starlight scattered from the disk surface. The strongest scattering happens at the rim, producing the ring structure outward of 0.5 au. The spiral structure due to the vortex is also visible. At larger radii (R > 1 au), the intensity drops by orders of magnitude and a shadow is visible. The vortex increases locally the inner rim height, throwing a nonaxisymmetric shadow onto the outer disk. Almost all the scattered 0.3 μm flux of the system comes from the inner rim. As recently discussed by Dong (2015), the shadow structure shows a smooth profile, without any sharp transitions. Although we do not expect such a structure to be observed given the spatial resolutions that can be reached with current telescope facilities, such shadowing by an inner vortex might affect the disk temperature (and therefore its dynamical response) through its impacts on heating and cooling.

4.3. Variability

We now investigate potential variability using the results of model RMHD_P1_6. We focus on two aspects. The first is the variability of the NIR emission caused by variations of the rim surface and shape. The second is related to the star’s occultation by the inner rim.

4.3.1. NIR Intensity Variability

We start with the variability of the NIR emission, which we calculate for a system viewed with an inclination of 45°. The light curve is plotted in Figure 16 for different wavelengths. At
1.25 μm, the variations are smaller than 1%. At this wavelength, most of the emission is coming from the optically thin and hot material close to the midplane position of the inner rim. Larger variations become visible at wavelengths 2.2 and 4.8 μm, reaching up to ±5% in relative amplitude. At longer wavelengths, e.g., at 7 μm, the fluctuation amplitude decreases again. Figure 16 also shows clearly that the variations at different wavelengths are correlated.
The NIR emission exhibits two different types of variations. During the early evolution (0–10 yr), Figure 16 shows low-frequency variations with a period of 2 yr (which roughly corresponds to 10 Keplerian orbits at 0.5 au). These variations could be connected to the oscillations of the mean toroidal magnetic field, which happen to display a similar timescale of 10 orbits (see Figure 16, bottom panel, where we plot the mean toroidal magnetic field at a radius of 0.5 au and a height of $Z/R = 0.05$). Oscillations of the mean toroidal magnetic field such as reported here are known to be a robust outcome of MRI-driven MHD turbulence in disks (Stone et al. 1996; Miller & Stone 2000; Lesur & Ogilvie 2008; Gressel 2010; Simon et al. 2011; Flock et al. 2012a). Our results thus potentially suggest an indirect signature of this dynamical feature in the NIR emission variability of Herbig stars. At later time during the simulation ($t > 10$ yr), the frequency of the variability changes and the NIR emission starts to display monthly time variations. These are due to the vortex rotating around the star and depend on the combination of vortex azimuthal angle and disk inclination.

4.3.2. Stellar Occultation by the Inner Rim

Finally, we investigate the variability associated with the occultation of the star due to variations, in both space and time, of the inner rim height. Such height variations will produce a time-varying absorption of the stellar light, which we study here. To do so, we calculate a time series of the relative intensity (i.e., normalized by the mean intensity) received by an observer at 0.3 μm when viewing the disk at an inclination $\theta = 81.1^\circ$. We chose that particular inclination because this is the value of $\theta$ for which the variability is the largest. The wavelength at 0.3 μm was chosen to represent the variations at the peak emission flux for this type of star.

The time evolution of the 0.3 μm intensity is shown in Figure 17 (top panel), with a time sampling of 0.1 yr (~1/6 of an orbital period at 1 au for this type of star). The amplitude of the variability is initially (i.e., at times $t < 10$ yr) of the order of 50% and displays an irregular pattern. It is caused by the turbulent motions at the rim surface. In addition, the mean field oscillations reported in Figure 16 are also able to increase the density along the line of sight for a given time. At later times during the evolution ($t > 10$ yr), the vortex causes the variations to become more periodic with intensity fluctuations up to an order of magnitude. To obtain a finer sampling of both occultation patterns, we make two additional series of Monte Carlo radiative transfer calculations, one for a representative snapshot from the pre-vortex stage of the disk’s evolution, and the other for the later stage. For each, we simulate the time changes by systematically increasing the azimuthal angle from which we view the disk. The results are shown in Figure 17 (bottom panel). At $t = 4.5$ yr (dashed curve), we find variations of the order of 20% with a corresponding timescale of about 10 days. They are due to turbulent structures located at the rim surface and correspond to the high-frequency fluctuations seen at early times on the top panel of Figure 17. At $t = 14.5$ yr (solid curve), we recover the periodic modulation of the intensity, with an amplitude of roughly one order of magnitude, seen at late times on the top panel of Figure 17. As discussed previously (see the variations of the $\tau_e = 1$ line of Figure 10), this is due to the rim height locally increasing by about 10% at the location of the vortex.

5. Discussion

In this section, we discuss some limitations of our modeling.

5.1. Zero-net-flux Models

In Section 3.1 we have shown that the disk structure remains stable for the simulation runtime. However, the accretion stress inside the dead zone that is found for models RMHD_PQ_4 and RMHD_P1_6 is orders of magnitude lower than what was assumed to generate the initial conditions. The value of the surface density inside the dead zone should therefore be taken with care. Figure 18 shows the surface density evolution over time at the dead-zone inner edge at 0.85 au for model RMHD_PQ_4. There we observe the fastest surface density variation. The surface density at the dead-zone inner edge increases around 10% over the runtime. Over the accretion flow timescale we would expect a gradual increase of the surface density in the dead zone. Spanning such timescales is not feasible in 3D simulations.
fully treated in that paper. In our models we find the rim’s shape accurately using Equation (9). Most of the emission in the $J$ and $K$ band is then coming from a narrow region that is not much affected by magnetic fields, except in the outer parts of the rim. As a result, we find an NIR flux increase of about 20% at 2 $\mu$m when adding a strong and uniform vertical magnetic field. An even stronger magnetized corona would be needed to explain the NIR excess.

5.5. Observed Variability

Variability of young star–disk systems has been the focus of intense research for decades (Joy 1945; Carpenter et al. 2001; Morales-Calderón et al. 2011). Large sets of month-long simultaneous optical and infrared light curves became available recently through surveys of low-mass T Tauri stars with the CoRoT and Spitzer space telescopes (Cody et al. 2014; Stauffer et al. 2016). A few Herbig stars have been examined through imaging and/or spectroscopic time series. Sitko et al. (2012) studied the variability of the gas and dust emission from the Herbig system SAO 206462, reporting spectral line changes connected with variations in the accretion rate, and NIR dust flux changes on monthly timescales with amplitudes of 10%–20%. Our models match the observed timescales very well, but the MRI turbulence yields somewhat lower amplitudes below 10%. Wagner et al. (2015) investigated the Herbig system HD 169142 at two epochs separated by 10 yr. They reported NIR variability of 45%, explaining it by a structural change in the inner dust rim. These observations suggest that there may be an additional variability mechanism, perhaps associated with a disk wind (Bans & Königl 2012), which could be driven by the MRI (Miyake et al. 2016). Further linking the variability to the inner rim shape are scattered-light observations of HD 163296 by Wisniewski et al. (2008). They report that shadows cast by the inner rim vary on timescales of several years. We finally note that occultation by vortices might be observed in highly inclined systems. An example is AA Tau, which is inclined about 75° and still undergoing a strong occultation event that began in 2013 (Bouvier et al. 2013). Such an event could be due to a local thickening of the disk at a vortex like that on the inner rim in the models we present, but located farther from the star. Highly inclined disks appear well suited to observe the rim occulting the star, especially in cases where the outer disk is dust depleted by radial drift or settling (Bertout 2000). Other studies relating flux dips in highly inclined systems to occultation by dusty material include those by Alencar et al. (2010), Morales-Calderón et al. (2011), and Cody et al. (2014).

Such an event could be due to a vortex located at larger disk radii, increasing locally the height of the disk, similar to the vortex at the inner rim in the models we present. Such highly inclined disk systems might be ideally suited to observe the star occultation by the rim (Bertout 2000), especially in cases where the outer disk is dust depleted by the radial drift or settling. The studies by Alencar et al. (2010), Morales-Calderón et al. (2011), and Cody et al. (2014) related dipping events to dust occultation, which was observed in highly inclined systems. Recently, Ansdell et al. (2016) showed that such events could also occur for less inclined systems.
We have presented the first global 3D radiation nonideal MHD models of the innermost reaches of protostellar disks, using them to investigate the dynamics and thermodynamics of the planet-forming material. Our models include the transfer of the starlight into the dust and gas, where the heating impacts the dust sublimation and deposition and the ohmic resistivity. The starting conditions come from axisymmetric radiation viscous hydrodynamical models of the disk around a typical Herbig Ae star, with a radially independent mass accretion rate of $10^{-8} \dot{M}_\odot$ yr$^{-1}$. Magnetic fields either with or without a net vertical flux yield magnetorotational turbulence. The inner disk’s structure divides naturally into four zones:

1. Between the star and the silicate front, the gas is turbulent with rms speeds of 400–800 m s$^{-1}$, depending on the initial magnetic field configuration. The accretion stress-to-pressure ratio $\alpha$ is between 3% and 10%, and the turbulent magnetic field strengths are several gauss. The gas is hotter than the silicate sublimation threshold.

2. Lower temperatures let silicate dust exist beyond a curved front that is closest to the star in the midplane at about 0.5 au. Dust and strong turbulence coexist at 0.5–0.8 au, where temperatures are about 1000 K. The stress-to-pressure ratios are similar to those nearer the star, but the turbulence is slightly slower, due to the lower temperatures, at 300–700 m s$^{-1}$. High-speed collisions should substantially limit the grains’ maximum size.

3. Beyond about 0.8 au, temperatures are low enough and collisional ionization slow enough that the magnetic fields decouple from the gas motions. This region is the dead zone. From 0.8 to 1.1 au, turbulent speeds decline quickly with distance. Density waves propagating from the turbulent region are quickly damped, leaving laminar gas with turbulent velocities below 1 m s$^{-1}$. A local pressure maximum lies in the weakly turbulent dead zone near 1 au. This pressure peak is able to halt solid particles’ radial drift.

4. Beyond 1.1 au, well inside the dead zone, the disk is quasi-laminar with very low turbulent speeds. This region lies partly in the shadow cast by the sublimation front.

The 3D calculations let us investigate nonaxisymmetric stability. We find that RWI develops over timescales of 20 local orbits into a vortex located at the dead zone’s inner edge and close to the upper rim of the curved silicate sublimation front. The vortex moves the disk’s surface up and down over its orbital period.

We post-process our results using Monte Carlo radiative transfer tools to compare against a variety of observational constraints:

1. Our models with strong magnetic fields have NIR fluxes that are 5%–20% greater than the viscous version, because the magnetically supported disk atmosphere raises the sublimation front, reprocessing more of the starlight into wavelengths near 2 and 3 $\mu$m. Magnetorotational turbulence could thus be a factor in the long-standing puzzle of Herbig stars’ anomalously large NIR excesses (Vinković et al. 2006; Acke et al. 2009; Dullemond & Monnier 2010).

2. The vortex that develops near the sublimation front’s high point locally raises the height where the starlight is absorbed, thus casting a longer shadow on the disk beyond. The fraction of the stellar luminosity intercepted by the sublimation front at this stellar longitude is increased by about 10%. Such shadow-casting vortices could potentially be related to the variability observed in scattered-light imaging of Herbig disks (Wisniewski et al. 2008).

3. The NIR flux varies up to 10%, due to the movements of the inner rim, on timescales of months to years. The regular component of the variations is larger relative to the irregular component when the vortex is present. Further development of this picture could help in understanding why young stars with protostellar disks have such diverse optical and infrared light curves (Sitko et al. 2012; Cody et al. 2014).

Radiation MHD models of the kind we have demonstrated here open a new window for investigating protoplanetary disks’ central regions. They are ideally suited for exploring young planets’ formation environment, interactions with the disk, and orbital migration, in order to understand the origins of the close-in exoplanets.

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Appendix A

Comparison of $\Delta \phi = 0.4$ versus $\Delta \phi = 1.6$

We previously reported stronger accretion stress in a smaller azimuthal domain due to stronger mean fields (Flock et al. 2012b). Here we compare the two models with different azimuthal domains. In the left panel of Figure 19, we show the radial profiles of $\alpha$ in the models RMHD$\_P_0\_4$ and RMHD$\_P_1\_6$ averaged over the same time period of 50 inner orbits. The two models present similar radial profiles with no significant differences. However, we note that we consider here a zero-net-flux field while a net-flux field was used in our previous simulations (Flock et al. 2012b). In addition, we think that the short azimuthal domain still can be an issue for model RMHD$\_P_0\_4\_BZ$, which uses a net vertical flux field. Here, the mean field becomes nearly as large as the turbulent component (Section 3.3), which could be a sign that the azimuthal domain is too small.
In the right panel of Figure 19, we take a final look at the density perturbations of models RMHD\_P\_4 and RMHD\_P\_6. Here, we calculate the Fourier transform of the density along azimuth at the midplane at 0.5 au using the same time average as before. The right panel of Figure 19 shows that the profiles look very similar, from which we conclude that both models represent similar turbulent characteristics.

### Appendix B

#### Generating Initial Magnetic Field Configurations

In the following steps we explain how to generate the initial random magnetic field. Such a field has the advantage that the MRI turbulence quickly reaches a steady state.

1. Calculate a random vector potential for the component $A_r = A^\text{rand} f_r r$, with $r$ being the radius, and $f_r$ being a parabolic damping factor proportional to $(r - r_0)^2$ to set $A_r = 0$ at the inner and outer radial boundary. $f_r$ is a parabolic factor that decreases the potential from the midplane to the $\theta$ boundary by a factor of 50 to account for the decrease of the magnetic field in the disk corona.
2. The amplitude of the vector potential $A_r$ is set to match a plasma beta value of 100 at the midplane.
3. Apply a Gaussian filter ($\sigma = 2\delta r$) to smooth out fluctuations on the grid level to obtain comparable scales as the turbulent field in the steady state.
4. Calculate $\nabla \times A$ to obtain an initial $B_\theta$ and $B_\phi$.

It is important to define the vector potential with a periodic boundary condition in the $\phi$ direction. Otherwise, there will be a violation of the $\nabla \times B = 0$ condition at the $\phi = 0$ boundary. Initially the amplitudes of $B_\theta$ and $B_\phi$ are equal. A snapshot of the initial magnetic field is shown in Figure 1.

For model RMHD\_P\_4\_B2, we add to the vector potential a constant value of $A_\phi$. The value of $A_\phi$ is chosen to match a magnetic field strength of 100 mG at 1 au, which corresponds to a plasma beta $\beta = 2P/B^2$ of $\beta = 3.5 \times 10^4$ at 1 au at the midplane. The resulting vertical field has a radial profile of $r^{-1}$. The strength of the field corresponds to a relatively high value of vertical magnetic flux (Okuzumi et al. 2014).

### Appendix C

#### Wave Damping at the Dead-zone Inner Edge

There are several damping mechanisms for the density waves, generated in the MRI turbulent regions and which are traveling into the dead zone. The most important one is the nonlinear damping by shocks as soon as the wavelength is comparable to the disk scale height (Heinemann & Papaloizou 2009b). A similar wave dissipation by weak shocking in the dead zone was found in global MHD simulations at the inner dead-zone edge by Faure et al. (2014). One difference from previous simulations is the fact that the local $H/R$ is much smaller, meaning that waves traveling over a given radial distance are stronger damped. Another difference is the radially changing thermal diffusion. The density waves travel through a region with increasing surface density and hence increased optical thickness. At the same time, in this region the MRI is switched off and there is no excitation of density waves anymore.

The efficiency of wave damping by thermal diffusion is highest if the diffusion timescale is comparable to the typical timescale of the density wave. The turbulent correlation time of the MRI is roughly 1/10 of the orbital period for length scales comparable to $H$. At the same time, Heinemann & Papaloizou (2009b) report that the largest-density waves fitting in the azimuthal domain carry most of the energy. The characteristic timescale of thermal diffusion can be estimated with the radiation diffusion in the gas-pressure-dominated regime (Flaig et al. 2010):

$$\Delta t_{\text{diff}} = \left(1 + \frac{\rho c}{4E_R}\right) \frac{3\kappa L^2}{c},$$

with the characteristic length scale $L$, which we set to the disk scale height $H$. In Figure 20 we plot the midplane diffusion timescale for this length scale, normalized over the dynamical timescale. The yellow bar marks the region in which the diffusion timescale becomes comparable to the dynamical timescale, for which we expect highest damping. The zone matches the region in which the Reynolds stress quickly drops.
We summarize that the combination of a small $H/R$ and a thermal diffusion timescale comparable to the dynamical timescale at the dead-zone inner edge leads to an efficient damping of the density waves and hence the Reynolds stress in the dead zone.

**Appendix D**

**RT Setup and Dust Halo**

We briefly summarize the setup for RADMC3D to post-process the 3D data sets. For the Monte Carlo runs we use 210 million photon packages. We first transfer the grid values from the radiation MHD calculation to the RADMC grid structure. Then we recalculate the thermal structure using the wavelength-dependent dust opacity table. This ensures that the SED and the temperatures are consistent for the given dust opacity. For the dust opacity we assume the same grain size distribution as for the 2D models (Appendix A in Flock et al. 2016). All grains have the same size distribution, including those in the dust halo in front of the dust rim. In reality, larger grains would be more likely to survive the hotter temperatures in front of the inner rim, due to their higher emission-to-absorption ratio (Kama et al. 2009).

We have checked that the temperature of the Monte Carlo run and the global RMHD models match exactly at the inner rim. As we neglect the gas opacity in the Monte Carlo runs, we observe small deviations in the temperature for the very optically thin layers of the global models. In addition, we have already shown in our previous models that the effect of the accretion heating remains small for these model parameters (Flock et al. 2016).

We also want to discuss again the dust halo that appears in our models (Flock et al. 2016). The main reason for this halo is the difference between the gas and dust temperatures in the optically thin environment. For the case $T > T_{\text{ev}}$, the dust starts to evaporate; however, pure gas alone would lead to a temperature below the evaporation temperature. The solution is that a tiny amount of dust condenses to balance the temperature drop. The result is a small dust halo in which the temperature is close to the evaporation temperature. A similar result was found by Kama et al. (2009); however, in their model, larger dust grains are responsible as they have a larger emission-to-absorption ratio and so survive in front of the rim. In our models, the gas component has a larger $\epsilon$ value, which leads to a temperature that is cooler than dust in an optically thin environment.

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**Figure 20.** Thermal diffusion timescale along the midplane for the snapshot at 50 inner orbits for model RMHD_P1_6. The profile follows roughly the profile of the dust density, which determines the opacity and hence the local optical depth. The yellow bar marks the region in which the diffusion timescale becomes comparable to the dynamical timescale (0.1–10 times the orbital time), for which we expect highest damping.

**Figure 21.** Quality factor, time averaged and mass weighted in the vertical direction. The dead-zone edge is annotated with the yellow line. The black dotted lines emphasize the eight-cell limit.

**Appendix E**

**MRI Quality Factor**

Following the work by Noble et al. (2010) and Sorathia et al. (2011), we determine the quality factor $Q$, which shows the number of grid cells per fastest MRI growing mode. The quality factor $Q_B$ for the azimuthal field is defined as

$$Q_B = 2\pi \left( \frac{16}{15} \right) \frac{|B_r|}{\Omega} \frac{1}{r \Delta \phi} .$$

In Figure 21 we plot the quality factor for models RMHD_P4_4 and RMHD_P4_4_BZ. Space and time averaging follows the same strategy as in Sections 3.2 and 3.3. The plot shows that both models resolve very well the MRI in the region with high ionization with 16 or more grid cells per fastest-growing MRI wavelength. Model RMHD_P4_4_BZ shows an even higher-quality factor, due to the stronger field (Figures 6 and 7).
