Dynamics of small grains in transitional discs

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\textbf{ABSTRACT}

Transitional discs have central regions characterised by significant depletion of both dust and gas compared to younger, optically-thick discs. However, gas and dust are not depleted by equal amounts: gas surface densities are typically reduced by factors of \(\sim 100\), but small dust grains are sometimes depleted by far larger factors, to the point of being undetectable. While this extreme dust depletion is often attributed to planet formation, in this paper we show that another physical mechanism is possible: expulsion of grains from the disc by radiation pressure. We explore this mechanism using 2D simulations of dust dynamics, simultaneously solving the equation of radiative transfer with the evolution equations for dust diffusion and advection under the combined effects of stellar radiation and hydrodynamic interaction with a turbulent, accreting background gas disc. We show that, in transition discs that are depleted in both gas and dust fraction by factors of \(\sim 100\) to \(\sim 1000\) compared to minimum mass Solar nebular values, radiative clearing of any remaining \(\sim 0.5\) \(\mu\)m and larger grains is both rapid and inevitable. The process is size-dependent, with smaller grains removed fastest and larger ones persisting for longer times. Our proposed mechanism thus naturally explains the extreme depletion of small grains commonly-found in transition discs. We further suggest that the dependence of this mechanism on grain size and optical properties may explain some of the unusual grain properties recently discovered in a number of transition discs. The simulation code we develop is freely available.

\textbf{Key words:} accretion, accretion discs – infrared: planetary systems – protoplanetary discs – radiative transfer – submillimetre: planetary systems

\section{INTRODUCTION}

Transitional discs are so-named as the stage in evolution of a single star’s protoplanetary disc in-between the optically thick Class II and the optically thin Class III stage, within the framework of inside-out disc clearing (Alexander et al. 2014). Although sometimes confused with circumbinary discs (Espaillat et al. 2007; Ireland & Kraus 2008), these discs remain an important stage in single star evolution (e.g. Ruiz-Rodriguez et al. 2016) and may be a signpost for giant planet or multiple giant planet formation (Zhu et al. 2011; Dodson-Robinson & Salyk 2011). Even if they are not a sign of planet formation in all systems, the phase when the disc is transitioning from optically thick to thin disc in the giant planet formation region is generally when giant planets are at their most detectable from high contrast surveys, as the recent example of PDS 70 has shown (Keppler et al. 2018; Wagner et al. 2018).

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However, many disc features are ambiguous, and the planetary nature of such features remains highly debated in numerous discs including T Cha (Huélamo et al. 2011; Cheetham et al. 2015), the infrared emission in LkCa 15 (Kraus & Ireland 2012; Thalmann et al. 2016), HD 100546 (Quanz et al. 2013; Rameau et al. 2017) and HD 169142 (Biller et al. 2014; Reggiani et al. 2014; Ligi et al. 2018). Much of the confusion surrounding these features is attributable to the inadequacy of simple dust models to explain the observed scattered light emission. T Cha had very bright emission from forward scattering, LkCa 15 had both bright and red emission appearing in a forward scattering geometry (Ireland & Kraus 2014; Thalmann et al. 2015; Currie et al. 2019), and HD 169142 required emission from extremely small or quantum heated grains in a disc where micron sized grains were largely absent (Birchall et al. 2019). These observed complex grain distributions motivates this paper, which considers grain segregation processes in transitional discs.

Most previous work on grain segregation in gaseous discs considers the effects of either settling or gas pres-
ure gradients combined with variable dust stopping times. For example, Takeuchi & Lin (2002) considered the radial flow of dust particles in a disc where radiation pressure was neglected, and the disc evolved viscously with a constant α prescription. In transition discs, the lower gas densities mean that significantly smaller grains settle to the midplane, and as the disc becomes optically thin, radiation pressure on grains can become important. Takeuchi & Artymowicz (2001) considered the joint effects of a gas pressure gradient and radiation pressure in a disc that is optically thin throughout, neglecting the effects of gas accretion. They found that radiation could remove <100 µm dust grains from the inner 10s of AU of a 10 M_⊕ disc on ~kyr timescales, and segregate grains according to their size. Takeuchi & Lin (2003) modeled the combined effects of radiation pressure and accretion, focusing on discs similar to a minimum mass solar nebula, where surface outward dust motion was almost negligible compared to the motion of the bulk of the disc inwards with the gas accretion. Tazaki & Nomura (2015) considered the motion of grains with a large radiative cross section in the surface layers of a minimum mass solar nebula (10 M_⊕ disc). They found that compact grains were not efficiently transported by radiation pressure, while smaller grains could be. Kenyon et al. (2016) considered a variety of mechanisms to remove dust from transition discs, and concluded either that planet formation must leave behind far fewer small grains than one might naively expect, or that some other mechanism, for example drag-induced accretion, must be available to clear dust from discs.

In this paper, we extend previous work by jointly considering the effects of gas pressure gradients and gas flows, stopping times that depend on grain radius, radiation and turbulent diffusion in order to study the dust temporal evolution during the transitional disc period of a protoplanetary disc. In this period, gas masses within ~30AU are between ~10 M_⊕ and 10 M_⊕ and small grains have been depleted through settling and growth. Evidence for gas disc depletion comes primarily from CO observations (van der Marel et al. 2016), where typical gas depletion of order 10^{-3} are found for transition discs. We note that masses derived from HD (McClure et al. 2016) are significantly higher than CO derived disc gas masses, but HD is more sensitive than CO to mass in the outer disc, so the HD results are less relevant to the region of interest for us. Even more significant depletions in both micron and mm sized grains are found, and can be attributed to grain growth beyond mm sizes in the inner disc (Birnstiel et al. 2012) and perhaps planetesimal formation. In this paper, we begin with initial conditions of a depleted gas disc that is partly depleted of dust, and show that the combined effects of radiation pressure and accretion are able to reduce the dust content much further, to the almost negligibly small levels seen in transition discs.

The code we use to carry out all of the simulations presented in this paper is available from https://bitbucket.org/krumholz/dustevol/ under an open source license. Full simulation outputs are available upon request from the authors, but are not included in the public repository due to their size.

## 2 Dust Evolution Model

We are interested in modeling the evolution of a population of dust grains orbiting a central star of mass M and luminosity L in a background gas disc. We will treat grains as simple spheres of radius a and density ρ_d ≈ 1 g cm^{-3}, and we ignore coagulation and shattering, so that the total mass of dust grains of any given size is conserved. The grains move in response to radiation forces and to drag forces exerted by the gas; below we will assume that the stopping time of grains is small, so that these forces are always in balance and the grains are at their terminal velocity. We further separate grain motion into two types: systematic drift at a terminal velocity determined by force balance considering only the bulk velocity of the gas, and random motions as a result of local drag forces due to turbulent motions in the gas, which we approximate as a diffusion process. Under these assumptions, the density ρ_{d,a} of dust grains of radius a evolves following an advection-diffusion equation,

\[ \frac{\partial \rho_{d,a}}{\partial t} + \nabla \cdot (\rho_{d,a} \mathbf{v}_{d,a} + \mathbf{j}_{d,a}) = 0. \]

(1)

Here \( \mathbf{v}_{d,a} \) is the bulk velocity and \( \mathbf{j}_{d,a} \) is the flux due to turbulent diffusion. This formulation of the evolution equations is identical to that proposed by Takeuchi & Lin (2002).

We now proceed to calculate the bulk velocity and diffusion coefficient. In the following discussion, we use σ and z to denote the radial and vertical position in a cylindrical coordinate system centred on the star, and \( r = \sqrt{\sigma^2 + z^2} \) and \( \theta = \cos^{-1} (z/r) \) to denote the corresponding radius and polar angle in a spherical coordinate system. We assume that the system is symmetric in the azimuthal angle. In the equations that follow, we aim to differentiate between radial and cylindrical components; a novel aspect of our model is the full treatment of two dimensional drift in the presence of radiation pressure.

### 2.1 Gas disc model

As a first step, we specify our model for the gas disc through which the grains flow. We treat the gas disc as constant in time. The run of surface density and temperature through the disc are described by powerlaws,

\[ \Sigma_\sigma (\sigma) = \epsilon \Sigma_{\text{MMSN}} \left( \frac{\sigma}{\text{AU}} \right)^p \]

(2)

\[ T(\sigma) = T_0 \left( \frac{\sigma}{\text{AU}} \right)^q \]

(3)

where \( \epsilon \) is a dimensionless factor that scales the mass in the disc to that of the minimum mass Solar nebula (MMSN), \( \Sigma_{\text{MMSN}} \approx 2200 \) g cm^{-2}, \( T_0 \) is the disc temperature at 1 AU \( (T = 120 \text{ K for a Sun-like star}) \), and \( p \) and \( q \) are constant. We are interested in transition discs, for which \( \epsilon < 1 \). Standard values for us are \( p = -3/2 \) and \( q = -3/7 \), as expected for a Chiang & Goldreich (1997) passive disc profile, but we will also consider the case of discs that have been depleted at small radii, and thus have \( p = 0 \). Our temperature profile neglects the effects of dust settling, and we further simplify the situation by assuming that the gas is vertically isothermal. Under this assumption the sound speed \( c_s \) is constant with \( \sigma \), and the scale height \( h_g \) follows the usual relation
where the gas radial velocity $v_p$ is the velocity of a gas particle at a distance $r$ from the central star. We choose an approximation of an ideal gas, where density, and the final equation contains fiducial MMSN values and scalings (Chiang & Youdin 2009). Also assuming hydrostatic equilibrium in the radial direction, we have (Chiang & Youdin 2009)

$$\Omega_\mathrm{g} = \Omega_{\mathrm{K, mid}} \left[ 1 + \frac{1}{2} \left( \frac{h_g}{r} \right)^2 \left( \rho - (q+3)/2 + q + \frac{q}{2} \frac{z^2}{h_g^2} \right) \right] \tag{8}$$

This is conveniently expressed as:

$$\Omega_\mathrm{K} \approx \Omega_{\mathrm{K, mid}} \left( 1 - \frac{3}{4} \frac{z^2}{r^2} \right) \tag{9}$$

$$\Omega_\mathrm{g} = \Omega_{\mathrm{K}} (1 - \eta)^{1/2} \tag{10}$$

$$\eta = -\left( \frac{h_g}{r} \right)^2 \left( \rho - \frac{q+3}{2} + q + \frac{q+3}{2} \frac{z^2}{h_g^2} \right). \tag{11}$$

Here $\Omega_\mathrm{K}$ is the Keplerian speed a height $z$ above the mid-plane, and $\Omega_\mathrm{g}$ is the gas angular velocity, which is smaller than the Keplerian velocity by a factor of $\sqrt{1 - \eta}$ due to the effects of pressure support.

In order to solve for the dust velocity, we will require an expression for the gas radial velocity. Specifically, we have a height-dependent velocity to be self-consistent. For simplicity, we choose an $\alpha$-disc model for this purpose, though since the gas radial velocity $v_{\phi, g}$ is generally small, the details of the model will not be tremendously important. We begin with the azimuthal component of the momentum equation:

$$\frac{2\pi \rho_g}{v_{\phi, g}} \left( \frac{\partial}{\partial \sigma} + v_{\phi, g} \frac{\partial}{\partial z} \right) \left( \sigma^2 \Omega_\mathrm{g} \right) = 2\pi \left[ \frac{\partial}{\partial \sigma} \left( \sigma^2 \rho_g v \frac{\partial \Omega_\mathrm{g}}{\partial \sigma} \right) + \frac{\partial}{\partial z} \left( \sigma^2 \rho_g v \frac{\partial \Omega_\mathrm{g}}{\partial z} \right) \right], \tag{12}$$

where $v$ is the kinematic viscosity. The term $v_{\phi, g} \partial / \partial \sigma (\sigma^2 \Omega_\mathrm{g})$ is smaller than $v_{\phi, g} \sigma / \Omega_\mathrm{g}$, so can be neglected (Takeuchi & Lin 2002). Solving for radial gas velocity, and retaining terms up to order $(h_g/r)^2$, we find

$$v_{g, \phi} = -\frac{h_g}{r} c_s \left[ 3 \left( \rho - 2 + \frac{3}{2} \right) + 2q + 6 + \frac{q}{2} \left( \frac{z}{h_g} \right)^2 \right]. \tag{13}$$

where $\alpha = v/(c_s h_g)$ is the usual dimensionless viscosity (see also Keller & Gail 2004). Equation 13 gives the gas radial velocity as a function of cylindrical radius $\sigma$ (implicitly, through $r$ and $z$) and height $z$ above the midplane.

### 2.2 Dust velocity

Now consider a dust grain, working in a reference frame co-rotating with the grain at azimuthal velocity $v_{d, \phi}$. In this frame, the equation of motion in the ($\sigma, z$) plane, considering only the bulk velocity of the gas and not its small-scale turbulent motion, and neglecting Poynting-Robertson drag, is

$$\frac{d}{d\tau} v_{d, \sigma} = \frac{v_{d, \phi}^2}{\sigma} \frac{d}{d\sigma} \left( \frac{\sigma^2 \rho_d v}{\sigma} \right) + \frac{F_{\text{drag}}}{\rho_d v_s} \tag{14}$$

where $\beta$ is the ratio of outward radiation pressure force to inward gravitational force and $F_{\text{drag}}$ is the force exerted by gas drag. The first term here represents the centrifugal force, the second is the radiative minus gravitational force, and the third is the gas drag force. We omit the Coriolis force because it exerts forces only in the azimuthal direction.

#### 2.2.1 Radiation force

In general the radiation pressure force must be determined by integrating in frequency. Following Wolfire & Cassinelli (1987), if the central star has specific luminosity $L_*$ and we neglect the scattered and dust-reprocessed component of the radiation field compared to the direct stellar field, then the radiation pressure force on a grain is

$$F_{\text{rad}} = \int \frac{L_*/c}{4\pi} \left( \frac{a}{\lambda} \right)^2 \left( Q_{\text{A}, \nu} + (1 - g_{\text{A}, \nu}) Q_{\text{S}, \nu} \right) d\nu, \tag{15}$$

where $Q_{\text{A}, \nu}$ and $Q_{\text{S}, \nu}$ are the absorption and scattering efficiencies for grains of size $a$ at frequency $\nu$, and $g_{\text{A}, \nu}$ is the cosine of the mean scattering angle (with $g_{\text{A}, \nu} = 1$ indicating complete forward scattering). The optical depth from the stellar surface at radius $r_s$ to the radial distance $r$ of the grain is

$$\tau_\nu = \int_{r_s}^{r} \int_{0}^{\infty} \frac{3}{4a} \rho_{d, a} \left( Q_{\text{A}, \nu} + Q_{\text{S}, \nu} \right) da d\nu, \tag{16}$$

where $\rho_{d, a}$ is the density of the grains. Evaluation of Equation 15 in general must be done numerically, and is numerically expensive if one requires high frequency resolution. However, the simplest application and one with broad applicability is for grains of size $a$ much larger than the wavelength of photons at the peak of the stellar spectral energy distribution. Specifically, if the stellar effective temperature is $T_*$, yielding a wavelength of peak emission per unit wavelength $\lambda_\nu \approx h c / (4.966 g_T) (T_*)$, grains will be in the limit of geometric optics, $Q_{\text{A}, \nu} + (1 - g_{\text{A}, \nu}) Q_{\text{S}, \nu} = 1$, if their size obeys

$$a \gg \frac{\lambda_\nu}{2\pi} \approx 0.077 \left( \frac{T_*}{6000 \text{ K}} \right) \mu m. \tag{17}$$
For such grains, the radiation force and optical depth reduce to

\[ F_{\text{rad}} = \frac{L_c}{c} e^{-\tau} \frac{a^2}{4\pi^2} \]

(18)

\[ \tau = \int_0^\infty \frac{3}{4a} \int_{R_c}^\infty \frac{\rho_d a}{\rho}\, dr' \, da \equiv \tau. \]

(19)

With this simplification, it is convenient to express the ratio of radiation pressure force to gravitational force as simply

\[ \beta = \beta_{a,0} e^{-\tau}, \]

(20)

where

\[ \beta_{a,0} = \frac{3L}{16\pi GM c \rho_d a} \approx 0.57 \left( \frac{L/M}{L_\odot/M_\odot} \right) \left( \frac{\rho}{1 \text{ g cm}^{-3}} \right)^{-1} \left( \frac{a}{1 \mu\text{m}} \right)^{-1} \]

(21)

is the ratio of radiative to gravitational force for a grain of size \( a \) exposed to the full, unshielded luminosity of the star.

### 2.2.2 Drag force

We compute the drag force under the assumption that the grains are small enough to obey the Epstein drag law,

\[ F_{\text{drag}} = \frac{4}{3} \pi \rho_d c_s^2 c_s \Delta v. \]

(22)

where \( \rho_d \) is the gas density, \( c_s \) is the gas sound speed, and \( \Delta v \) is the relative velocity of the gas and dust. Combining the radiative and drag terms, the total equation of motion for a single grain of size \( s \) is

\[ \frac{d}{dt} v_d = \frac{v_d^2}{\sigma} + (\beta - 1) \frac{G M}{r^2} - \frac{\Delta v}{t_s}, \]

(23)

where

\[ t_s = \frac{\rho_s a}{\rho_g c_s} \]

(24)

is the usual stopping time. Below it will be more convenient to work with the dimensionless stopping time

\[ T_s = t_s \Omega_K. \]

(25)

Note that, although we will not write this out explicitly for reasons of compactness, it is important to recall that \( T_s \) is a function of the grain size \( a \).

If we limit ourselves to considering grains of size \( a \) such that \( T_s \ll 1 \) near the midplane, then over timescales longer than an orbit the left hand side of Equation 23 approaches zero in the radial and vertical direction as the grains reach terminal velocity. The condition for this to hold is that

\[ a \ll \frac{\rho_g \Omega_K}{\rho_s \Omega_K_{\text{mid}}}, \]

(26)

where \( \rho_g \Omega_K \) is the midplane gas density, and in the second step we have taken \( M = M_\odot \) and inserted our fiducial value for \( \rho_g \) (Equation 6). Thus our approximations that grains can be treated in the geometric optics limit and that they reach terminal velocity quickly are valid over a wide range of grain sizes – from \( \approx 0.1 \mu\text{m} \) up to cm to m, depending on the value of \( \epsilon \).

In the vertical direction we find the dust terminal velocity to first order is

\[ \Delta v_z = t_s (\beta - 1) \frac{v_K^2 z}{r} \]

(27)

\[ v_{d,z} = T_s (\beta - 1) \Omega_K z, \]

(28)

where we have taken \( v_K \approx 0 \) to arrive at the second equation. To obtain an expression for the radial drift, first consider the azimuthal component of the dust momentum equation. Because the dominant source of angular momentum is simply Keplerian motion, we can relate the rate of angular momentum change to the drift rate of solids (Pinilla & Youdin 2017):

\[ \frac{d(\sigma v_{d,\phi})}{dt} = -\frac{d(\sigma v_K)}{dt} v_{d,\sigma} = -\frac{1}{2} \Omega_K v_{d,\sigma}, \]

(29)

We can use this relation to replace the L.H.S of the \( \phi \) component of Equation 23, which simplifies to

\[ (v_{d,\phi} - v_{g,\phi}) = -\frac{T_s}{2} v_{d,\sigma}. \]

(30)

We can use this relative velocity in the azimuthal direction to solve for the dust terminal velocity in the (cylindrical) radial direction. From Equation 23 we have:

\[ \Delta v_{d,\sigma} = t_s \left[ \frac{v_{d,\phi}^2}{\sigma} + (\beta - 1) \Omega_K^2 \right]. \]

(31)

We require a linearized expression for the dust azimuthal velocity \( v_{d,\phi} \). Following Takeuchi & Lin (2002) and Pinilla & Youdin (2017), we can remove higher order terms by relating \( v_{d,\phi} \) and \( v_K \)

\[ v_{d,\phi} - v_K^2 = (v_{d,\phi} + v_K)(v_{d,\phi} - v_K) \]

(32)

\[ = 2v_K \left( v_{d,\phi} - v_{g,\phi} \right) - \left( v_K - v_{g,\phi} \right) \]

(33)

\[ = 2v_K \left( v_{d,\phi} - v_{g,\phi} \right) - \eta v_K / 2 \]

(34)

Solving for \( v_{d,\phi} \) and inserting back into Equation 31, we finally arrive at the cylindrical terminal velocity:

\[ v_{d,\sigma} = v_{g,\sigma} T_{s,1} + \left[ \frac{\Omega_K}{T_s} - \eta \right] v_K, \]

(35)

where \( v_K = \pi \Omega_K \) is the Keplerian velocity at the position of the grain.

### 2.3 Turbulent diffusion

Having solved for the bulk velocity of the gas, we next calculate the rate of turbulent mixing. Following Takeuchi & Lin (2002), we model the diffusive flux of dust as

\[ \dot{J}_{d,a} = -\frac{1}{1 + T_s} \frac{a^2}{\Omega_K} \rho_g \frac{\rho_d}{\rho_g} \nabla \left( \frac{\rho_d}{\rho_g} \right) \equiv -D_{d,a} \rho_g \nabla \rho_{d,a} \]

(36)

where \( a \) is the dimensionless viscosity, and we have defined \( \dot{J}_{d,a} = \rho_d a / \rho_g \) as the dust mass fraction for grains of size \( a \), and

\[ D_{d,a} = a \frac{\sigma^2}{\Omega_K} \left( \frac{1}{1 + T_s} \right) \]

(37)

as the diffusion coefficient for dust grains of size \( a \). Note, however, the \( D_{d,a} \) is the diffusion coefficient for grain concentration, rather than grain density.
3 SIMPLIFIED 1D SYSTEM

3.1 Derivation

Before proceeding to full numerical solution of Equation 1, it is helpful to gain insight by considering a simplified system that we can solve semi-analytically. We do so by making the following approximations. First, we neglect the vertical structure of the disc, and focus on a small radial section so that we can neglect curvature (i.e., we treat the coordinate system as Cartesian, with the x direction aligned with the radial direction), and can treat the initial dust density distribution, background gas disc, and Keplerian speed as uniform (i.e., $\rho_D$, $v_k$, and $c_s$ are all constant). Second, we consider only a single size of dust grain $a$, with constant stopping time $t_s$. Third, we neglect both the radial inflow of the gas and the slow inward drift of dust compared to gas as a result of drag, i.e., we set $v_{g,\infty} = 0$ and $\eta = 0$. While these assumptions are obviously oversimplifications, they retain the essence of the problem: the radial evolution of the dust will be determined by the competition between radiation pressure forces, which attempt to sweep the dust up into an outward-moving shell, and diffusion, which attempts to force the dust distribution back towards uniform.

Under the approximations we have described, Equation 1 reduces to the one-dimensional PDE

$$\frac{\partial \rho_d}{\partial t} + \left( \frac{\beta_0 v_k}{T_s + T'_s} \right) \frac{\partial}{\partial x} \left( \rho_d e^{-\tau} \right) - D_d \frac{\partial^2 \rho_d}{\partial x^2} = 0,$$

(38)

where we have dropped the subscript $a$’s since we are considering only a single grain size, and we orient our coordinate system so the star lies at position $x = 0$. As an initial condition we take $\rho_d = 0$ for $x < 0$ and $\rho_d = \rho_{d,0}$ for $x > 0$, i.e., the dust initially occupies the positive half-plane. With this initial condition, we can write the optical depth to position $x$ as

$$\tau = \frac{3}{4a\rho_s} \int_0^x \rho_d(y) \, dy.$$

(39)

The first step in solving Equation 38 is to non-dimensionalise it. We normalise the density to the initial density, measure length in units of the optical depth at the initial density, and measure time in units such that the diffusion coefficient is unity. Mathematically, this amounts to making a change of variables $\rho'_d = \rho_d/\rho_{d,0}$, $x' = x/x_d$, $t' = t/t_d$, where

$$x_d = \frac{4}{3} a \frac{\rho_s}{\rho_{d,0}} \quad t_d = \frac{x_d^2}{D_d}.$$

(40)

Here $x_d$ and $t_d$ are the characteristic length and time scales for the problem. This allows us to rewrite Equation 38 as

$$\frac{\partial \rho'_d}{\partial t'} + \frac{\partial}{\partial x'} \left( \rho'_d e^{-\tau} \right) - \frac{\partial^2 \rho'_d}{\partial x'^2} = 0,$$

(41)

where

$$\tau = \int_0^{x'} \rho'_d(y') \, dy'$$

(42)

$$\chi = \frac{4}{3} \left( \frac{\beta_0}{a\rho_{d,0}} \right) \left( \frac{\rho_s}{\rho_{d,0}} \right)^2 \left( \frac{a}{r} \right)^2 \left( \frac{v_k}{c_s} \right)^3.$$

(43)

Here we have used Equation 25 and Equation 37 for $D_d$ and $T_s$, respectively, and $r = v_k/Dk$ is the radial location of our region of interest, and $f_{d,0} = \rho_{d,0}/\rho_S$ is the initial dust fraction. The interstellar dust abundance is $f_{d,0} \approx 0.01$, but the transition discs in which we are interested have undergone considerable grain agglomeration into larger bodies, and have observed dust abundances that lie more in the range $10^{-3} - 10^{-4}$ (e.g., van der Marel et al. 2016).

Thus we see that our simplified 1D system represents a single-parameter family of PDEs. The parameter $\chi$ characterises the relative importance of advection by radiation forces (the second term in Equation 38) and diffusion by the gas (the third term). Intuitively, we expect that radiation forces on the exposed face of the dust at $x = 0$ will begin to sweep dust into an advancing wave, which will be spread out to a characteristic width determined by diffusion. The parameter $\chi$ controls the characteristic speed with which the wave moves, sweeping up dust as it goes. The value of $\chi$ in a real disc obviously varies significantly depending on the local properties, as we discuss in further detail in Section 3.4, but for the cases of greatest interest to us we will have $\chi$ in the range tens to thousands.

3.2 Semi-analytic Solution

We cannot obtain an exact analytic solution even to Equation 38, but we can derive some analytic constraints on the asymptotic behaviour of the solution, which we can use to derive a semi-analytic model. First note that for material at high optical depth, i.e., any dust that begins at $x' > 1$, the advection term is negligible because it is proportional to $e^{-\tau}$. Thus the equation reduces to

$$\frac{\partial \rho'_d}{\partial t'} - \frac{\partial^2 \rho'_d}{\partial x'^2} = 0,$$

(44)

which can we can solve via the usual similarity transformation for diffusion problems, $\zeta = x'/2\sqrt{t'}$. This reduces the problem to an ODE, which has the solution

$$\rho'_d = c_1 + c_2 \text{erf}(\zeta).$$

(45)

The two constants of integration $c_1$ and $c_2$ are determined by the boundary conditions. One of them can be fixed by requiring that $\rho'_d \to 1$ as $\zeta \to x'/2\sqrt{t'} \to \infty$, i.e., that the density approach the initial density far upstream of the advancing dust wave. Applying this condition, the analytic solution at large $\tau$ must approach

$$\rho'_d = 1 + k \text{erf} \left( \frac{x'}{2\sqrt{t'}} \right),$$

(46)

where $k$ is a constant that depends on $\chi$, and $\text{erf}(x) = 1 - \text{erf}(x)$ is the complementary error function.

Thus the solution will consist of a low-optical depth, low-density downstream region over which the dust wave has already passed, a transition zone where $\tau \approx 1$ located at position $s(t')$, and an upstream region where the solution approaches Equation 46. At late times, when $\rho'(t') \gg 1$, the great majority of the dust mass that was initially at $x' < s(t')$ must be in the upstream region, since by definition the downstream and transition regions contain a mass per unit area of order unity in our dimensionless variables. Thus conservation of mass requires that for $s(t') \gg 1$ we
have
\[
s(t') = \int_{s(t')}^{\infty} k \text{erfc} \left( \frac{x' - \sqrt{2\lambda t'}}{\sqrt{2\lambda t'}} \right) dx'
\]
\[
= k \left\{ \text{erfc} \left[ \frac{s(t')}{\sqrt{2t'}} \right] - \frac{1}{\sqrt{\pi}} e^{-s(t')^2/4t'} \right\}.
\]
(47)

This equation can be satisfied for arbitrary \( t \) only if we have
\[
s(t') = 2\sqrt{\lambda t'}
\]
\[
k = \left[ \text{erf}(1) - 1 + \frac{e^{-1^2}}{\sqrt{\pi}} \right]^{-1}.
\]
(49)

Thus we learn that the position of the dust wave at late times must be proportional to \( \sqrt{t'} \), with a constant of proportionality that depends on \( \lambda \).

### 3.3 Numerical Solution

We can verify this analytic calculation, and calibrate the dependence of \( \lambda \) on \( \chi \), using numerical solutions to Equation 41. We solve the system using a 1D finite volume method that is second order accurate in both space and time; we give a full description of the method in Appendix A. In Figure 1 we show an example solution to Equation 41 for log \( \chi = 1.5 \). The parameters for this run are included in Table 1. As predicted, the position of the dust front (defined here by the location of maximum dust density) as a function of time is fit extremely well by \( \text{erf} \left( \frac{s(t')}{\sqrt{2t'}} \right) \); a simple least-squares fit to the solution shown in Figure 1 gives \( \lambda = 3.81 \).

In order to determine the dependence of \( \lambda \) on \( \chi \), we solve the system numerically at a range of \( \chi \) values. We list all the simulations we carry out in Table 1; the domain sizes \( L \) and simulation times \( t_{\text{max}} \) are chosen to ensure that the width of the dust wave is \( \ll L \) at all times, and that the dust wave advances to \( x \approx 20 \), by which point the wave position as a function of time has always converged very well to the asymptotic \( s \propto t^{1/2} \) behaviour we predict analytically. We ensure that our results are converged in resolution by carrying out a convergence study: for every case, we first run the simulation at a resolution of 64 cells and then 128 cells, compute \( \lambda \) via a least-squares fit to the front position as a function of time at both resolutions, and compare the results. If they differ by more than 1%, we double the resolution again, to 256 cells, and repeat the process. We continue doubling the resolution until either (1) we reach a resolution of 4096 cells or (2) for the highest two resolutions, the two values of \( \lambda \) that emerge from our fit differ by < 1%. We then use a Richardson extrapolation of the resolution-dependent results to generate our final estimate for \( \lambda \) for that value of \( \chi \); we do this in two steps. First, we estimate the order of convergence by fitting the difference between the outcome at

### Table 1.
Parameters and results for simulations of the simplified 1D system. Here \( \chi \) is the dimensionless advection to diffusion ratio, \( t_{\text{max}} \) is the dimensionless time \( t' \) for which we run the simulation, \( L \) is the dimensionless size of the simulation domain, \( \Delta x_{\text{min}} \) is the spatial resolution of the best-resolved run, \( k \) is the estimated order of convergence (error \( \propto \Delta x^k \)), \( \lambda \) is our best estimate for \( \lambda \) based on Richardson extrapolation, and \( \text{Err}(\lambda) \) is the estimated fractional error on \( \lambda \). See main text for details of how \( \Delta x_{\text{min}} \), \( k \), \( \lambda \), and \( \text{Err}(\lambda) \) are computed.

| \( \log \chi \) | \( t_{\text{max}} \) | \( L \) | \( \Delta x_{\text{min}} \) | \( k \) | \( \lambda \) | \( \text{Err}(\lambda) \) |
|-----------------|----------------|-------|----------------|-----|--------|----------------|
| 1.0             | 20.0           | 16.0  | 1/32           | 1.40| 1.96   | 7.3 \times 10^{-3} |
| 1.25            | 12.0           | 16.0  | 1/64           | 1.33| 2.76   | 5.9 \times 10^{-3} |
| 1.5             | 8.0            | 8.0   | 1/128          | 1.32| 3.80   | 5.0 \times 10^{-3} |
| 1.75            | 4.0            | 8.0   | 1/256          | 1.25| 5.16   | 4.0 \times 10^{-3} |
| 2.0             | 2.0            | 4.0   | 1/256          | 1.36| 6.94   | 7.3 \times 10^{-3} |
| 2.25            | 2.0            | 4.0   | 1/512          | 1.24| 9.31   | 6.5 \times 10^{-3} |
| 2.5             | 2.0            | 4.0   | 1/1024         | 1.13| 12.46  | 5.5 \times 10^{-3} |
| 2.75            | 1.6            | 4.0   | 1/1024         | 1.03| 16.59  | 9.1 \times 10^{-3} |
| 3.0             | 1.0            | 4.0   | 1/1024         | 0.87| 22.03  | 2.1 \times 10^{-3} |

Figure 1. Top: dimensionless density \( \rho'_{d} \) as a function of position \( x' \) at five different times, for the case log \( \chi = 1.5 \) at a resolution \( \Delta x = 1/128 \). Note that the region plotted is larger than the domain size \( L \) due to our sliding grid; see Appendix A for details. Bottom: position of the dust front \( s(t') \) as a function of dimensionless time \( t' \). The blue points show the simulation results, where we define the front location as the position of maximum dust density (every 5th time plotted, to avoid clutter), while the black dashed line shows the best-fitting semi-analytic solution, \( s(t') = 2\sqrt{\lambda t'} \).
that would be required for radiation pressure to move the
dust clearing time
$\tau_{\text{clr}}$ at that position a distance comparable to its current
solution
solution in a disc, we can compute
applications of this finding. For any specified dust and gas
density, where $\tau_{\text{clr}}$ is the dust to gas ratio. For any given choices of param-
ers describing the star ($M$, $L$) and the disc ($\epsilon$, $f_{\text{dust}}$, $T_D$
and the dust ($a$, $\rho_d$), we can use this expression to compute the
dust and gas densities at every point, and then
use these to compute $\chi$ and $t_{\text{clr}}$.

In Figure 3 we show an example map of $\chi$ and $t_{\text{clr}}$ for a
transition disc with $\epsilon = 10^{-2}$, $f_{\text{dust}} = 10^{-4}$. In the example
shown, the midplane is quite resistant to dust clearing ($t_{\text{clr}} >$
1 Myr, but above the midplane significant clearing is possible
on timescales well under a Myr. Recall, however, that we
have the near-proportionality $t_{\text{clr}} \propto f_{\text{dust}} \rho_d^2$. Thus we expect
clearing to become much more rapid as we move to discs that
are more dust- or gas-depleted than the example shown in
Figure 3. Conversely, for richer discs clearing will be much slower.

which is the (dimensional) time that would be required for a
dust wave following the semi-analytic solution derived in the
previous section to move a distance $r$. For small grains, $T_s \ll$
1, in a thin, moderately-accreting disc, $v_K/c_s \sim 10^2$ and $a \sim$
$10^{-2}$, significant dust sweeping in $\lesssim 10^6$ orbits is expected
for $\lambda \sim 1 - 10$, corresponding to $\chi$ of tens to hundreds.

We can also write the clearing timescale in terms of the
classical viscous accretion timescale $t_{\text{acc}} = r^2/v$, where
$v = \alpha c_s^2 / \Omega_K$ is the kinematic viscosity. Then we simply have

$$ t_{\text{clr}} = \frac{1 + T_s^2}{4 T_s^2} t_{\text{acc}} \quad (52) $$

and we again see that we expect grains to be cleared faster
than they accrete only for $\lambda \gtrsim 1$, meaning $\chi \gtrsim 10$.

Finally, it is instructive to insert our best-fit scaling for $\lambda$
as a function of $\chi$, Equation 50, into Equation 53, and
then to substitute for $\chi$ using Equation 43. Doing so gives

$$ t_{\text{clr}} = 0.46 \left( 1 + T_s^2 \right)^{-0.02} \left( \frac{d_{\text{dust}}}{\beta_0} \right)^{1.02} \left( \frac{\rho_g}{\rho_d} \right)^{2.04} \left( \frac{\epsilon_s}{v_K} \right)^{1.06} \Omega_K^{-1} \quad (53) $$

Thus we see that the dust clearing timescale is very sensitive
to both the grain size (roughly $t_{\text{clr}} \propto a^{-2}$) and the
background dust density ($t_{\text{clr}} \propto \rho_d^2$). Thus smaller grains
in denser gas are much more resistant to clearing, while larger
grains are easier to clear.

To give a sense of the numerical values implied by Equation
53, let us consider a disc in which the dust and gas
are initially in equilibrium in the absence of radiative forces
or radial transport (i.e., with $v_{\text{dust}} = 0$, $f_{\text{dust}} = 0$, and
$\beta = 0$ in Equation 1). Takeuchi & Lin (2002) show that the
steady-state vertical distribution of size $a$ in such a disc has
a steady-state solution

$$ \rho_{\text{dust}}(z) = \rho_{\text{dust}}(0) \exp \left( -\frac{z^2}{2h_g^2} - \frac{\alpha}{\alpha} \frac{T_{s,\text{mid}}}{\alpha} \left[ \exp \left( \frac{-z^2}{2h_g^2} \right) - 1 \right] \right) $$

where $T_{s,\text{mid}}$ is the stopping time evaluated at the midplane
gas density, $\alpha = 1 + T_{s,\text{mid}}$ is the Schmidt number for a
particular grain size $a$, and the midplane density $\rho_{\text{dust}}(0)$ is set by requiring that

$$ 2 \int_0^{\infty} \rho_{\text{dust}}(z) \, dz = f_{\text{dust}} \Sigma_g $$

Here $\Sigma_g$ is the gas column density at cylindrical radius $\sigma$, $f_{\text{dust}}$
is the dust to gas ratio. For any given choices of parameters
describing the star ($M$, $L$) and the disc ($\epsilon$, $f_{\text{dust}}$, $T_D$,
$a$, $p$, $q$) and the dust ($a$, $\rho_d$), we can use this expression to compute the
dust and gas densities at every point, and then
use these to compute $\chi$ and $t_{\text{clr}}$.

In Figure 3 we show an example map of $\chi$ and $t_{\text{clr}}$ for a
transition disc with $\epsilon = 10^{-2}$, $f_{\text{dust}} = 10^{-4}$. In the example
shown, the midplane is quite resistant to dust clearing ($t_{\text{clr}} >$
1 Myr, but above the midplane significant clearing is possible
on timescales well under a Myr. Recall, however, that we
have the near-proportionality $t_{\text{clr}} \propto f_{\text{dust}} \rho_d^2$. Thus we expect
clearing to become much more rapid as we move to discs that
are more dust- or gas-depleted than the example shown in
Figure 3. Conversely, for richer discs clearing will be much slower.

3.4 Astrophysical Implications

We are now in a position to consider the astrophysical
implications of this finding. For any specified dust and gas
distribution in a disc, we can compute $\chi$ from Equation 43
at any point in the disc, and then from our semi-analytic
solution $s(t) = 2t\sqrt{\tau}$, we can compute the characteristic time
t that would be required for radiation pressure to move the
dust at that position a distance comparable to its current
distance from the star. To be precise, at any point a radial
distance $r$ from the star, we define the dimensionless radiative
dust clearing time $t'$ by the condition that $r/\chi d = 2t\sqrt{\tau}$.

The corresponding dimensionless time is

$$ t_{\text{clr}} = \frac{t_d}{4a^2} \left( \frac{\tau}{\chi d} \right)^2 = \frac{1 + T_s^2}{4a \Omega^2} \left( \frac{v_K}{c_s} \right)^2 \Omega_K^{-1} \quad (51) $$

Formally our method is second-order accurate for smooth flows.
However, the flow is not smooth in the vicinity of the maximum
dust density, where $\tau = 1$. Since the behaviour in this region is
critical to determining the solution, the actual accuracy will be
worse than second order. We find typical convergence orders of
1 – 2 depending on $\chi$.

Figure 2. Dust front speed parameter $\lambda$ as a function of advection
to diffusion ratio $\chi$. Blue circles show the numerical results
from Table 1 (error bars are too small to be seen), while the black
dashed line shows the best-fitting powerlaw.
4 2D SIMULATIONS

Armed with the general understanding provided by the simplified 1D system solved in Section 3, we now proceed with full numerical solutions to Equation 1 in 2D, including the full spatial dependence of the background gas disc. We summarise the properties of the runs we carry out in Table 2. Motivated by Figure 3, we take $\epsilon = 10^{-2}$, $f_{\text{dust}} = 10^{-4}$ as our most gas- and dust-rich case, and explore from those values downward.

4.1 Numerical Method

We solve Equation 1 using a conservative finite volume method that we fully describe in Appendix B. Our method is second-order accurate in time, second-order accurate in space for the diffusion terms, and third-order accurate for the advection terms. The calculation operates on a 2D spherical polar grid defined by coordinates $(r, \theta)$, which we divide in $N_r \times N_\theta$ cells. For convenience, since we will go back and forth between polar and cylindrical coordinates, we will use $\mu = \cos \theta = z/r$ as our coordinate rather than $\theta$; $z$ and $\mu$ both increase in the same direction, and $\mu = 0$ corresponds to $z = 0$. The inner and outer radial edges of the grid lie at $r = r_{\text{min}}$ and $r_{\text{max}}$, respectively, and in the polar direction the edges of the outermost cells are at $\mu = 0$ and $\mu_{\text{max}}$. We assume symmetry about the midplane at $\mu = 0$. All the simulations we present here use $N_r = 512, N_\theta = 256$, $r_{\text{min}} = 0.1$ AU, $r_{\text{max}} = 50$ AU, and $\mu_{\text{max}} = 0.1$.

In each computational cell we track the density of $N_a$ logarithmically-spaced grain size bins, each with mean grain size $a_k$. That is, the density of grains in size bin $k$ represents the total density of grains with sizes from $\sqrt{a_k a_{k+1}}$ to $\sqrt{a_{k+1} a_{k+2}}$, where $k = 1 \ldots N_a$, and $a_0$ and $a_{N_a+1}$ are set so that bins 1 and $N_a$ contain the same logarithmic range of grain sizes as all other bins. For all simulations we present here, we adopt $N_a = 4$ with $a_k = 10^{(k-1)/2} \mu$m, so grain sizes go from $10^{-0.5} - 10^{0.5} \mu$m in steps of 0.5 dex.

We adopt zero flux boundary conditions across both the midplane at $\theta = 0$ and the top of the disc at $\theta = \theta_{\text{min}}$. At the inner and outer radial boundaries of our computational domain we adopt diode boundary conditions. At the inner edge we set the diffusive mass flux to zero, and we set the mass flux across the boundary to zero in any location where the velocity is into the computational domain, but we allow mass to flow inward radially if the velocity at the domain edge is inward. For the outer boundary, we similarly set the diffusive mass flux to zero, and anywhere the radial velocity is out of the domain we allow mass to flow out freely, but no mass to enter.

4.2 Initial Conditions

We initialise all simulations using the analytic solution derived by Takeuchi & Lin (2002), given by Equation 54. However, unlike in Section 3, we now consider multiple grain size bins, and thus the constraint on the initial midplane density $\rho_{d,0}(0)$ becomes

$$2 \int_0^\infty \rho_{d,0} dz = f_{\text{dust}} f_a \Sigma_g,$$

(56)

where $\Sigma_g$ is the gas column density at cylindrical radius $\sigma$, $f_{\text{dust}}$ is the initial total dust to gas ratio summed over all grain sizes, and $f_a$ is the fraction of the total grain mass found in grains in the size bin whose mean size is $a$. We set the initial fractional masses $f_a$ in each grain size bin.
by assuming that grains follow a size distribution consistent with a collisional cascade, \(\frac{dn}{dm} \propto m^\alpha\), where \(m \propto a^3\) is the mass of an individual grain and \(q_d \approx -11/6\), as expected for a collisional cascade after larger bodies have started to form (Dohnanyi 1969). From this choice, we have \(f_{a,k} \propto (a_{k+1} a_k)^{3/2} q_d/2 - (a_{k-1} a_k)^{3/2} q_d/2\) for size bin \(k\), which together with the constraint \(\sum_k f_{a,k} = 1\) fully specifies the initial mass in each bin.

We carry out six simulations, using the parameters shown in Table 2. The first three of these use our fiducial \(p = -1.5\) density profile for the initial gas and dust disc, with varying amounts of gas and dust depletion. The most gas- and dust-rich of these cases (case 1 in the table, with \(\epsilon = 10^{-2}\), and \(f_{\text{dust}} = 10^{-4}\)) corresponds to the parameters shown in Figure 3, and roughly to the highest column density inner transition disc in the sample of van der Marel et al. (2016); case 2 has a lower initial dust-to-gas ratio by a factor of 10, while case 3 has the same dust-to-gas ratio as case 1, but a factor of 10 lower disc mass overall.

The next three simulations use a flat gas density profile \(p = 0\), as might be expected to prevail late in disc evolution after the majority of the gas in an inner disc accretes onto the host star. These are interesting both because they potentially represent the evolution at such late stages of accretion, and because the choice \(p = 0\) implies that there is no radial drift of grains into the star, and thus no other grain removal mechanism operates. For these cases we fix the ratio of mass relative to the MMSN at 1 AU to quantify the rate at which grains are lost from the inner disc. We show snapshots of our simulation results for cases 1, 2, and 3 in Figure 4, Figure 5, and Figure 6, respectively.

| Parameter | Meaning | Case 1 | Case 2 | Case 3 | Case 4 | Case 5 | Case 6 |
|-----------|---------|-------|-------|-------|-------|-------|-------|
| \(p\)     | Gas density index | -1.5  | -1.5  | -1.5  | 0     | 0     | 0     |
| \(\epsilon\) | Mass relative to MMSN at 1 AU | \(10^{-2}\) | \(10^{-2}\) | \(10^{-3}\) | \(10^{-2.5}\) | \(10^{-2.5}\) | \(10^{-2.5}\) |
| \(f_{\text{dust}}\) | Initial D/G ratio | \(10^{-4}\) | \(10^{-4}\) | \(10^{-4}\) | \(10^{-4}\) | \(10^{-4}\) | \(10^{-4}\) |

### 4.3 Simulation results

#### 4.3.1 Cases with a radial gas gradient

We show snapshots of our simulation results for cases 1, 2, and 3 in Figure 4, Figure 5, and Figure 6, respectively. Comparing the runs, we see some common features and some differences. As expected, our initial distribution of grains places the largest grains at the smallest scale height. Because of their small scale height, the largest grains at the outer edge of the disc are completely shielded from radiation by the dense inner disc. As a result the grains drift inward from the outer edge of the disc at 50 AU, leaving a void behind them; this is the usual result of gas drag, and is fastest for the largest grains because they are nearest to being critically-damped, \(T_r \approx 1\). At smaller radii, where grains are exposed to radiation pressure, the situation is very different. In case 1, which is our most gas- and dust-rich, the inner disc is close to static over the duration of our simulation. This is simply a consequence of the small values of \(\chi\) for the inner part of the disc shown in Figure 3: due to the strong drag forces imposed by high gas densities, the net rate of grain drift is small. The smallest grains that are lofted well above the disc plane and that are exposed to radiation can drift at appreciable speeds, but the mass of grains in regions that are subject to drift is negligible compared to the much larger mass in regions where drift is negligible. Consequently any grains that are pushed outward by radiation are immediately replaced as turbulence causes the much larger reservoir of low-altitude grains to diffuse upward.

In cases 2 and 3, on the other hand, the outcome is very different. Case 2 has lower shielding against radiation due to its lower dust mass, while case 3 has both lower shielding and reduced drag. Both lead to a substantially higher value of \(\chi\), and a shorter dust clearing time, such that dust is driven back from the disc inner edge on timescales of \(\sim 100\) kyr. The smallest grains are swept up most rapidly, because their greater height within the disc leaves them both more exposed to stellar radiation, and less slowed by gas drag.

**Table 2.** Summary of 2D simulation parameters

}[MNRAS 000, 1–18 (2019)]
Larger grains that sit lower in the disc move outward more slowly, and form a sharper ring of dust due to the stronger drag forces in the regions where they reside. Consequently, radiation sorts the grains by size; this sorting is especially apparent for case 3 (Figure 6). However, the entire structure of sorted grains moves outward over time, eventually colliding with the outer edge of shielded grains drifting inward due to gas drag. At this point all the grains are collected into rings that radiation pushes outward. If we allow the simulation to run long enough, eventually all the dust leaves the computational domain.

\[ \mu \leq 2 \mu \leq 3 \mu \leq 0.3 \mu m \]

\( \log \Sigma [g/cm^3] \)

| 0 kyr | 67 kyr | 133 kyr | 200 kyr |
|-------|-------|--------|--------|
| 0.3 µm | 0.3 µm | 0.3 µm | 0.3 µm |
| 1.0 µm | 1.0 µm | 1.0 µm | 1.0 µm |
| 3.2 µm | 3.2 µm | 3.2 µm | 3.2 µm |
| 10.0 µm | 10.0 µm | 10.0 µm | 10.0 µm |

| 0 kyr | 67 kyr | 133 kyr | 200 kyr |
|-------|-------|--------|--------|
| 0.3 µm | 0.3 µm | 0.3 µm | 0.3 µm |
| 1.0 µm | 1.0 µm | 1.0 µm | 1.0 µm |
| 3.2 µm | 3.2 µm | 3.2 µm | 3.2 µm |
| 10.0 µm | 10.0 µm | 10.0 µm | 10.0 µm |

\[ \log \Sigma [g/cm^3] \]

4.3.2 Cases without a radial gas gradient

In Figure 7, Figure 8, and Figure 9 we show the results for cases 4, 5, and 6, respectively, our three cases without an initial radial gradient in the gas or dust surface density. These runs show a qualitatively different evolution from the previous cases, in that there is no inward migration of dust caused by drag. Instead, there is only outward flow of the dust caused by radiation pressure, which sweeps up an outward-moving front. Grains sort by size, but by a smaller amount than in the cases with \( p = -1.5 \).

Moreover, the radius of the front versus time is quite different than in cases 1 - 3. In the cases with \( p = -1.5 \), the most difficult part of the disc to evacuate is the centre. Once the central regions are clear, however, the process tends to run away: the declining density with radius, and thus the decrease in both mass to be swept up and strength of diffusive mixing, makes it relatively easy to clear the entire disc inside a few hundred kyr. For the cases with \( p = 0 \), neither
Figure 6. Same as Figure 4, but for the run with \( \epsilon = 10^{-3}, f_{\text{dust}} = 10^{-4}, p = -1.5 \) (case 3 in Table 2); note that the colour scales in the two figures are not the same. The order of magnitude reduction in gas density compared to case 2 facilitates the collection of dust into rings, whose location and shape are grain-size dependent. An animated version of this figure is included in the Supplementary material (online).

Figure 7. Same as Figure 4, but for the run with \( \epsilon = 10^{-2.5}, f_{\text{dust}} = 10^{-3}, p = 0 \) (case 4 in Table 2); note that the colour scales in the two figures are not the same. The absence of radial density (and pressure) gradients inhibits the formation of rings and an inner hole when the gas mass is non-negligible. An animated version of this figure is included in the Supplementary material (online).

5 DISCUSSION

5.1 Astrophysical Implications

In our simplified one-dimensional case, we found that grains clear faster than they accrete for a dimensionless parameter \( \chi \geq 10 \) (Equation 43). Considering now the 2D models of Section 4, it is helpful to keep in mind that the accretion timescale \( t_{\text{acc}} \) in physical units was \( \sim 3 \) Myr for our relatively low viscosity parameter \( \alpha = 10^{-4} \), so a more relevant criterion for whether radiative dust clearing is significant is arguably whether the clearing timescale \( t_{\text{clr}} \) is on the same order of magnitude as the \( 0.1 \) Myr timescale for the transitional disk phase as constrained by population studies (Alexander et al. 2014). This timescale \( t_{\text{clr}} \) has no dependence on \( \alpha \) for high \( \chi \), and is proportional to \( \epsilon^2 f_d \) (Equation 53, noting that \( \rho_g \propto \epsilon \)). For our case with gas surface density power law index \( p = -1.5 \), in our most gas- and dust-rich case, case 1, we have \( \epsilon^2(f_d/0.01) = 10^{-4} \), while the values are \( 10^{-5} \) for case 2 and \( 10^{-6} \) for case 3. The simu-
lations show that a transition to rapid dust clearing occurs around $\epsilon^2(f_d/0.01) \sim 10^{-5}$. For our $p = 0$ cases, models 4 - 6, we also find a transition to efficient clearing around $\epsilon^2(f_d/0.01) \sim 10^{-5}$, corresponding to case 5 (c.f. Table 2). Thus our simulations, together with our analytical calculation of timescales and their dependence on disc dust and gas properties, support the general hypothesis that radiative dust clearing is a significant process in any disc satisfying $\epsilon^2(f_d/0.01) \leq 10^{-5}$.

In the critical inner ~ 10 AU, gas power law densities have not been carefully measured for Class II objects, although it appears possible to do so in the coming years with ALMA (Miotello et al. 2018). For transitional discs, gas density models that combine spectra with partially resolved observations in CO isotopologs result in only moderately satisfactory fits (van der Marel et al. 2016), but clearly indicate very significant depletion of CO in the inner ~ 10 AU. This CO depletion is further supported by simultaneous modelling of spectra and spectro-astrometry (Pontoppidan et al. 2008), where the complete lack of CO gas at high velocities is strong evidence of cleared CO within ~ 5 AU of SR 21 in particular. Typical values of $\epsilon$ around $10^{-2.5}$ and power law indices between 0 and $-1.5$, i.e., precisely the range spanned by our simulations, are consistent with those papers. Small dust grains are also severely depleted in these discs, with depletions in the very inner disc between $10^2$ and $10^6$; indeed, spectral energy distribution modelling is consistent with there being no dust at all at moderate radii ($\sim 10$ AU; van der Marel et al. 2016). The mechanisms we have explored in this paper provide a natural explanation for these results, since we show that the combination of radiative acceleration, gas drag and turbulent viscosity could start from the small grain dust distribution of a Class II T Tauri star and produce an inner hole largely cleared of small grains, so long as some grain growth ($f_d \sim 10^{-4}$) and accretion-based gas clearing ($\epsilon \sim 10^{-2.5}$) occurs during the Class II phase.
5.2 Model Limitations

We end this discussion by pointing out some of the limitations of the models we have explored thus far, which point to the directions required in future work. First, our calculation is limited to grains whose interaction with radiation can be approximated by geometric optics. Although this is an excellent starting point, since it applies to almost all grains larger than a few tenths of a micron, it does not represent the situation in the most evolved of discs, where for example there is evidence for very small grains (Oph IRS 48 and HD 169142, Birchall et al. 2019) or unusually bright scattering indicative of unusual optical properties (LkCa 15, Thalmann et al. 2016). Indeed, the mechanism proposed in this paper provides a natural explanation for clearing out grains with a “normal” optical properties, and thus high ratio of radiative to gravitational acceleration $\beta$, leaving unusually low $\beta$ grains behind.

A second limitation of our models is that we considered a static background disc, rather than one whose structure is self-consistently generated as a result of viscous accretion and similar processes that shape the gas distribution. This makes it difficult to directly relate our model parameters to the stellar accretion rate, which is a key measurable parameter of real star-disk systems. We chose not to evolve a model where the gas was in a viscous steady state because although turbulent diffusion is certainly a key driver of the evolution of the dust density distribution, turbulent viscosity (Shakura & Sunyaev 1973) is not the leading candidate for driving gas accretion in cool, evolved disks approaching or in the transitional phase (Bai & Stone 2013; Turner et al. 2014). Ideally, the work in this paper could be coupled with a plausible gas accretion mechanism. We note that gas clearing may be coupled with dust clearing, as the dust density distribution directly feeds back to the true gas scale height and dynamics – another physical mechanism beyond the scope of this paper.

6 CONCLUSIONS

We have shown in this paper that grain growth and accretion processes naturally clear a protoplanetary disc, there is a transition point where the combination of radiation pressure and gas drag can move the grains outwards. Using 2D simulations in which we simultaneously include radiative forces, turbulent diffusion of dust by gas, and inward flow of dust due to gas accretion and radial pressure gradients, we show that the disc clearing is not simply a surface effect, and can affect the entire small grain dust disc structure. This process had not been studied in depth before, because the mechanism alone is not effective for a minimum mass solar nebula, and requires the disc to already have evolved significantly. Conversely, however, once these evolutionary processes drive the gas and dust density low enough, radiative clearing becomes both unavoidable and rapid.

Our proposed physical clearing process has a number of appealing features. It does not invoke planet formation directly, and can take place even in a disc that does not form planets. It leaves behind a structure that is consistent with current transitional disc observations. Notably, this process clears dust and not gas, so is consistent with transitional discs still having moderately large gas discs while having an inner cavity that is almost completely devoid of dust.

The primary limitation of our work thus far is that, while we have considered a range of dust grain sizes, we have thus far limited our calculations to grains whose interaction with starlight can be described by geometric optics. Future work will involve relaxing this assumption allowing us to consider not just grains smaller than $\sim 0.1 \mu\text{m}$ that are too small for geometric optics, but also grains with differing radiative properties, for example high degrees of scattering asymmetry. This will also enable radiative transfer models to see how effectively the dust structures produced by this model can reproduce real observations.

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APPENDIX A: NUMERICAL METHOD FOR 1D SYSTEMS

Here we describe the numerical method we use to solve the simplified 1D system, Equation 41. To avoid clutter in this appendix we drop the primes on all the terms in this equation, but all the quantities listed are the non-dimensionalised ones.

A1 Spatial discretisation, initial conditions, and boundary conditions

We use a uniform grid with constant cell size $\Delta x$, with the left edge of cell 0 at $x = 0$ and the right edge of cell $N - 1$ at $x = x_{\text{max}}$; we use $x_{i-1/2}$ and $x_{i+1/2}$ to denote the positions of the left and right edges of cell $i$. We use a finite volume discretisation on this grid; integrating Equation 41 over cell $i$, we have

$$\frac{\partial}{\partial t} \rho_{di} = \Delta x^{-1} \left[ \left( \rho_{di} e^{-\tau} \right)_{i+1/2} - \left( \rho_{di} e^{-\tau} \right)_{i-1/2} \right] - \frac{\partial \rho_i}{\partial x} \left|_{i+1/2} \right| + \frac{\partial \rho_i}{\partial x} \left|_{i-1/2} \right|, \quad \text{(A1)}$$

where $\rho_{di} = \Delta x^{-1} \int^{x_{i+1/2}}_{x_{i-1/2}} \rho_d \, dx$ is the average of $\rho_d$ over cell $i$, and the subscripts $i+1/2$ and $i-1/2$ indicate that a particular quantity is to be evaluated the corresponding cell edge.

We initialise the simulation with $\rho_{di} = 1$ in every cell, and adopt boundary conditions whereby both the advective and diffusive fluxes out of the domain are set to zero. To ensure that these choices do not affect the result, we always choose the size of our domain large enough so that the right edge of the domain is well beyond the dust wave, and thus the flux through cells near it is negligibly small in any event.

As the simulation evolves, and the dust front moves to larger $x$, an increasingly large fraction of the computational domain becomes filled with cells for which $\rho_{di} \approx 0$. To avoid expending CPU cycles needlessly updating these nearly-empty cells, at the end of each time step (see next section) we shift our grid to the left, removing the leftmost cells within which $\rho_{di} < 10^{-6}$. We keep the number of cells constant by adding an equal number of new cells on the right hand side of the domain, all initialised to $\rho_{di} = 1$; since our domains extend well past the edge of the dust wave at all times, the existing cells adjacent to those being added also have $\rho_{di} \approx 1$, and thus the newly-added cells blend smoothly with the existing ones.

A2 Time discretisation and time-stepping strategy

We advance the calculation in time using an explicit-explicit update step with Strang (1968) splitting between the advective terms, which we handle explicitly, and the diffusion terms, which we handle implicitly. To advance the calculation from time $t_n$ to time $t_{n+1} = t_n + \Delta t$, starting from the dust densities $\rho_{di}^{(n)}$ in every cell at time $n$, we carry out the following steps:

(i) Advance the diffusion subsystem (the $\partial \rho_{di}/\partial x$ terms in Equation A1) for a time $\Delta t/2$ using an implicit method that is second-order accurate in space and time (Section A3.1). We denote the state after this step as $\rho_{di}^{(e)}$.

(ii) Advance the advection subsystem (the $\rho_d e^{-\tau}$ terms in Equation A1), starting from state $\rho_{di}^{(e)}$ for a time $\Delta t$ using an explicit method that is second-order accurate in time and third-order accurate in space (Section A3.2). We denote the state that results from this procedure as $\rho_{di}^{(s)}$.

(iii) Starting from state $\rho_{di}^{(s)}$, carry out a final diffusion advance, using the same method as in step (i), through time $\Delta t/2$. This yields the final state $\rho_{di}^{(n+1)}$ at the new time.

The overall scheme is second-order accurate in time. We set the time step based on a Courant-Friedrichs-Lewy (CFL)
condition as applied to the advection step, which we describe in Section A3.2. This condition guarantees positivity during the first advection update, but is not sufficient to guarantee positivity through the full Strang-split time step. Thus on occasion our update scheme yields a negative density. If this occurs, we simply reduce the time step by factors of 2 and retry until the step succeeds.

### A3 Subsystems

Here we describe our procedures for advancing the advection and diffusion subsystems.

#### A3.1 Diffusion

We evaluate the diffusion terms in Equation A1 using second-order accurate centered differences,

$$\left( \frac{\partial \rho_d}{\partial x} \right)_{i+1/2} = \rho_{d,i+1} - \rho_{d,i} \frac{\Delta t}{\Delta x},$$

(A2)

and similarly for cell edge $i - 1/2$. We discretise the diffusion subsystem in time using a second-order accurate Crank-Nicolson method. Defining $\Theta = 1/2$ as the time centring parameter, for time step $\Delta t$ we obtain the usual second-order Cartesian diffusion discretisation:

$$\rho_{d,i}^{(n+1)} = \rho_{d,i}^{(n)} + \Delta t \frac{\Delta x^2}{4} \left( (1 - \Theta)(\rho_{d,i+1} - 2\rho_{d,i} + \rho_{d,i-1})^{(n)} \right) + \Theta(\rho_{d,i+1} - 2\rho_{d,i} + \rho_{d,i-1})^{(n+1)} \right),$$

(A3)

where the superscript $(n)$ indicates the state at the start of the update and $(n+1)$ indicates the state after the diffusion update. This equation can be rewritten as a linear system

$$\mathbf{M} \rho_d^{(n+1)} = \rho_d^{(n)} + \Delta t \rho_d^{(\text{diff})},$$

(A4)

where $\rho_d$ is an $N$-element vector containing the densities in all cells,

$$\rho_d^{(n)} = (1 - \Theta) \left( \rho_{d,i+1} - 2\rho_{d,i} + \rho_{d,i-1} \right)^{(n)} \frac{\Delta x^2}{4}$$

(A5)

is the rate of change of $\rho_d$ due to diffusion evaluated at the old time, and the $\mathbf{M}$ is an $N \times N$ tridiagonal matrix whose elements are

$$M_{ij} = \left( 1 + 2\Theta \frac{\Delta t}{\Delta x^2} \right) \delta_{ij} - \Theta \frac{\Delta t}{\Delta x^2} \left( \delta_{i,j+1} + \delta_{i,j-1} \right).$$

(A6)

We solve Equation A4 using the standard Thomas algorithm for tridiagonal matrices.

#### A3.2 Advection

Since the velocities are non-local functions of the density coupled via the radiation field, we cannot obtain second-order accuracy in time using standard predictor-corrector methods. Instead, following Skinner et al. (2018), we use a Shu & Osher (1988) TVD time discretisation. Given a starting state $\rho_{d,i}^{(n)}$, we advance the calculation from $t_n$ to $t_{n+1} = t_n + \Delta t$ via

$$\rho_{d,i}^{(n+1)} = \rho_{d,i}^{(n)} + \Delta t \left( \rho_{d,i}^{(\text{adv})} \right),$$

(A7)

where

$$\rho_{d,i}^{(\text{adv})} = \frac{1}{2} \left( \rho_{d,i}^{(n)} + \rho_{d,i}^{(n+1)} \right) \frac{\Delta t}{\Delta x} \left( \delta_{i,j+1} + \delta_{i,j-1} \right).$$

(A8)

We evaluate these terms in three steps. First, for the initial density field $\rho_{d,i}^{(n)}$ or $\rho_{d,i}^{(n+1)}$ we compute a piecewise-parabolic method (PPM) reconstruction of the density field (Colella & Woodward 1984). Specifically, we approximate the dust density in cell $i$ with a parabolic function

$$\rho_d(x) = c_0 + c_1 x + c_2 x^2,$$

(A10)

where the reconstruction has the property that $\Delta x = \int_{x_{i-1/2}}^{x_{i+1/2}} \rho_d(x) dx = \rho_{d,i}$, and the function $\rho_d(x)$ is monotonic for $x \in (x_{i-1/2}, x_{i+1/2})$. The reconstruction coefficients $c_0$, $c_1$, and $c_2$ are functions of $\rho_{d,i-1}$, $\rho_{d,i}$, and $\rho_{d,i+1}$. Second, we calculate the optical depths to cell edges

$$\tau_{i+1/2} = \sum_{j=0}^{i} \rho_{d,i}.$$ 

(A11)

From the optical depths we can derive the velocities $v_{i+1/2} = \chi e^{k_{i+1/2}}$ at each cell face. Third, we evaluate the mass per unit area transported across cell face $i + 1/2$ over time $\Delta t$, which is $\Delta t \rho_d e^{k_{i+1/2}}$, by evaluating the amount of mass contained in the region between the cell edge and the position of a contact discontinuity propagating at speed $v_{i+1/2}$ away from that cell edge:

$$\Delta t (\rho_d e^{k_{i+1/2}})_{i+1/2} = \int_{x_{i+1/2} - \Delta t v_{i+1/2}}^{x_{i+1/2}} \rho_d(x) dx.$$ 

(A12)

This procedure allows us to evaluate $(\dot{\rho}_{d,i})$ in every cell. We set the overall time step as

$$\Delta t = C \min \left( \frac{\tau_{i+1/2}}{v_{i+1/2}}, \frac{\tau_{i+1/2}}{v_{i+1/2}} \right),$$

(A13)

where the minimum is over all cells $i$, and $C$ is the CFL number. The scheme is stable for $C < 0.5$.

### APPENDIX B: NUMERICAL METHOD FOR 2D SYSTEMS

Here we describe the full details of the method we use to solve the advection-diffusion equation, Equation 1. Our strategy here is a 2D generalisation of that described in Appendix A.

#### B1 Computational grid and discretisation

We adopt a 2D spherical polar grid with $(r, \theta)$ as our basic coordinates, but we will specify our grid in terms of the radial and angular variables $x$ and $\mu$, where $x = \log r / r_{\text{min}}$. 

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\[ \mu = \cos \theta, \text{ and } r_{\text{min}} \] is the inner edge of the computational domain. The centre of cell \(ij\) is located at coordinates \(x_i\) and \(\mu_j\), and its upper right corner is located at \(x_{i+1/2}\) and \(\mu_{j+1/2}\). In the radial direction the grid starts at \(r_{-1/2} = r_{\text{min}}\) and ends at \(r_{N_r-1/2} = r_{\text{max}}\), and in the azimuthal direction it extends from \(\mu_{-1/2} = 0\) to \(\mu_{N_{\mu}-1/2} = \mu_{\text{max}}\); the grid is \(N_r \times N_{\mu}\) cells in size, and is uniformly spaced so that the sizes of cells are \(\Delta r = (x_{N_r-1/2} - x_{-1/2})/N_r\) and \(\Delta \mu = \mu_{N_{\mu}-1/2}/N_{\mu}\). For this grid, cell volumes and radial and angular cell face areas are

\[ V_{ij} = \frac{2}{3} \pi \left( r_{i+1/2}^3 - r_{i-1/2}^3 \right) \Delta \mu \tag{B1} \]
\[ A_{i+1/2,j} = 2 \pi r_j \Delta \mu \tag{B2} \]
\[ A_{i,j+1/2} = \pi \left( r_{i+1/2}^2 - r_{i-1/2}^2 \right) \Delta \theta \tag{B3} \]

respectively.

We also discretize in bins of grain size, by defining a logarithmically-spaced set of grain size bins. Specifically, we use \(N_d\) grain size bins, with \(a_{-1/2} = a_{\text{min}}\) representing the smallest size grains in the smallest bin, and \(a_{N_d-1/2}\) the largest grains in the largest bin, \(\Delta a = \log(a_{N_d-1/2}/a_{-1/2})/N_d\) constant, and \(a_k = \sqrt{a_{k-1/2} a_{k+1/2}}\) representing the mean size of grains in the \(k\)th size bin. We let \(\rho_{d,k}\) represent the mean density of grains in the size range from \(a_{k-1/2}\) to \(a_{k+1/2}\).

We adopt a finite-volume spatial discretization strategy. Integrating Equation 1 over the volume of cell \(ij\), and making use of the divergence theorem, we have

\[ \frac{\partial}{\partial t} \rho_{d,ijk} = -V_{ij} \cdot \] 
\[ \left[ F_{\text{adv},i+1/2,j,k} A_{i+1/2,j} - F_{\text{adv},i-1/2,j,k} A_{i-1/2,j} + F_{\text{adv},i,j+1/2,k} A_{i,j+1/2} - F_{\text{adv},i,j-1/2,k} A_{i,j-1/2} + F_{\text{diff},i+1/2,j,k} A_{i+1/2,j} - F_{\text{diff},i-1/2,j,k} A_{i-1/2,j} + F_{\text{diff},i,j+1/2,k} A_{i,j+1/2} - F_{\text{diff},i,j-1/2,k} A_{i,j-1/2} \right], \tag{B4} \]

where \(F_{\text{adv}}\) and \(F_{\text{diff}}\) are the advective and diffusive fluxes at the cell faces, defined by

\[ F_{\text{adv},i+1/2,j,k} = \int_{A_{i+1/2,j}} \rho_{d,k} d\mu d\theta dA \tag{B5} \]
\[ F_{\text{adv},i,j+1/2,k} = \int_{A_{i,j+1/2}} \rho_{d,k} d\mu d\theta dA \tag{B6} \]
\[ F_{\text{diff},i+1/2,j,k} = -\int_{A_{i+1/2,j}} D_{d,k} \rho_{d,k} \frac{df_{d,k}}{dr} dA \tag{B7} \]
\[ F_{\text{diff},i,j+1/2,k} = -\int_{A_{i,j+1/2}} D_{d,k} \rho_{d,k} \frac{1}{r} \frac{df_{d,k}}{d\theta} dA \tag{B8} \]

Here, for each size bin \(k\), \(\rho_{d,ijk}\) is the mean dust density in cell \(ij\), \(v_{r,ijk}\) and \(v_{\theta,ijk}\) are the \(r\) and \(\theta\) velocities, and \(D_{d,k}\) is the diffusion coefficient evaluated for grains of size \(a_k\). Note that Equation B4 is exact. We defer discussion of how we evaluate the fluxes to Section B2.

We discretise the equations in time and advance using the same approach as in the 1D case, as described in Appendix A2. Specifically, we break the problem into advective and diffusive subsystems, and use Strang (1968) splitting to advance them alternately while retaining second-order accuracy in time.

### B2 Subsystems

Here we describe our procedures for advancing the advection and diffusion subsystems.

#### B2.1 Diffusion

The diffusion subsystem of Equation B4 is

\[ \frac{\partial}{\partial t} \rho_{d,ijk} = -V_{ij} \cdot \]
\[ \left[ F_{\text{diff},i+1/2,j,k} A_{i+1/2,j} - F_{\text{diff},i-1/2,j,k} A_{i-1/2,j} + F_{\text{diff},i,j+1/2,k} A_{i,j+1/2} - F_{\text{diff},i,j-1/2,k} A_{i,j-1/2} \right], \tag{B9} \]

We evaluate the diffusive fluxes using second-order accurate centred finite differences:

\[ F_{\text{diff},i+1/2,j,k} = -D_{d,i+1/2,j,k} \rho_{g,i+1/2,j} - D_{d,i+1/2,j,k} \rho_{g,i-1/2,j} + \]
\[ \sqrt{\frac{1 - \mu_{j+1/2}}{\mu_{j+1/2}}} D_{d,i+1/2,j,k} \rho_{g,i,j+1/2} - D_{d,i+1/2,j,k} \rho_{g,i,j-1/2} \] 
\[ \frac{df_{d,k}}{dx} \bigg|_{i+1/2,j} \]
\[ \frac{df_{d,k}}{dx} \bigg|_{i,j+1/2} \tag{B10} \]

\[ \left( \frac{df_{d,k}}{dx} \right)_{i+1/2,j} = 1 \Delta x \left( \rho_{d,ijk+1,k} - \rho_{d,ijk} \right) \tag{B11} \]

and similarly for the \(\mu\) derivatives. The subscripts indicate the cell face or centre at which all quantities are to be evaluated, and we note that \(\rho_g\) and \(D\) are known analytically at all positions.

We discretise the diffusion subsystem in time using a second-order accurate Crank-Nicolson scheme. Defining, \(\Theta = 1/2\) as the time-centring parameter, for a time step \(\Delta t\) we have

\[ \frac{\rho_{d,ijk}^{(n+1)} - \rho_{d,ijk}^{(n)}}{\Delta t} = -V_{ij} \cdot \]
\[ \left[ \frac{1 - \Theta}{2} F_{\text{diff},i+1/2,j,k} A_{i+1/2,j} - \frac{1 + \Theta}{2} F_{\text{diff},i-1/2,j,k} A_{i-1/2,j} + \frac{1 - \Theta}{2} F_{\text{diff},i,j+1/2,k} A_{i,j+1/2} - \frac{1 + \Theta}{2} F_{\text{diff},i,j-1/2,k} A_{i,j-1/2} \right], \tag{B13} \]

where \(\rho_{d,ijk}^{(n)}\) and \(\rho_{d,ijk}^{(n+1)}\) denote quantities evaluated at the previous and new times, respectively.

We can rearrange Equation B13 to obtain a sparse linear system for each grain species \(k\),

\[ \text{M}_k \dot{\rho}_{d,k}^{(n+1)} = \dot{\rho}_k^{(n)} + \Delta \dot{\rho}^{(n)}_{d,k} \]

Here \(\dot{\rho}_k^{(n)}\) is the vector with \(N_d N_{\mu}\) elements ordered so that element \(\ell\) contains the dust density in cell \((i,j) = (\ell \mod N_r, \ell/N_r)\), i.e.,

\[ \dot{\rho}_k^{(n)} = \dot{\rho}_{d,\ell \mod N_r, \ell/N_r} \tag{B14} \]

and similarly for \(\dot{\rho}_k^{(n)}\). The term \(\dot{\rho}_{d,k}^{(n)}\) represents the rate of
change in density due to diffusion evaluated at the old time, and is given by
\[
(\rho_{\text{diff},ij}^{(n)})_k = \frac{1}{V_{ij}} (1 - \Theta) \cdot 
\]
\[
\left[ F_{\text{adv},i+1/2,j,k}^{(n)} A_{i+1/2,j} - F_{\text{adv},i-1/2,j,k}^{(n)} A_{i-1/2,j} + 
F_{\text{adv},i,j+1/2,k}^{(n)} A_{i,j+1/2} - F_{\text{adv},i,j-1/2,k}^{(n)} A_{i,j-1/2} \right] 
\]  \hspace{1cm} (B16)

We solve Equation B14 using a biconjugate gradient stabilised solver (BiCGSTAB) as implemented in the Eigen software package (Guennebaud & Benoît 2010).

B2.2 Advection

The advection subsystem of Equation B4 is
\[
\frac{\partial}{\partial t} \rho_d^{(n)}_{ijk} = -v_T \cdot \nabla \rho_d^{(n)}_{ijk} 
\]
\[
\left[ F_{\text{adv},i+1/2,j,k}^{(n)} A_{i+1/2,j} - F_{\text{adv},i-1/2,j,k}^{(n)} A_{i-1/2,j} + 
F_{\text{adv},i,j+1/2,k}^{(n)} A_{i,j+1/2} - F_{\text{adv},i,j-1/2,k}^{(n)} A_{i,j-1/2} \right] 
\]  \hspace{1cm} (B17)

We solve this subsystem using the same TVD approach described in Appendix A3.2. Given a starting state \( \rho_d^{(n)}_{ijk} \), we advance the calculation from \( t_n \) to \( t_{n+1} = t_n + \Delta t \) via
\[
\rho_d^{(n+1)}_{ijk} = \rho_d^{(n)}_{ijk} + \Delta t (\rho_{\text{adv}}^{(n)}_{ijk}) 
\]  \hspace{1cm} (B18)

\[
\rho_{\text{adv}}^{(n)}_{ijk} = -\frac{1}{V_{ij}} \cdot 
\left[ F_{\text{adv},i+1/2,j,k}^{(n)} A_{i+1/2,j} - F_{\text{adv},i-1/2,j,k}^{(n)} A_{i-1/2,j} + 
F_{\text{adv},i,j+1/2,k}^{(n)} A_{i,j+1/2} - F_{\text{adv},i,j-1/2,k}^{(n)} A_{i,j-1/2} \right] 
\]  \hspace{1cm} (B19)

where
\[
(\rho_{\text{adv}}^{(n)}_{ijk})^{(s)} = \frac{1}{2} (\rho_{\text{adv}}^{(n)}_{ijk}) + \frac{1}{2} \Delta t (\rho_{\text{adv}}^{(s)}_{ijk}) 
\]

is the rate of change in \( \rho_{\text{adv}}^{(n)}_{ijk} \) evaluated using the density field \( \rho_d^{(n)}_{ijk} \) and similarly for \( \rho_{\text{adv}}^{(s)}_{ijk} \). We evaluate these terms in three steps.

First, for the initial density field \( \rho_d^{(n)}_{ijk} \) or \( \rho_d^{(s)}_{ijk} \), we compute a piecewise-parabolic method (PPM) reconstruction of the density field using the generalised PPM method of Skinner et al. (2018), which extends the classical Colella & Woodward (1984) PPM method to curvilinear, non-uniform coordinates. Specifically, in the radial direction we approximate the density of grains in size bin \( k \) as a function of position within cell \( ij \) with a parabolic function
\[
\rho_{d,k}(r) = c_{0,ijk} + c_{1,ijk} x(r) + c_{2,ijk} x(r)^2, 
\]  \hspace{1cm} (B21)

where the reconstruction has the property that the average of \( \rho_{d,k}(r) \) over the volume of cell \( ij \) is \( \rho_{d,ijk} \), and the function \( \rho_{d,k}(r) \) is monotonic for \( r \in (r_{i-1/2}, r_{i+1/2}) \). The reconstruction coefficients \( c_0 \), \( c_1 \), and \( c_2 \) are functions of \( \rho_{d,i-1/2,j,k}, \rho_{d,i,j-1,k}, \rho_{d,i,j,k} \), and \( c_{d,i+1,j,k} \), and chosen via the procedure described by Skinner et al. (2018). The reconstruction is third-order accurate for smooth flows. We use the same procedure to obtain a PPM reconstruction of the density field in the \( \mu \) direction.

Second, we calculate the velocities at cell faces. For each grain size bin we define \( B_k \) by using \( a_k \) in Equation 21, and we discretize Equation 19 for the optical depth to cell edge \( i + 1/2 \) along angle \( j \) as
\[
\tau_{i+1/2,j} = \sum_k \frac{3}{4a_k} \int_{r_i}^{r_{i+1/2}} \left( c_{0,ijk} + c_{1,ijk} x(r) + c_{2,ijk} x(r)^2 \right) dr. 
\]  \hspace{1cm} (B22)

The integrals are trivial to evaluate analytically in each cell, since \( x(r) \) is a known function. Given \( \rho_{d,k} \) and \( \tau_{i+1/2,j} \), along with the local Keplerian speed \( \Omega_k \), gas velocity \( v_g, \sigma_r \), and stopping time \( t_s \) (computed from our analytic background gas model), we can use Equation 28 and Equation 35 to evaluate the \( \sigma_r \) and \( z \) velocities each face \( i + 1/2, j \), which we can trivially transform into the velocities \( v_{d,r,i+1/2,j,k} \) and \( v_{d,\sigma_r,i+1/2,j,k} \) that we require. Our strategy for cell faces \( i, j + 1/2 \) in the \( \theta \) direction is similar, except that we cannot use the PPM reconstruction of the density field for rays along cell edges in the \( \theta \) direction because it is not guaranteed to be continuous at cell edges. For this reason, we instead use an appropriately modified version of Equation B22 to evaluate the optical depth to cell centres \( ij \), and then take \( \tau_{i+j+1/2} = (\tau_{ij} + \tau_{ij+1/2})/2 \). This then provides the velocities at the \( i, j + 1/2 \) faces.

The third and final step is to calculate the rate of change terms. Consider the upper radial cell face, \( i + 1/2, j \), at which the velocity is \( v_r = v_{r,i+1/2,j} \). After time \( \Delta t \), the contact discontinuity between the two cells adjoining the face will be displaced from its initial location \( r_c = r_{i+1/2,j} \) to a new location \( r'_{c} = r_{c} - v_{r} \Delta t \), and thus, using our PPM reconstruction, the mass transported across the cell face during this time is
\[
\Delta M_{i+1/2,j,k} = 2\pi \Delta r. \quad \left\{ \begin{array}{ll}
\int_{r'_{c}}^{r_{c}} [c_{0,ijk} + c_{1,ijk} x(r) + c_{2,ijk} x(r)^2] r^2 dr, & v_c > 0 \\
\int_{r_{c}}^{r'_{c}} [c_{0,ijk} + c_{1,ijk} x(r) + c_{2,ijk} x(r)^2] r^2 dr, & v_c < 0
\end{array} \right. 
\]  \hspace{1cm} (B23)

The corresponding mass flux is \( F_{\text{adv},i+1/2,j,k} = \Delta M_{i+1/2,j,k}/A_{i+1/2,j} \). The expressions for the other three cell faces are analogous.

This completes a specification of the spatial discretization of Equation 1; the full scheme we have described is second-order accurate in space.

B3 Boundary conditions

Evaluation of the fluxes at the domain boundaries requires specification of boundary conditions. In the angular direction, we enforce zero advective and diffusive flux both across the midplane at \( \mu = 0 \) and out of the top of the disc at \( \mu = \mu_{\text{max}} \). In terms of our spatial discretisation, this amounts to setting \( v_{d,i+1/2,j,k} = 0 \) and \( D_{d,j,k} = 0 \) for all \( j = -1/2 \) and \( j = N_{\theta} - 1/2 \). In the radial direction, we use closed box boundary conditions for diffusion, and therefore set \( D_{d,j,k} = 0 \) for all \( i = -1/2 \) and \( i = N_r - 1/2 \).

The advective radial flux requires a more sophisticated treatment. We wish to allow material to be advected inward across the inner radial boundary by drag, and to be pushed outward through the outer radial boundary by radiation. However, we do not wish new material to be able to enter the domain. We therefore adopt diode boundary...
conditions. At the inner boundary, we solve for the velocity across the innermost cell face \( v_{d\,-1/2,\,j,\,k,\,r} \) as described in the previous section, but if \( v_{d\,-1/2,\,j,\,k,\,r} > 0 \) (i.e., if the velocity is radially outward, and thus into the domain), we set \( v_{d\,-1/2,\,j,\,k,\,r} = 0 \) so that no mass enters the domain from smaller radii. We treat the outer boundary in the same way: we compute \( v_{d\,N,\,-1/2,\,j,\,k,\,r} \), but if the resulting value is negative, indicating flow into the computational domain, we reset the value to zero.

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