Inhomogeneous dust formation due to turbulent motion in Brown Dwarf atmospheres

Christiane Helling[1], Marcus Lüttke[1], Michael Oevermann[2], Rupert Klein[2], Erwin Sedlmayr[1]
[1]Zentrum für Astronomie & Astrophysik, Technische Universität Berlin, Germany
[2]Fachbereich Mathematik & Informatik, Freie Universität Berlin, Germany

Brown Dwarfs are very faint, low mass star-like objects possibly bridging the gap between stars and planets. Their interior is dominated by convective energy transport which deposits energy, momentum, and matter into the atmosphere. Brown Dwarf atmospheres furthermore provide favorable conditions for the gas–solid phase transition due to their low temperatures and high densities since they are cool and compact objects. Brown Dwarfs are therefore an excellent test bed to study dust formation under turbulent conditions.

In Brown Dwarfs, dust-free convective cells originating from the interior convective zone travel radially outward and decay into smaller and smaller eddies. Following Kolmogoroff's assumption, energy is transfered from the largest scales into smaller and smaller scales until the energy is finally dissipated on the Kolmogoroff scale ($\eta \approx 10^{-2}$cm for $l_{\rm ref} \approx 10^4$cm) by the viscosity of the gas. Considering that the large scale turbulent motions have a characteristic Mach number $M \approx 1$, resulting acoustic waves create a turbulent temperature and density field in the atmosphere which influences the dust complex due to its high temperature and density sensitivity. Combining *asymptotic techniques* and *time-dependent, multi-dimensional numerical simulations*, we show that on microscopic scales acoustic waves can initiate dust nucleation in otherwise dust-hostile environments. An *instable feedback loop* occurs which is started by small temperature disturbances which allow the first dust particles to form. These particles grow to macroscopic sizes and thereby intensify the temperature decrease due to the radiative cooling which in turn re-initiates and henceforth intensifies dust formation. This runaway effect is stopped if all condensible material is consumed or the radiative equilibrium is reached.

The model problem

The model problem is twofold:
A: *The hydro- and thermodynamics* which are described following the classical approach for an inviscid, compressible fluid write in dimensionless form:

$$(\rho)_t + \nabla\cdot(\rho\boldsymbol{v}) = 0 \tag{1}$$

$$(\rho\boldsymbol{v})_t + \nabla\cdot(\rho\boldsymbol{v}\circ\boldsymbol{v}) = -\frac{1}{\mathrm{M}^2}\nabla P - \frac{\mathrm{M}^2}{\mathrm{Fr}^2}\rho\boldsymbol{g} \tag{2}$$

$$(\rho e)_t + \nabla\cdot(\boldsymbol{v}[\rho e + P]) = \mathrm{Rd}\,\kappa(T_{\rm RE}^4 - T^4) \tag{3}$$

$$\rho e = \mathrm{M}^2\left(\frac{\rho\boldsymbol{v}^2}{2} + \frac{1}{\mathrm{Fr}^2}\rho g y\right) + \frac{P}{\gamma-1}. \tag{4}$$

The quantities and the characteristic numbers have their usual meaning. Additionally, $T_{\rm RE}$ is the radiative equilibrium temperature, κ the total absorption coefficient, $\boldsymbol{g}$ the gravitational acceleration acting in the y direction. Assuming local thermal equilibrium, the interaction between matter and radiation field (radiative heating/cooling) can be described by a relaxation ansatz on the r.h.s. of the energy equation (Eq. 3).
B: *The chemistry and dust formation.* The dust formation is a two step process – nucleation and growth (Gail et al. 1984, Gail & Sedlmayr 1988) – and depends by the amount of condensible

species on the local temperature and density of the gas which are determined by Complex A. The dimensionless dust moment and element consumption equations write ($j \in$ N):

$$(\rho L_0)_t + \nabla\cdot(\boldsymbol{v}\,\rho L_0) = \mathrm{Da}_\mathrm{d}^\mathrm{nuc}\,J_* \tag{5}$$

$$(\rho L_\mathrm{j})_t + \nabla\cdot(\boldsymbol{v}\,\rho L_\mathrm{j}) = \mathrm{Da}_\mathrm{d}^\mathrm{nuc}\,\mathrm{Se_j}\,J_* + \mathrm{Da}_\mathrm{d}^\mathrm{gr}\frac{\mathrm{j}\chi^\mathrm{net}}{3}\rho L_\mathrm{j-1} \tag{6}$$

$$(\rho\epsilon_\mathrm{x})_t + \nabla\cdot(\boldsymbol{v}\,\rho\epsilon_\mathrm{x}) = -\mathrm{El}\sum_{\mathrm{r}=1}^{\mathrm{R}}(\nu_\mathrm{r}^\mathrm{nuc}\,\mathrm{Da}_\mathrm{d}^\mathrm{nuc}N_l J_* + \nu_\mathrm{r}^\mathrm{gr}\,\mathrm{Da}_\mathrm{d}^\mathrm{gr}n_\mathrm{x,r}v_\mathrm{rel,x}\alpha_\mathrm{r}\,\rho L_2). \tag{7}$$

ϵ_x is the element abundance of the chemical element x (e.g. Ti, Si, O) in mass fractions, which is consumed by nucleation (first term, r.h.s.) and growth (second term, r.h.s.) with the stoichiometric factor ν_r due to the reaction r. $n_\mathrm{x,r}$ is the particle density of the atoms and molecules containing the element x which are involved in nucleation (Eq. 5) and/or growth (Eq. 6) by reaction r, L_j ($[L_\mathrm{j}] = \mathrm{cm^j/g}$) are the dust moments in mass fractions of the grain size distribution function $f(V)$ with V the grain volume. The number of dust particles $n_\mathrm{d} = \rho L_0$ [$\mathrm{cm^{-3}}$] is determined by the nucleation rate J_* [$\mathrm{cm^{-3}\,s^{-1}}$] which is calculated from

$$J_* = \frac{n_\mathrm{x}}{\tau}\exp\left[-\frac{4}{27}\left(\frac{T_\Theta}{T}\right)^3\frac{1}{\ln S^2}\right] \tag{8}$$

by applying classical nucleation theory; T_Θ is a material quantity containing e.g. the surface tension of the clusters. The nucleation process inherents a *threshold characteristic*: efficient nucleation is only possible if a temperature T_S is reached for which the supersaturation ratio $S \gg 1$, therefore $T_\mathrm{S} < T(S=1)$. The growth process is determined by the heterogeneous net growth velocity χ^net which contains e.g. the sticking coefficient of the growth species (e.g. SiO, $\mathrm{TiO_2}$).

The governing equations of our model problem are those of an *inviscid, compressible fluid* (Eqs. 1–3) coupled to stiff dust moment equations ($\mathrm{Da}_\mathrm{d}^\mathrm{nuc}$, $\mathrm{Da}_\mathrm{d}^\mathrm{gr} \gg 1$; Eqs. 5,6) and a singular radiative energy transfer in the presents of dust (Rd $\gg 1$). $\mathrm{Da}_\mathrm{d}^\mathrm{nuc}$ and $\mathrm{Da}_\mathrm{d}^\mathrm{gr}$ are Damköhler-like numbers for the dust nucleation and growth. El is the characteristic number for element consumption. Se is the Sedlmaÿr number characterizing the dust size distribution, and Rd is the characteristic number for radiative heating/cooling. Since the microscopic regime ($l_\mathrm{ref} < H_\rho$) is considered here only, $Fr \gg 1$ and gravitational effects (e.g. grain sedimentation) are negligible.

Inhomogeneous dust formation

Asymptotic consideration: A key observation for the following analysis is that the nucleation rate J_* strongly depends on temperature with a reverse activation energy type characteristic. The number of dust nuclei formed during the interaction time Δt of two waves is given by the time integral $n_\mathrm{d} = \int_{\Delta t} J_*(T(t))\,dt$. Under typical dust forming conditions the parameter Θ in

$$J_* = \frac{n_\mathrm{x}}{\tau}\exp\left(-\frac{\Theta}{T(T_S-T)^2}\right),\qquad \Theta = \frac{4}{27}\frac{1}{B^2}T_S^2T_\Theta^3, \tag{9}$$

is very large, here $\Theta = \mathcal{O}(10^9)$. The supersaturation ratio S can be approximated by some material quantity B (see Helling et al. 2001). This allows an asymptotic approximation of the integral:

$$\int_t J_*\,dt = \int f(t)\exp(\Theta g(t))\,dt \approx \frac{\sqrt{2\pi}f(t_*)}{\sqrt{-\Theta g''(t_*)}}\exp(\Theta g(t_*)), \tag{10}$$

where $f(t) = n_\mathrm{x}/\tau(T(t))$ and $g(t) = -\frac{1}{T(T_s-T)^2}$. t_* is the time of the minimum temperature during the interaction of two waves. Assuming linear acoustic waves (e.g. Gaussian) with given temperature disturbances ΔT, we can analytically evaluate the integral. Excellent agreement between a numerical computation of the integral and the asymptotic approximation for different temperature amplitudes has been shown.

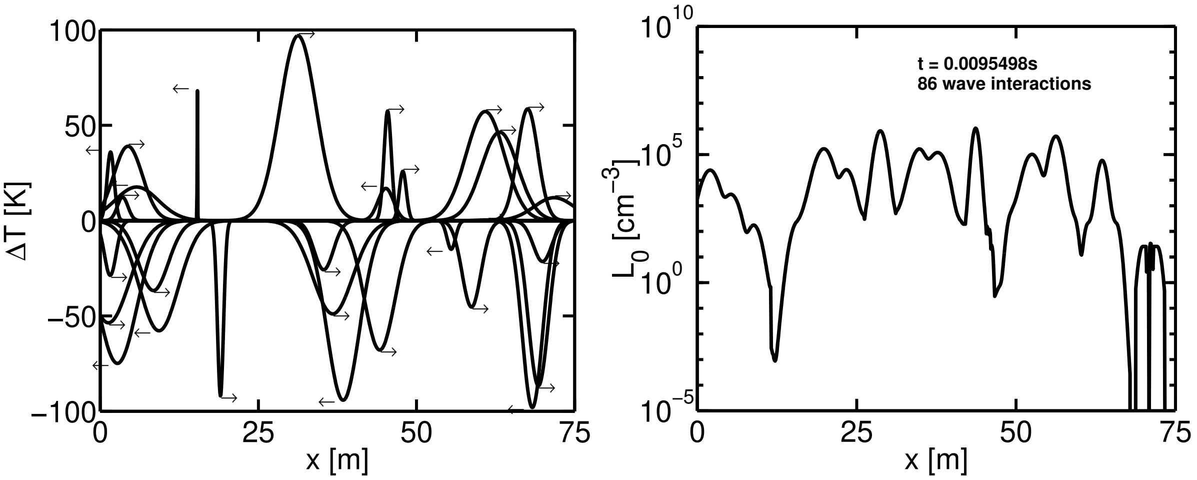

Figure 1: **Left:** Stochastic interaction of 86 Gaussian acoustic waves. **Right:** Resulting spatial distribution of dust nuclei of 86 Gaussian acoustic waves ($T_{\rm ref} = 1900\,{\rm K}$, $\rho_{\rm ref} = 10^{-4}{\rm g\,cm^{-3}}$).

To study the effects of multiple stochastic interactions of this type, we consider 86 Gaussian-shaped acoustic waves with random amplitudes ΔT [K] $\in [-100, 100]$, wavelengths λ [cm] $\in [0, 500]$, and propagation directions (Figure 1, l.h.s.). Since every wave travels with the same speed of sound here, only waves moving in opposite directions interact. If two waves with a negative temperature fluctuation collide, seed nucleation occurs during the time of interaction. Figure 1 (r.h.s.) displays the spatial distribution of $(TiO_2)_N$ dust nuclei on a logarithmic scale, represented by the zeroeth dust moment L_0, after the interaction of all the acoustic waves: *inhomogeneous nucleation events result in an intermittent distribution of dust.* For the computation of the spatial nuclei distribution we used the asymptotic Eq. (10) assuming linear superposition of the waves.

Numerical Simulations: A second-order Godunov-type multi-dimensional hydro-code (Smiljanovski et al. 1997), where an operator splitting method has been used for the spatial directions, dust formation (nucleation, growth, element consumption), chemistry, radiative cooling, and gravity, has been applied for solving our model equations for the microscopic scale regime ($l_{\rm ref} < H_\rho$) in two dimensions with a spatial resolution of 100×100 grid points. Two-dimensional Gauss-like pressure pulses create an inhomogeneous distribution of pulses of various wavelength ($\lambda = 300 \ldots 600\,{\rm cm}$) and temperature amplitudes ($\Delta T = 50 \ldots 70\,{\rm K}$) in a 2D test volume with open boundaries (von Neumann). The size of the domain is $l_{\rm ref}/2 = 0.5 \cdot 10^5$cm. These studies have been performed regarding the formation of core-mantel grains ((TiO_2) core, SiO/TiO_2 mantel) under typical conditions of a hot and dense part in a Brown Dwarf atmosphere.

The interacting pressure pulses cause two scenarios to appear: 1) the randomly interacting *acoustic expansion waves create* thermodynamic conditions (i.e. *low temperatures*) in regions usually unfavorable for dust formation, and 2) corresponding *compression waves suppress* dust formation in regions appropriate for dust formation due to an *increase of temperature*.

The first scenario is characterized by a short period of wave interaction when the local gas temperature drops below the threshold temperature $T_{\rm S}$ of efficient nucleation. A small number of particles is formed and an *instable feedback loop* is started. Subsequent growth causes an increase of size and therefore also an increased absorption coefficient κ which in turn causes an intensified radiative cooling (see Eq. 3). Temperature drops again, and again $T < T_{\rm S}$ and efficient nucleation is re-initiate. Consequently, the number of dust particles increases. A *run-away effect* of intensified radiative cooling by more particles formed with subsequent grow continues until all the condensible material is consumed or the radiative equilibrium is reached. This feedback loop causes an *inhomogeneous formation of dust particles depending on the site and on the time of constructive interference of the acoustic expansion waves* (compare also Fig. 1). The events of efficient dust

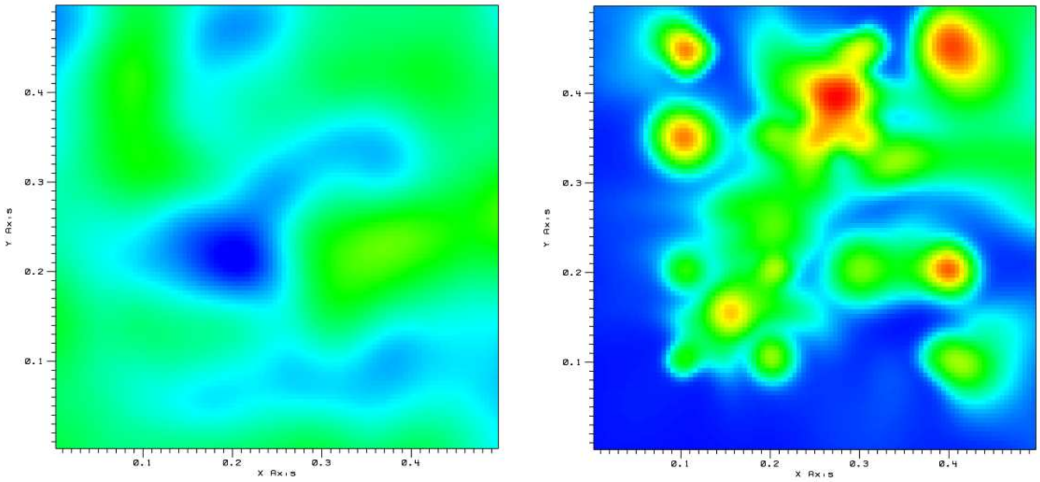

Figure 2: **Left:** Nucleation rate $\log J_{*,\mathrm{TiO_2}}$ [$\mathrm{cm^{-3}}$] after $t = 5 \cdot 10^{-3}$s ($\log J_{*,\mathrm{min}} = -21$ (blue/black), $\log J_{*,\mathrm{max}} = -17$ (green/lightest grey)). The maximum value achieved during the whole computation was $\log J_* = -13$ [$\mathrm{cm^{-3}}$].
Right: Dust particle number density $\log n_\mathrm{d}$ [$\mathrm{cm^{-3}}$] after $t = 5 \cdot 10^{-3}$s ($n_{\mathrm{d,min}} = 0$ (blue/black), $\log n_{\mathrm{d,max}} = 3.0$ (red/dark grey - only inside the inhomogeneities)).
($T_\mathrm{ref} = 19000\,\mathrm{K}$, $\rho_\mathrm{ref} = 10^{-4}\mathrm{g\,cm^{-3}}$)

nucleation appear in Fig. 2 with the largest dust particle number density n_d.

Meanwhile, the acoustic waves pass through the 2D test volume and also compression waves develop which cause an increase of the temperature. Due to the temperature sensitivity of J_*, the formation of dust particles will locally be suppressed which results again in an inhomogeneous distribution of the dust component.

As time proceeds, a stationary situation may be reached regarding the hydrodynamical quantities: T, ρ, and p become homogeneous and $u \approx 0$ on the microscopic scale regime considered. Consequently, also the nucleation rate homogenizes (Fig.2, l.h.s.) and becomes negligible if $T > T_\mathrm{S}$. The previously inhomogeneously formed dust particles continue to grow until all condensible material is consumed. Since an equal amount of condensible material per volume is available, smaller mean particle sizes result in regions with many particles. Hence, beside an inhomogeneous distribution of the number of dust particles, also inhomogeneous mean particle sizes are the result of interacting acoustic waves.

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