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A general multi-component method for the description of dust grain processing

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Abstract. We derive a special differential form of a balance or conservation equation for the grain size distribution function. This equation describes the evolution of the grain size spectrum in one-dimensional stationary flows also taking into account possible size dependent drift velocities of the grains relative to the gas flow. Various physical and chemical processes acting differently on grains of different size and velocities can be treated simultaneously: grain condensation, growth and evaporation, mechanical and chemical sputtering, grain coagulation and shattering.

A corresponding computational multi-component method is presented and we provide some details on efficient implementation.

As a test calculation the numerical scheme is applied to investigate mechanical sputtering of grains due to dense shocks.

Key words: dust processing – methods: numerical – hydrodynamics – shock waves

1. Introduction

Dust is an ubiquitious component of the interstellar medium (ISM). It is found in the winds of late-type stars and thought to be responsible for the heavy mass loss of these objects, which make the largest contribution to the matter injected into the ISM (Gehrz 1989). Furthermore, dust is intimately linked with the question of the origin of life, since every theory of star and planetary system formation has to account for the role of dust as a cooling agent during cloud collapse and as constituting material of planets.

Thus, dust plays a key role in the cosmic cycle of matter, and the structure, composition and size distribution of cosmic dust grains are of considerable importance for the understanding of many interesting astrophysical issues. Unfortunately, observation yields little direct information about the nature of the dust; a consistent modelling of the most important cosmic dust production and processing sites seems necessary to supplement observations and make possible their correct interpretation.

Consequently, we are in need of a detailed knowledge of the physical and chemical processes the dust grains are involved in, as well as efficient computational methods to describe these processes and the dust component itself.

There already exist a variety of methods that mainly concentrate on the description of certain aspects of dust formation and processing. All of these methods either assume the center of mass of the dust component to be comoving with the gas or even treat the dust-gas mixture as a one-fluid, i. e. under the assumption of negligible net motion of the grains relative to the bulk of the gas (position coupling). We will give a short overview of these methods as far as we are aware of their publication and without claim to completeness.

Gail & Sedlmayr (1984, 1988) have developed a rapid moment method to calculate dust formation and growth. This method was successively improved by including evaporation (Gauger et al. 1990), the treatment of heterogeneous and core-mantle grains (Dominik et al. 1993) and a formalism to derive the shape of the grain size spectrum (Dominik et al. 1989). However, for growth or destruction processes to be included in this scheme their efficiency has to vary proportional to some integer power of the grain radius a. Furthermore, the treatment of discontinuous processes which eliminate grains from the size distribution function is not possible. Thus, coagulation or fragmentation due to grain-grain collisions cannot be described by means of the moment method.

In another approach Monte Carlo simulations are used to determine the grain size distribution (Daniels & Hughes 1981, Fulle 1992). In principle, this allows for the treatment of virtually any desired growth or destruction process. However, Monte Carlo calculations require a large amount of computing time. It thus seems difficult to

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use these methods in combination with iterative solution schemes for e. g. the hydrodynamic equations describing the astrophysical object under consideration.

The effects of grain-grain collisions on the grain size distribution are described by an integro-differential equation (Smoluchowsky 1917). This coagulation equation has been solved analytically in the steady state case (Dorschner 1982, Hayakawa & Hayakawa 1988). Elaborate time-dependent numerical calculations have been performed by Kessel'man & Frolov (1986).

An advanced method for the description of dust processing in contracting protostellar clouds has been presented by Rossi et al. (1991), including grain-grain collisions and grain growth. A similar method has been used by McKee et al. (1987) and Jones et al. (1994) to model grain destruction in shocks in the ISM. However, both schemes draw on the hypothesis that the mean velocity of the dust fluid is the same as that for the gas.

It is the aim of this paper to provide a general method of describing dust formation and processing and a corresponding numerical scheme that allows for the simultaneous consideration of a multitude of processes acting on the grains in case of a stationary one-dimensional (1D) flow. The grains are *not assumed* to be position coupled to the gas and we explicitly allow for a size-dependent, directed drift velocity inducing effects such as the dynamical dilution of the dust component (Krüger et al. 1994).

In Sect. 2 we derive a special differential form of a balance or conservation equation for the grain size distribution function. A corresponding computational multi-component scheme is presented in Sect. 3 and we provide some details on efficient implementation. A test calculation involving grain sputtering behind dense shocks is presented in Sect. 4. Some brief conclusions are given in Sect. 5.

2. Evolution of the grain size distribution function

In this section we will derive an equation for the value of the size distribution function as modified by processes affecting the dust component. The dust particles are assumed to be characterized by a single, quasicontinuous parameter. In the following we will identify this parameter with the grain radius a, although other choices, e. g. the grain mass or volume are also conceivable. If the grains are, for instance, spherical and of uniform chemical composition, they are in fact characterized by this sole parameter a.

Concerning the chemical and physical processes affecting a dust grain we will in the following distinguish between continuous and discontinuous processes, respectively. Discontinuous processes abruptly change the size of the affected grains and/or their *number*, e. g. coagulation, shattering or (possibly complete) vaporization following grain-grain collisions.

In contrast, continuous processes are incessantly acting on the surface of a grain, slowly eroding or covering the outermost layer of monomers and thus smoothly changing the size of a grain. These processes include mechanisms such as homogeneous or heterogeneous (chemical) growth, thermal evaporation, chemical and mechanical sputtering etc. (cf. e. g. Gauger et al. 1990). Usually, continuous processes are those arising from interaction of the grain with the gas phase.

2.1. Flow assumptions and topology

We consider a stationary flow and assume that an appropriate coordinate system (p, q, r) can be chosen such that the flow is symmetric with respect to p and q. The sole independent variable is designated by r (1D formulation). Simple examples of such a flow geometry are a plan-parallel shock wave or a spherically symmetric outflow or infall, respectively. The description of thin viscous accretion disks is also possible. The hydrodynamics of such disks are considered one-dimensional, because the flow is independent of the angular coordinate and the coordinate perpendicular to the disk can be discarded.

In order to mimic certain two-dimensional flows, e. g. collimated bipolar outflows, an equivalent quasi-spherical model can be adopted (Ruden et al. 1990). By means of this simplification of more complicated flow geometries the otherwise prohibitive computation of, for instance, non-equilibrium chemistry and dust formation is made possible.

The set of state variables describing the gas and the velocities $\boldsymbol{v}_\mathrm{d}(a, r)$ of grains with radius a are assumed to be known or obtained otherwise, i. e. by the solution of the corresponding equations.

2.2. The size evolution of a sample grain

Refraining from discontinuous processes, the net growth of a single dust grain of spatial dimension d and radius a consisting of N monomers is described by (Gauger et al. 1990)

$$\frac{\mathrm{d}N}{\mathrm{d}t} = \frac{1}{\tau_\mathrm{net}(N,t)} N^{\frac{d-1}{d}} \tag{1}$$

or, equivalently,

$$\frac{\mathrm{d}a}{\mathrm{d}t} = \frac{1}{\tau_\mathrm{net}(a,t)} \frac{a_0}{d} \tag{2}$$

where τ_net^{-1} denotes the net growth rate and a_0 is the hypothetical radius of a monomer. τ_net^{-1} comprises all types i of continuous processes to be considered and is simply given by

$$\tau_\mathrm{net}^{-1} = \sum_i \tau_i^{-1}. \tag{3}$$

In the stationary case Eq. (2) for the grain growth can be written as

$$\frac{\mathrm{d}a}{\mathrm{d}r} = \frac{1}{v_{\mathrm{d}}(a,r)} \frac{1}{\tau_{\mathrm{net}}(a,r)} \frac{a_0}{d} \tag{4}$$

where $v_{\mathrm{d}}(a,r)$ is the velocity component in r-direction of a grain of radius a. In the following we will refer to the grain radius a as grain "size" in order to avoid confusion with the independent variable r.

There are essentially two possibilities of modelling grain "creation" (cf. also Fig. 1): First, a dust particle of size a_* may be injected at the base r_0 of the flow, where the calculation starts. This will be the case when the processing of a given grain size spectrum (e. g. that of the ISM) is to be investigated. On the other hand, for explicitly modelling grain *formation*, e. g. in the cool envelopes of red giants, small clusters condense out of the gas phase at $r = r_*$ (this process is refered to as nucleation). We introduce a lower limit a_ℓ of the size of macroscopic particles, thus separating the dust component from the molecular domain and the growth species (cf. Gauger et al. 1990). If a cluster exceeds the size a_ℓ it is considered a newly created dust particle.

In order to keep a uniform notation and since both cases may occur in the same flow, we introduce the combined parameter ζ which is equal to either a_* or r_* depending on the specific model of grain "creation". The parameter ζ thus characterizes the initial condition upon "creation" of a grain.

At position r in the flow a specific sample grain will have grown to a size $a_r(\zeta)$ given by integration of Eq. (4)

$$a_r(\zeta) = a_* + \frac{a_0}{d} \int\limits_{r_*}^{r} \frac{1}{v_{\mathrm{d}}(a_{r'}(\zeta), r')} \frac{1}{\tau_{\mathrm{net}}(a_{r'}(\zeta), r')} \mathrm{d}r' \tag{5}$$

where $r_* \equiv r_0$ if the particle is merely injected at the base of the flow and $a_* \equiv a_\ell$ for $r_* > r_0$, i. e. in case of nucleation. Equation (5) is well defined as long as $a_r(\zeta) \geq a_\ell$, otherwise the considered sample grain will be regarded as removed from the dust component by destructive continuous processes, e. g. due to evaporation.

It is important to notice here that in a stationary flow any grain created at a position $\hat{r}_* > r_*$ further downstream than an exemplary reference grain or with a smaller initial size $\hat{a}_* < a_*$ will at no point be larger than this reference grain, since as soon as it has grown up to the size of the reference grain all continuous growth and destruction processes for the two grains will be equal. In other words, grains can not "overtake" one another with respect to their size.

2.3. The fundamental balance equation

As stated above we are considering a stationary 1D flow in a spatial domain

$$\mathcal{V} = [p_0; p_{\mathrm{max}}] \times [q_0; q_{\mathrm{max}}] \times [r_0; r_{\mathrm{max}}] \equiv \mathcal{P} \times \mathcal{Q} \times \mathcal{R}. \tag{6}$$

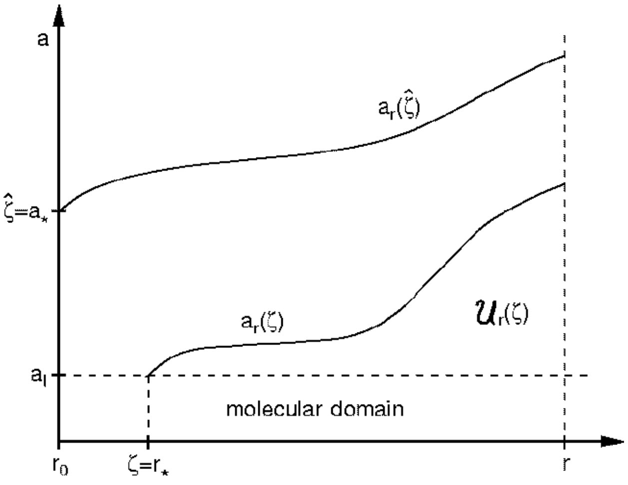

Fig. 1. Size evolution of sample grains injected with size $\hat{\zeta} = a_*$ at r_0 or condensed from the gas phase at $\zeta = r_*$, respectively

Let $f(a,r)$ be the size distribution of dust particles such that $f(a,r)\mathrm{d}a$ equals the number of particles per unit spatial volume in the grain size interval between a and $a+\mathrm{d}a$. In the four-dimensional vector space

$$\mathcal{W} = [a_\ell; a_{\mathrm{max}}] \times \mathcal{V} \equiv \mathcal{A} \times \mathcal{V} \tag{7}$$

the following balance or conservation equation holds for the size distribution function f in any subset $\mathcal{U} \subseteq \mathcal{W}$

$$\int_{\mathcal{U}} \nabla \bullet (\boldsymbol{u}(a,r) f(a,r))\, \mathrm{d}\mathcal{U} = \int_{\mathcal{U}} q(a,r)\, \mathrm{d}\mathcal{U} \tag{8}$$

where in the 1D formulation the nabla operator ∇ collapses to $(\partial/\partial a, 0, 0, \partial/\partial r)$ and $\boldsymbol{u} = (\dot{a}, \dot{p}, \dot{q}, \dot{r})$ denotes the four-velocity of grains in the vector space $\mathcal{W}$. Discontinuous processes creating or destroying grains of size a at r are described by the source term $q(a,r)$.

The volume element $\mathrm{d}\mathcal{U}$ of the four-dimensional vector space is given by

$$\mathrm{d}\mathcal{U} = \mathrm{d}a\, \mathrm{d}x\, \mathrm{d}y\, \mathrm{d}z \tag{9}$$

$$= \mathrm{d}a \left| \frac{\partial(x,y,z)}{\partial(p,q,r)} \right| \mathrm{d}p\, \mathrm{d}q\, \mathrm{d}r \tag{10}$$

where x, y, z signify cartesian coordinates. In order to perform the integration within a specific coordinate system (p,q,r) we are in need of the Jacobian determinant Δ of the corresponding spatial transformation

$$\Delta = |J| = \left| \frac{\partial(x,y,z)}{\partial(p,q,r)} \right|. \tag{11}$$

In the 1D case this determinant can be factorized into two parts $\Delta_{p,q}$ and Δ_r. For spherical symmetry (i. e. $(p,q,r) = (\theta, \phi, r)$) for instance, $\Delta_{\theta,\phi} = \sin\theta$ and $\Delta_r = r^2$.

The balance equation (8) can thus be rewritten in the following way

$$\int_p \mathrm{d}p \int_q \mathrm{d}q\, \Delta_{p,q} \cdot \int_a \mathrm{d}a \int_r \mathrm{d}r\, \nabla \bullet (\boldsymbol{u}(a,r) f(a,r))\Delta_r$$
$$= \int_q \mathrm{d}q \int_q \mathrm{d}q\, \Delta_{p,q} \cdot \int_a \mathrm{d}a \int_r \mathrm{d}r\, q(a,r)\Delta_r \qquad (12)$$

where the first double integrals on both sides are identical and can be omitted.

Now consider a specific subset $\mathcal{U}_r(\zeta) \subseteq \mathcal{W}$ chosen such that its upper boundary with respect to $\mathcal{A}$ is given by the size of a sample grains $a_r(\zeta)$ (cf. Fig. 1 showing a projection of $\mathcal{U}$ onto $\mathcal{A} \times \mathcal{R}$). Formally, $\mathcal{U}_r(\zeta)$ is given by

$$\mathcal{U}_r(\zeta) = \{(a, r') \mid r' \in [r_*; r] \wedge a \in [a_\ell; a_{r'}(\zeta)]\} \times \mathcal{P} \times \mathcal{Q} \qquad (13)$$

This choice of a trajectory $a_{r'}(\zeta)$ of a sample grain as one of the boundaries of $\mathcal{U}_r(\zeta)$ has the advantage that no flux of dust particles crosses that boundary of $\mathcal{U}_r(\zeta)$ (cf. Sect. 2.2). Refraining from discontinuous processes, grains are entering or leaving the subset $\mathcal{U}_r(\zeta)$ only via the boundaries where the dust particles are created and across the boundary at r where the size distribution function is to be evaluated.

By means of the Gauss law the balance equation (8) or (12), respectively, then reads

$$\Delta_r \int_{a_\ell}^{a_r(\zeta)} \mathrm{d}a'\, v_\mathrm{d}(a', r) f(a', r) - \Delta_{r_0} \int_{a_\ell}^{a_*} \mathrm{d}a'\, J_0(a')$$
$$- \int_{r_*}^{r} \mathrm{d}r'\, J_\ell(r')\Delta_{r'} = \int_{r_*}^{r} \mathrm{d}r'\, \Delta_{r'} \int_{a_\ell}^{a_{r'}(\zeta)} \mathrm{d}a'\, q(a', r') \qquad (14)$$

where we have introduced the flux-like quantities $J_0(a) \equiv v_\mathrm{d}(a, r_0) f(a, r_0)$ and $J_\ell(r) \equiv \dot{a}|_{a_\ell} f(a_\ell, r)$. The latter can be identified with the rate of nucleation or evaporation, respectively, as defined by Gail & Sedlmayr (1988). The second term on the l. h. s. of Eq. (14) is equal to zero if the sample grain has been created by condensation from the gas phase at $r_* > r_0$. In the absence of discontinuous processes the integral on the r. h. s. vanishes.

In order to arrive at an expression for the value of the distribution function $f(a, r)$ we formally differentiate Eq. (14) with respect to ζ, noting that some limits of the integrals also depend on ζ. This finally yields the special differential balance or conservation equation for the grain size distribution

$$-\Delta_{r_0} \frac{\mathrm{d}a_*}{\mathrm{d}\zeta} J_0(a_*) + \Delta_{r_*} \frac{\mathrm{d}r_*}{\mathrm{d}\zeta} J_\ell(r_*)$$
$$+\Delta_r \frac{\mathrm{d}a_r(\zeta)}{\mathrm{d}\zeta} v_\mathrm{d}(a_r(\zeta), r) f(a_r(\zeta), r)$$
$$= \int_{r_*}^{r} \mathrm{d}r'\, \Delta_{r'} \frac{\mathrm{d}a_{r'}(\zeta)}{\mathrm{d}\zeta} q(a_{r'}(\zeta), r') \equiv Q(a_r(\zeta), r). \qquad (15)$$

If the sample grain has been "created" by injection, i. e. if $\zeta \equiv a_*$, the second term on the l. h. s. vanishes and $\mathrm{d}a_*/\mathrm{d}\zeta = 1$, while for a sample grain condensed at $r_* > r_0$ the first term is identical to zero and $\mathrm{d}r_*/\mathrm{d}\zeta = 1$.

In principle, the size distribution f can be calculated from this equation at any point r and for every size $a = a_r(\zeta)$. However, as $a_r(\zeta)$ is actually an integrated quantity (cf. Eq. (5)) depending on $a_{r'}(\zeta)$ for $r' < r$, Eq. (15) represents an integro-differential equation and the derivatives of $a_r(\zeta)$ are not readily obtained. Our computational multi-component scheme presented in Sect. 3 comprises the evaluation of these derivatives by finite differences on a non-uniform $a_r(\zeta_i)$-grid which is moving in the grain size space $\mathcal{A}$. This grid is constructed by following the size evolution of a large, variable number of grains injected at r_0 and/or originating from appropriately chosen radii $r_* = r_i$.

2.4. Processes affecting the grains size distribution

For a review of grain growth and destruction processes see, for example, Seab (1987). As stated above we are distinguishing between continuous and discontinuous processes acting on a grain. In this subsection we will describe briefly how these classes of processes can be taken into account in the general balance equation.

2.4.1. Continuous processes

The treatment of continuous processes such as growth or sputtering is an inherent feature of the approach presented above. These processes are taken into consideration by simply including their corresponding grain growth or reduction rates, respectively, in Eq. (4) for the evolution of a sample grain size. The derivative of this sample grain size directly affects the value of the size distribution via the basic Eq. (15). Explicit expressions for the rates of the most important continuous processes are given in Gauger et al. (1990) and Woitke et al. (1993). The necessary modifications of chemical sputtering and growth rates due to possible drift motion of the grains relative to the gas are derived in Krüger & Sedlmayr (1995).

2.4.2. Discontinuous processes

Grain processing due to discontinuous processes such as coagulation, (possibly complete) vaporization or shattering is represented by a source term $q(a, r)$. Unfortunately, there seems to be little or no experimental data on reaction probabilities or yields available (cf. Seab 1987). On the other hand, coagulation has been thoroughly studied by Chokshi et al. (1993) by means of an analytical theory. In a recent paper Tielens et al. (1994) also determine the fraction of a grain vaporized by a grain-grain collision .

Here, we restrict ourselves to state an expression for $q(a, r)$ corresponding to coagulation as an exemplary source function. Actually, $q(a,r)$ is a Boltzmann type collision term accounting for gains and losses from the size range $[a; a+\mathrm{d}a]$. According to Völk et al. (1980) it is of the form

$$q(a,r) = -f(a,r)\int_{a_\ell}^{a_{\max}} \mathrm{d}a'\, f(a',r)\Omega(a,a',r) + \frac{1}{2}\int_{a_\ell}^{a} \mathrm{d}a'\, f(a',r)f(\bar{a},r)\left(\frac{a}{\bar{a}}\right)^2 \Omega(a',\bar{a},r) \qquad (16)$$

where $\bar{a}^3 \equiv a^3 - a'^3$ due to mass conservation. The reaction frequency $\Omega(a,a',r)$ per unit density is given by the product of the collisional cross-section and the r.m.s. of the sticking probability α and the relative velocity v_{rel} of the grains

$$\Omega(a,a') = \pi(a+a')^2\langle[\alpha(a,a',r)v_{\mathrm{rel}}(a,a',r)]^2\rangle^{1/2}. \qquad (17)$$

In the limit case of high size dependent drift velocities in r-direction $v_{\mathrm{rel}}(a,a',r) = v_{\mathrm{d}}(a,r) - v_{\mathrm{d}}(a',r)$. Please note, however, that according to the results of Chokshi et al. (1993) the sticking probability of colliding grains is zero for $|v_{\mathrm{rel}}| > v_{\mathrm{cr}} \sim 10^2$ cm s^{-1}. In the opposite case of vanishing drift in r-direction, v_{rel} may be given by isotropic relative velocities due to a Brownian motion of the grains or turbulent gas motion (cf. Völk et al. 1980).

3. The computational multi-component scheme

So far our approach was completely analytic; no errors due to discretization etc. have been introduced during the derivation of the fundamental balance or conservation equation (15). However, in order to evaluate this equation, i. e. to calculate the size distribution at r and for $a = a_r(\zeta)$, we have to calculate the derivatives of $a_r(\zeta)$ with respect to ζ. To do this, we follow the size evolution of a large number of sample grains, i. e. for each sample grain we solve an ordinary differential equation (ODE) of type (4) with increasing r. In this way a moving, non-uniform grid in grain size space $\mathcal{A}$ is constructed, its points being identified with the momentary sizes $a_r(\zeta_i)$ of sample grains.

If nucleation or complete thermal evaporation of grains is to be considered, the number of sample grains and, hence, the number of ODE's to be solved successively increases or decreases, respectively. The grid in grain size space $\mathcal{A}$ then not only varies in position but also in size.

3.1. Grid generation

It is obviously difficult to give some general advice on an appropriate choice of grid points since this strongly depends on the specific problem to be solved. In case of the mere processing of a given size distribution, i. e. if all sample grains are injected at the base r_0 of the flow and no further nucleation takes place, a logarithmically spaced a_i-grid serving as initial conditions $a_{*,i}$ for the system of ODE's of type (4) (henceforth called grid point equations) should suffice. The number of grid points I, i. e. the dimension of the system of ODE's, then depends on the desired resolution.

If, additionally or instead, nucleation is to be treated the number of grid points I is not constant anymore. During the integration of the grid point equations their number is successively incremented whenever we choose to add a new grid point $a_r(\zeta_i)$ at $r_i \equiv r_{*,i}$. This is done to account for the continuous increase of the number density of grains due to condensation of small clusters from the gas phase.

There are several possible criteria to decide whether a new grid point should be added: for example, whenever the state variables of the gas have changed by a certain fraction or whenever a certain amount of dust has been newly formed. An estimate for the expected final size $a_\infty(r_i)$ of a grains formed at r_i may also serve as a useful guide. For example, Dominik et al. (1989) derived a final grain size estimate in quickly expanding flows

$$a_\infty(r) \approx \left(\frac{\mathrm{d}\tau_{\mathrm{net}}(r)}{\mathrm{d}r}\right)^{-1} \Big/ v_{\mathrm{d}}(r)a_0 \qquad (18)$$

where τ_{net} and v_{d} have been assumed to be independent of the grain size a by these authors.

Now, given the availability of a final grain size estimate, a new grid point is added when the estimated final size of a grain condensing at the momentary position r is smaller than a certain fraction of the estimated final size of the previous sample grain created at r_I

$$\text{create grid point:} \quad \log a_\infty(r_I) - \log a_\infty(r) > \delta. \qquad (19)$$

The value of δ is chosen according to the desired resolution of the grain size distribution at infinity. In order to achieve a final number $I_{\max}$ of grid points we put

$$\delta = \frac{\log a_\infty(r_1) - \log a_0}{I_{\max} - 1} \qquad (20)$$

corresponding to a roughly logarithmically equidistant grid in grain size space $\mathcal{A}$ at the end of computation.

As stated in Sect. 2.2 sample grains may also be removed from the gas phase due to destructive continuous processes like sputtering or thermal evaporation. This will happen, for instance, in the accretion disks around protostellar objects. In this case, the number I of grid equations will be successively decremented as the smaller grains are destroyed.

$$\text{remove grid point:} \quad a_r(\zeta_I) < a_\ell \qquad (21)$$

Since the grain size grid points are identified with the momentary size $a_r(\zeta_i)$ of sample grains, the grid points move through the grain size space $\mathcal{A}$ according to the evolution of the dust component and the size distribution function f should always be well resolved. In the rare case where neighbouring grid points become to far apart or to close, finer or coarser resolution can be easily achieved by insertion or removing, respectively, of grid points.

Concerning the insertion of grid points this remapping or rezoning procedure involves simple linear interpolation of the grain size distribution function at the desired new grid point $a_r(\hat{\zeta})$. This introduces discretization errors of second order in the grain size separation $a_r(\zeta_i) - a_r(\zeta_{i+1})$ as do all other numerical schemes employed in our multi-component approach. The corresponding initial parameter $\hat{\zeta}$ of the new sample grain is obtained through integration of Eq. (4) backward in r-direction until $r = r_0$ or $a_r(\hat{\zeta}) = a_\ell$.

3.2. Numerical differentiation by finite differences

The relevant derivatives in the fundamental balance equation (15) can now be approximated by the analytic derivative of the Lagrange interpolating polynomial of degree two passing through the set of points $\{\zeta_j, a_r(\zeta_j)\}$ with $j = i-1, i, i+1$

$$\frac{\mathrm{d}a_r(\zeta_i)}{\mathrm{d}\zeta_i} = -\frac{h_i}{h_{i-1}(h_{i-1}+h_i)} a_r(\zeta_{i-1}) + \frac{h_i - h_{i-1}}{h_i h_{i-1}} a_r(\zeta_i) + \frac{h_{i-1}}{h_i(h_{i-1}+h_i)} a_r(\zeta_{i+1}) \tag{22}$$

where $h_i \equiv \zeta_{i+1} - \zeta_i$. At the first and at the last grid point ($i = 1$ and $i = I$, respectively) the set of points is adjusted by choosing $j = 1, 2, 3$ and $j = I-2, I-1, I$ yielding similar formulae. The discretization error of this finite difference scheme is of second order in h_i.

Obviously, I has to be larger than 2 for this scheme to be applied at all. Thus, in case of an initially dust-free medium no information about the size distribution can be obtained during the starting of the multi-component method. Consequently, the first three grid points should be generated in rather quick succession after the onset of nucleation.

3.3. Discontinuous processes

For the treatment of discontinuous processes due to grain-grain collisions the quantity $Q(a_r(\zeta_i), r)$ in the fundamental balance equation (15) needs to be calculated. This is most efficiently done by solving one additional ODE per grid point, namely

$$\frac{\mathrm{d}Q(a_r(\zeta_i), r)}{\mathrm{d}r} = \Delta_r \frac{\mathrm{d}a_r(\zeta_i)}{\mathrm{d}\zeta_i} q(a_r(\zeta_i), r) \tag{23}$$

where the derivative of $a_r(\zeta_i)$ with respect to ζ_i is evaluated as described in Sect. 3.2. The initial value of Q upon grid point creation is always zero.

3.4. Derived macroscopic quantities of the dust component

We are now in the position to calculate the size distribution function by means of the fundamental balance equation (15). We only have to keep track of the evolution of the sample grain sizes $a_r(\zeta_i)$ and of the quantities $Q(a_r(\zeta_i), r)$ accounting for discontinuous processes and to take care of storing the quantities ζ_i and $\Delta_{r_0} J_0(a_i)$ or $\Delta_{r_i} J_\ell(r_i)$, respectively.

Given the size distribution f on the non-uniform grid $a_r(\zeta_i)$ any macroscopic quantity given as a linear functional of the grain size spectrum can be calculated by simple integration, e. g. the total dust opacity, the collisional drag force exerted by the drifting grains or the consumption rate of condensable material from the gas due to grain growth. The following equation holds for any macroscopic property $P_\mathrm{d}(r)$ of the dust component given the microscopic property $p(a, r)$ of a single grain of size a

$$\begin{aligned} P_\mathrm{d}(r) &= f(a_r(\zeta_1), r)\, p(a_r(\zeta_1), r)\, [a_r(\zeta_1) - a_r(\zeta_2)]/2 \\ &+ \sum_{i=2}^{I-1} f(a_r(\zeta_i), r)\, p(a_r(\zeta_i), r)\, [a_r(\zeta_{i-1}) - a_r(\zeta_{i+1})]/2 \\ &+ f(a_r(\zeta_I), r)\, p(a_r(\zeta_I), r)\, [a_r(\zeta_{I-1}) - a_r(\zeta_I)]/2 \end{aligned} \tag{24}$$

where the integral was approximated by the extended trapezoidal rule. The discretization error of this rule is of second order in grain size separation $a_r(\zeta_i) - a_r(\zeta_{i+1})$. Thus, our integration scheme is accurate to the same order as our numerical differentiation scheme (cf. Sect. 3.2).

More complicated, non-linear functionals of the grain size distribution function can be calculated in an analogue manner to Eq. (24) though some, e. g. the second integral of the coagulation source term (16), may involve some interpolation of f on the grain size grid $a_r(\zeta_i)$. Fortunately, linear interpolation (which again involves discretization errors of second order in grain size separation) is sufficient here.

3.5. Error estimation

The underlying fundamental principle of our approach is the flux conservation of the dust component (cf. Eq. (8))

$$\Delta_r \int_{a_\ell}^{a_\mathrm{max}} \mathrm{d}a'\, v_\mathrm{d}(a', r) f(a', r) = \Delta_{r_0} \int_{a_\ell}^{a_\mathrm{max}} \mathrm{d}a'\, J_0(a') + \int_{r_0}^{r} \mathrm{d}r'\, J_\ell(r') \Delta_{r'} + \int_{r_0}^{r} \mathrm{d}r'\, \Delta_{r'} \int_{a_\ell}^{a_\mathrm{max}} \mathrm{d}a'\, q(a', r'). \tag{25}$$

It therefore seems plausible to define the estimated error $\epsilon(r)$ of the computational multi-component method by the deviation of the "theoretical" flux $j_\mathrm{tot}(r)$ given by the r. h. s. of Eq. (25) from the numerical grain flux $j_\mathrm{tot}^\mathrm{num}$ as calculated according to Eq. (24) with $p(a, r) \equiv v_\mathrm{d}(a, r)$, which represents the the r. h. s. of Eq. (25)

$$\epsilon(r) = |1 - j_\mathrm{tot}^\mathrm{num}(r)/j_\mathrm{tot}(r)|. \tag{26}$$

If this error exceeds or falls below some user-specified thresholds, grid points can be inserted or removed, respectively, in order to adjust the achieved accuracy of the multi-component method (cf. Sect. 3.1).

4. A test calculation: Grain sputtering behind dense shocks

The computational multi-component method outlined above is applied in a test calculation to model the processing of a given grain size distribution due to mechanical sputtering behind a dense shock. This test calculation is not intended to give new astrophysical insights but rather serves as a worked example for the multi-component method and as a test for its validity.

For a more elaborate application see the paper of Krüger & Sedlmayr (1995). They model dust driven stellar winds and investigate the influence of grain drift on dust formation and on the shape of the size distribution function.

4.1. Adopted shock structure

In order to discuss the effects of grain sputtering independent of a complicated hydro- and thermodynamical structure, a very simple model of a jump-type or J-type shock of velocity v_s will be used here. We adopt and slightly simplify the results of Neufeld & Hollenbach (1994) who thoroughly investigated a dense shock of preshock density $n_0 = 10^9$ cm s^{-1} and $v_\mathrm{s} = 50$ km s^{-1}. After the immediate jump of the gas velocity v_g to 1/4 v_s behind the shock front, the gas further decelerates as it cools.

The initial grain velocity $v_\mathrm{d}(a)$ just behind the shock is given by v_s. According to the results of Neufeld & Hollenbach (1994) no significant deceleration of the grains takes place for $N_\mathrm{H} < 10^{16}$ cm^{-2} where N_H is the column densities of hydrogen nuclei behind the shock front. Similarly, it turns out (cf. Sect. 4.6) that grain sputtering is negligble in this region.

Hence, we start our computation at $N_\mathrm{H} \approx 10^{16}$ cm^{-2}. The value of the gas velocity for $N_\mathrm{H} < 10^{16}$ cm^{-2} does not influence the outcome of the calculations, since grain deceleration and sputtering sets in at $N_\mathrm{H} \approx 10^{16}$ cm^{-2}.

According to the results of Neufeld & Hollenbach (1994) the gas density is varying only slowly for 10^{16} cm$^{-2} \lesssim N_\mathrm{H} \lesssim 10^{21}$ cm^{-2}. Thus, we assume a constant postshock density of $n_\mathrm{H} = 5\,10^{10}$ cm^{-3} in this region, corresponding to a gas velocity $v_\mathrm{g} = 1$ km s^{-1}. For $N_\mathrm{H} > 10^{21}$ cm^{-2} no further grain processing takes places and the computation is stopped.

4.2. Grain dynamics

In the present test calculation N_H takes the place of the independent flow variable r. Due to the plan-parallel geometry the transformation determinant $\Delta \equiv 1$.

For sufficiently high preshock densities the grains follow nearly linear trajectories and are stopped before they can be significantly accelerated by the betatron mechanism (Neufeld & Hollenbach 1994). Assuming the grains to be decelerated solely by collisional drag of the gas particles the equation of motion for a grain can be written as (cf. Woitke et al. 1993, henceforth WDS)

$$\frac{\mathrm{d}v_\mathrm{d}(a)}{\mathrm{d}N_\mathrm{H}} = -\frac{3\mu m_\mathrm{u}}{4a\rho_\mathrm{s}}\frac{(v_\mathrm{d}(a)-v_\mathrm{g})^2}{v_\mathrm{d}(a)} \tag{27}$$

where ρ_s denotes the mass density of the grain material, m_u is the atomic mass unit and $\mu = 1.4$ is the mean molecular weight corresponding to complete dissociation of the gas and solar elemental abundances. In Eq. (27) and the remainder of this section we omit the functional dependency of physical quantities on N_H.

4.3. Grain sputtering

In the present test calculation we limit ourselves to the inclusion of mechanical sputtering as the sole processing mechanism of the grains. With N_H being the independent variable of the flow Eq. (4) for the grain size evolution can then be written as (cf. also WDS)

$$\frac{\mathrm{d}a}{\mathrm{d}N_\mathrm{H}} = -\pi a_0^2\frac{v_\mathrm{d}(a)-v_\mathrm{g}}{v_\mathrm{d}(a)}\overline{Y}_\mathrm{sp}\frac{a_0}{d} \tag{28}$$

where $\overline{Y}_\mathrm{sp} \equiv \overline{Y}_\mathrm{sp}(v_\mathrm{d}(a)-v_\mathrm{g})$ denotes the mean sputtering yield, i. e. the number of lattice particles removed from the grain surface per incident gas particle.

As has been argued by WDS it suffices to take into account H, He and an artificial species (denoted by "C/N/O") for all metals in order to determine the mean sputtering yield. It is then given by

$$\overline{Y}_\mathrm{sp} = Y_\mathrm{sp,H} + \epsilon_\mathrm{He}Y_\mathrm{sp,He} + \epsilon_\mathrm{CNO}Y_\mathrm{sp,CNO} \tag{29}$$

where ϵ_i denotes the abundance of the sputtering species i relative to hydrogen. In our test calculation we have used semianalytical yields derived from experimental data (for details see Tielens et al. (1994) and references therein).

4.4. Initial grain size distribution and chemical composition of the gas phase

We have investigated the processing of spherical ice coated dust grains. For the sake of simplicity we assumed the grain to consist of a small core coated by a thick layer of ice ($\rho_s \approx 1$ g/cm^{-3}, $a_0 = 1.9\,10^{-8}$ cm). The initial size distribution is given by

$$f(a) \propto a^{-3.5} \tag{30}$$

in the size range $10^{-2}\,\mu$m $< a < 1\,\mu$m as suggested by the results of Mathis et al. (1977).

The adopted abundances of the sputtering species are $\epsilon_\mathrm{He} = 10^{-1}$ and $\epsilon_\mathrm{CNO} = 10^{-3}$.

4.5. Method of solution

Considering grain sputtering behind plane-parallel shocks the fundamental balance equation (15) simplifies to

$$f(a) = \frac{J_0(a_*)}{v_\mathrm{d}(a)} \bigg/ \frac{\mathrm{d}a}{\mathrm{d}a_*} \tag{31}$$

For the multi-component method we follow the size evolution of I sample grains with their initial sizes $a_* = a_i$ chosen to be

$$\log_{10}(a_i/\mu\mathrm{m}) = -2 + 2(i - 1/I - 1)^2. \tag{32}$$

This corresponds to a modified logrithmic grid with higher resolution of the smaller grain sizes and thus accounts for the fact that 95% of the grains are smaller than $2.5\ 10^{-2}\,\mu$m.

The grid point equations (28) and the corresponding equations of motions (27) for the sample grains form a system of $2I$ ODE's. They are solved by means of an embedded, explicit fourth order Runge-Kutta scheme (Hairer et al. 1987). Our calculations have been performed on a Silicon Graphics IRIS Indigo R 4000 workstation. The results presented below have been calculated with $I = 30$. This takes less than a second of computing time.

4.6. Results and discussion

Figure 2 shows the grain velocities v_d behind the shock front for three different initial grain sizes a_i. We confirm the well known fact that the distance required to slow down the grains to the gas velocity is proportional to their size (cf. WDS).

The size evolution of three sample grains relative to their initial size a_i is shown in Fig. 3. The larger a grain the longer it suffers from sputtering, since it maintains a significant drift velocity well beyond the shock front. However, the *relative* amount of dust material returned to the gas phase is the same for all grains irrespective of their initial size. This has also been shown analytically by WDS.

The evolution of the grain size distribution $f(a)$ (multiplied by $a^{3.5}$) is presented in Fig. 4 by a sequence of snapshots taken at various column densities N_H behind the shock. The final size distribution is obtained if all grains have decelerated to zero drift velocity. Compared to the initial size distribution the final distribution is shifted upwards due to the compression of the gas. The distribution is also shifted horizontally towards smaller grain sizes, since *all* grain sizes have been uniformly reduced by $\sim 55\%$ due to sputtering.

To summarize, in Fig. 4 the size distribution performs an upward movement combined with a shift to the left. Moreover, it does so in a certain order: sections of the distribution representing smaller grains (which are decelerated faster than larger ones) approach the final distribution at lower column densities. This is reflected in the snapshots for $N_\mathrm{H} = 10^{17}, 10^{18}, 10^{19}, 10^{20}$ cm^{-2}.

The shape of these inbetween size distributions during grain deceleration and sputtering can be explained as follows: For every column density there is a grain size a such that the separation Δa of neighbouring grain sizes is temporarily increased, since grains smaller than a already almost completed the sputtering process while grains larger than a not yet experienced a significant change of size (cf. also Fig. 3). As a result, the derivative $\mathrm{d}a/\mathrm{d}a_*$ is large and, consequently, $f(a)$ is small (cf. Eq. (31)), i.e. the corresponding section of the size distribution drops below the initial distribution. When the grains are decelerated to drift velocities smaller than about 10 km s^{-1} grain sputtering ceases. During the further deceleration of the grains the compression of the dust fluid, however, continues and the considered section of the distribution function rises towards the final distribution (cf. Eq. (31)).

Finally, Fig. 5 depicts the estimated local error ϵ as defined in Eq. (26) for three different numbers of grid points I. The maximum deviation from flux conservation does not accumulate towards the end of the calculation but rather occurs at $N_\mathrm{H} \sim 10^{18}$ cm^{-2}, when the majority of the grains, namely the small ones, are processed. However, this error only amounts to a few percent, even if as few as 10 grid points are distributed over the whole size spectrum.

If the number I of grid points is increased, the mean separation in grain size space decreases accordingly in an antiproportional manner. During the derivation of the computational multi-component scheme in Sect. 3 we have taken care of all discretization errors to be of second order in grain size separation. This can also be seen in Fig. 5 where a tenfold increase in the number of grid points leads to a reduction of the estimated local error by 10^2.

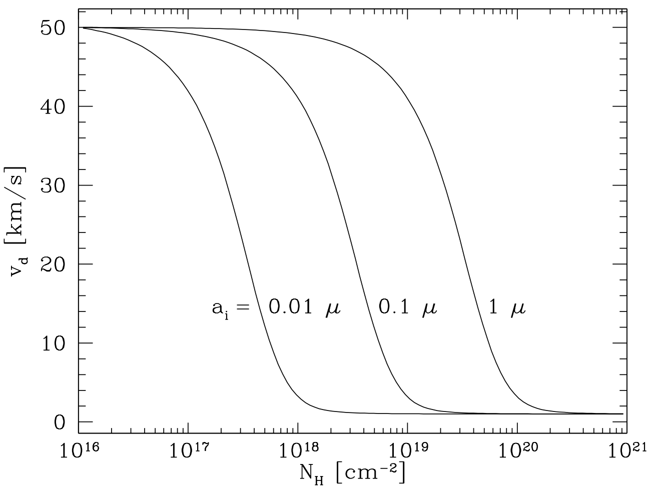

Fig. 2. Velocities of dust particles of initial size $a_i = 0.01\,\mu$m, $0.1\,\mu$m and $1\,\mu$m

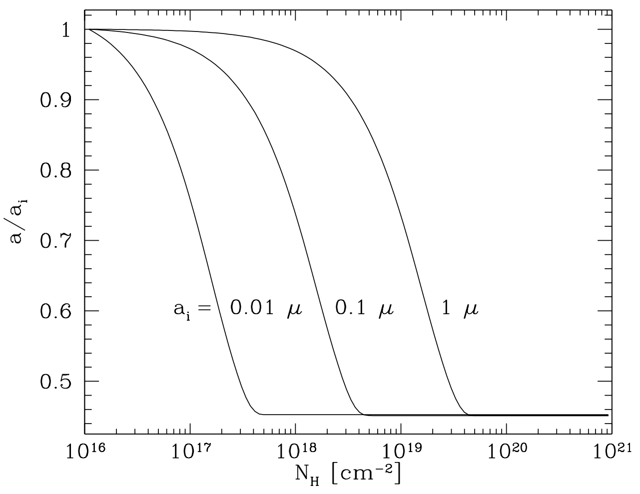

Fig. 3. Size evolution of grains relative to their initial size $a_i = 0.01\,\mu$m, $0.1\,\mu$m and 1 μm

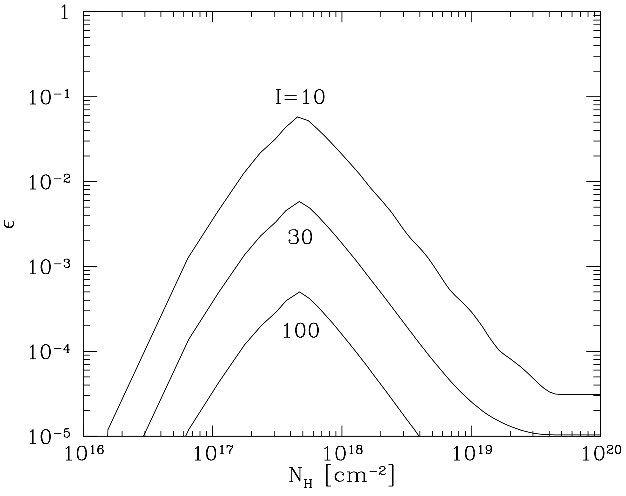

Fig. 5. Estimated local error of the multi-component method for $I = 10, 30$ and 100 grid points

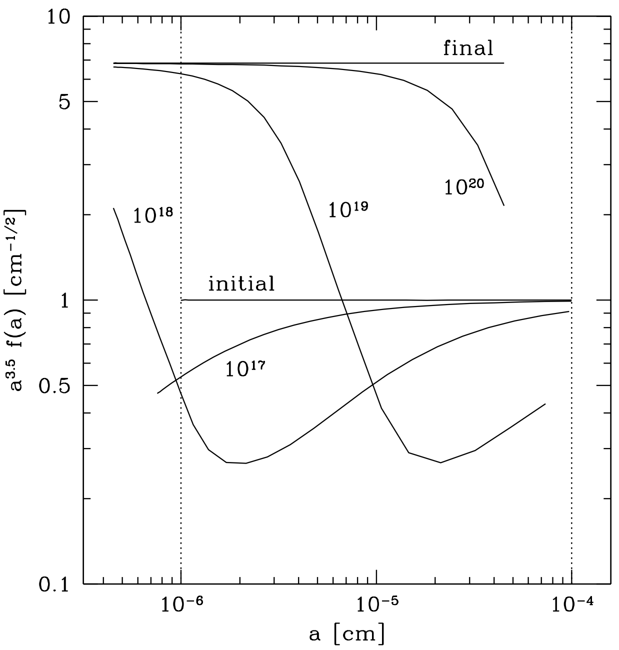

Fig. 4. Grain size distribution (apart from an arbitrary scaling factor) multiplied by $a^{3.5}$ at various positions $N_{\rm H} = 10^m$ cm^{-2} behind the shock front

5. Conclusions

In this paper we have derived a special differential form of a balance or conservation equation for the grain size distribution function. In contrast to other approaches on the subject of grain processing, this equation not only holds in those regimes where either growth or coagulation dominates the evolution of the size distribution. Instead, all processes acting on the grains can be treated simultaneously, taking furthermore into account that grains of different size may move and be processed differently. This makes possible a more detailed treatment of such effects as the size dependence of grain temperature and charge on the processing of the distribution function. Moreover, distinct spatial geometries and symmetries of the flow can be taken into account as long as there is only one independent spatial coordinate.

A corresponding computational multi-component method was presented. Here, the essential idea was to discretize the size distribution on a Lagrange-like grid in grain size space which moves according to the size evolution of selected sample grains. In this way the grid is self-adapting to the way the size distribution is evolving which seems more natural than the use of a static grid. The treatment of continuous changes in grain size thus is an inherent feature of the multi-compontent method, since such processes simply amount to an adjustment of the grid in grain size space.

Another distinguished feature of our method is that we do not try to approximate the size distribution function by a linear combination of simple box-car or square puls size distributions refered to as bins. Instead, the grain size spectrum is sampled at selected grid points only, which can be compared to the discretization approach taken in radiative transfer calculations. This allows for a straightforward inclusion of coagulation and other discontinuous processes.

We also performed a test calculation involving grain sputtering behind dense shocks in order to assess the validity and reliability of our multi-component method. It turned out that the corresponding code is very efficient and that the results expected from a theoretical point of view could be reproduced. Furthermore, additional insight of how exactly the grain size distribtution evolves was gained.

In summary, we have provided a new and efficient method for the modelling of grain processing which we feel is capable of being applied to a wide range of astrophysical problems, e. g. dust formation in circumstellar dust shells (Krüger & Sedlmayr 1995), grain growth and coagulation in dense clouds, formation of planetesimals and processing of chondrule precursor grains in the solar nebula or other protostellar disks.

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