

Mixing and Settling in Disks

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1 Vertical equilibrium between mixing and settling

Mulders and Dominik (2012) write down the continuity equation for the size-dependent dust mass density $\rho_d(a)$ as

$$\frac{\partial \rho_d}{\partial t} = \underbrace{\frac{\partial}{\partial z} \left(\rho D_d \frac{\partial}{\partial z} \left(\frac{\rho_d}{\rho} \right) \right)}_{j_{\text{diff}}} - \underbrace{\frac{\partial}{\partial z} \left(\rho_d \overset{\circ}{v}_{\text{dr}} \right)}_{j_{\text{set}}} \quad (1)$$

where ρ is the gas mass density, t the time and z the vertical coordinate. It is assumed that

- there is no bulk motion of the gas $\vec{v} = 0$,
- grains are transported downwards by gravitational settling with their size-dependent equilibrium settling velocity $\overset{\circ}{v}_{\text{dr}}(a)$,
- grains are transported upwards by eddy diffusion according to the size-dependent dust diffusion coefficient $D_d(a)$, driven by dust particle concentration gradients $\frac{\partial}{\partial z} \left(\frac{\rho_d(a)}{\rho} \right)$,
- grains are passive tracers in this model, their size and mass is assumed not to change, e.g. due to coagulation, shattering or ice formation.

The latter assumption is not quite so obvious. Grains could, for example, be shattered in the midplane, then mixed up by turbulence where they would re-grow and settle back to the midplane. Assuming that the grains have relaxed towards a steady state, we have for each size $\frac{\partial \rho_d}{\partial t} \rightarrow 0$ and zero net flux $j_{\text{diff}} - j_{\text{set}} \rightarrow 0$

$$\rho D_d \frac{\partial}{\partial z} \left(\frac{\rho_d}{\rho} \right) = \rho_d \overset{\circ}{v}_{\text{dr}}, \quad (2)$$

from which we find

$$\boxed{\frac{\partial}{\partial z} \left(\ln \frac{\rho_d}{\rho} \right) = \frac{\overset{\circ}{v}_{\text{dr}}}{D_d}}. \quad (3)$$

Equation (3) addresses the speed at which the *dust densities falls off quicker than the gas* with increasing height. Integration from 0 to z results in

$$\ln \frac{\rho_d(z)/\rho_d(0)}{\rho(z)/\rho(0)} = \int_0^z \frac{\overset{\circ}{v}_{\text{dr}}(z')}{D_d(z')} dz' \quad (4)$$

As long as the integral on the right side is small ($\ll 1$), the dust densities follow the gas densities. Otherwise (keeping in mind that $\overset{\circ}{v}_{\text{dr}}$ is downward, hence negative), the dust densities will subside sooner than the gas. Larger particles have larger $\overset{\circ}{v}_{\text{dr}}$, so they are more affected than small grains.

2 Basic processes

2.1 Gravitational settling

For large Knudsen numbers and subsonic particle velocities (Epstein regime), the equilibrium settling velocity, also called terminal fall speed, is given by Schaaf (1963)

$$\overset{\circ}{v}_{\text{dr}} = -\frac{g_z \rho_m a}{\rho v_{\text{th}}} = -g_z \tau_{\text{stop}} \quad (5)$$

where g_z is the vertical gravitational acceleration, a is the particle radius, ρ_m the dust material density, and where the thermal velocity is given by

$$v_{\text{th}} = \sqrt{\frac{8kT}{\pi\mu}} = \sqrt{\frac{8}{\pi}} c_s . \quad (6)$$

k the Boltzman constant, T the local gas temperature, μ the mean molecular mass, c_s the local isothermal speed of sound, and $p = c_s^2 \rho$ the local gas pressure. Equation (5) seems widely incorrect in the literature, where often c_s is sloppily used instead of the correct mean of the magnitude of the thermal velocities of gas particles v_{th} , as required in Schaaf's formula, see Woitke and Helling (2003). The second part of Eq. (5) follows from a general relaxation ansatz

$$\tau_{\text{stop}} = m \left(\left. \frac{\partial F_{\text{fric}}}{\partial v_{\text{dr}}} \right|_{v_{\text{dr}}} \right)^{-1} = \frac{\rho_m a}{\rho v_{\text{th}}} , \quad (7)$$

where τ_{stop} is the stopping or frictional coupling timescale, m the mass of a dust particle, $F_{\text{fric}}(\rho, a, v_{\text{dr}})$ the frictional force for large Knudsen numbers and subsonic particle drift $v_{\text{dr}} \ll c_s$, see Eq. (21) in Woitke and Helling (2003).

2.2 Gas diffusion

Eddy diffusion (“turbulent mixing”) is assumed to be dominant over gas-kinetic diffusion. The eddy diffusion coefficient in general is given by a characteristic velocity times a characteristic length

$$D_{\text{gas}} = \langle v_z \rangle L \quad (8)$$

where L is the size of the largest eddies (“mixing length”) and $\langle v_z \rangle$ the root-mean square average of the fluctuating part of the vertical gas velocities.

2.3 Dust diffusion

In a Kolmogorov type of power spectrum $P(k) \propto k^{-5/3}$, there are different turbulent modes associated with different wave-numbers k or different spatial eddy sizes l . Any given particle of size a tends to co-move with all sufficiently large and slow turbulent eddies whereas its inertia prevents following the short-term, small turbulence modes. In order to arrive at an effective particle diffusion coefficient, the advective effect of all individual turbulent eddies has to be averaged, and thereby transformed into a collective particle diffusion coefficient. This procedure is carried out with different methods and approximations, see Dubrulle et al. (1995), Schr apler and Henning (2004) and Youdin and Lithwick (2007). The result of Schr apler and Henning (2004, see their Eq. 27), reads

$$D_d = \frac{D_{\text{gas}}}{1 + St} \quad (9)$$

where St is the Stokes number given by

$$St = \frac{\tau_{\text{stop}}}{\tau_{\text{eddy}}} . \quad (10)$$

τ_{eddy} is the eddy turnover or turbulence correlation timescale in consideration of the largest eddy, which is assumed to equal the mixing length L .

$$\tau_{\text{eddy}} = \frac{L}{\langle v_z \rangle} . \quad (11)$$

Our basic equation (3) for the balance of upward mixing against gravitational settling is hence

$$\boxed{\frac{\partial}{\partial z} \left(\ln \frac{\rho_d}{\rho} \right) = - \frac{g_z \tau_{\text{stop}}}{D_{\text{gas}}} (1 + St)} . \quad (12)$$

3 Disk physics

So far, our approach is quite general, describing an equilibrium between settling and mixing in a relaxed 1D structure, as long as our dust particles are in the Epstein regime and chemically/physically passive. In the following, we introduce a bit of disk jargon which will enable us to make the connections to the disk literature. On Keplerian orbits, at pressure-supported height z above the midplane, the zentrifugal force caused by the rotation around the symmetry axis is balanced by the radial component of gravity

$$\frac{v_K^2}{r} = \Omega^2 r = g_r, \quad (13)$$

where v_K is the Keplerian velocity and the gravity has components

$$g = \frac{GM_\star}{r^2 + z^2} \quad \text{with components} \quad \frac{g_r}{g} = \frac{r}{\sqrt{r^2 + z^2}} \quad \text{and} \quad \frac{g_z}{g} = \frac{z}{\sqrt{r^2 + z^2}} \quad (14)$$

r is the distance from the symmetry axis and z the height above the midplane. We find

$$\Omega^2 = \frac{GM_\star}{(r^2 + z^2)^{3/2}} \approx \frac{GM_\star}{r^3} \quad (15)$$

$$v_K^2 = \frac{GM_\star r^2}{(r^2 + z^2)^{3/2}} \approx \frac{GM_\star}{r} \quad (16)$$

$$g_z = \frac{GM_\star z}{(r^2 + z^2)^{3/2}} = z \Omega^2 \quad (17)$$

The approximations on the right side are called the “thin disk” approximation. Ω is the Keplerian circular frequency. The condition of vertical hydrostatic equilibrium can be expressed by

$$\frac{\partial p}{\partial z} = -\rho g_z = -\rho z \Omega^2. \quad (18)$$

For thin disks with vertically constant temperature T and vertically constant mean molecular weight μ , we can write $\frac{\partial p}{\partial z} = c_s^2 \frac{\partial \rho}{\partial z}$ which allows us to integrate Eq. (18) as

$$\frac{\partial}{\partial z} \ln \rho = -z \frac{\Omega^2}{c_s^2} \quad \Rightarrow \quad \rho(z) = \rho_0 \exp\left(-\frac{z^2}{2 H_p^2}\right) \quad (19)$$

$$\text{with pressure scale height} \quad H_p = c_s / \Omega, \quad (20)$$

and our basic equation (12) reads

$$\boxed{\frac{\partial}{\partial z} \left(\ln \frac{\rho_d}{\rho} \right) = -\frac{z \Omega^2 \tau_{\text{stop}}}{D_{\text{gas}}} (1 + St)}. \quad (21)$$

According to an α disk model (Shakura and Sunyaev, 1973), the typical vertical length scale is $L = H_p$ and the turbulent velocity is $\langle v_z \rangle = \alpha c_s$, so the eddy diffusion coefficient is given by

$$D_{\text{gas}} = \alpha c_s H_p \quad (22)$$

$$\tau_{\text{eddy}} = \frac{H_p}{\alpha c_s} = \frac{1}{\alpha \Omega} \quad (23)$$

$$\tau_{\text{stop}} = St \tau_{\text{eddy}} = \frac{St}{\alpha \Omega}. \quad (24)$$

Something strange happens here, as Dubrulle et al. (1995), Schr apler and Henning (2004) and Riols and Lesur (2018) all have $\tau_{\text{eddy}} = H_p / c_s = 1 / \Omega$ which I don’t understand. The eddy turnover

timescale must be much larger than this, because typical turbulent velocities are αc_s , i.e. much smaller than c_s , because $\alpha \ll 1$. According to Eq. (24) we then have

$$\frac{\partial}{\partial z} \left(\ln \frac{\rho_d}{\rho} \right) = - \frac{z \Omega St}{\alpha D_{\text{gas}}} (1 + St), \quad (25)$$

which is not quite as general as Eq. (21), because $c_s = H_p \Omega$ has been used, which requires $T = \text{const}$ and $\mu = \text{const}$. All quantities on the right hand side of Eq. (25), Ω , St , α and D_{gas} , as well as T , c_s , μ and ρ_m , will in general depend on height z . In addition, St and τ_{stop} depend on grain size a .

4 Application in disks

4.1 Dubrulle et al. (1995)

Dubrulle et al. (1995) ignore all z -dependences on the r.h.s. of Eq. (21) and replace all those variables by their mid-plane values. They apparently drop the $(1 + St)$ term and assume $St = \tau_{\text{stop}}(0) \Omega$, i.e. without the α . In that case, we carry out the z -integration over

$$\frac{\partial}{\partial z} \left(\ln \frac{\rho_d}{\rho} \right) = - \frac{z \Omega^2 \tau_{\text{stop}}(0)}{\alpha c_s(0) H_p} \quad (26)$$

which results in

$$\ln \frac{\rho_d / \rho_d(0)}{\rho / \rho(0)} = - \frac{\Omega^2 \tau_{\text{stop}}(0)}{\alpha c_s(0) H_p} \int_0^z z' dz' = - \frac{z^2}{2 H_p^2} \frac{\Omega^2 \tau_{\text{stop}}(0) H_p}{\alpha c_s(0)} = - \frac{z^2}{2 H_p^2} \frac{\Omega \tau_{\text{stop}}(0)}{\alpha}. \quad (27)$$

We introduce the size-dependent dust scale height H_a via $\rho_d(a, z) = \rho_d(a, 0) \exp(-\frac{z^2}{2 H_a^2})$ to find

$$\Rightarrow - \frac{z^2}{2 H_a^2} + \frac{z^2}{2 H_p^2} = - \frac{z^2}{2 H_p^2} \frac{\Omega \tau_{\text{stop}}(0)}{\alpha} \quad (28)$$

$$\Rightarrow \boxed{\frac{H_p^2}{H_a^2} = 1 + \frac{\Omega \tau_{\text{stop}}(0)}{\alpha}} \quad (29)$$

Notes about the implementation in ProDiMo:

In ProDiMo there are variables called

$$St' = \frac{\Omega \rho_m a}{\rho(0) c_s(0)} \quad \text{and} \quad \text{Hh2} = \sqrt{3} \frac{St'}{\alpha} \quad \text{and} \quad \text{reduce} = \frac{H_a^2}{H_p^2} = \frac{1}{1 + \text{Hh2}}$$

so the Dubrulle midplane-settling is currently implemented as

$$\frac{H_p^2}{H_a^2} = 1 + \frac{\sqrt{3} \Omega \rho_m a}{\alpha \rho(0) c_s(0)} = 1 + \sqrt{3} \frac{v_{\text{th}}}{c_s(0)} \frac{\Omega \tau_{\text{stop}}(0)}{\alpha} \quad (30)$$

Comparison to Eq. (29) reveals a mismatch of a factor $\sqrt{\frac{3 \times 8}{\pi}} \approx 2.76$ for Hh2, which is substantial as it enters in the exponential, equivalent to the viscosity parameter α being off by that factor.

For hydrostatic models, an additional complication is that one should interpret H_p as an actual pressure scaleheight rather than a density scaleheight, so considering (partial) pressures rather than densities, we write

$$\frac{f(a, z) c_s^2(z)}{f(a, 0) c_s^2(0)} = \exp \left(\frac{\ln(p(z)/p(0))}{\text{reduce}} \right) = \exp \left(\frac{\ln p(z)}{\text{reduce}} - \frac{\ln p(0)}{\text{reduce}} \right) \quad (31)$$

This is done to ensure a monotonic decrease of $f(a, z)$ with height in the hydrostatic mode, where $p(z)$ decreases monotonically, but $\rho(z)$ may not, because of sudden changes in $T(z)$ or $\mu(z)$. Since $C = f(a, 0) c_s^2(0)$ is a constant normalisation factor, and $\text{const} = \ln p(0)/\text{reduce}$ is constant, too, we calculate the dust size distribution function $f(a)$ from

$$f(a, z) \propto \frac{1}{c_s^2(z)} \exp\left(\frac{\ln p(z)}{\text{reduce}} - \text{const}\right). \quad (32)$$

In the mostly used MCFOST-like mode, where $\rho(r, z)$ is set parametrically, H_p is constant and hence well-defined, $c_s(z) = c_s(0)$ is assumed, and $c_s(0) = H_p \Omega$ is used to determine $c_s(0)$, the “pressure” is computed as $p(z) = c_s^2(0)\rho(z)$, and we simply have

$$\frac{f(a, z)}{f(a, 0)} = \exp\left(-\frac{z^2}{2 H_p^2 \text{reduce}}\right) \quad (33)$$

but we use Eq. (32) instead, also in the MCFOST-like mode, where it is equally valid. Equation (33) explains the meaning of “reduce”, namely the factor by which the gas scale height² is reduced for size a . Eventually, $f(a, 0)$ is fixed by the normalisation condition to have the same dust column density before/after settling in each size bin.

4.2 Riols & Lesur (2018)

Riols and Lesur (2018) also drop the $(1 + St)$ term and start with Eq. (25), taking into account that St is, and Ω and D_{gas} might be, z -dependent. They furthermore explicitly assume a Gaussian for the vertical gas density distribution, $\rho = \rho(0) \exp\left(-\frac{z^2}{2 H_p^2}\right)$, and since $St \propto 1/\rho$ they write

$$St = St(0) \exp\left(\frac{z^2}{2 H_p^2}\right) = \alpha \Omega \tau_{\text{stop}}(0) \exp\left(\frac{z^2}{2 H_p^2}\right), \quad (34)$$

Equation (25) hence becomes

$$\frac{\partial}{\partial z} \left(\ln \frac{\rho_d}{\rho} \right) = -\frac{z \Omega St}{\alpha D_{\text{gas}}} = -\frac{z \Omega St(0)}{\alpha D_{\text{gas}}} \exp\left(\frac{z^2}{2 H_p^2}\right) \quad (35)$$

and integration yields

$$\ln \frac{\rho_d/\rho_d(0)}{\rho/\rho(0)} = -\int_0^z \frac{z' \Omega St(0)}{\alpha D_{\text{gas}}} \exp\left(\frac{z'^2}{2 H_p^2}\right) dz', \quad (36)$$

which reproduces Eq. (33) in Riols and Lesur (2018) if one keeps in mind that their definition of St misses the α .

$$\frac{\rho_d}{\rho_d(0)} = \exp\left(-\frac{z^2}{2 H_p^2}\right) \exp\left(\int_0^z \frac{z' \Omega St(0)}{\alpha D_{\text{gas}}} \exp\left(\frac{z'^2}{2 H_p^2}\right) dz'\right). \quad (37)$$

With the additional assumption that Ω , D_{gas} and α are z -independent we find

$$\ln \frac{\rho_d}{\rho_d(0)} = -\frac{z^2}{2 H_p^2} - \frac{\Omega St(0)}{\alpha D_{\text{gas}}} \int_0^z z' \exp\left(\frac{z'^2}{2 H_p^2}\right) dz' \quad (38)$$

$$-\frac{z^2}{2 H_a^2} = -\frac{z^2}{2 H_p^2} - \frac{\Omega St(0)}{\alpha D_{\text{gas}}} H_p^2 \left(\exp\left(\frac{z^2}{2 H_p^2}\right) - 1 \right) \quad (39)$$

$$\frac{H_p^2}{H_a^2} = 1 + \frac{\Omega St(0) H_p^2}{\alpha D_{\text{gas}}} \left(\frac{2 H_p^2}{z^2}\right) \left(\exp\left(\frac{z^2}{2 H_p^2}\right) - 1 \right) \quad (40)$$

$$\Rightarrow \boxed{\frac{H_p^2}{H_a^2} = 1 + \frac{\tau_{\text{stop}}(0)\Omega}{\alpha} \left(\frac{2H_p^2}{z^2}\right) \left(\exp\left(\frac{z^2}{2H_p^2}\right) - 1\right)} \quad (41)$$

which clearly shows the improvement with respect to the Dubrulle et al. (1995) formula (Eq. 29). The decrease of the dust scaleheight H_a with respect to Eq. (29) is remarkable, the function $(2/x^2)(\exp(x^2/2) - 1)$ is 3.19 at $x = 2$, 20 at $x = 3$, 370 at $x = 4$ and 21000 at $x = 5$. Infrared emission lines from disks, for example, are quite typically emitted from layers located at about 3–4 scaleheights, see e.g. Woitke et al. (2018), their Fig. 8, where lines from OH, H₂O, CO₂ and HCN are emitted from $z/r \approx 0.15 - 0.2$ and the scale height at 1 au is $H_p = 10 \text{ au} \left(\frac{1 \text{ au}}{100 \text{ au}}\right)^{1.15} = 0.05 \text{ au}$.

Notes about the implementation in ProDiMo:

In ProDiMo the following variables are used

$$St'(0) = \frac{\Omega \rho_m a}{\rho(0) c_s(0)} \quad \text{and} \quad \text{Hh2} = \sqrt{3} \frac{\Omega St'(0) H_p^2}{D_{\text{gas}}} \quad \text{and} \quad D_{\text{gas}} = \alpha c_s H_p$$

$$\text{fak} = \left(\frac{2H_p^2}{z^2}\right) \left(\exp\left(\frac{z^2}{2H_p^2}\right) - 1\right) \quad \text{and} \quad \text{reduce} = \frac{H_a^2}{H_p^2} = \frac{1}{1 + \text{Hh2 fak}}$$

The same inconsistency of a factor $\sqrt{\frac{3 \times 8}{\pi}} \approx 2.76$ occurs. It remains unclear to me why both Dubrulle et al. (1995) and Riols and Lesur (2018) have not taken into account the $(St + 1)$ factor in the dust diffusion coefficient.

Riols & Lesur in hydrostatic models

In the hydrostatic case, where $T_{\text{gas}}(z)$, $\mu(z)$ and $p(z)$ are consistently calculated from the chemistry and gas energy balance, and where consequently the scale height H_p is not constant and ill-defined, we follow the same concept

$$\frac{\partial}{\partial z} \left(\ln \frac{f(a, z) c_s^2(z)}{p(z)} \right) = - \frac{z \Omega^2 \tau_{\text{stop}}(a, z)}{D_{\text{gas}}(z)} (1 + St(a, z)) . \quad (42)$$

With the same simplifications used above, i.e. drop $(1 + St)$, use $\tau_{\text{eddy}} = 1/\Omega$, use $\tau_{\text{stop}} = \sqrt{3} \rho_m a / (\rho c_s)$, use $D_{\text{gas}} = \alpha c_s H_p = \alpha c_s^2 / \Omega$, the result is

$$\ln \frac{f(a, z) c_s^2(z)}{f(a, 0) c_s^2(0)} = \ln \frac{p(z)}{p(0)} - \underbrace{\frac{\sqrt{3} a}{\alpha} \int_0^z z' \frac{\Omega^3 \rho_m(z')}{c_s^3(z') \rho(z')} dz'}_{F(z)} \quad (43)$$

$$f(a, z) \propto \frac{1}{c_s^2(z)} \exp\left(\ln \frac{p(z)}{p(0)} - F(z)\right) \quad (44)$$

Since $\rho(z)$ becomes small as z increases, $F(z)$ will reach the order of unity at some point, and then soon becomes $\gg 1$, which means that $f(a, z)$ rapidly declines, by orders of magnitude, beyond that point. Equations (43) and (44) are implemented in ProDiMo for the case of hydrostatic models with Riols and Lesur (2018)-settling. The integral in Eq. (43) is solved numerically from bottom to top in each column for each dust size bin.

If we rather believe in the equations explained in this article, we would have

$$\ln \frac{f(a, z) c_s^2(z)}{f(a, 0) c_s^2(0)} = \ln \frac{p(z)}{p(0)} - \frac{a}{\alpha} \int_0^z z' \frac{\Omega^3 \rho_m(z')}{v_{\text{th}}(z') c_s^2(z') \rho(z')} (1 + St(a, z')) dz' \quad (45)$$

with $St = \alpha \Omega \tau_{\text{stop}}$, which, because of the additional $(1 + St)$ -factor, would lead to even more extreme settling results.

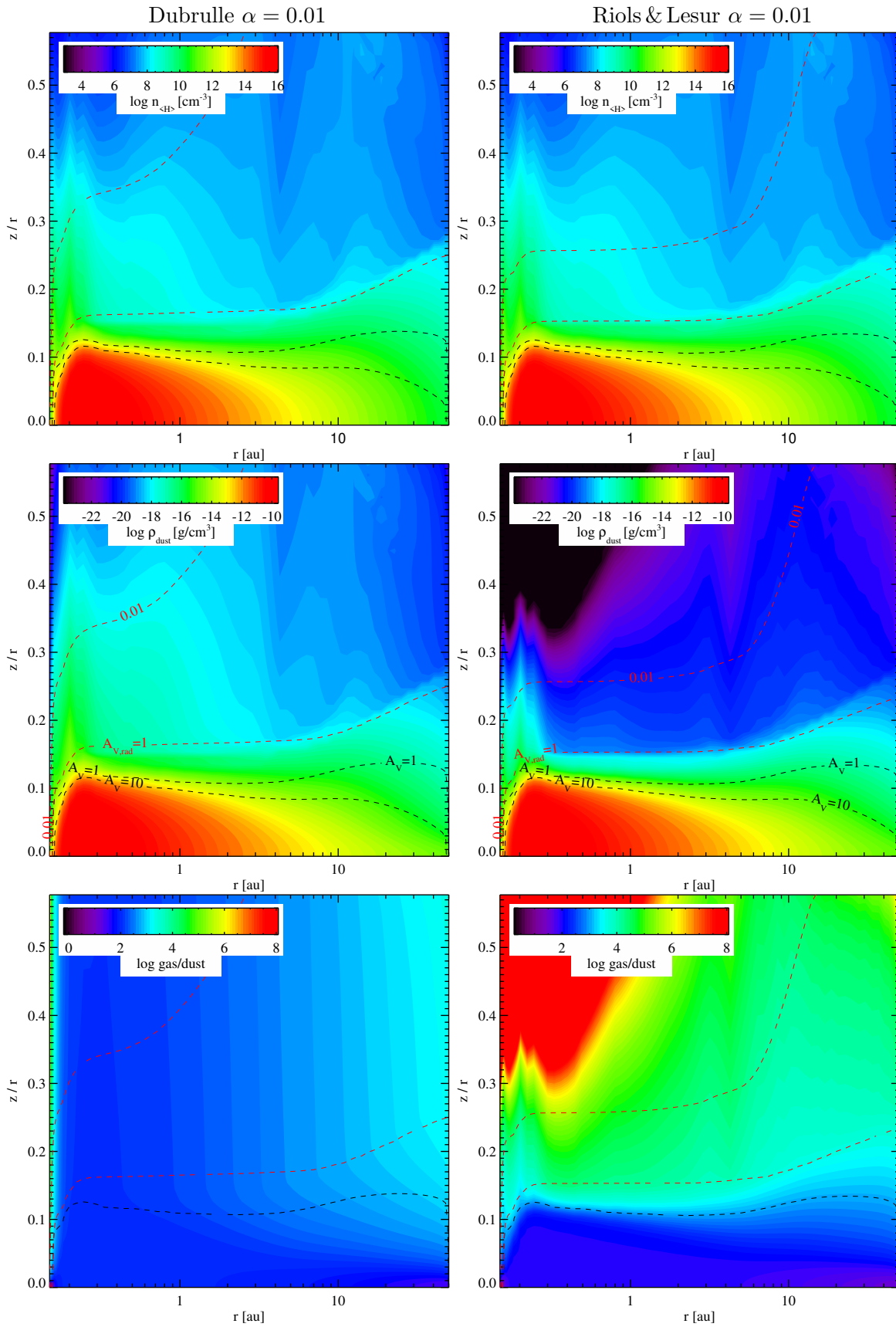


Figure 1: Results for the Dubrulle et al. (1995) and the Riols and Lesur (2018) settling, both with $\alpha = 0.01$. The model is for a MMSN-type hydrostatic disk around an 1Myr old T Tauri star ($M = 1 M_{\odot}$, $L_{\star} = 2.24 L_{\odot}$, $T_{\text{eff}} = 4280 \text{ K}$) with $\Sigma_{\text{dust}}(1 \text{ au}) = 1700 \text{ g/cm}^2$, $\epsilon = 1.5$ and $\dot{M}_{\text{acc}} = 10^{-8} M_{\odot}/\text{yr}$ with viscous heating. The gas density, temperature, and pressure distributions are the same in both models, they are taken from the consistent model with Dubrulle-settling, but then frozen for the right model with Riols & Lesur settling.

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