Disk physical model for Nautilus

V. Wakelam, L. Majumdar

Feb 2017

We present the physical model used as input for Nautilus. The temperature, density and visual extinction profiles are computed in the vertical direction at a specific radius from the central star. The dust temperature can also be provided. To mimic the grain sedimentation and growth, the abundance of grains, size and AV/NH conversion factor can be given for each altitude. This code computes these quantities from some specific parameters. A fortran procedure has been created to produce a file containing all these quantities at each height, starting from the most external point of the envelop. This document shows the exact calculations that are being done. For more physical description, we refer to Hersant et al. (2009); Wakelam et al. (2016).

1 Input parameters

The input parameters for the IDL procedure are the following:

- Number of spatial points in the vertical direction (resolution of the grid): nbpoints.
- Radius in disk from the star where we want the vertical structure in AU: r.
- Mass of the central object in g: M_*.
- Mid-plane temperature (in K) of the gas at radius (R) in AU constrained by the observations: T_{midplanR}.
- Gas temperature (in K) in the atmospheric limit (at 4 scale height) at radius (R) constrained by the observations : T_{atmosR}.
- Surface density at R AU (in g.cm^{-2}): Σ_R. This is constrained by observations.
- UV irradiation field coming from the central star at R AU: UV_R. In our model, we assume that the UV spectrum of the central star has the same as the ISM. Thus this parameter is a factor of Draine's ISM UV field.
- Exponent of the radial variation of temperature: q. This parameter is constrained by observations.
- Stiffness of the vertical temperature profile: σ.

- Exponent of the radial variation of density: d. This is constrained by observations.

- Dust to gas mass ratio: dtogm_up. This is usually taken to 10^{-2}. In the case of homogeneous grains, this value is used for all altitudes. In the case of sedimentation, this parameter is the dust to gas mass ratio in the upper part of the disk.

- Grain sizes (in cm): small_grains and big_grains. We assume that the small grains are in the upper atmosphere while the big grains are in the lower atmosphere.

- Transition altitude (in z/H): transition_altitude. This is the altitude of transition of small grains to big grains.

2 Constants

Here are the constants that are used for the calculation:

- Boltzmann constant: $k_B = 1.38054 \times 10^{-16}$ in erg.K^{-1}.

- Conversion factor from AU to cm: autocm=1.49597×10^{13}.

- Mean molecular weight of the gas: μ=2.4. The mean molecular weight of the gas is by default equal to the solar metallicity value μ=2.4 but can be varied between μ=2 (pure molecular hydrogen) and μ=3 (highly metal rich). See Mayer et al. (2008) for more discussions.

- Atomic mass unit: amu=1.66043×10^{-24} g

- Gravitational constant: G=6.668×10^{-8} cm^{3}g^{-1}s^{-2}

- Conversion factor of H column density to Av: $AV/NH_0 = 6.25 \times 10^{-22}$. From Wagenblast & Hartquist (1989).

3 Computation of mid-plane and atmospheric temperatures at a given radius r

If the mid-plane and atmospheric temperatures are observationally constrained at R AU, then mid-plane and atmospheric temperatures at the selected radius r are computed through:

$$\mathrm{T_{midplan}} = \mathrm{T_{midplanR}} \times \left(\frac{\mathrm{r}}{\mathrm{R}}\right)^{-\mathrm{q}} \tag{1}$$

$$\mathrm{T_{atmos}} = \mathrm{T_{atmosR}} \times \left(\frac{\mathrm{r}}{\mathrm{R}}\right)^{-\mathrm{q}} \tag{2}$$

4 Computation of the scale heights H and H_{atmos}

H is the scale height (in cm) defined by the mid-plane temperature and assuming vertical static equilibrium. H is computed by the equation:

$$\mathrm{H} = \sqrt{\frac{\mathrm{k_B \times T_{mid-plan} \times (r \times autocm)^3}}{\mathrm{\mu amuGM_*}}} \tag{3}$$

H_{atmos} is the scale height defined by T_{atmos}:

$$\mathrm{H_{atmos}} = \sqrt{\frac{\mathrm{k_B T_{atmos} \times (rautocm)^3}}{\mathrm{\mu amuGM_*}}} \tag{4}$$

5 Computation of the vertical grid

The total size of the box is 4H. z will be a table of spatial points vertically distributed and equally spaced. z is computed with the formula given by Franck Hersant:
for i=0,nbpoints-1 do $\mathrm{z(i)} = (1 - \frac{2\times \mathrm{i}}{2\times \mathrm{nbpoints}-1}) \times 4\mathrm{H}$

6 Computation of the 1D vertical temperature profile

We are using the definition by Williams & Best (2014) meaning that T is constant above 4H. Below this height, the temperature is computed using a sinus:

$$\mathrm{Tz(i)} = \mathrm{T_{midplan}} + (\mathrm{T_{atmos}} - \mathrm{T_{midplan}}) \times \left(\sin\left(\frac{\pi \mathrm{z(i)}}{2\mathrm{z(0)}}\right)\right)^{2\sigma} \tag{5}$$

7 Computation of the 1D vertical density profile

The density is computed assuming the hydrostatic equilibrium.
We first compute: $\Omega = \frac{G \times M_*}{(r \times au-conv)^3}$.

We compute the maximum $\mathrm{H_2}$ density (in $\mathrm{cm^{-3}}$), i.e. the density in the mid-plane from the surface density.

$$\mathrm{nzH2_{midplan}} = \Sigma_\mathrm{R} \times \left(\frac{\mathrm{r}}{\mathrm{R}}\right)^{-\mathrm{d}} \times \frac{1}{\mathrm{\mu amuH}\sqrt{2\pi}} \tag{6}$$

The most external point of the atmosphere $\mathrm{nzH2_0}$ will have a density of 1 for the moment.

We then compute the $\mathrm{H_2}$ density (in $\mathrm{cm^{-3}}$) for each z point:

$$\mathrm{int(i)} = \mathrm{int(i-1)} - (\ln \mathrm{Tz(i)} - \ln \mathrm{Tz(i-1)}) - \frac{\Omega \mu \mathrm{amu}}{\mathrm{k_B Tz(i) z(i)(z(i) - z(i-1))}} \tag{7}$$

$$\mathrm{nzH2(i) = \exp{(int)}} \tag{8}$$

Then a rescaling of the density is done so that the maximum density of the distribution is $\mathrm{nzH2}_{midplan}$:
for i=0,nbpoints-1 do nzH2(i) $= \frac{nzH2(i)}{max(nzH2) \times nzH2_{midplan}}$

8 Computation of the 1D vertical visual extinction profile

In the previous version of the code, we would compute the H column density above 4H (the most external point of our grid) assuming an ercf to the gaussian distribution above that point:

$$\mathrm{int} = \frac{\mathrm{4H}}{\sqrt{2} \times \mathrm{H_{atmos}}} \tag{9}$$

$$\mathrm{NH(0)} = 2 \times \frac{\mathrm{nzH2(0)} \times \mathrm{H_{atmos}} \times \sqrt{2} \times \exp{(-\mathrm{int}^2)}}{\mathrm{int} + \sqrt{\mathrm{int}^2 + 2}} \tag{10}$$

The factor of 2 is to take into account the fact that we compute total H column density from H2 densities. There is here an approximation since at this altitude, part of hydrogen will be atomic.
This formula was however wrong (the density should not be nzH2(0) and a π was missing. Thus we have decided to assume a null NH(0). After some tests, we have found that it did not make any difference except for the first point. This has no impact on the model and it simplifies the calculation.
From NH(0), we compute Avz(0):

$$\mathrm{Avz(0)} = \mathrm{NH(0)} \times \mathrm{AV/NH_0} \times \frac{\mathrm{dtogm}}{10^{-2}} \times \frac{10^{-5}}{\mathrm{r_{grain}}} \tag{11}$$

So Avz(0) = 0.
Computation of Avz for other points:
for i=1,nbpoints-1 do

$$\mathrm{Avz(i)} = \mathrm{Avz(i-1)} + 2 \times \mathrm{nH2z(i)} \times (\mathrm{z(i-1)} - \mathrm{z(i)}) \times \mathrm{AV/NH_0} \times \frac{\mathrm{dtogm}}{10^{-2}} \times \frac{10^{-5}}{\mathrm{r_{grain}}} \tag{12}$$

with r_{grain} the grain radius (in cm). This is to change the Av according to the radius of the grains while changing it.

9 Computation of the UV irradiation factor

We also compute the UV irradiation factor at the requested radius. The initial UV is divided by two because since we do not make a full 3D transfer, we assume that only half of the photons irradiated from the star diffuse into the disk, the other half diffuse in the opposite direction. The UV flux coming from the star is

Table 1: List of parameters used for our disk models

	LkCa15[a]	DMTAU[b]	MWC 480[c]	GG Tau[d]	TW Hya[e]
R (AU)	100	100	100	200	10
UV Flux	2550	410	8500	1500[f]	3400
Age (Myr)	3-5	5	7	1-5	3-10
Stellar Mass (g)	2×10^{33}	1.054×10^{33}	3.640×10^{33}	2.53×10^{33}	0.80×10^{33}
$\mathrm{T_{midplanR}}$ (K)	15	15	30	14	20
$\mathrm{T_{atmosR}}$ (K)	20	30	48	30	104
Disk mass (solar mass)	0.03	0.03	0.18	0.12	0.06
r_{out} (AU)	550	800	500	800	172
Total surface density at R (g.cm^{-2})	0.9	0.75	5.7	14.9	0.79
Temperature exponent (q)	0.5	0.5	0.5	1.1	0.55
Density exponent (d)	1.5	1.5	1.5	2.75	1.5
Temperature Stiffness (σ)	2	2	2	2	2

Notes: a-b-c: Guilloteau et al. (2011); Pitu et al. (2007); Bergin et al. (2004); Guilloteau & Dutrey (1998)

d: Guilloteau et al. (1999); Dutrey et al. (2014)

e: Andrews et al. (2012); Herczeg et al. (2004), Qi et al. (2006)

f. No measurement. Other canonical values could be used as well: 500, 3000 by discussing with A. Dutrey

assumed to have the same spectrum as the interstellar DRAINE field multiplied by a certain amount and diluted as $1/\mathrm{r}^2$.

$$\mathrm{UVfactor} = \frac{\mathrm{UVR}}{2 \times \sqrt{(\mathrm{r/R})^2 + (4\mathrm{H}/(\mathrm{R} \times \mathrm{au} - \mathrm{conv})^2)}} \tag{13}$$

10 Calculation of the total surface density at radius R

The total surface density Σ depends on the total mass of the disk and the outer radius. The mass of the disk is:

$$\mathrm{M} = \int_0^\infty 2\pi \times \mathrm{r} \times \Sigma(\mathrm{r})\mathrm{dr} \tag{14}$$

If d is 1.5, the final total surface density at R AU is:

$$\Sigma_R = \frac{M \times (R)^{-1.5} \times 0.5}{2 \times \pi \times (r_{out})^{0.5}} \tag{15}$$

11 Typical results

We here show results for the following parameters (for DMTAU):

- r = 300 AU,
- $\mathrm{M}_* = 1.054 \times 10^{33}$ g,
- $\mathrm{T}_{midplan,100} = 15$ K,

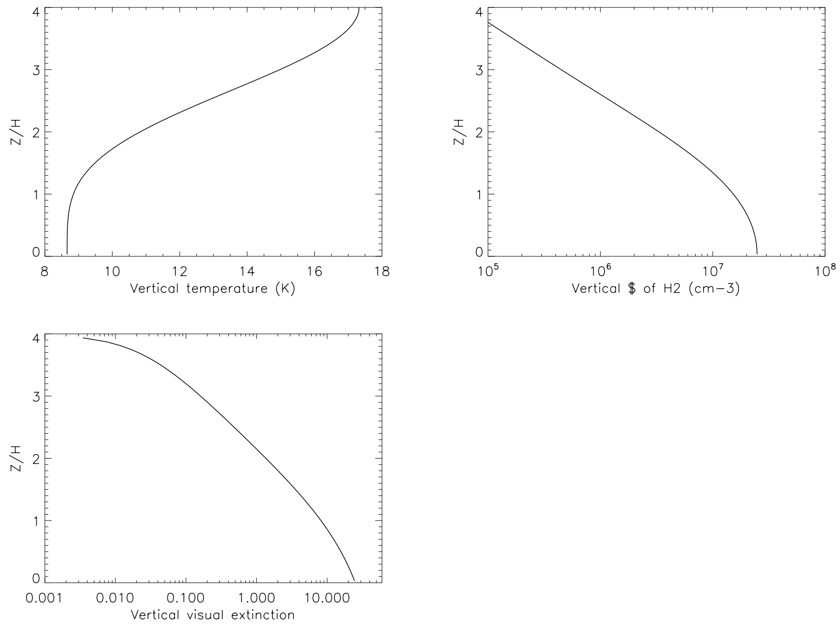

Figure 1: Physical model computed from the described equations are for the parameters given in section 11.

- $T_{midplan,100}$ = 30 K,
- UV100AU = 410,
- q = 0.5,
- $\sigma = 2$,
- $\Sigma_{100} = 0.8$ g.cm^{-2},
- d = 1.5,
- dtogm = 10^{-2}

12 Dust properties

To simulate different grain characteristics with the altitude (grain growth and sedimentation), we can read in the file 1D_static.dat file the gas-to-dust density number (GTODN, this is the inverse of the abundance of grains with respect to the total proton density), the AV to NH conversion factor (which depends on the dust to gas mass ratio) and the sizes of the grains. Only one size of grains is assumed at each altitude but they can be different at each altitude.

The dust to gas mass ratio (dtogm_up or $\frac{\rho_g}{\rho_d}$) is first changed to remove the Helium mass:

$$\frac{\rho_g}{\rho_d} = \frac{\rho_g}{\rho_d} * (1 + 4 \times Y(He)) \tag{16}$$

with Y(He) the Helium abundance indicated in the input parameter and used in the chemical model.

For the size, we will assume small grains (with radius r_{sg}, for instance 10^{-5} cm) above a certain altitude ($z_{transition}$) and big grains (r_{bg}) below this altitude. The grain radius directly influence the sticking (cross section of collision). It determines also the number of sites. This number does not change the adsorption but it changes the time for a species to scan the surface of the grains and so the time to react. The larger this value, the smaller the reactivity.

For GTODN: This parameter is directly used in the model to determine the efficiency of sticking and the mean number of species per grain. The larger 1/GTODN, the larger the reactivity. This parameter is computed from the dust-to-gas mass ratio and the size of the grains.

$$GTODN = \frac{n_H}{n_d} = \frac{\rho_g}{\rho_d} \times \frac{4\pi r_{gr}^3 \rho_{gr}}{3 m_H} \tag{17}$$

where n_H and n_d are the densities of proton and of grains, $\frac{\rho_g}{\rho_d}$ the gas to dust mass ratio, r_{gr} the radius of the grains, ρ_{gr} the density of one grain in g.cm^{-3} (commonly assumed to be 3) and m_H the atomic mass unit.

For the AV to NH conversion factor, we have used the following scaling according to the gas-to-dust mass ratio:

$$AV/NH = (AV/NH)_0 \times \frac{dtogm}{10^{-2}} \times \frac{10^{-5}}{r_{grain}} \tag{18}$$

This parameter is used for the computation of the H_2 and CO self-shielding.

12.1 Example of dust layering

As an example, we have considered two different layers of dust: small grains of 10^{-5} cm (0.1 μm) above Z/H=1 and big grains of 3×10^{-3} (30 μm) below. The dust-to-gas mass ratio (dgt1) is 10^{-3} above Z/H=1.

To have conservation of the total mass of dust in the vertical direction, the gas-to-dust mass ratio below this altitude is: $dgt2 = (10^{-2} \times (mass1 + mass2) - dgt1 \times mass1)/mass2$ with mass1 and mass2 the integrated mass of gas above and below the transitional Z/H.

In our example, mass1 is 6.28×10^{-16} g while mass2 is 1.36×10^{-15} g so that dgt2 is 0.014. This leads to an AV/NH of 6.25×10^{-23} above and 3.96×10^{-24} below.

The main consequence is on GTODN and the vertical visual extinction. The visual extinction in the mid-plan is approximately multiplied by $6 \times 10^{-3}(= \frac{dtogm}{10^{-2}} \times \frac{10^{-5}}{r_{grain}})$ (see figure 2).

The two values of GTODN are:

$$GTODN_{above} = 1/10^{-3} \times \frac{4\pi(10^{-5})^3 \times 3}{3 \times 1.66043 \times 10^{-24}} = 7.57 \times 10^{12} \tag{19}$$

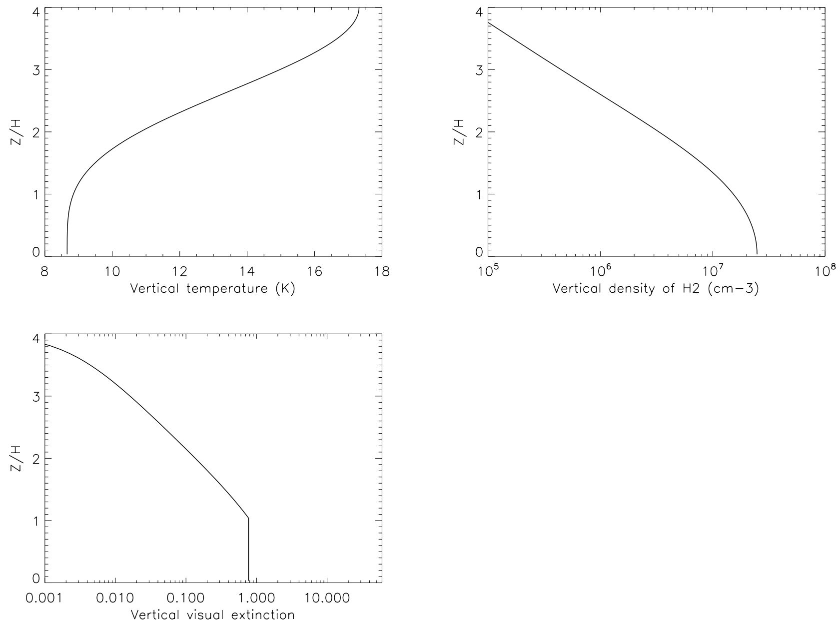

Figure 2: Physical model computed for two different layers of dust: small grains of 10^{-5} cm above Z/H=1 and big grains of 3×10^{-3} below. The dust-to-gas mass ratio is 10^{-3} above Z/H=1 and 1.9×10^{-2} below.

$$GTODN_{below} = 1/(1.4 \times 10^{-2}) \times \frac{4\pi(3.10^{-3})^3 \times 3}{3 \times 1.66043 \times 10^{-24}} = 10^{19} \qquad (20)$$

So the abundance of grains in the mid plan is 10^6 times less abundant than in the upper part.

13 References

Pitu, V., Dutrey, A., & Guilloteau, S. 2007, A&A, 467, 163

Guilloteau, S. & Dutrey, A. 1998, A&A, 339, 467

Guilloteau, S., Dutrey, A., Pitu, V., & Boehler, Y. 2011, A&A, 529, A105

Bergin, E., Calvet, N., Sitko, M. L., et al. 2004, ApJ, 614, L133

Herczeg, G. J., Wood, B.E., Linsky, J. L., Valenti, J. A., & JohnsKrull, C. M. 2004, ApJ, 607, 369

Dutrey et al., 2014, nature , 514, 600

Hersant et al., 2009, A&A, 493, L49

Andrews S.M et al., 2012. ApJ, 744, 162

Qi C., Wilner D. J., Calvet N., Bourke T. L., Blake G. A., Hogerheijde M. R., Ho P. T. P., Bergin E., 2006, ApJL, 636, L157

Mayer, L., Lufkin, G., Quinn, T., & Wadsley, J. 2007, ApJL, 661, L77