

Dust in brown dwarfs

II. The coupled problem of dust formation and sedimentation

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Abstract. In this paper, we quantify and discuss the physical and surface chemical processes leading to the formation, temporal evolution and sedimentation of dust grains in brown dwarf and giant gas planet atmospheres: nucleation, growth, evaporation and gravitational settling. Considering dust particles of arbitrary sizes in the different hydrodynamical regimes (free molecular flow, laminar flow, turbulent flow), we evaluate the equilibrium drift velocities (final fall speeds) and the growth rates of the particles due to accretion of molecules. We show that a depth-dependent maximum size of the order of $a_{\max} \approx 1 \mu\text{m}$ (upper regions) . . . $100 \mu\text{m}$ (lower regions) exists, which depends on the condensate and the stellar parameters, beyond which gravitational settling is faster than growth. Larger particles can probably not be formed and sustained in brown dwarf atmospheres. We furthermore argue that the acceleration towards equilibrium drift is always very fast and that the temperature increase of the grains due to the release of latent heat during the growth process is negligible. Based on these findings, we formulate the problem of dust formation coupled to the local element depletion/enrichment of the gas in brown dwarf atmospheres by means of a system of partial differential equations. These equations state an extension of the moment method developed by Gail & Sedlmayr (1988) with an additional advective term to account for the effect of size-dependent drift velocities of the grains. A dimensionless analysis of the new equations reveals a hierarchy of nucleation \rightarrow growth \rightarrow drift \rightarrow evaporation, which characterises the life cycle of dust grains in brown dwarf atmospheres. The developed moment equations can be included into hydrodynamics or classical stellar atmosphere models. Applications of this description will be presented in a forthcoming paper of this series.

Key words. stars: atmospheres – stars: low-mass, brown dwarfs – dust, extinction – molecular processes – methods: numerical

1. Introduction

Brown dwarfs are the only stars known so far that are cool enough to host small solid particles or fluid droplets (henceforth called *dust* or *dust grains*) in their atmospheres. The dust has a strong influence on the opacity and hence on the structure of the atmosphere as well as on the spectral appearance of brown dwarfs (Allard et al. 2001; Marley et al. 2002; Tsuji 2002; Cooper et al. 2002), e.g. by smoothing out molecular bands and thermalising the radiation, by increasing the temperature below optically thick cloud layers, and in particular, by affecting the element composition of the gas depth-dependently.

Furthermore, the dust component seems to be responsible for a wealth of variability phenomena recently observed (Bailer-Jones & Mundt 2001a,b; Bailer-Jones 2002; Martín et al. 2001; Eislöffel & Scholz 2001). The observed light variations are partly non-periodic and, thus, cannot be explained solely by rotation and magnetic spots.

In order to study the atmospheres of these ultra-cool stars and giant gas planets, a consistent physical description of the formation, temporal evolution and gravitational settling of dust grains is required, which states a new fundamental problem to the classical theory of stellar atmospheres. A better physical description of the dust component is likely to provide the key not only to understand the variability of brown dwarfs, but also the structure of their atmospheres and the observations of brown dwarfs in general.

In comparison to other astronomical sites of effective dust formation (Sedlmayr 1994), the atmospheres of brown dwarfs provide special conditions for the dust formation process. The convection replenishes the gas in the upper layers with fresh uncondensed gas from the deep interior, probably in a non-continuous and spatially inhomogeneous way. The convection energises turbulence which creates strongly varying thermodynamical conditions on small scales, causing an inhomogeneous and time-dependent distribution of the dust (Helling et al. 2001, henceforth called Paper I). Three further points are to be mentioned:

(i) The stellar gravity ($\log g \approx 5$) is about a hundred times larger than in the earth's atmosphere and roughly 10^4

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to 10^5 times larger than in the circumstellar envelopes of red giants. This strong gravity puts severe physical constraints on the dynamical behaviour of the forming dust component. Once formed from the gas phase, dust grains are immediately forced to sink downwards. The atmosphere can be expected to clean up from dust grains via gravitational settling on time-scales ranging in minutes to months, depending on the dust grain size. This is just the opposite as encountered in the circumstellar envelopes of red giants, where the forming dust grains are accelerated outwards due to radiation pressure.

(ii) The dust forming gas in brown dwarf atmospheres is very dense, $\rho \approx 10^{-7} \dots 10^{-3} \text{ g cm}^{-3}$. On the one hand side, these high densities simplify a physical description of the dust formation process, since chemical equilibrium in the gas phase can be assumed. On the other hand side, the large densities lead to a quite different molecular composition of the gas (for example a simultaneous occurrence of CH_4 , H_2O and CO_2 , i.e. no CO-blocking), like in planetary atmospheres (e.g. Lodders & Fegley 1994). Consequently, different chemical preconditions for the dust formation process are present as e.g. in M-type giants (Gail & Sedlmayr 1998). Other nucleation species and other surface chemical reactions can be important for the dust growth process. Other solid compounds and even fluid phases can be stable in a brown dwarf atmosphere.

(iii) The high densities lead furthermore to a qualitatively different dynamical behaviour of the gas flow around a dust grain. The mean free path lengths of the gas particles can be smaller than a typical diameter of a grain, leading to small Knudsen numbers $Kn < 1$. This affects the range of applicability of certain physical descriptions at hand, concerning for example the drag force or the growth of a dust grain due to accretion of molecules from the gas phase, which may be limited by the diffusion of the molecules toward the grain's surface.

One of the key processes to understand the structure of planetary and brown dwarf atmospheres – including element depletion and weather-like features – is the dust sedimentation, which means a non-zero relative motion between the dust particles and the surrounding gas, known as *the drift problem*. Various approaches have been carried out to simulate the dynamics of dust/gas mixtures, e.g. in the circumstellar envelopes of late-type stars (Gilman 1972; Berruyer & Frisch 1983; MacGregor & Stencel 1992; Krüger et al. 1994, 1997). Mostly, two-fluid approaches have been applied, assuming a constant dust grain size, where nucleation is disregarded or assumed to be followed by an instantaneous growth to the mean particle size. Simis et al. (2001) and Sandin & Höfner (2003) have relaxed this approach by allowing for a varying mean grain size, according to the results of a time-dependent treatment of the dust nucleation and growth according to (Gail et al. 1984; Gail & Sedlmayr 1988). However, an unique velocity of the dust component is assumed. Assuming stationarity, Krüger et al. (1995) have developed a bin method for the 1D drift problem in stellar winds including a full time-dependent description of the dust component, which explicitly allows for a size-dependent drift velocity. This powerful approach has inspired Lüttke (2002) to develop an adaptive bin tracking algorithm where the evolution of each

bin is followed in time and space, using the multi-grid method of Nowak (1993).

In the business of fitting the spectra of brown dwarfs and extra-solar gas planets, much simpler approaches have been adopted so far in order to study the effects of element depletion and dust sedimentation by gravitational settling. In the frame of static model atmospheres with frequency-dependent radiative transfer, the usual procedure is to remove heavy elements like Ti, Fe, Mg, . . . from the object's atmosphere, assuming that these elements have been consumed by dust formation guided by stability arguments (Burrows et al. 1997; Burrows & Sharp 1999; Saegers & Sasselow 2000). Depending on the purpose of the model, dust formation is either simply disregarded, the dust is assumed to be fully present or to have rained out completely, leaving behind a saturated gas. An extensive time-scale study of dust formation and sedimentation for the atmospheres of Jupiter, Venus, and Mars has been presented by Rossow (1978). Ackermann & Marley (2001) have extended these time-scale considerations to the turbulent regime for large dust Reynolds numbers by adopting various data fits. Cooper et al. (2002) have presented further time-scale arguments in consideration of an atmosphere with prescribed supersaturation to arrive at a maximum size of dust particles as function of depth, emphasising the influence of particles sizes on the resulting spectra. However, usually much simpler *ad-hoc* assumptions about the grain size distribution are made, e.g. relying on the size distribution function known from the interstellar medium (e.g. Allard et al. 2001). Very recently, Tsuji (2002) has published photospheric models based on the assumption that the dust particles remain very small (smaller than the critical cluster size) such that the particles are continuously evaporating and reforming. In this case, the problem of the gravitational settling does not occur. All these simple approaches allow for an easy use of up-to-date solid opacity data in the simulations, but a consistent theoretical description of the dust component is still not at hand.

In this paper, we aim at a solution of this new problem in stellar atmospheres. We formulate a physical description of the formation, the temporal evolution and the gravitational settling of dust grains in brown dwarf atmospheres, consistently coupled to the element consumption from the gas phase, by modifying and extending the moment method developed by Gail & Sedlmayr (1988). This description is based on partial differential equations for the moments of the dust grain size distribution function in conservation form, which avoids an elaborate and time-consuming binning of the size distribution function, thus making a straightforward inclusion into hydrodynamics and classical stellar atmosphere calculations possible.

After the outline of the *forces* in the equation of motion, the concept of *equilibrium drift* is discussed in Sect. 2. Section 3 contains a physical description of the *dust growth* by accretion of molecules in the free molecular flow ($Kn \gg 1$) and in the viscous case ($Kn \ll 1$). Section 4 investigates the influence of the *latent heat of condensation* and the frictional heating due to particle drift on the growth process. In Sect. 5, our new description of the dust component by means of *moment equations* is developed. The character of these equations is discussed by

analysing the corresponding *dimensionless equations* and *characteristic numbers* in Sect. 6. Section 7 comprises our conclusions and future aims.

2. The equation of motion

The trajectory $\mathbf{x}(t)$ of a spherical dust particle of radius a and mass $m_d = \frac{4\pi}{3}a^3\rho_d$, floating in a gaseous environment like a stellar atmosphere, is determined by Newton's law

$$m_d\ddot{\mathbf{x}} = \mathbf{F}_{\text{grav}}(\mathbf{x}, a) + \mathbf{F}_{\text{rad}}(\mathbf{x}, a) + \mathbf{F}_{\text{fric}}(\mathbf{x}, a, \mathbf{v}_{\text{dr}}). \quad (1)$$

\mathbf{F}_{grav} is the gravitational force, \mathbf{F}_{rad} the radiative force due to absorption and scattering of photons, and \mathbf{F}_{fric} the frictional force exerted by the surrounding gas via collisions. The frictional force depends on the relative velocity (drift velocity) between the dust particle and the gas $\mathbf{v}_{\text{dr}} = \dot{\mathbf{x}} - \mathbf{v}_{\text{gas}}$. The gas is hereby considered as a hydrodynamic ensemble with velocity \mathbf{v}_{gas} . ρ_d is the density of the dust grain material.

2.1. Force of gravity

The gravitational force on the grain is given by

$$\mathbf{F}_{\text{grav}}(\mathbf{x}, a) = m_d \mathbf{g}(\mathbf{x}), \quad (2)$$

where $\mathbf{g}(\mathbf{x}) = -g_*(R_*/r)^2\mathbf{e}_r$ is the gravitational acceleration and \mathbf{e}_r the unit vector in radial direction. Because of the small extension of the atmospheres of brown dwarfs ($H_p/R_* \approx 10^{-5} \dots 10^{-4}$), the radial distance r is about equal to the stellar radius R_* , and \mathbf{g} becomes a constant.

2.2. Force of radiation

The radiative force is given by the momentum transfer from the ambient radiation field to the grain due to absorption and scattering of photons

$$\mathbf{F}_{\text{rad}}(\mathbf{x}, a) = \frac{4\pi}{c} \int_0^\infty \pi a^2 Q_{\text{ext}}(a, \lambda) \mathbf{H}_\lambda(\mathbf{x}) d\lambda, \quad (3)$$

where $\mathbf{H}_\lambda(\mathbf{x})$ is the Eddington flux of the radiation field at wavelength λ and site \mathbf{x} . Q_{ext} is a dimensionless extinction efficiency of the grain, which can be calculated from the optical properties of the grain material (real and imaginary part of the refractory index) by applying Mie theory, see e.g. Bohren & Huffman (1983).

However, as the following rough estimation will demonstrate, the radiative force is small compared to the other forces in brown dwarf atmospheres and can be neglected. We simplify the integral in Eq. (3) by pulling out the flux mean extinction efficiency $\overline{Q}_{\text{ext}}^H(a)$. The wavelength integrated Eddington flux is given by $\mathbf{H}(\mathbf{x}) = \frac{1}{4\pi}\sigma T_{\text{eff}}^4 (R_*/r)^2 \mathbf{e}_r$, where σ is the Stefan-Boltzmann constant and T_{eff} is the effective temperature of the star. Considering furthermore the small particle limit (SPL) of Mie theory $2\pi a \ll \lambda$ (Rayleigh limit), the extinction efficiency is proportional to the grain size $Q_{\text{ext}}(a, \lambda) = a \widehat{Q}_{\text{ext}}^{\text{SPL}}(\lambda)$, and Eq. (3) results in

$$|\mathbf{F}_{\text{rad}}(\mathbf{x}, a)| \lesssim \frac{\pi a^3}{c} \overline{Q}_{\text{ext}}^{\text{SPL}H} \left(\frac{R_*}{r} \right)^2 \sigma T_{\text{eff}}^4. \quad (4)$$

Table 1. Estimation of the gravitational and the radiative forces acting on small dust grains in the atmospheres of a red giant and a brown dwarf. A mass density of the dust grain material of $\rho_d = 2 \text{ g cm}^{-3}$ is assumed.

$\widehat{Q}_{\text{ext}}^{\text{SPL}} [\text{cm}^{-1}]$	$ \mathbf{F}_{\text{rad}} [\text{dyn}]$	$ \mathbf{F}_{\text{grav}} [\text{dyn}]$
Red Giant:		
$T_{\text{eff}} = 3000 \text{ K}, \log g_* = 0, r = 2 R_*$		
10^1	$a^3 \cdot 1.2 \times 10^0$	$a^3 \cdot 2.1 \times 10^0$
10^4	$a^3 \cdot 1.2 \times 10^4$	$a^3 \cdot 2.1 \times 10^0$
Brown Dwarf:		
$T_{\text{eff}} = 2000 \text{ K}, \log g_* = 5, r = 1 R_*$		
10^1	$a^3 \cdot 9.5 \times 10^{-1}$	$a^3 \cdot 8.4 \times 10^5$
10^4	$a^3 \cdot 9.5 \times 10^3$	$a^3 \cdot 8.4 \times 10^5$

For large grains, the radiative force is smaller than in the small particle limit and asymptotically scales as $\sim a^2$. Therefore, we put the relation sign “ \lesssim ” in Eq. (4). The flux mean extinction coefficient is roughly given by a typical value of Q_{ext} around the maximum of the stellar flux (see Table 1). Considering a wavelength interval from $1 \mu\text{m}$ to $10 \mu\text{m}$, typical values of the extinction efficiency $\widehat{Q}_{\text{ext}}^{\text{SPL}}$ are found to vary between 10 cm^{-1} (crystalline, glassy materials like $\text{Al}_2\text{O}_3, \text{TiO}_2$) and 10^4 cm^{-1} (e.g. amorphous carbon, iron bearing solid materials like MgFeSiO_4), see Mutschke et al. (1998), Tamanai (1998), Andersen et al. (1999), Posch et al. (1999) or, for an overview, see Woitke (1999).

Table 1 demonstrates that the radiative force on dust grains in brown dwarf atmospheres is always much smaller than the gravity, even in case of light but opaque grains¹. Consequently, the radiative force can be neglected, and the dust grain's equation of motion (Eq. (1)) simplifies to

$$m_d\ddot{\mathbf{x}} = \mathbf{F}_{\text{grav}}(\mathbf{x}, a) + \mathbf{F}_{\text{fric}}(\mathbf{x}, a, \mathbf{v}_{\text{dr}}). \quad (5)$$

2.3. Force of friction

An unique description of the frictional force (drag force) is difficult to obtain for brown dwarf atmospheres. These difficulties arise from the fact that the behaviour of the gas flow around the moving dust grain changes qualitatively with changing grain size, changing drift velocity and/or changing thermodynamic state of the gas. There are transitions from freely impinging gas particles to a viscous flow, from a subsonic to a supersonic behaviour, and from a laminar flow to turbulence. The physical conditions in brown dwarf atmospheres are such that all transitions may possibly occur. Reliable physical descriptions of the drag force are only available in certain limited regimes and an unique description must be compiled from these special cases.

In order to quantify the behaviour of the streaming gas flow, the following characteristic numbers are introduced: the Knudsen number Kn and the dust Reynolds number Re_d . The Knudsen number Kn is defined by the ratio of the mean free path length of the gas particles $\bar{\ell}$ to a typical dimension ℓ_{ref} of

¹ In contrast, the radiative force generally dominates in the circumstellar envelopes of red giants.

the gas flow under consideration, here given by the diameter of the grain

$$Kn = \frac{\bar{\ell}}{2a}. \quad (6)$$

Kn expresses the influence of inter-molecular collisions. In case $Kn \gg 1$ (e.g. small gas densities), inter-molecular collisions are rare in the streaming flow. Consequently, the drag force results from a simple superposition of independent, elementary collisions where the velocity distribution of the impinging gas particles resembles a Maxwellian distribution characterised by the gas temperature T which is shifted in velocity space by \mathbf{v}_{dr} (*free molecular flow*).

In contrast, if $Kn \ll 1$, inter-molecular collisions are frequent and the stream of gas particles colliding with the dust grain becomes viscous. In this case, the drag force cannot be obtained via reduction to elementary collisions. This is the regime of continuum theory for which well-tested empirical formulae are available, e.g. from engineering science (*viscous case or slip flow*), depending on whether the gas flow around the dust grain is laminar or turbulent. In order to characterise the transition from laminar (Stokes) friction to turbulent (Newtonian) friction, the dust grain's Reynolds number Re_d is introduced

$$Re_d = \frac{2a\rho|\mathbf{v}_{\text{dr}}|}{\mu_{\text{kin}}} \quad (7)$$

with the characteristic properties $l_{\text{ref}} = 2a$, $v_{\text{ref}} = |\mathbf{v}_{\text{dr}}|$, and $\rho_{\text{ref}} = \rho_{\text{gas}} = \rho$. For large Reynolds numbers ($Re_d \gtrsim 1000$) the flow around a dust particle is turbulent, whereas for small Reynolds numbers ($Re_d \lesssim 1000$) the flow is laminar (for a discussion on these limits see e.g. Großmann 1995).

In order to evaluate the kinematic viscosity of the gas μ_{kin} we follow the considerations of Jeans (1967) for a mixture of ideal gases

$$\mu_{\text{kin}} = \sum_i \frac{0.499 n_i m_i v_i^{\text{th}}}{\sum_j n_j \pi (r_i + r_j)^2 \sqrt{1 + \frac{m_i}{m_j}}}, \quad (8)$$

where n_i , m_i , r_i and $v_i^{\text{th}} = \sqrt{8kT/(\pi m_i)}$ are the gas particle densities, masses, radii and thermal velocities, respectively. Assuming a mixture of H_2 and He with particle ratio 5:1 and particle radii derived from friction experiments ($r_{\text{H}_2} = 1.36 \text{ \AA}$ and $r_{\text{He}} = 1.09 \text{ \AA}$; Jeans 1967), we find the viscosity to be

$$\mu_{\text{kin}} = 5.877 \times 10^{-6} \frac{\text{g}}{\text{cm s}} \sqrt{T[\text{K}]}. \quad (9)$$

The mean free path $\bar{\ell}$ entering into Eq. (6) is calculated backwards from Eq. (9), using the general relation $\mu_{\text{kin}} = \frac{1}{3} \rho \bar{v}_{\text{th}} \bar{\ell}$ in consideration of mean gas particles only², where $\bar{v}_{\text{th}} = \sqrt{8kT/(\pi \bar{\mu})}$ is the mean thermal velocity and $\bar{\mu} = \sum n_i m_i / \sum n_i \approx 2.35 \text{ amu}$ is the mean molecular weight

$$\bar{\ell} = 1.86 \times 10^{-4} \text{ cm} \cdot \left(\frac{\rho}{10^{-5} \text{ g cm}^{-3}} \right)^{-1}, \quad (10)$$

² Accordingly, the product of the characteristic numbers Kn and Re_d is given by $Kn \cdot Re_d = 3|\mathbf{v}_{\text{dr}}|/\bar{v}_{\text{th}}$.

which corresponds to a value of the mean collisional cross section of the H_2/He -mixture defined by

$$\bar{\ell} = \frac{1}{n \bar{\sigma}} \quad (11)$$

of $\bar{\sigma} = \bar{\mu}/(\rho \bar{\ell}) = 2.1 \times 10^{-15} \text{ cm}^2$, which is more than three times larger as $\pi r_{\text{H}_2}^2 = 5.8 \times 10^{-16} \text{ cm}^2$.

Free molecular flow ($Kn \gg 1$): Considering the mechanics of rarefied gases, Schaaf (1963) derives a formula for the drag force by freely impinging gas particles due to elastic collisions, equally applicable in the subsonic as well as in the supersonic range,

$$\mathbf{F}_{\text{fric}}^{\text{Sch}} = -\pi a^2 \rho |\mathbf{v}_{\text{dr}}| \mathbf{v}_{\text{dr}} \cdot \left[\left(1 + \frac{1}{s^2} - \frac{1}{4s^4} \right) \text{erf}(s) + \left(\frac{1}{s} + \frac{1}{2s^3} \right) \frac{e^{-s^2}}{\sqrt{\pi}} \right], \quad (12)$$

with abbreviations $s = |\mathbf{v}_{\text{dr}}|/c_T$ and $c_T = \sqrt{2kT/\bar{\mu}}$. The error function is defined by $\text{erf}(s) = \frac{2}{\sqrt{\pi}} \int_0^s e^{-s'^2} ds'$. Equation (12) has the following asymptotic behaviour

$$\mathbf{F}_{\text{fric}}^{\text{Sch}} \rightarrow \begin{cases} -\frac{8\sqrt{\pi}}{3} a^2 \rho c_T \mathbf{v}_{\text{dr}} & , |\mathbf{v}_{\text{dr}}| \ll c_T \\ -\pi a^2 \rho |\mathbf{v}_{\text{dr}}| \mathbf{v}_{\text{dr}} & , |\mathbf{v}_{\text{dr}}| \gg c_T \end{cases}. \quad (13)$$

Viscous case ($Kn \ll 1$): In this regime, continuum theory is valid for which well-tested empirical formulae exist. Lain et al. (1999), carrying out experimental studies on bubbly flows, arrive at the following empirical expression for the drag force

$$\mathbf{F}_{\text{fric}}^{\text{LBS}} = -\pi a^2 c_D \frac{\rho}{2} |\mathbf{v}_{\text{dr}}| \mathbf{v}_{\text{dr}} \quad (14)$$

where the drag coefficient c_D is given by

$$c_D = \begin{cases} \frac{24}{Re_d} (1 + 0.15 Re_d^{0.687}) & , Re_d \leq 500 \\ 9.5 \times 10^{-5} Re_d^{1.397} & , 500 < Re_d \leq 1500 \\ 2.61 & , Re_d > 1500. \end{cases} \quad (15)$$

Comparable formulae can be found in (Huber & Sommerfeld 1998), studying spherical coal particles in pipes, and in (Macek & Polasek 2000), modelling the inverse problem of porous media in combustion engineering for elliptical particles³. We note that Eqs. (12) and (14) are strictly valid only for perfectly rigid, spherical particles. Deviations from this ideal case, e.g. shape distortions of liquid grains, porosity and non-spherical shapes of solid grains, generally lead to an *increase* of the effective surface area and hence to a *decrease* of the gravitational fall speed as defined in Sect. 2.4 (for further details see Rossow 1978, p. 14). Such second order effects might roughly be accounted for by reducing the dust material density ρ_d .

³ We note that such empirical formulae cannot be derived from first principles without additional assumptions about the physics of the microscopic interactions which can only be introduced as phenomenological values (Sedlmayr 1976).

Using Eq. (7), the drag force in the viscous case according to Eq. (14) is found to have the following asymptotic behaviour

$$\mathbf{F}_{\text{fric}}^{\text{LBS}} \rightarrow \begin{cases} -6\pi a \mu_{\text{kin}} \mathbf{v}_{\text{dr}} & , Re_d \ll 1 \\ -1.3 \pi a^2 \rho |\mathbf{v}_{\text{dr}}| \mathbf{v}_{\text{dr}} & , Re_d > 1500 \end{cases} \quad (16)$$

which reveals the classical formulae for Stokes friction (laminar flow) and Newtonian friction (turbulent flow), respectively.

The general case: For flows with an intermediate Knudsen number ($Kn \approx 1$), so-called transition flows, reliable expressions for the drag force are difficult to obtain. We therefore define a critical Knudsen number Kn^{cr} where $\mathbf{F}_{\text{fric}}^{\text{Sch}}$ equals $\mathbf{F}_{\text{fric}}^{\text{LBS}}$. Considering the limiting cases of subsonic drift velocities and small Re_d in Eqs. (13) and (16), respectively, the result is exactly

$$Kn^{\text{cr}} = \frac{1}{3}. \quad (17)$$

In order to arrive at a general formula for arbitrary Knudsen numbers we adopt a simple interpolation scheme⁴

$$\mathbf{F}_{\text{fric}} = \mathbf{F}_{\text{fric}}^{\text{Sch}} \left(\frac{Kn'}{Kn' + 1} \right)^2 + \mathbf{F}_{\text{fric}}^{\text{LBS}} \left(\frac{1}{Kn' + 1} \right)^2 \quad (18)$$

where $Kn' = Kn/Kn^{\text{cr}}$. We note that a Cunningham factor $(1 + \beta Kn)$ has been introduced in the literature (see e.g. Rossow 1978) in order to extrapolate the resulting formula for the final fall speed valid in the $Kn \ll 1$ case (see Eq. (72)) into the $Kn \gg 1$ regime. The constant β is usually fixed by measurements. However, it is questionable whether the theoretically known friction law for the limiting case $Kn \rightarrow \infty$ is revealed in this way. Our finding is consistent with $\beta = 3$ (or $\beta = 1.5$ if the Knudsen number is defined as $Kn = \bar{\ell}/a$, compare Eqs. (6) and (63)).

2.4. Equilibrium drift

Considering a dust particle of constant radius a floating in a gas at constant thermodynamical conditions (ρ , T) and a constant velocity \mathbf{v}_{gas} , the particle will be accelerated until a force equilibrium is reached, where the gravitational acceleration is balanced by frictional deceleration

$$m_d \mathbf{g}(\mathbf{x}) + \mathbf{F}_{\text{fric}}(\mathbf{x}, a, \dot{\mathbf{v}}_{\text{dr}}) = 0. \quad (19)$$

Equation (19) states an implicit definition for the gravitational fall speed (or, more precisely, the equilibrium drift velocity⁵) $\dot{\mathbf{v}}_{\text{dr}}$. The equilibrium drift velocity is determined by \mathbf{g} , a , ρ and T , and is always directed towards the centre of gravity, even within a horizontal gas flow. Whether or not this equilibrium state is reached in a realistic situation will be discussed in Sect. 2.5. In the general case, $\dot{\mathbf{v}}_{\text{dr}}$ cannot be obtained from an analytical inversion of Eq. (19), but must be calculated by finding the root of Eq. (19) numerically, applying iterative methods.

⁴ The interpolation coefficients in Eq. (18) do not sum up to 1, because at $Kn = Kn^{\text{cr}}$ (where $\mathbf{F}_{\text{fric}}^{\text{Sch}} = \mathbf{F}_{\text{fric}}^{\text{LBS}}$) the true \mathbf{F}_{fric} is *smaller* than in both limiting cases.

⁵ Rossow (1978) uses the term “terminal velocity” for $\dot{\mathbf{v}}_{\text{dr}}$, Ackermann & Marley (2001) use “terminal fall speed”.

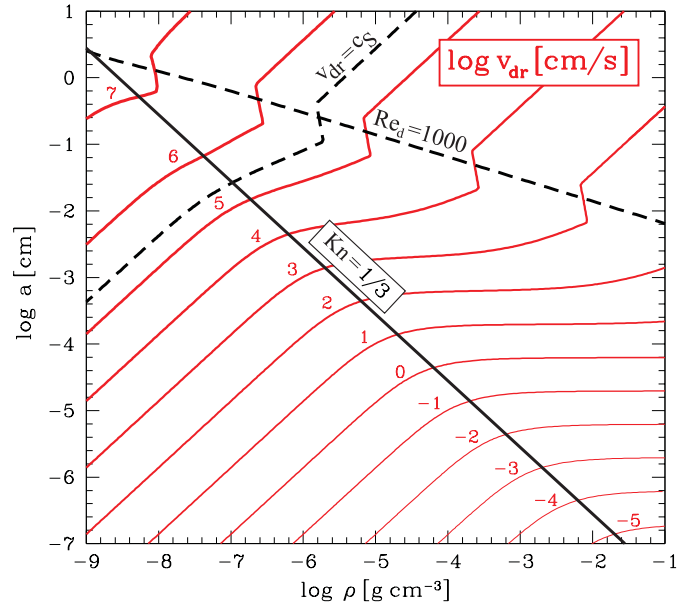


Fig. 1. Contour plot of the equilibrium drift velocity $\log \dot{v}_{\text{dr}}$ [cm s⁻¹] as function of grain radius a and gas density ρ at constant temperature $T = 1500$ K and gravitational acceleration $g = 10^5$ cm s⁻². A mass density of the dust grain material of $\rho_d = 2.65$ g cm⁻³ (quartz – SiO₂) is assumed.

Figure 1 shows the resulting values of \dot{v}_{dr} in a brown dwarf’s atmosphere with $\log g = 5$. The equilibrium drift velocities roughly range in $[10^{-4}, 10^{+6}]$ cm s⁻¹ and are generally smaller for small particles and large densities. The small bendings of the contour lines around $Re_d \approx 1000$ are no numerical artifacts but result from the measured re-increase of the drag coefficient of spherical particles c_D between $Re_d = 500$ and $Re_d = 1500$ (Eq. (15)), associated with the transition from laminar to turbulent friction.

Small dust particles can sustain longer in the respective atmospheric layers, whereas large grains will “rain out” sooner. Only dust particles $\geq 100 \mu\text{m}$ at gas densities $\leq 10^{-7}$ g cm⁻³ can hereby reach a drift velocity beyond the local velocity of sound $\dot{v}_{\text{dr}} > c_s = \sqrt{\gamma kT/\bar{\mu}}$. However, such particles will remove themselves so quickly from the respective atmospheric layers ($\tau_{\text{sink}} < 4$ s) that this case seems very unlikely to be relevant for any part of the atmosphere, unless there exists a physical process (convective streams or atmospheric winds) which is capable to produce supersonic upwinds. The time-scale for gravitational settling is hereby defined as

$$\tau_{\text{sink}} = H_p / |\dot{v}_{\text{dr}}|. \quad (20)$$

$H_p = kT/(\bar{\mu}g) \approx 10^6$ cm is the pressure scale height of the brown dwarf’s atmosphere.

Figure 1 demonstrates furthermore that even the smallest dust particles cannot sustain forever but will slowly sink into deeper layers. Assuming that the dust particles do not grow along their way down the atmosphere (which would increase their drift velocity), a $0.1 \mu\text{m}$ -particle starting in an atmospheric layer with $\rho = 10^{-5}$ g cm⁻³ needs about $\tau_{\text{sink}} \approx 2 \times 10^7$ s

(8 months) to pass one scale height. A dust particle with $a = 100 \mu\text{m}$ needs only $\sim 1/4$ hour⁶.

The destiny of those particles drifting inward is to finally reach an atmospheric layer where the temperature is high enough to evaporate them thermally. This sets free the elements the dust grains are composed off and thereby *enriches* the surrounding gas in this layer. Hence, the rain-out will tend to saturate the gas below the cloud base, where the “cloud base” is identified with the level in the atmosphere where the dust grains are just thermodynamically stable ($S = 1$, see Sect. 3).

2.5. Accelerated drift

The actual relative velocity of the dust particle with respect to the gas, $\mathbf{v}_{\text{dr}}(a, \mathbf{x}, t)$, can of course deviate from its equilibrium value defined in Sect. 2.4. It will only asymptotically reach $\hat{\mathbf{v}}_{\text{dr}}(a, \mathbf{x})$ for $t \rightarrow \infty$, if the parameters a , \mathbf{v}_{gas} , ρ and T are constant. However, considering a dust particle created in a brown dwarf atmosphere, the particle may grow by accretion of molecules ($da/dt \neq 0$, see Sect. 3) and the physical state of the surrounding gas may change with time (e.g. $d\rho/dt \neq 0$) as the particle sinks into deeper layers of the atmosphere. Turbulence may furthermore create a time-dependent velocity field ($d\mathbf{v}_{\text{gas}}/dt \neq 0$), which provides an additional cause for temporal deviations between $\mathbf{v}_{\text{dr}}(a, \mathbf{x}, t)$ and $\hat{\mathbf{v}}_{\text{dr}}(a, \mathbf{x})$.

Thus, an important question for the discussion of the dynamical behaviour of the dust component in brown dwarf atmosphere is, whether or not $\mathbf{v}_{\text{dr}}(a, \mathbf{x}, t)$ can be replaced by $\hat{\mathbf{v}}_{\text{dr}}(a, \mathbf{x})$, at least approximately.

In order to discuss this question, we consider the dust particle acceleration time-scale τ_{acc} towards equilibrium drift. Expressing the dust particle’s equation of motion (Eq. (5)) in terms of the first-order differential equation $dy/dt = f(y)$ with $y = v_{\text{dr}}$ and $f(y) = F_{\text{fric}}(v_{\text{dr}})/m_{\text{d}} - g$, and assuming small deviations δy from the stability point \hat{y} (where $f(\hat{y}) = 0$), the temporal change of y is $dy/dt = f(\hat{y} + \delta y) \approx f(\hat{y}) + f'(\hat{y})\delta y$. Accordingly, the acceleration time-scale is given by $\tau_{\text{acc}} = \delta y / (dy/dt) = 1 / f'(\hat{y})$, or

$$\tau_{\text{acc}} = m_{\text{d}} \left(\frac{\partial F_{\text{fric}}}{\partial v_{\text{dr}}} \Big|_{\hat{v}_{\text{dr}}} \right)^{-1}. \quad (21)$$

This time-scale is to be compared with the other characteristic time-scales inherent in the ambient medium. A hydrodynamical time-scale $\tau_{\text{hyd}} = l_{\text{ref}}/v_{\text{ref}}$ results to be ≈ 10 s when the so-called micro-turbulence velocity $v_{\text{micro}} \approx c_{\text{S}} \approx 10^5 \text{ cm s}^{-1}$, introduced to fit otherwise unidentified line broadening effects, is considered on macroscopic scales $l_{\text{ref}} = H_{\text{p}} \approx 10^6 \text{ cm}$. About the same value is found when mean convective velocities derived from mixing length theory $v_{\text{MLT}} \approx 10^3 \text{ cm s}^{-1}$ are considered on microscopic scales $l_{\text{ref}} \approx 10^4 \text{ cm}$. Comparison to Fig. 2 shows that usually $\tau_{\text{acc}} \ll \tau_{\text{hyd}}$ in brown dwarf atmospheres, unless

⁶ Pushing these simple time-scale arguments forward, one could arrive at the wrong conclusion that brown dwarf’s atmosphere with lifetimes $> 10^9$ yrs must be completely dust-free. The error in this conclusion is that brown dwarf’s atmospheres are not static, but turbulent, and the convection leads to a non-continuous replenishment of the upper atmosphere with condensable elements.

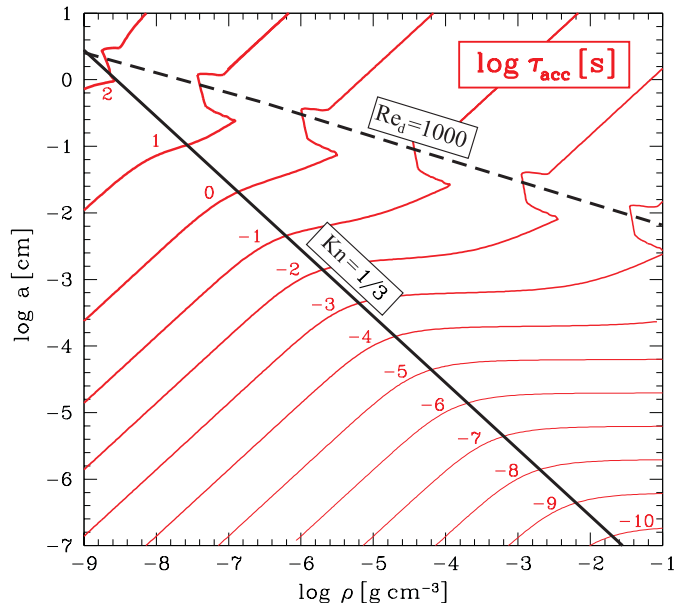


Fig. 2. Contour plot of the acceleration time-scale towards equilibrium drift τ_{acc} [s] as function of grain radius a and gas densities ρ . Other parameters are the same as in Fig. 1.

very large grains with supersonic fall speeds are considered. This implies that the dust particles will reach their equilibrium drift velocity much faster than usual hydrodynamical changes occur.

For a powerlaw dependence $F_{\text{fric}} \propto v_{\text{dr}}^{\beta}$, Eqs. (20) and (21) result in $\tau_{\text{acc}}/\tau_{\text{sink}} = \frac{\gamma}{\beta} \left(\frac{v_{\text{dr}}}{c_{\text{S}}} \right)^2$, i.e. we find $\tau_{\text{acc}} \ll \tau_{\text{sink}}$ for $v_{\text{dr}} \ll c_{\text{S}}$. Since Sect. 3 will demonstrate that also the growth of the dust particles is slow in comparison to τ_{acc} , we may conclude that the concept of equilibrium drift provides a good approximation for the description of the size-dependent relative velocities between dust and gas in brown dwarf atmospheres.

3. Dust growth and evaporation

A fundamental process for the consideration of the time-dependent behaviour of the dust component in brown dwarf atmospheres is the growth of the dust particles by accretion of molecules. The respective reverse process (thermal evaporation, in view of more complex surface reactions also sometimes denoted by chemical sputtering) is important at high temperatures⁷. Considering the thermodynamical conditions in brown dwarf atmospheres, we are again faced with the problem of qualitative changes of the dynamical behaviour of the gas component due to different Knudsen numbers.

⁷ We will not discuss coagulation caused by dust-dust collisions in this paper. According to Cooper et al. (2002), coagulation (also denoted as “coalescence” if the dust-dust collisions are caused by the size-dependent drift velocities) generally operates on larger time-scales than the growth. We note, however, that the coagulation remains the only active physical process influencing the dust size distribution if the supersaturation ratio S is very close to unity, where growth and nucleation vanish.

Free molecular flow ($Kn \gg 1$): For large Knudsen numbers (lKn), gas molecules of all kinds are freely impinging onto the surface of the grain. Some of these dust-molecule collisions (sometimes a certain sequence of them) will initiate a chemical surface reaction which causes a growth step (or an evaporation step) of the dust particle. This case has been extensively studied in the circumstellar envelopes of AGB stars (Gail & Sedlmayr 1988; Gauger et al. 1990; Dominik et al. 1993).

The accretion rate, expressed in terms of the increase of the particle's volume $V = 4\pi a^3/3$ due to chemical surface reactions for large Knudsen numbers is given by

$$\frac{dV}{dt}{}^{lKn} = 4\pi a^2 \sum_r \Delta V_r n_r v_r^{\text{rel}} \alpha_r \left(1 - \frac{1}{S_r}\right), \quad (22)$$

where “r” is a general surface reaction index, ΔV_r is the increase of the dust particle's volume V caused by one reaction “r”. n_r is the particle density of a key gas species whose collision rate limits the rate of the surface reactions of index “r”. This gas species has to be identified by considering the particle densities present in the ambient gas and stoichiometric constraints. Equation (22) explicitly allows for the consideration of *heterogeneous growth*, where different solid phases can grow simultaneously on the same surface, resulting in “dirty” grains. The relative velocity is here defined as $v_r^{\text{rel}} = \sqrt{kT/(2\pi m_r)}$ where m_r is the mass of the key species. α_r is a sticking coefficient which contains more detailed knowledge about the surface chemical process, if available.

The last term on the r.h.s. of Eq. (22) takes into account the reverse chemical processes, namely the thermal evaporation rates. It determines the sign of dV/dt and hence decides whether the dust particle grows or shrinks. $S_r = n_r/\dot{n}_r$ is a generalised supersaturation ratio of the surface reaction “r” (Dominik et al. 1993) where \dot{n}_r is the particle density of the key species in phase-equilibrium over the condensed dust material. S_r is not known a priori. In the case of simple surface reactions, which transform m_r units of the solid material \mathcal{A} from the gaseous into the condensed phase (and vice versa), e.g. $[\text{TiO}_2]_{\text{N}}(\text{s}) + \text{TiO}_2 \rightleftharpoons [\text{TiO}_2]_{\text{N+1}}(\text{s})$ ($\mathcal{A} = \text{TiO}_2$, $m_r = 1$) or $\text{C}_{\text{N}}(\text{s}) + \text{C}_2\text{H}_2 \rightleftharpoons \text{C}_{\text{N+2}}(\text{s}) + \text{H}_2$ ($\mathcal{A} = \text{C}$, $m_r = 2$), the generalised supersaturation ratio S_r is related to the usual supersaturation ratio $S = n_{\mathcal{A}}kT/p_{\mathcal{A}}^{\text{vap}}(T)$ of the dust grain material \mathcal{A} (Gauger et al. 1990) by

$$S_r = S^{m_r}. \quad (23)$$

$p_{\mathcal{A}}^{\text{vap}} = \dot{n}_{\mathcal{A}}kT$ denotes the saturation vapour pressure of the molecule \mathcal{A} over a flat surface of the condensed state, which is a pure temperature function determined by the Gibbs free energies of the solid and the gaseous species \mathcal{A} . The supersaturation ratio S is well-defined even if \mathcal{A} is not stable as a free molecule (Woitke 1999).

It is principally possible to account for additional effects caused by a fast relative motion of the grain within the scope of this description for grain growth and evaporation. These effects comprise an enlargement of v_r^{rel} as well as a decrease of α_r in the case of super-thermal collisions (see Krüger et al. 1996). However, such effects become only relevant for supersonic drift velocities which, following the discussion in Sect. 2.4, are not

very likely to be relevant for brown dwarf atmospheres due to the fast self-removal of the respective dust particles.

Viscous case ($Kn \ll 1$): For small Knudsen numbers (sKn), the transport of gas molecules to the surface of the grain (or the transport of evaporating molecules away from the grain's surface) is not a simple free flight with thermal velocity as assumed in Eq. (22), but is hindered by inter-molecular collisions. Consequently, the grain growth and evaporation is limited by the diffusion of molecules towards or away from the grain's surface, considering growth or evaporation in the laminar case, respectively (we disregard here convection as transport process for the molecules, expected to occur in the turbulent case). We consider the following particle conservation equation with a diffusive transport term (see Landau & Lifschitz 1987, Eq. (38.2) ff)

$$\frac{\partial}{\partial t}(\rho c_i) + \nabla \cdot (\mathbf{v}_{\text{gas}} \rho c_i) = -\nabla \cdot \mathbf{j}_i^{\text{diff}}. \quad (24)$$

$c_i = n_i/\rho$ [g^{-1}] is the concentration of gaseous molecules of kind i in the gas with mass density ρ and velocity \mathbf{v}_{gas} . The diffusive particle flux is given by

$$\mathbf{j}_i^{\text{diff}} = -\rho D_i \nabla c_i, \quad (25)$$

where D_i is the diffusion constant of gas particles of the kind i in the gas mainly composed of H_2 molecules (we neglect He atoms here), as given by Jeans (1967, Eq. (260))

$$D_i = \frac{v_{\text{th},i}^{\text{red}}}{3\pi (r_{\text{H}_2} + r_i)^2 n}. \quad (26)$$

$v_{\text{th},i}^{\text{red}} = \sqrt{8kT/(\pi m_{\text{red}})}$ is the thermal velocity of a gas particle of kind i with reduced mass $1/m_{\text{red}} = 1/m_{\text{H}_2} + 1/m_i$, where m_{H_2} and m_i are the masses of H_2 and i , respectively. $n = \rho/\bar{\mu}$ is the total gas particle density. The particle radii r_i can be derived from friction experiments (see Jeans 1967, p. 183) and vary between the values for hydrogen $r_{\text{H}_2} = 1.36 \text{ \AA}$, carbon monoxide $r_{\text{CO}} = 1.89 \text{ \AA}$, water and carbon dioxide $r_{\text{H}_2\text{O}} = r_{\text{CO}_2} = 2.33 \text{ \AA}$ to benzene $r_{\text{C}_6\text{H}_6} = 3.75 \text{ \AA}$.

Considering the static case ($\mathbf{v}_{\text{gas}} = 0$) and assuming stationary ($\partial(\rho c_i)/\partial t = 0$) and spherical symmetry, Eq. (24) results in

$$\nabla \cdot (\rho D_i \nabla c_i) = \frac{1}{r^2} \frac{\partial}{\partial r} \left(r^2 \rho D_i \frac{\partial c_i}{\partial r} \right) = 0. \quad (27)$$

Assuming furthermore constant ρ and D_i , we find

$$r^2 \rho D_i \frac{\partial c_i}{\partial r} = \text{const}_i. \quad (28)$$

In order to solve the second order diffusion equation (27), two boundary conditions must be specified. First, considering the asymptotic behaviour for $r \rightarrow \infty$, we assume that the concentration c_i approaches the undisturbed value n_i/ρ in the distant gas. Second, at the lower integration boundary $r = a$, we assume phase equilibrium

$$c_i(\infty) = \frac{n_i}{\rho} \quad (29)$$

$$c_i(a) = \frac{\dot{n}_i}{\rho} = \frac{n_i}{\rho} \frac{1}{S_i}, \quad (30)$$

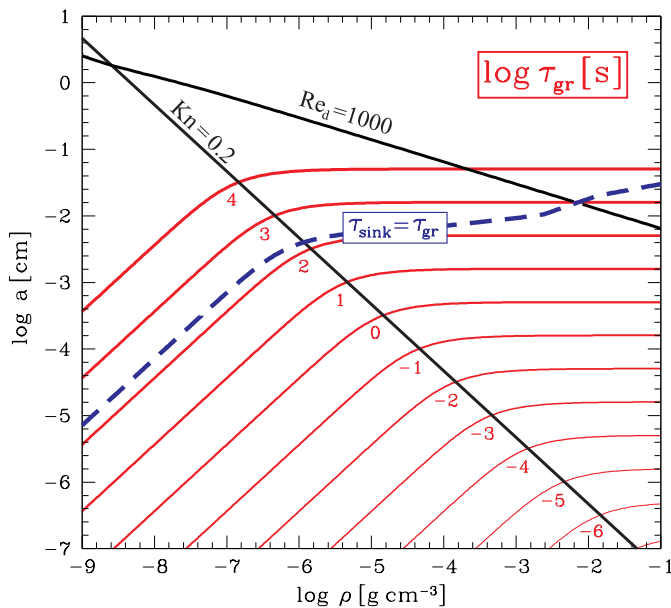


Fig. 3. Contour plot of the growth time-scale $\log \tau_{\text{gr}}$ [s] as function of the grain radius a and the gas density ρ at constant temperature $T = 1500$ K for quartz (SiO_2 , $\rho_d = 2.65 \text{ g cm}^{-3}$). We assume growth by accretion of the key species SiO with solar particle density $n_{\text{SiO}} = 10^{(7.55-12)} n_{(\text{H})}$ and extreme supersaturation ($S \rightarrow \infty$). $r_{\text{SiO}} = 2 \times 10^{-8} \text{ cm}$ is estimated.

i.e. we assume that the chemical surface reactions responsible for the growth and evaporation of the dust particle are sufficiently effective to completely exhaust or enrich the gas in the boundary layer with molecules of kind i for growth and evaporation, respectively. As in the last paragraph, $S_i = n_i / \dot{n}_i$ is the supersaturation ratio.

The solution of Eq. (28) with the boundary conditions (29) and (30) is

$$c_i(r) = \frac{n_i}{\rho} \left(1 - \frac{a}{r} \left(1 - \frac{1}{S_i} \right) \right) \quad (31)$$

and the total volume accretion rate of the grain for small Knudsen numbers, summing up the contributions of several surface reactions of index r (like in Eq. (22)) with net rate $-4\pi r^2 j_i^{\text{diff}}$, according to Eqs. (25) and (31), is

$$\frac{dV^{\text{sKn}}}{dt} = 4\pi a \sum_r \Delta V_r D_r n_r \left(1 - \frac{1}{S_r} \right). \quad (32)$$

The description of the volume accretion rate according to Eq. (32) again allows for the simultaneous growth of different solid materials on the same surface, resulting in “dirty” grains (heterogeneous growth).

The general case: For arbitrary Knudsen numbers we apply the same interpolation scheme as outlined in Sect. 2.3. We define a critical Knudsen number Kn^{cr} by equating Eqs. (22) with (32)

$$a v_r^{\text{rel}} \alpha_r = D_r. \quad (33)$$

Using Eqs. (26) and (11), the result is

$$Kn_r^{\text{cr}} = \frac{\bar{\ell}}{2a} = \frac{3\pi(r_{\text{H}_2} + r_r)^2 \alpha_r}{8\bar{\sigma} \sqrt{1 + \frac{m_r}{m_{\text{H}_2}}}}. \quad (34)$$

Assuming perfect sticking ($\alpha_r = 1$) and considering typical molecular radii and masses between $r_{\text{CO}} = 1.89 \text{ \AA}$ and $r_{\text{H}_2\text{O}} = 2.33 \text{ \AA}$, and between $m_{\text{CO}} = 28 \text{ amu}$ and $m_{\text{H}_2\text{O}} = 18 \text{ amu}$, respectively, the resulting critical Knudsen numbers for growth Kn_r^{cr} are found to range in 0.15 to 0.24, independent of density and temperature. Thus, we simply adopt an unique critical Knudsen number for all growth and evaporation species

$$Kn^{\text{cr}} \approx 0.2. \quad (35)$$

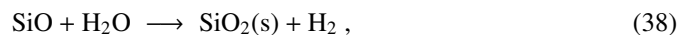
Our ansatz of the general volume accretion rate for arbitrary Knudsen numbers with $Kn' = Kn / Kn^{\text{cr}}$ is

$$\frac{dV}{dt} = \frac{dV^{\text{lKn}}}{dt} \left(\frac{Kn'}{Kn' + 1} \right)^2 + \frac{dV^{\text{sKn}}}{dt} \left(\frac{1}{Kn' + 1} \right)^2. \quad (36)$$

Figure 3 shows the resulting growth time-scale

$$\tau_{\text{gr}} = \frac{4\pi a^3}{3} \left/ \frac{dV}{dt} \right. \quad (37)$$

as function of particle size a and gas density ρ for the example of quartz grains in an extremely supersaturated gas ($S \rightarrow \infty$) of solar abundances, where all Si is bound to SiO. We consider the explicit growth reaction



where SiO is identified as the key educt.

The particle growth is found to be typically 3 orders of magnitude slower than the acceleration which allows us to assume instantaneous acceleration (equilibrium drift). For large Knudsen numbers, we find $\tau_{\text{gr}} \propto a/\rho$ whereas for small Knudsen numbers the growth time-scale increases faster for larger grains and becomes density-independent, $\tau_{\text{gr}} \propto a^2$. Note that the influence of the drift velocities on the particle growth has not been considered in Eqs. (22) and (32) such that for supersonic drift velocities or large dust Reynolds numbers, the presented physical description is not valid.

3.1. Maximum grain size

An additional dashed line is depicted in Fig. 3, where $\tau_{\text{gr}} = \tau_{\text{sink}}$. This line defines a maximum dust grain size a_{max} in a brown dwarf atmosphere. For larger particles ($a > a_{\text{max}}$ above the dashed line), the growth time-scale exceeds the time-scale for gravitational settling ($\tau_{\text{gr}} > \tau_{\text{sink}}$) which means that such particles are already removed from the atmosphere before they can be formed. Consequently, such particles cannot exist. The maximum grain size a_{max} varies between $\approx 1 \mu\text{m}$ in the thin, outer atmospheric regions ($\rho \approx 10^{-8} \text{ g/cm}^3$) and $\approx 100 \mu\text{m}$ in the dense, inner regions ($\rho \geq 10^{-5} \text{ g/cm}^3$). These values depend on the stellar parameters and the considered dust material density.

Note, that an absolute minimum of τ_{gr} has been considered in Fig. 3 since extreme supersaturation ($S \rightarrow \infty$) and solar abundance of silicon in the gas phase have been assumed. In the case

of an Si-depleted or nearly saturated gas ($S \gtrsim 1$), τ_{gr} becomes larger and the maximum particle radius a_{max} becomes smaller. Furthermore, the values for a_{max} are relatively independent of temperature, but will shift as $a_{\text{max}} \propto g$ in the free molecular flow case and $a_{\text{max}} \propto \sqrt{g}$ in the laminar viscous case, remembering that $\dot{v}_{\text{dr}} \propto g$ in both cases and that $H_p \propto 1/g$ (see also Eq. (81)).

Figure 3 demonstrates furthermore that dust particles moving with supersonic drift velocities cannot be expected in brown dwarf atmospheres. Similarly, the turbulent flow regime with dust Reynolds numbers $Re_d > 1000$ is barely reached at very large densities. Therefore, we can conclude that for dust grains in brown dwarf atmospheres the *subsonic free molecular flow* and the *laminar viscous flow* are the important cases to be investigated.

4. Energy balance of dust grains

The surface chemical reactions responsible for the growth of a dust particle liberate the latent heat of condensation $\Delta_t H$ [erg/g] which causes a heating of the grain as

$$Q_{\text{cond}} = \frac{dV}{dt} \rho_d \Delta_t H. \quad (39)$$

It has been proposed (Cooper et al. 2002) that this heating can increase the internal dust temperature T_d substantially, until the sublimation temperature is reached (where $S = 1$). In that case, the growth rate is limited by the need to remove the latent heat of condensation from the grain and Eqs. (22) and (32) are not valid.

A further heating process of the dust particle is given by the friction caused by the motion relative to the gas,

$$Q_{\text{fric}} = \alpha_{\text{fric}} |\mathbf{F}_{\text{fric}} \cdot \mathbf{v}_{\text{dr}}| = \alpha_{\text{fric}} m_d \mathbf{g} \cdot \dot{\mathbf{v}}_{\text{dr}}. \quad (40)$$

Hereby, we assume that the total work done by the frictional force per time, $|\mathbf{F}_{\text{fric}} \cdot \mathbf{v}_{\text{dr}}|$, is converted into heat, from which the fraction α_{fric} is delivered to the grain. For the r.h.s. expression, the condition of equilibrium drift $|\mathbf{F}_{\text{fric}}| = |\mathbf{F}_{\text{grav}}|$ is used (Eq. (5)). Since elastic collisions do not transfer any energy, we assume $\alpha_{\text{fric}} = \alpha_{\text{acc}}$ (see Eq. (43))⁸.

In order to determine the dust temperature increase, we balance these heating processes with the net energy losses due to radiation and due to inelastic collisions. The net radiative cooling rate of a single dust grain is given by

$$Q_{\text{rad}} = 4\pi \int \pi a^2 Q_{\text{abs}}(a, \lambda) [B_\lambda(T_d) - J_\lambda] d\lambda, \quad (41)$$

where Q_{abs} is the absorption efficiency, B_λ the Planck function and J_λ the mean intensity of the radiation field.

The cooling due to inelastic collisions with gas particles, in particular with H_2 , depends again on the Knudsen number. For large Knudsen numbers ($Kn \gg 1$) the collisional cooling rate is given by

$$Q_{\text{coll}}^{\text{Kn}} = \pi a^2 n \bar{v}_{\text{th}} \alpha_{\text{acc}} 2k(T_d - T_g), \quad (42)$$

⁸ Schaaf (1963) provides an exact formula for the total collisional net heating rate $Q = Q_{\text{fric}} - Q_{\text{coll}}$ for large Knudsen numbers, but unfortunately we are not aware of a comparable expression for small Kn . We have checked that our approach is in agreement with the Schaaf formula, by order of magnitude, for large Kn .

where T_g is the gas temperature, \bar{v}_{th} the mean thermal velocity introduced on page 300 and α_{acc} the efficiency for thermal accommodation, given by Burke & Hollenbach (1983)

$$\alpha_{\text{acc}} = 0.1 + 0.35 \cdot \exp\left(-\sqrt{\frac{T_d + T_g}{500 \text{ K}}}\right). \quad (43)$$

For small Knudsen numbers ($Kn \ll 1$), the removal of heat from the grain's surface in the laminar case⁹ is limited by the heat conductivity of the ambient gas. We consider the energy equation of an ideal fluid

$$\frac{\partial}{\partial t}(\rho e) + \nabla(\mathbf{v}_{\text{gas}}[\rho e + P]) = -\nabla j_{\text{HC}} \quad (44)$$

where e is the internal energy of the gas including kinetic and gravitational potential energies (Paper I) and P the thermal gas pressure. The energy flux by heat conduction is given by

$$j_{\text{HC}} = -\kappa \nabla T. \quad (45)$$

κ [erg K⁻¹cm⁻¹s⁻¹] is the heat conductivity of the gas which according to Jeans (1967) equals

$$\kappa = \frac{9\gamma-5}{4} \mu_{\text{kin}} C_V, \quad (46)$$

where $\gamma = (f+2)/f = 7/5$ is the adiabatic index, f the number of degrees of freedom, μ_{kin} the kinematic viscosity (Eq. (9)) and $C_V = (fk)/(2\bar{\mu}) \approx 8.845 \times 10^7$ erg g⁻¹ K⁻¹ the isochoric heat capacity of the gas, resulting in

$$\kappa = 988 \frac{\text{erg}}{\text{K cm s}} \sqrt{T_g[\text{K}]} \quad (47)$$

The further derivation of the cooling rate by heat conduction is analogous to the derivation of the viscous growth rate on page 303. We consider the static case ($\mathbf{v}_{\text{gas}} = 0$) and assume stationary ($\partial(\rho e)/\partial t = 0$) and spherical symmetry, such that Eq. (44) becomes

$$r^2 \kappa \frac{\partial T}{\partial r} = \text{const.} \quad (48)$$

Regarding κ as a constant, the solution of Eq. (48) with boundary conditions $T(a) = T_d$ and $T(\infty) = T_g$ is

$$T(r) = T_g - \frac{a}{r} (T_g - T_d) \quad (49)$$

and the collisional cooling rate $Q_{\text{coll}}^{\text{sKn}} = 4\pi r^2 j_{\text{HC}}$, according to Eqs. (45) and (49), results in

$$Q_{\text{coll}}^{\text{sKn}} = 4\pi \kappa a (T_d - T_g). \quad (50)$$

The general collisional cooling rate with $Kn' = Kn/Kn^{\text{cr}}$ is again approximated by

$$Q_{\text{coll}} = Q_{\text{coll}}^{\text{Kn}} \left(\frac{Kn'}{Kn' + 1}\right)^2 + Q_{\text{coll}}^{\text{sKn}} \left(\frac{1}{Kn' + 1}\right)^2 \quad (51)$$

where Kn^{cr} results from equating Eqs. (42) with (50). We find a value of 0.023 at 1000 K and a value of 0.019 at 2000 K.

⁹ In the turbulent regime, the grains will be efficiently cooled by heat transport due to convection.

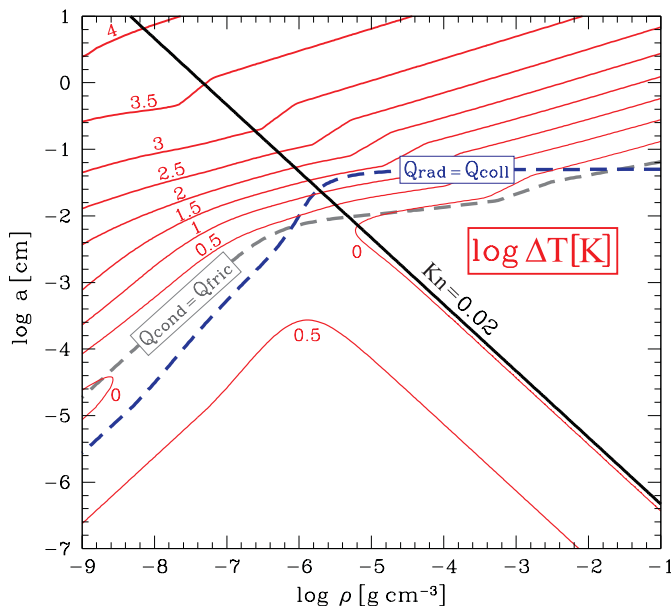


Fig. 4. Contour plot of the temperature increase $\log \Delta T$ [K], due to the liberation of latent heat during grain growth and frictional heating, as function of the grain radius a and gas density ρ at constant gas temperature $T = 1500$ K for quartz grains with the same parameters as in Fig. 3. We assume growth by accretion of the key species SiO with maximum particle density $n_{\text{SiO}} = 10^{(7.55-12)} n_{\text{(H)}}$ and extreme supersaturation ($S \rightarrow \infty$). The two dashed lines indicate where the two considered heating and cooling rates are equal. Above these lines, $Q_{\text{fric}} > Q_{\text{cond}}$ and $Q_{\text{rad}} > Q_{\text{coll}}$, respectively.

For simplicity, we apply a constant value for the critical Knudsen number as $Kn^{\text{cr}} = 0.02$ in the following.

The energy balance of a single dust grain is finally given by

$$Q_{\text{cond}} + Q_{\text{fric}} = Q_{\text{rad}} + Q_{\text{coll}}, \quad (52)$$

which states an implicit equation for the temperature increase $\Delta T = T_{\text{d}} - T_{\text{g}}$ due to the liberation of latent heat during grain growth and frictional heating.

Figure 4 shows an example for the resulting temperature increase ΔT of quartz grains. We assume $J_{\lambda} = B_{\lambda}(T_{\text{g}})$ and again consider the explicit growth reaction (Eq. (38)) with a release of latent heat of $\Delta_r H = 5.73$ eV per reaction at 1000 K, 5.61 eV at 1500 K and 5.49 eV at 2000 K (data reduced from the enthalpies of formation of the involved molecules and the solid, source: JANAF-tables, electronic version, Chase et al. 1985).

For the sake of simplicity, we furthermore assume

$$Q_{\text{abs}}(a, \lambda) \approx \min \left\{ 1, a \widehat{Q}_{\text{ext}}^{\text{SPL}}(\lambda) \right\} \quad (53)$$

for this calculation, where the extinction efficiency over a in the small particle limit of Mie theory is given by

$$\widehat{Q}_{\text{ext}}^{\text{SPL}} = \frac{8\pi}{\lambda} \text{Im} \left\{ \frac{m(\lambda)^2 - 1}{m(\lambda)^2 + 2} \right\}. \quad (54)$$

$m(\lambda)$ is the complex refractory index of the dust grain material and Im the imaginary part. The optical constants for amorphous SiO₂ (quartz glass) are taken from H. R. Philipp's section in (Palik 1985) and the resulting $\widehat{Q}_{\text{ext}}^{\text{SPL}}$ -values are log-interpolated between the measured wavelengths points.

Despite these simplifications, Fig. 4 clearly indicates that the warming of the dust grains due to the release of latent heat is negligible, being less than 3.5 K all over the relevant parts of the size-density-plane, where $\tau_{\text{gr}} \leq \tau_{\text{sink}}$ (compare Fig. 3). Here, we find that this heating is balanced by collisional cooling $Q_{\text{cond}} \approx Q_{\text{coll}}$. Since both heating/cooling rates scale as $\propto a^2 \rho$ for large Knudsen numbers and as $\propto a$ for small Knudsen numbers, a constant value for ΔT tunes in for both cases, $\Delta T \approx 3.5$ K for large Kn , and $\Delta T \approx 0.5$ K for small Kn . Note that the calculated temperature differences are always an upper estimate. The actual temperature differences may be much smaller because we have assumed solar, undepleted abundances of Si in the gas phase and $S \rightarrow \infty$ for the calculation of dV/dt .

For larger particles (roughly at $a \gtrsim a_{\text{max}}$ as defined in Sect. 3.1), the character of the energy balance of the dust particles changes. Here, the frictional heating due to the rapid relative motion and the radiative cooling dominate, i.e. $Q_{\text{fric}} \approx Q_{\text{rad}}$. Much larger temperature deviations up to 10 000 K result in this case. However, as argued before, such large grains cannot be formed in brown dwarf atmospheres.

Thus, the resulting increase of the dust temperature T_{d} is by far too small to reach the sublimation temperature T_{sub} , unless gas temperatures very close to T_{sub} are considered and, therefore, Eqs. (22) and (32) remain valid.

5. Moment method for nucleation, growth, evaporation and equilibrium drift

The physical and chemical processes discussed so far (nucleation, growth, evaporation, gravitational settling and element depletion/enrichment) occur simultaneously in the atmosphere and may be strongly coupled. Therefore, our aim in this section is to derive a consistent time-dependent description of the dust component in brown dwarf or giant gas planet atmospheres. We will derive a system of partial differential equations which describes the evolution of the dust component by means of the moments of its size distribution function. This idea was originally developed by Gail & Sedlmayr (1988) and extended by Dominik et al. (1993) to core-mantle and dirty grains. The resulting differential equations are supposed to be simple and includable into hydrodynamics or classical stellar atmosphere calculations. In contrast, we want to avoid an elaborate and time-consuming multi-component treatment of the dust component, e.g. by using discrete bins for the dust size distribution function with individual drift velocities in this paper.

The master equation for dust particles $\in [V, V + dV]$, $f(V) dV$, where $f(V)$ [cm⁻⁶] is the distribution function of dust particles in volume space, is given by

$$\frac{\partial}{\partial t} (f(V) dV) + \nabla \left[\left(v_{\text{gas}} + v_{\text{dr}}(V) \right) f(V) dV \right] = \sum_k R_k dV. \quad (55)$$

The r.h.s. of Eq. (55) expresses the population and depopulation of the considered volume interval $[V, V+dV]$ with dust particles which are changing their size due to accretion or evaporation of molecules (see Fig. 5),

$$\sum_k R_k dV = \left(R_{\uparrow} - R^{\uparrow} + R^{\downarrow} - R_{\downarrow} \right) dV. \quad (56)$$

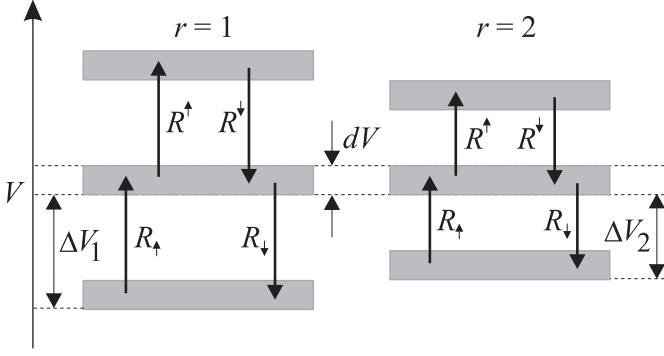


Fig. 5. Two surface chemical processes ($r=1$ and $r=2$) populating or depopulating an infinitesimal dust grain volume interval $[V, V+dV]$.

Multiplication of Eq. (55) with $V^{j/3}$ ($j=0, 1, 2, \dots$) and integration over V from a lower integration boundary $V = V_\ell$ to $V \rightarrow \infty$ results in

$$\frac{\partial}{\partial t}(\rho L_j) + \nabla(\mathbf{v}_{\text{gas}} \rho L_j) = \underbrace{\int_{V_\ell}^{\infty} \sum_k R_k V^{j/3} dV}_{\mathcal{A}_j} - \underbrace{\nabla \int_{V_\ell}^{\infty} f(V) V^{j/3} \mathbf{v}_{\text{dr}}(V) dV}_{\mathcal{B}_j}, \quad (57)$$

where the j th moment of the dust size distribution function L_j [cm^j/g] is defined by

$$\rho L_j(\mathbf{x}, t) = \int_{V_\ell}^{\infty} f(V, \mathbf{x}, t) V^{j/3} dV. \quad (58)$$

The source term \mathcal{A}_j expresses the effects of surface chemical reactions on the dust moments and \mathcal{B}_j is an additional, advective term in the dust moment equations which comprises the effects caused by a size-dependent drift motion of the grains, e.g. due to gravity.

The maximum grain sizes to be expected in brown dwarf atmospheres (Fig. 3) allow us to concentrate on two major cases in the following, namely the *subsonic free molecular flow* and the *laminar viscous flow*.

5.1. Subsonic free molecular flow ($Kn \gg 1 \wedge \mathbf{v}_{\text{dr}} \ll c_T$)

For large Knudsen numbers, the chemical rates depicted in Fig. 5 can be expressed according to Eq. (22):

$$R^\uparrow dV = \sum_r f(V) dV 4\pi[a(V)]^2 n_r v_r^{\text{rel}} \alpha_r \quad (59)$$

$$R_\uparrow dV = \sum_r f(V - \Delta V_r) dV 4\pi[a(V - \Delta V_r)]^2 n_r v_r^{\text{rel}} \alpha_r \quad (60)$$

$$R^\downarrow dV = \sum_r f(V + \Delta V_r) dV 4\pi[a(V)]^2 n_r v_r^{\text{rel}} \alpha_r \frac{1}{S_r} \quad (61)$$

$$R_\downarrow dV = \sum_r f(V) dV 4\pi[a(V - \Delta V_r)]^2 n_r v_r^{\text{rel}} \alpha_r \frac{1}{S_r}. \quad (62)$$

Applying detailed balance considerations (Milne relations), Gauger et al. (1990) and Patzer et al. (1998) have shown that

for simple types of surface reactions, denoted by homogeneous and heterogeneous growth, the (inverse) evaporation rates can be expressed by the related (forward) growth rates and the supersaturation ratio in the way written in Eqs. (61) and (62). For Eqs. (59) and (60), we have neglected a possible influence of a fast drift motion on the growth rates and for Eqs. (61) to (62), we have assumed thermal equilibrium (dust temperature \equiv gas temperature) and chemical equilibrium among the molecules in the gas phase.

Solving Eq. (19) with the frictional force according to Eq. (13, subsonic case) the equilibrium drift velocity is

$$\mathbf{v}_{\text{dr}} = -\frac{\sqrt{\pi} g \rho_d a}{2\rho c_T} \mathbf{e}_r. \quad (63)$$

By means of the Eqs. (59) to (63), the integrals on the r.h.s. of Eq. (57) can be evaluated as shown in more detail concerning the term \mathcal{A}^{IKn} in (Gail & Sedlmayr 1988). After some algebraic manipulations, including $a = (3V/4\pi)^{1/3}$, the approximation $\Delta V_r \ll V$ and partial integration, the results are

$$\mathcal{A}_j^{\text{IKn}} = V_\ell^{j/3} J(V_\ell) + \frac{j}{3} \chi_{\text{IKn}}^{\text{net}} \rho L_{j-1} \quad (64)$$

$$\mathcal{B}_j^{\text{IKn}} = -\xi_{\text{IKn}} \nabla \left(\frac{L_{j+1}}{c_T} \mathbf{e}_r \right), \quad (65)$$

where $J(V_\ell) = f(V_\ell) \frac{dV}{dr} \Big|_{V=V_\ell}$ is the current of dust particles in volume space at the lower integration boundary. In case of net growth, $J(V_\ell)$ [$\text{cm}^{-3} \text{s}^{-1}$] can be identified with the stationary nucleation rate J_\star (Gail & Sedlmayr 1988). The characteristic growth speed $\chi_{\text{IKn}}^{\text{net}}$ [cm/s] (an increase of radius per time) and the characteristic gravitational force density ξ_{IKn} [dyn/cm^3] are given by

$$\chi_{\text{IKn}}^{\text{net}} = \sqrt[3]{36\pi} \sum_r \Delta V_r n_r v_r^{\text{rel}} \alpha_r \left(1 - \frac{1}{S_r} \right) \quad (66)$$

$$\xi_{\text{IKn}} = \frac{\sqrt{\pi}}{2} \left(\frac{3}{4\pi} \right)^{1/3} g \rho_d. \quad (67)$$

5.2. Laminar viscous flow ($Kn \ll 1 \wedge Re_d < 1000$)

The derivation of the moment equations for the case of small Knudsen numbers is analogous to the previous subsection. We express the surface chemical rates according to Eq. (32) by

$$R^\uparrow dV = \sum_r f(V) dV 4\pi a(V) n_r D_r \quad (68)$$

$$R_\uparrow dV = \sum_r f(V - \Delta V_r) dV 4\pi a(V - \Delta V_r) n_r D_r \quad (69)$$

$$R^\downarrow dV = \sum_r f(V + \Delta V_r) dV 4\pi a(V) n_r D_r \frac{1}{S_r} \quad (70)$$

$$R_\downarrow dV = \sum_r f(V) dV 4\pi a(V - \Delta V_r) n_r D_r \frac{1}{S_r}, \quad (71)$$

again neglecting the influence of drift on growth and assuming thermal and chemical equilibrium. The equilibrium drift velocity results from Eq. (19) with the frictional force according to Eq. (16, small Re_d case)

$$\mathbf{v}_{\text{dr}} = -\frac{2g\rho_d a^2}{9\mu_{\text{kin}}} \mathbf{e}_r. \quad (72)$$

By repeating the procedure of the last subsection, the r.h.s. terms of the dust moment equations are

$$\mathcal{A}_j^{\text{sKn}} = V_\ell^{j/3} J(V_\ell) + \frac{j}{3} \chi_{\text{sKn}}^{\text{net}} \rho L_{j-2} \quad (73)$$

$$\mathcal{B}_j^{\text{sKn}} = -\xi_{\text{sKn}} \nabla \left(\frac{\rho L_{j+2}}{\mu_{\text{kin}}} \mathbf{e}_r \right). \quad (74)$$

The characteristic growth speed $\chi_{\text{sKn}}^{\text{net}}$ has now the unit $[\text{cm}^2 \text{s}^{-1}]$ (an increase of surface per time) whereas the characteristic gravitational force density ξ_{sKn} remains the same except for a different geometry factor.

$$\chi_{\text{sKn}}^{\text{net}} = \sqrt[3]{48\pi^2} \sum_r \Delta V_r n_r D_r \left(1 - \frac{1}{S_r} \right) \quad (75)$$

$$\xi_{\text{sKn}} = \frac{2}{9} \left(\frac{3}{4\pi} \right)^{2/3} g \rho_d. \quad (76)$$

6. Discussion

6.1. Dimensionless analysis

For the sake of analysis and discussion, we transform the dust moment equations derived in Sects. 5.1 and 5.2 into their dimensionless form by introducing reference values as $t \rightarrow t/t_{\text{ref}}$, $\nabla \rightarrow l_{\text{ref}} \nabla$, $\rho \rightarrow \rho/\rho_{\text{ref}}$, $\mathbf{v} \rightarrow \mathbf{v}/v_{\text{ref}}$, $\mathbf{g} \rightarrow \mathbf{g}/g_{\text{ref}}$, $J(V_\ell) \rightarrow J(V_\ell)/J_{\text{ref}}$, $L_j \rightarrow L_j/L_{j,\text{ref}}$, $\chi^{\text{net}} \rightarrow \chi^{\text{net}}/\chi_{\text{ref}}$, $\xi \rightarrow \xi/\xi_{\text{ref}}$, $\mu_{\text{kin}} \rightarrow \mu_{\text{kin}}/\mu_{\text{kin}}^{\text{ref}}$ following the procedure described in Paper I. The reference values are to be chosen according to the expected order of magnitude of the respective quantities and the length and time-scales under investigation. After this substitution, all quantities are dimensionless and can be compared by number.

This allows us to identify the leading terms in the equations, e.g. in the inner and outer regions of a brown dwarf atmosphere. The remaining constants (products of the reference values) can be summarised into characteristic numbers which provide an efficient way to describe the qualitative behaviour of the dust component.

The dimensionless dust moment equations for nucleation, growth, evaporation, and equilibrium drift write for a *subsonic free molecular flow* ($Kn \gg 1 \wedge v_{\text{dr}} \ll c_T$)

$$\begin{aligned} [Sr] \frac{\partial}{\partial t} (\rho L_j) + \nabla (\mathbf{v}_{\text{gas}} \rho L_j) &= [Sr \cdot Da_d^{\text{nuc}} \cdot Se_j] J(V_\ell) \\ &+ [Sr \cdot Da_{d,Kn}^{\text{gr}}] \frac{j}{3} \chi_{\text{sKn}}^{\text{net}} \rho L_{j-1} \\ &+ \left[\left(\frac{\pi\gamma}{32} \right)^{1/2} \frac{Sr \cdot M \cdot Dr}{Kn^{\text{HD}} \cdot Fr} \right] \xi_{\text{sKn}} \nabla \left(\frac{L_{j+1}}{c_T} \mathbf{e}_r \right) \end{aligned} \quad (77)$$

and for a *laminar viscous flow* ($Kn \ll 1 \wedge Re_d < 1000$)

$$\begin{aligned} [Sr] \frac{\partial}{\partial t} (\rho L_j) + \nabla (\mathbf{v}_{\text{gas}} \rho L_j) &= [Sr \cdot Da_d^{\text{nuc}} \cdot Se_j] J(V_\ell) \\ &+ [Sr \cdot Da_{d,\text{sKn}}^{\text{gr}}] \frac{j}{3} \chi_{\text{sKn}}^{\text{net}} \rho L_{j-2} \\ &+ \left[\left(\frac{\pi\gamma}{288} \right)^{1/2} \frac{Sr \cdot M \cdot Dr}{Kn \cdot Kn^{\text{HD}} \cdot Fr} \right] \xi_{\text{sKn}} \nabla \left(\frac{\rho L_{j+2}}{\mu_{\text{kin}}} \mathbf{e}_r \right). \end{aligned} \quad (78)$$

The equations are valid for $j = 0, 1, 2, \dots$. The constants in squared brackets are written in terms of characteristic numbers, which are further explained in Table 2. All other quantities and terms in Eqs. (77) and (78) are of the order of unity for an appropriate choice of the reference values.

The following discussion is based on a typical structure of a brown dwarf atmosphere with solar abundances *in the gas phase*, i.e. neglecting the possible depletion due to dust formation (see Table 2). As underlying (T, ρ) -structure we refer to a brown dwarf model atmosphere with $T_{\text{eff}} = 1000 \text{ K}$ and $\log g = 5$ which has been kindly provided by T. Tsuji (2002)¹⁰. As exemplary dust species we consider solid SiO_2 (amorphous quartz), growing by the accretion of SiO and H_2O (Eq. (38)). Since the nucleation of SiO_2 seems dubious (the monomer is rather unstable as a free molecule and hence not very abundant in the gas phase) we consider nucleation of TiO_2 instead¹¹.

6.2. Hierarchy of nucleation, growth and drift

An analysis of the characteristic numbers in front of the source terms in Eqs. (77) and (78) (see Table 2) reveals a hierarchy of nucleation \rightarrow growth \rightarrow drift:

- 1) In the cool outer layers, the gas is strongly supersaturated ($S \gg 1$) and nucleation is effective ($J(V_\ell) = J_\star > 0$). The products of the Damköhler number of nucleation Da_d^{nuc} with the Strouhal number Sr and the Sedlmayr numbers Se are as large as the products of the Damköhler numbers of growth Da_d^{gr} with the Strouhal number Sr (even larger for small j) and much larger than the combined drift numbers, indicating that the nucleation provides an important source term in Eqs. (77) and (78). Consequently, the condensable elements will be quickly consumed by the process of nucleation before the particles can grow much further. Hence, the dust particles remain very small in this *layer of effective nucleation*.
- 2) In the warmer layers, the gas is almost saturated ($S \gtrsim 1$) and nucleation is not effective ($J(V_\ell) \rightarrow 0$). The products of the Damköhler numbers of growth Da_d^{gr} with the Strouhal number Sr are large and the growth term (the second term on the r.h.s.) is the leading source term in the dust moment Eqs. (77) and (78). In comparison, the influence of the drift term is small as quantified by the combined drift numbers in Table 2. Consequently, *the dust growth process will substantially be completed before the dust grains start to settle gravitationally*. In these *growth-dominated layers*, a few existing particles will quickly consume all condensable elements from the gas phase and, thus, will reach much larger particle sizes. Since these particles cannot be created via nucleation here, they must have

¹⁰ The static model atmosphere results from frequency-dependent radiative transfer calculations and mixing length theory for the convective energy flux. Dust is included in form of three species (Fe, Al_2O_3 , MgSiO_3) following stability arguments and considering a prescribed grain size distribution.

¹¹ We are mainly interested in the qualitative behaviour of the dust component in this paper. The following estimates will be very similar for other refractory dust materials composed of abundant elements.

Table 2. Characteristic numbers and reference values used for the analysis of the dimensionless dust moment Eqs. (77) and (78). Hydro- and thermodynamic reference values are taken from a static brown dwarf model atmosphere (Tsuji 2002) with $T_{\text{eff}} = 1000$ K and $\log g = 5$, considering an inner ($T_{\text{ref}} = 1700$ K) and an outer ($T_{\text{ref}} = 1000$ K) layer, typical for the growth-dominated region and the region of effective nucleation, respectively (see text). We assume constant $\gamma = 7/5$ and $\bar{\mu} = 2.35$ amu (1 amu = 1.6605×10^{-24} g). In each layer, two reference length scales are considered: $l_{\text{ref}} = 10^4$ cm (microscopic scale) and $l_{\text{ref}} = 10^6$ cm ($\approx H_p$; macroscopic scale). The reference values for the dust complex have been adopted according to the experience of Paper I, considering an undepleted gas of solar abundances. The growth rates are calculated for SiO_2 via addition of SiO and H_2O (see Eq. (38)), assuming $S_r \gg 1$ and $\alpha_r = 1$. Further molecular and dust material quantities are listed in Table 3. Boldfaced numbers mark those values which are related to the proper Knudsen number case ($Kn \ll 1$ or $Kn \gg 1$).

Name	Characteristic Number	Value			
		inside		outside	
Mach number	$M = \frac{v_{\text{ref}}}{c_s}$	$\approx 1/10$			
Froude number	$Fr = \frac{v_{\text{ref}}}{l_{\text{ref}} g_{\text{ref}}}$	0.842	8.42×10^{-3}	0.495	4.95×10^{-3}
Strouhal number	$Sr = \frac{v_{\text{ref}}}{l_{\text{ref}} \omega_{\text{ref}}}$	≈ 1			
hydrodyn. Knudsen number	$Kn^{\text{HD}} = \frac{l_{\text{ref}}}{2\langle a \rangle_{\text{ref}}}$	$5 \times 10^{+6}$	$5 \times 10^{+8}$	$5 \times 10^{+9}$	$5 \times 10^{+11}$
Knudsen number (Eq. (6))	$Kn = \frac{l_{\text{ref}}}{2\langle a \rangle_{\text{ref}}}$	3.09×10^{-3}	$1.86 \times 10^{+1}$
Drift number	$Dr = \frac{\rho_d v_{\text{ref}}}{\rho_{\text{ref}}}$	$8.83 \times 10^{+3}$	$5.30 \times 10^{+4}$
combined drift number ($Kn \gg 1$)	$\left(\frac{\pi\gamma}{32}\right)^{1/2} \frac{Sr \cdot M \cdot Dr}{Kn^{\text{HD}} \cdot Fr}$	7.78×10^{-5}	7.93×10^{-7}
combined drift number ($Kn \ll 1$)	$\left(\frac{\pi\gamma}{288}\right)^{1/2} \frac{Sr \cdot M \cdot Dr}{Kn \cdot Kn^{\text{HD}} \cdot Fr}$	8.38×10^{-3}	1.42×10^{-8}
Sedlmayr number ($j \in \mathbb{N}_0$)	$Se_j = \left(\frac{\alpha_r}{\langle a \rangle_{\text{ref}}}\right)^j$	$j=0: 1$ $j=1: 2.08 \times 10^{-4}$ $j=2: 4.32 \times 10^{-8}$ $j=3: 8.99 \times 10^{-12}$		$j=0: 1$ $j=1: 2.08 \times 10^{-1}$ $j=2: 4.32 \times 10^{-2}$ $j=3: 8.99 \times 10^{-3}$	
Damköhler no. of nucleation	$Da_{\text{d}}^{\text{nuc}} = \frac{l_{\text{ref}} J_{\text{ref}}}{\rho_{\text{ref}} L_{0,\text{ref}}}$	0	0	$3.24 \times 10^{+4}$	$3.24 \times 10^{+6}$
Damköhler no. of growth ($Kn \gg 1$)	$Da_{\text{d,lKn}}^{\text{gr}} = \frac{l_{\text{ref}} \chi_{\text{ref,lKn}}}{\left(\frac{4\pi}{3} \langle a \rangle_{\text{ref}}^3\right)^{1/3}}$	3.95	$3.95 \times 10^{+2}$	$6.58 \times 10^{+2}$	$6.58 \times 10^{+4}$
Damköhler no. of growth ($Kn \ll 1$)	$Da_{\text{d,sKn}}^{\text{gr}} = \frac{l_{\text{ref}} \chi_{\text{ref,sKn}}}{\left(\frac{4\pi}{3} \langle a \rangle_{\text{ref}}^3\right)^{2/3}}$	9.24×10^{-2}	9.24	$9.24 \times 10^{+4}$	$9.24 \times 10^{+6}$

Name	Physical Quantity	Reference Value			
		inside		outside	
temperature	T_{ref} [K]	1700		...	1000
density	ρ_{ref} [g/cm^3]	3×10^{-4}		...	5×10^{-5}
thermal pressure	$P_{\text{ref}} = \frac{\rho_{\text{ref}} k T_{\text{ref}}}{\beta}$ [dyn/cm^2]	$1.80 \times 10^{+7}$...	$1.77 \times 10^{+6}$
velocity of sound	$c_s = \sqrt{\gamma \frac{P_{\text{ref}}}{\rho_{\text{ref}}}}$ [cm/s]	$2.90 \times 10^{+5}$...	$2.23 \times 10^{+5}$
velocity	v_{ref} [cm/s]	...		$\approx c_s/10$	
length	l_{ref} [cm]	10^{+4}	10^{+6}	10^{+4}	10^{+6}
hydrodyn. time	$t_{\text{ref}} = \frac{l_{\text{ref}}}{v_{\text{ref}}}$ [s]	3.45×10^{-1}	$3.45 \times 10^{+1}$	4.49×10^{-1}	$4.49 \times 10^{+1}$
gravitational acceleration	g_{ref} [cm/s^2]	...		10^{+5}	
mean particle radius	$\langle a \rangle_{\text{ref}}$ [cm]	10^{-3}		...	10^{-6} (\diamond)
0th dust moment ($= n_d/\rho$)	$L_{0,\text{ref}} = \frac{\Delta V_{\text{SiO}_2} n_{\text{ref,SiO}}}{\rho_{\text{ref}} \left(\frac{4\pi}{3} \langle a \rangle_{\text{ref}}^3\right)}$ [1/g]	$1.35 \times 10^{+5}$...	$1.35 \times 10^{+14}$ (\square)
nucleation rate	$J_{\text{ref}}/n_{\langle \text{H} \rangle_{\text{ref}}}$ [1/s]	0 (\dagger)		...	2.30×10^{-5} (\ddagger)
growth velocity ($Kn \gg 1$, Eq. (67))	$\chi_{\text{lKn}}^{\text{ref}}$ [cm/s]	1.85×10^{-2}		...	2.36×10^{-3} (Δ)
growth velocity ($Kn \ll 1$, Eq. (76))	$\chi_{\text{sKn}}^{\text{ref}}$ [cm^2/s]	6.96×10^{-7}		...	5.34×10^{-7} (Δ)
diffusion constant (Eq. (26))	D_{ref} [cm^2/s]	5.28×10^{-1}		...	2.43 (Δ)
mean free path (Eq. (10))	$\bar{\ell}_{\text{ref}}$ [cm]	6.19×10^{-6}		...	3.71×10^{-5}
total hydrogen number density	$n_{\langle \text{H} \rangle_{\text{ref}}} = \frac{\rho_{\text{ref}}}{1.427 \text{ amu}}$ [1/ cm^3]	1.27×10^{20}		...	2.11×10^{19}
molecular number density	$n_{\text{ref}} = n_{\text{ref,SiO}}$ [1/ cm^3]	4.49×10^{15}		...	7.49×10^{14} (Δ)

(\diamond): According to the experience of Paper I. (\square): We choose the reference value of the dust-to-gas mass ratio $\rho_d \cdot L_{3,\text{ref}}$ by considering the case when all Si is bound in solid SiO_2 and adapt the reference value for the total dust particle density $\rho_{\text{ref}} L_{0,\text{ref}}$ according to the assumed grain's reference size $\langle a \rangle_{\text{ref}}$: $L_{j,\text{ref}} = \left(\frac{4\pi}{3} \langle a \rangle_{\text{ref}}^3\right)^{j/3} L_{0,\text{ref}}$ (Gail & Sedlmayr 1999). (\dagger): We assume vanishing nucleation rates in this region around 1700 K, because the supersaturation ratios $S \gtrsim 1$ are either too small for efficient nucleation or the nucleation species have already been consumed by growth. (\ddagger): The reference value for the nucleation rate J_{ref} is chosen by considering homogeneous nucleation of TiO_2 according to Paper I. (Δ): SiO is considered as key growth species.

Table 3. Additional material quantities used to calculate the reference values listed in Table 2.

Name	Value		
dust material density	$\rho_{\text{d,SiO}_2}$	[g/cm ³]	2.65
monomer volume	ΔV_{SiO_2}	[cm ³]	3.76×10^{-23}
lower dust grain radius	a_{ℓ,SiO_2}	[cm]	2.08×10^{-7}
molecular radius	r_{SiO}	[cm]	2.0×10^{-8}

Table 4. Scaling of the physical processes, ordered by their appearance from left to right in Eqs. (77) and (78).

physical process	$Kn \gg 1$	$Kn \ll 1$
time-derivative		$\propto \frac{l_{\text{ref}}}{v_{\text{ref}} t_{\text{ref}}}$
advective term		1
nucleation term ^(Δ)		$\propto \frac{l_{\text{ref}} J_{\text{ref}}}{v_{\text{ref}} \rho_{\text{ref}} L_{0,\text{ref}} \langle a_{\text{ref}} \rangle^j}$
growth term ^(Δ)	$\propto j \cdot \frac{l_{\text{ref}} \rho_{\text{ref}} \sqrt{I_{\text{ref}}}}{v_{\text{ref}} \langle a_{\text{ref}} \rangle}$	$\propto j \cdot \frac{l_{\text{ref}} \sqrt{I_{\text{ref}}}}{v_{\text{ref}} \langle a_{\text{ref}} \rangle^2}$
drift term	$\propto \frac{g_{\text{ref}} \rho_{\text{d,ref}} \langle a_{\text{ref}} \rangle}{v_{\text{ref}} \rho_{\text{ref}} \sqrt{I_{\text{ref}}}}$	$\propto \frac{g_{\text{ref}} \rho_{\text{d,ref}} \langle a_{\text{ref}} \rangle^2}{v_{\text{ref}} \sqrt{I_{\text{ref}}}}$

(Δ): the importance of this process depends on the considered dust moment j with the following associated mean dust quantity: $j=0 \rightarrow$ dust particle density, $j=1 \rightarrow$ dust size, $j=2 \rightarrow$ dust surface area, $j=3 \rightarrow$ dust mass density.

been formed elsewhere and transported into these layers by winds or drift. The growth will either be terminated by element consumption or by the loss due to gravitational settling when the particles reach their maximum size as introduced in Sect. 3.1.

- 3) At the cloud base, the gas is hot and saturated ($S = 1$). Consequently, nucleation and growth vanish and the only remaining source term on the r.h.s. of Eqs. (77) and (78) is the additional advection of the particles due to their drift motion (drift term). The combined drift numbers, however, are small indicating that the drift term has a smaller influence than the hydrodynamical advection term.

6.3. Scaling laws

Table 4 shows some dependencies of the combined characteristic numbers (the squared brackets in Eqs. (77), (78)), which provides scaling laws for the importance of the different processes in the different regimes:

- 1) The drift term scales as $\propto \langle a_{\text{ref}} \rangle$ ($Kn \gg 1$) or $\propto \langle a_{\text{ref}} \rangle^2$ ($Kn \ll 1$) whereas the growth term scales as $\propto \langle a_{\text{ref}} \rangle^{-p}$ with different $p \geq 0$ for the different cases (Table 4). This means that at a certain large mean particle size, the drift term will start to dominate over growth, which in fact just occurs at the maximum particle size a_{max} introduced in Sect. 3.1.
- 2) Nucleation (always) and growth ($Kn \gg 1$) become increasingly important with increasing gas density ρ_{ref} (note that typically $J_{\text{ref}} \propto \rho_{\text{ref}}^{2+p}$ with $p > 0$), whereas the drift term ($Kn \gg 1$) diminishes for increasing ρ_{ref} , i.e. the drift is generally more important in a thin gas. However, the particles are expected to remain smaller in such a thin gas

situated in the upper layers, which has a stronger, opposite effect on the drift term.

- 3) The larger the considered length scale l_{ref} , the more stiff the dust moment equations become because of the increasingly large nucleation and growth terms. This may actually cause some numerical difficulties for models on macroscopic scales. In comparison, the advective and the drift term are independent on l_{ref} , which means that these terms gain importance on small scales in relation to the other terms.
- 4) The drift term scales as $\propto g_{\text{ref}} \rho_{\text{d,ref}}$, i.e. the drift is naturally more important for heavy grains in a strong gravitational field.

6.4. Control mechanisms

In Table 2, we have assumed $Sr = 1$, i.e. we have considered time-scales t_{ref} of the order of $l_{\text{ref}}/v_{\text{ref}}$, appropriate for disordered (e.g. turbulent) velocity fields, where the l.h.s. terms of Eqs. (77) and (78) are of comparable importance. However, if large-scale systematic motions are stable for a long time (e.g. a circulating thunderstorm or a stable convection roll), the system may reach a quasi-stationary situation where t_{ref} becomes much larger and hence $Sr \rightarrow 0$. In this case, the first term on the l.h.s. of Eqs. (77) and (78) vanishes (see Table 4) whereas all other terms remain unaffected.

An interesting special case occurs if additionally $v_{\text{gas}} \rightarrow 0$, i.e. when the dust-forming system reaches the static case. In this case, also the advective terms in Eqs. (77) and (78) vanish and the source terms must balance each other. In the $S > 1$ case, this means that the gain of dust by nucleation and growth must be balanced by the loss of dust due to rain-out, which means that the gas will be depleted. In the $S < 1$ case, just the opposite is true, i.e. the loss by evaporation must be balanced by the gain of dust particles raining in from above. Consequently, the gas in such undersaturated layers will be enriched by the condensable elements liberated by the evaporating grains.

However, both control mechanisms (in the static limit) result in an efficient transport of condensable elements from the cool upper layers into the warm inner layers, which cannot last forever. We may conclude that if the brown dwarf's atmosphere is truly static for a long time, there is no other than the trivial solution for Eqs. (77) and (78) where the gas is saturated ($S \equiv 1$) and dust-free ($L_j \equiv 0$). This situation changes, however, if the brown dwarf's atmosphere is turbulent or, in particular, when it is convective. In that case, the replenishment of the atmosphere with fresh uncondensed gas from the deep interior will counteract the downward transport of condensable elements by the formation and gravitationally settling of dust grains. Simulations of this quasi-static balance will be the subject of the forthcoming paper in this series.

6.5. Outlook

A dynamical modelling of the dust component in brown dwarf atmospheres by means of a moment method as proposed in this paper – consistently coupled to hydrodynamics, radiative transfer and element depletion in the scope of hydrodynamical

or classical stellar atmosphere calculations – seems straightforward as soon as two major problems can be solved:

Knudsen number fall differentiation: The structure of the dust moment Eqs. (77)/(78) changes with changing Knudsen number. The size distribution function $f(V)$, however, will generally include small and large grains simultaneously, which may possess large and small Knudsen numbers, respectively. A proper treatment of all dust grains by means of a moment method is hence possible only in one of the limiting cases $Kn \gg 1$ or $Kn \ll 1$, where *all* grains fall into one particular case. This situation may be relevant for the cool upper regions of a brown dwarf atmosphere, where the densities are small and the dust particles remain tiny. In general, however, a solution of this problem by means of a moment method can only be approximate in nature and will require additional numerical tricks, e.g. switching the case as soon as the Knudsen number according to the *mean* size of the particles reaches unity.

Open system of equations: The number of unknowns in Eqs. (77)/(78) exceeds the number of equations, since the drift term on the r.h.s. involves a higher dust moment L_{j+1} (for $Kn \gg 1$) or even L_{j+2} (for $Kn \ll 1$). Therefore, in order to benefit from the moment Eqs. (77)/(78), we require a physically reliable closure condition, as e.g.

$$L_{j+1} = F(L_0, L_1, \dots, L_j). \quad (79)$$

Such closure conditions are fastidious problems. We are optimistic, nevertheless, to find such a closure term, because the size distribution $f(V)$ is usually a very smooth function and the dust moments L_j often reveal a very simple functional dependency on the index j , indicating that the true number of the degrees of freedom for a parametric description of $f(V)$ is actually quite small.

One idea to construct such a closure condition has been developed by Deufelhard & Wulkow (1989) and Wulkow (1992), studying the kinetics of polyreaction systems. The size distribution function $f(V)$ is here approximated by a weight function $\Psi^\alpha(V)$, which describes the basic shape of $f(V)$, and modified by a sum of orthogonal polynomials $\{p_k(V)\}$ ($k = 0, 1, 2, \dots, n$) as

$$f(V, \mathbf{x}, t) = \Psi^\alpha(V) \sum_{k=0}^n a_k(\mathbf{x}, t) p_k^\alpha(V). \quad (80)$$

α is an additional parameter (dependent on \mathbf{x}, t) of the weight function and a_k are polynomial coefficients. The parameters α and a_k ($k = 0, 1, 2, \dots, n$) are stepwise adjusted in order to fit the known moments L_j ($j=0, 1, 2, \dots, n$) exactly, using the orthogonality relation $\int \Psi^\alpha(V) p_i^\alpha(V) p_k^\alpha(V) dV = \delta_{ik}$. Once these coefficients are known, all missing moments of the size distribution function can be reconstructed from Eq. (80), again utilising the orthogonality relation. This procedure leads to reliable results, if the weight function $\Psi^\alpha(V)$ is already close to the actual size distribution function $f(V)$, such that the polynomials only provide small corrections and the sum in Eq. (80) converges rapidly.

7. Conclusions

In this paper, we have investigated the basic physical and chemical processes which are responsible for the formation, the temporal evolution and the precipitation of dust grains in brown dwarf atmospheres.

In contrast to other astronomical sites of effective dust formation, the dust particles are embedded in such a dense gas that the Knudsen numbers may fall short of unity. This requires a careful fall differentiation for the different hydrodynamical regimes: *free molecular flow (subsonic and supersonic)* and *slip flow (laminar and turbulent case)*.

Compiling a general formula for the drag force from the different special cases, we have shown that the large gravity in brown dwarf atmospheres forces the dust particles to move with a considerably high downward drift velocity relative to the gas. The acceleration of the dust particles (on a time-scale τ_{acc}) towards the equilibrium drift velocity (final fall speed) results to be always much faster than any other considered process (nucleation, growth, hydrodynamical acceleration and sedimentation) such that an *instantaneous acceleration* of the particles to equilibrium drift can be assumed. In contrast, the outward acceleration of dust grains due to radiation pressure is completely negligible in brown dwarf atmospheres.

The large drift velocities are found to limit the residence time of the forming dust grains and hence their maximum size a_{max} as

$$a_{\text{max}} \approx \begin{cases} \left(\frac{6\rho H_p c_T}{\sqrt{\pi} g \rho_d} \sum_r \Delta V_r n_r v_r^{\text{rel}} \alpha_r \left(1 - \frac{1}{S_r}\right) \right)^{1/2}, & Kn \gg 1 \\ \left(\frac{27 H_p \mu_{\text{kin}}}{2 g \rho_d} \sum_r \Delta V_r n_r D_r \left(1 - \frac{1}{S_r}\right) \right)^{1/4}, & Kn \ll 1. \end{cases} \quad (81)$$

Typical values for a_{max} vary between $\approx 1 \mu\text{m}$ in the thin outermost atmospheric layers and $\approx 100 \mu\text{m}$ in the dense innermost layers. As soon as the particles come close to this limiting size, they rain out quickly. This maximum size does not allow for the existence of supersonic dust particles or dust particles with very high Reynolds numbers, such that the *subsonic free molecular flow* and the *laminar viscous flow* are the important main cases to be discussed for dust grains in brown dwarf atmospheres.

For small Knudsen numbers, the growth of the particles by accretion of molecules is limited by the diffusion of the molecules towards the grain surface, and the energy exchange with the surrounding gas is limited by heat conduction. The latter process co-works with the radiative gains and losses of the hot grains. According to our results, the release of latent heat during the growth does only lead to a small increase of the grain temperature ($< 5 \text{ K}$) and has no particular influence on the growth rates.

Based on these findings, we have formulated a system of partial differential equations for the consistent physical description of the dust component in brown dwarf and giant gas planet atmospheres. These *moment equations* represent a unique tool to model the *nucleation, growth and size-dependent equilibrium drift* of the dust particles, and the *element depletion/enrichment* of the gas. We consider such a description as essential, because these processes occur simultaneously and are strongly coupled. The description allows for an inclusion into

hydrodynamics or classical stellar atmosphere calculations, although a few unsolved questions still remain, e.g. a reliable closure condition and a clean Knudsen number fall differentiation.

A dimensionless analysis of the moment equations reveals the existence of the following three regimes associated with the formation of a cloud layer:

- 1) At high altitudes the temperatures are much lower than the sublimation temperatures of the various solid materials and the gas is highly supersaturated. Consequently, nucleation is effective and we find the following relation between the time-scales inherent in the different physical processes:

$$\tau_{\text{acc}} \ll \tau_{\text{nuc}} \lesssim \tau_{\text{gr}} \ll \tau_{\text{hyd}} \ll \tau_{\text{sink}} \quad (S \gg 1).$$

This means that the dust particles are mainly created *here* (by nucleation) as consequence of hydrodynamical enrichment events, e.g. due to the mixing caused by the convection. The particles in this *region of efficient nucleation* remain much smaller than a_{max} . The gravitational settling of the grains is very slow such that they form a rather passive component, subject to hydrodynamical streams (e.g. winds).

- 2) At lower altitudes where the temperatures are close to the sublimation temperatures (the cloud layer is expected to reach its maximum opacity here), nucleation is inefficient and the particle growth is the leading physical process

$$\tau_{\text{acc}} \ll \tau_{\text{gr}} < \tau_{\text{hyd}} \lesssim \tau_{\text{sink}} \quad (S \gtrsim 1).$$

In this *growth-dominated region*, the dust particles may reach much larger sizes, only limited by element consumption or, eventually, by gravitational settling when they even reach a_{max} . Anyway, *the dust growth will be essentially completed before the particles are influenced by drift*. The dust grains are not created here (by nucleation) but are transported into these layers by winds or rain in from above. The efficient growth will consume most of the condensable elements from these layers and thereby bring the supersaturation ratio close to unity in this region.

- 3) Below the cloud base, the temperatures are higher than the sublimation temperatures, and the dust grains that rain in from above will quickly evaporate

$$\tau_{\text{acc}} \ll \tau_{\text{evap}} \approx \tau_{\text{sink}} \lesssim \tau_{\text{hyd}} \quad (S \lesssim 1),$$

thereby releasing the condensable elements of the grains and enriching the surrounding gas.

It remains to be pointed out, however, that in a turbulent fluid field considerable variations of the thermodynamical conditions may occur. For example, the nucleation of dust particles may take place even in a dust-hostile environment, if interfering expansion waves temporarily cause low temperatures, i.e. high supersaturation ratios (Paper I). In such turbulent environments, the correlation between the supersaturation ratio S and the atmospheric height (as assumed in the upper item list) is loosened. Thus, the regimes are characterised by S rather than by the atmospheric height, and may possibly occur also on small scales.

The *life cycle of dust grains in brown dwarf atmospheres* is finally completed by convective streams which mix up gas from the deep interior into the upper layers. On a large scale, we expect an intricate balance of this upward mixing of condensable elements by convection with the downward gravitational settling of the condensing dust grains, which will determine the large-scale structure of the element abundances in the atmosphere related to the observation of the various molecular features.

This work will be continued in the next paper of this series by solving the dust moment equations for the special case of a static atmosphere.

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