Definitions

symbol	description	unit
z	vertical coordinate	cm
$n_{\langle\mathrm{H}\rangle}$	hydrogen nuclei density	cm^{-3}
$\rho = \mu_\mathrm{H}\, n_{\langle\mathrm{H}\rangle}$	gas mass density	$\mathrm{g\,cm}^{-3}$
T	gas temperature	K
a	dust particle radius	cm
$V = \frac{4\pi}{3}a^3$	volume of a dust particle	cm^3
V_ℓ	miminum volume of a dust particle	cm^3
$f(V)$	size distribution function	cm^{-6}
$\rho L_j = \int_{V_\ell}^\infty f(V) V^{j/3}\,dV$	dust moments	cm^{j-3}
L_j	dust moments	$\mathrm{cm}^j\,\mathrm{g}^{-1}$
$J_\star$	nucleation rate	$\mathrm{cm}^{-3}\mathrm{s}^{-1}$
D	diffusion coefficient	$\mathrm{cm}^2\,\mathrm{s}^{-1}$

1 General Equations

The dust moment equations are given by (see derivation in Woitke & Helling, 2003, section 3)

$$\frac{\partial(\rho L_j)}{\partial t} + \nabla(\vec{v}\,\rho L_j) \;=\; \underbrace{V_\ell^{j/3}\sum_s J_\star^s}_{\text{nucleation}} \;+\underbrace{\frac{j}{3}\,\chi\,\rho L_{j-1}}_{\text{growth}} \;+\underbrace{\nabla\left(D_d\,\rho\nabla L_j\right)}_{\text{diffusion}} \;+\underbrace{\nabla\left(\xi\frac{\rho_\mathrm{d}}{c_T}L_{j+1}\,\hat{r}\right)}_{\text{drift}} \tag{1}$$

where the first term on the r.h.s. accounts for the increase of the dust moments due to nucleation, the second term accounts for the growth and evaporation of the dust particles (χ can be negative), the third term is for diffusive mixing, and the forth term accounts for the downward equilibrium drift of the grains in a gravitational field, $\xi = \sqrt[3]{\frac{3}{4\pi}}\frac{\sqrt{\pi}}{2}\,g$, for the case of small Knudsen numbers, see Woitke & Helling (2003, section 5.1). $\hat{r}$ is the unit vector away from the center of gravity. The idea of diffusive mixing due to convection and overshoot is introduced in Woitke & Helling (2004, Sect. 2.1 and, in particular, Sect. 4.2).

All dust grains are assumed to be perfect spheres with well-mixed material composition, independent of size. We can then introduce $\rho L_3^s = \int_{V_\ell}^\infty f(V)V^s\,dV$ (Helling et al., 2008) and write

$$V = \sum_s V^s \quad , \quad L_3 = \sum_s L_3^s \quad , \quad b^s = \frac{L_3^s}{L_3}\;. \tag{2}$$

In the following, $s = 1\ldots S$ is an index running over the different solid species, $r = 1\ldots R$ is an index running over the surface reactions and $j = \{0,1,2,3,4\}$ is the index of the dust moments. We introduce the following abbreviation for the surface reaction rates [number of net reactions per surface area and per time]

$$c_r^s \;=\; \sqrt[3]{36\pi}\,\frac{\nu_r^s\,n_r^\mathrm{key}\,v_r^\mathrm{rel}\,\alpha_r}{\nu_r^\mathrm{key}}\left(1-\frac{b^s}{S_r}\right)\;, \tag{3}$$

where n_r^key is the particle density [cm^{-3}] of the key species of surface reaction r, ν_r^key its stoichiometric factor in that reaction, $v_r^\mathrm{rel} = \sqrt{kT/(2\pi\,m^\mathrm{key})}$ its thermal relative velocity, m^key its mass, α_r its sticking probability, and S_r is the reaction supersaturation ratio. For example, in this reaction

$$2\,\mathrm{CaH} \;+\; 2\,\mathrm{Ti} \;+\; 6\,\mathrm{H_2O} \;\longrightarrow\; 2\,\mathrm{CaTiO_3[s]} \;+\; 7\,\mathrm{H_2} \tag{4}$$

the key species is either key=CaH or key=Ti (depending on which species is less abundant), $\nu_r^{\rm key}=2$ in both cases, $s=$CaTiO$_3$[s] is the solid species, and $\nu_r^s=2$ units of CaTiO$_3$[s] are produced by one reaction. Using this definition, we can express the net growth velocity of all grains χ [cm/s] as

$$\chi = \sum_s \sum_r c_r^s V_0^s \ , \tag{5}$$

where V_0^s is the volume of one solid unit of material kind s. We can now separate the third moment equation and can express the element conservation equations as follows

$$\frac{\partial(\rho L_3^s)}{\partial t} + \nabla(\vec{v}\,\rho L_3^s) \;=\; V_\ell J_\star^s \;+ \rho L_2 \sum_r V_0^s c_r^s \;+ \nabla\left(D_d\,\rho \nabla L_3^s\right) \;+ \nabla\left(\xi \frac{\rho_{\rm d}}{c_T}\, b^s L_4\,\hat{r}\right) \tag{6}$$

$$\frac{\partial(n_{\langle{\rm H}\rangle}\epsilon_k)}{\partial t} + \nabla(\vec{v}\,n_{\langle{\rm H}\rangle}\epsilon_k) \;=\; -\sum_s \nu_k^s N_\ell J_\star^s \;- \rho L_2 \sum_s \sum_r \nu_k^s c_r^s \;+ \nabla\left(D\,n_{\langle{\rm H}\rangle}\nabla\epsilon_k\right) \ , \tag{7}$$

where ν_k^s is the stoichiometric factor of element k in solid s, for example $\nu_{\rm Ti}^{\rm TiO2[s]}=1$ and $\nu_{\rm O}^{\rm TiO2[s]}=2$.

2 Static planeparallel atmosphere

Next we assume that the gas in the atmosphere is static $\vec{v}=0$ and that all processes are stationary $\frac{\partial\,\cdot}{\partial t}=0$. Also assuming plane-parallel geometry $\nabla \to \frac{d}{dz}$, we find

$$0 \;=\; V_\ell^{j/3} \sum_s J_\star^s \;+ \frac{j}{3}\,\chi\,\rho L_{j-1} \;+ \frac{d}{dz}\left(D_d\,\rho \frac{dL_j}{dz}\right) \;+ \frac{d}{dz}\left(\xi \frac{\rho_{\rm d}}{c_T} L_{j+1}\right) \tag{8}$$

$$0 \;=\; V_\ell J_\star^s \;+ \rho L_2 \sum_r V_0^s c_r^s \;+ \frac{d}{dz}\left(D_d\,\rho \frac{dL_3^s}{dz}\right) \;+ \frac{d}{dz}\left(\xi \frac{\rho_{\rm d}}{c_T}\, b^s L_4\right) \tag{9}$$

$$0 \;=\; -\sum_s \nu_k^s N_\ell J_\star^s \;- \rho L_2 \sum_s \sum_r \nu_k^s c_r^s \;+ \frac{d}{dz}\left(D\,n_{\langle{\rm H}\rangle} \frac{d\epsilon_k}{dz}\right) \ . \tag{10}$$

2.1 Dust mixing – yes or no?

The assumed mixing by turbulence is described by a diffusion approximation where the effective diffusion coefficients is much larger than the gas-kinetic one

$$D_{\rm micro} \;=\; \frac{1}{3}\frac{v_{\rm th}}{\sigma\, n} \tag{11}$$

where $1/(\sigma\, n)$ is the mean free path, n would be the total gas particle density and $\sigma \approx 3\times 10^{-15}\,{\rm cm}^2$ would be a typical cross-section for gas-gas collisions (Woitke & Helling, 2003). Instead, the turbulent diffusion coefficient is roughly given by

$$D \;\approx\; \langle v_z\rangle\, H_p \;\gg\; D_{\rm micro} \ , \tag{12}$$

where $\langle v_z\rangle$ is the root-mean-square average of vertical velocities in the atmosphere, at height z. In the convective layer, $\langle v_z\rangle \approx v_{\rm conv}$ is the convective velocity which is a part of the stellar atmosphere model and results from the application of mixing length theory. Above the convective layer, where the Schwarzschild criterion for convection is false, $\langle v_z\rangle$ will decrease rapidly with increasing z, but will not be entirely zero due to convective overshoot. We apply a powerlaw in $\log p$ to approximate this behaviour

$$\log\langle v_z\rangle = \log v_{\rm conv} - \beta\cdot\max\{0, \log p_{\rm conv} - \log p(z)\} \tag{13}$$

with free parameter $\beta \approx 1.5\,...\,2.2$ (Ludwig et al., 2002; Lee et al., 2015). Due to their inertia, dust particles are less effected by turbulence, namely only via the slower and bigger turbulent modes (larger eddies). The dust diffusion coefficient is hence expected to be bracketed by the gas diffusion coefficient as

$$0 \;<\; D_d \;\le\; D \;. \tag{14}$$

We cannot fully account for these effects, because we need an average dust diffusion coefficient which we can pull out of the dust size integrals. However, we can consider the following two limiting cases

$$\begin{array}{lll} \textbf{case 1:} & \text{small grains} & D_d = D \\ \textbf{case 2:} & \text{large grains} & D_d = 0 \end{array} \tag{15}$$

For case 2, we are left with

$$0 \;=\; V_\ell^{j/3} \sum_s J_\star^s \;+\frac{j}{3}\,\chi\,\rho L_{j-1} \;+\frac{d}{dz}\left(\xi\frac{\rho_\mathrm{d}}{c_T}L_{j+1}\right) \tag{16}$$

$$0 \;=\; V_\ell J_\star^s \;+\rho L_2 \sum_r V_0^s c_r^s \;+\frac{d}{dz}\left(\xi\frac{\rho_\mathrm{d}}{c_T}\,b^s L_4\right) \tag{17}$$

$$0 \;=\; -\sum_s \nu_k^s N_\ell J_\star^s \;-\rho L_2 \sum_s\sum_r \nu_k^s c_r^s \;+\frac{d}{dz}\left(D\,n_{\langle\mathrm{H}\rangle}\frac{d\epsilon_k}{dz}\right) \;. \tag{18}$$

2.2 The total flux of elements

An important realisation is that in the static case, the total vertical flux of elements (due to vertical dust settling *and* due to turbulent mixing) must be zero everywhere in the atmosphere and for each element. We can derive this conclusion formally by summing up (Eq. 18) and $\sum_s$ (Eq. 17) $\cdot\,\nu_k^s/V_0^s$. The nucleation and growth terms cancel out exactly in this case, and we find

$$\frac{d}{dz}\left(D\,n_{\langle\mathrm{H}\rangle}\frac{d\epsilon_k}{dz}\right) \;+\; \frac{d}{dz}\left(\xi\frac{\rho_\mathrm{d}}{c_T}L_4\sum_s\frac{\nu_k^s\,b^s}{V_0^s}\right) \;=\; 0 \;, \tag{19}$$

thus,

$$D\,n_{\langle\mathrm{H}\rangle}\frac{d\epsilon_k}{dz} \;+\; \xi\frac{\rho_\mathrm{d}}{c_T}L_4\sum_s\frac{\nu_k^s\,b^s}{V_0^s} \;=\; \mathrm{const}_k \tag{20}$$

This equation stills allow for constant (time-independent and height-independent) fluxes of elements through the atmosphere. Since this case would require very strange boundary conditions (where do these elements come from / where do they go?) we exclude that possibility here and demand $\mathrm{const}_k = 0$ instead, finding

$$\underbrace{D\,n_{\langle\mathrm{H}\rangle}\frac{d\epsilon_k}{dz}}_{-j_k^\mathrm{mix}} \;+\; \underbrace{\xi\frac{\rho_\mathrm{d}}{c_T}L_4\sum_s\frac{\nu_k^s\,b^s}{V_0^s}}_{-j_k^\mathrm{drift}} \;=\; 0 \tag{21}$$

$j_k^\mathrm{drift} < 0$ is the element flux [1/cm^2/s] due to the downward gravitational settling of all dust particles. Equation (21) means that this flux must be balanced by an upward directed diffusive mixing flux $j_k^\mathrm{mix} > 0$ due to turbulence, at each height z in the atmosphere and for all elements k. We conclude

$$\frac{d\epsilon_k}{dz} \;=\; -\,\frac{\xi\rho_\mathrm{d}L_4}{c_T D\,n_{\langle\mathrm{H}\rangle}}\sum_s\frac{\nu_k^s\,b^s}{V_0^s} \qquad \le\; 0 \tag{22}$$

Whenever dust is present ($L_4 > 0$) and gravity is active ($\xi > 0$), the gas element gradients must be negative, i.e. the abundance of all elements k involved in dust formation *must monotonically decrease* toward the top of the atmosphere.

3 Solution method

Using Eq. (22), we can write the system of coupled differential equations for dust and gas as

$$\boxed{\begin{array}{rcll} -\dfrac{d}{dz}\left(\xi\dfrac{\rho_{\rm d}}{c_T}L_{j+1}\right) &=& V_\ell^{j/3}\displaystyle\sum_s J_\star^s \,+\dfrac{j}{3}\,\chi\,\rho L_{j-1} & (j=0,1,2) \\ -\dfrac{d}{dz}\left(\xi\dfrac{\rho_{\rm d}}{c_T}\,b^s L_4\right) &=& V_\ell J_\star^s \,+\rho L_2\displaystyle\sum_r V_0^s c_r^s & (s=1,\dots,S) \\ -\dfrac{d\epsilon_k}{dz} &=& \xi\dfrac{\rho_{\rm d}}{c_T}\dfrac{L_4}{D\,n_{\langle{\rm H}\rangle}}\displaystyle\sum_s\dfrac{\nu_k^s\,b^s}{V_0^s} & (k=1,\dots,K) \end{array}} \tag{23}$$

3.1 Closure condition

The moment equation system is completed by a closure condition of the form

$$L_0 = \mathcal{F}(L_1, L_2, L_3, L_4)\ , \tag{24}$$

see Woitke & Helling (2004, section 2.4.1).

3.2 ODE system

Our equation system (23) has the standard form of a system of Ordinary Differential Equations (ODE) as

$$\frac{d\vec{y}}{dx} \;=\; \vec{F}(x,\vec{y})\ . \tag{25}$$

We will denote $\vec{y}$ as the *solution vector* and $\vec{F}$ as the *right-hand-side vector* in the following. The solution vector has dimension $(3+S+K)$ and is given by

$$\vec{y} = \{\xi\frac{\rho_{\rm d}}{c_T}L_1\ ,\ \xi\frac{\rho_{\rm d}}{c_T}L_2\ ,\ \xi\frac{\rho_{\rm d}}{c_T}L_3\ ,\ \xi\frac{\rho_{\rm d}}{c_T}b^1L_4\ ,\ \dots\ ,\ \xi\frac{\rho_{\rm d}}{c_T}b^SL_4\ ,\ \epsilon_1\ ,\ \dots\ ,\ \epsilon_K\} \tag{26}$$

3.3 Boundary Conditions

- The element abundances are given deep inside the star, well below the cloud layers, say at $z=0$.
- All dust quantities can be assumed to be zero both at the top and the bottom of the atmosphere
- I seems to me that the equations can only be integrated from top to bottom, following the natural direction of the settling dust particles
- I tried to solve the equations with a ODE-solver with a shooting method, but it looks to be very unstable and not working so far.

Huston, we have a problem.

References

Helling, C., Woitke, P., Thi, W.-F. (2008, July). Dust in brown dwarfs and extra-solar planets. I. Chemical composition and spectral appearance of quasi-static cloud layers. *A&A* **485**, 547–560.

Lee, G., Helling, C., Dobbs-Dixon, I., Juncher, D. (2015, August). Modelling the local and global cloud formation on HD 189733b. *A&A* **580**, A12.

Ludwig, H.-G., Allard, F., Hauschildt, P. H. (2002, November). Numerical simulations of surface convection in a late M-dwarf. *A&A* **395**, 99–115.

Woitke, P., Helling, C. (2003, February). Dust in brown dwarfs. II. The coupled problem of dust formation and sedimentation. *A&A* **399**, 297–313.

Woitke, P., Helling, C. (2004, January). Dust in brown dwarfs. III. Formation and structure of quasi-static cloud layers. *A&A* **414**, 335–350.