Description of the Cometary Model of Dust Environments (ComMoDE).

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List of Symbols

t	time of flight
v	velocity
θ	emission angle
Φ	phase angle
t	time
a	particle radius/size
L	side length of cell
x	x-coordinate of cell
y	y-coordinate of cell
R	cometocentric distance
κ	power-law index
θ	emission angle

1 Introduction

The goal of this work is to provide a flexible, time-efficient and accurate dust coma model for cometary missions. It is designed to allow for a wide range of user inputs.

2 User Inputs

2.1 Size Distribution

- **Switch for default size distribution**
  Description: The user decides if the default size distribution should be used.
  Range: Yes/No

- **Number of size bins**
  Description: Specifies the number of logarithmic size bins
  Range: [10,80]

- **Largest size**
  Description: Specifies the largest considered particle size
  Range: [10^{-3},10^{-1}] m.

- **Smallest size**
  Description: Specifies the smallest considered particle size
  Range: [10^{-7},10^{-5}] m.

- **Power-law index**
  Description: Specifies the exponent κ describing the dust particle size distribution ejected from the nucleus $n_d(a) \propto a^{-\kappa}$.
  Range: [3.1,4.5]

2.2 Scattering Properties

- **Material**
  Description: The user decides which material is used.
  Range: Water ice, enstatite, astronomical silicate and troilite

- **Phase angle**
  Description: Specifies the phase angle.
  Range: [0,180] $^\circ$

- **Heliocentric distance**
  Description: Specifies the distance between the sun and the comet.
  Range: [0.5,2.0] AU

2.3 Dust production rate

- **Switch for dust production rate estimation based on $Af\rho$**
  Description: The user decides if the dust production rate should be estimated based on the input of $Af\rho$.
  Range: Yes/No

- ***Afρ***
  Description: Specifies $Af\rho$ (refer to more detailed explanation later in document). This input parameter is mutually exclusive to an input of the dust production rate.
  Range: [25,300] m

- **Dust production rate**
  Description: Specifies the global dust production rate of the comet. This input parameter is mutually exclusive to an input of $Af\rho$.
  Range: [1000,40000] kg/s

2.4 Estimation of bulk dust outflow velocity

- **Gas production rate**
  Description: Specifies the gas production rate.
  Range: [1000,40000] kg/s

- **Radius of comet nucleus**
  Description: Specifies the radius of the comet.
  Range: [1000,30000] m

- **Nucleus surface temperature**
  Description: Specifies the temperature on the surface of the nucleus.
  Range: [280,340] K

- **Bulk dust density**
  Description: Specifies the bulk dust density of the dust particles.
  Range: [400,800] kg/m^3

2.5 Day-night asymmetry

- **Day-Night asymmetry switch**
  Description: User decides if there is a day- to night-side asymmetry. In the isotropic case the dust densities can be calculated analytically which decreases the running time by orders of magnitude.
  Range: Yes/No

- **Angular asymmetry function**
  Description: The user decides which function is used to model the emission angle dependence of the outflow velocity and the dust production rate.
  Range: Cosine, Gaussian and Half-Maxwell

- **Amplitude of cosine**
  Description: Specifies the amplitude of the cosine used to introduce an emission angle dependence. At the maximum amplitude the dust production rate at the anti-solar point is 0. This input parameter can only be set if the angular asymmetry function is the cosine.
  Range: [0,1]

2.6 Rotational variability

- **Rotational variability switch**
  Description: User decides if the dust production rate varies due to the rotation of the comet nucleus.
  Range: Yes/No

- **Amplitude of rotational variability**
  Description: Specifies the amplitude of the rotational variability relative to the average dust production rate.
  Range: [0,1]

- **Rotational period**
  Description: Specifies the rotational period of the comet nucleus.
  Range: [0,50] h

2.7 Grid

- **Maximum distance**
  Description: Specifies the maximum cometocentric distance.
  Range: [10000,100000] km

- **Resolution**
  Description: Specifies the sidelength of the grid cells.
  Range: [10,100] km

2.8 Spacecraft trajectory

- **Impact parameter**
  Description: Specifies cometocentric distance of the spacecraft at closest approach
  Range: [100,5000] km

- **Phase angle of approach**
  Description: Specifies the phase angle of approach.
  Range: [-90,90] $^\circ$

- **Altitude angle**
  Description: Specifies the phase angle of the spacecraft at the point it crosses the sun-comet line.
  Range: [-90,90] $^\circ$

- **Spacecraft velocity**
  Description: Specifies the magnitude of the spacecraft velocity relative to the comet nucleus.
  Range: [10,80] km/s

- **Spacecraft frontal area**
  Description: Specifies the frontal area of the spacecraft.
  Range: [0.01,10] m^2

3 Assumptions and Simplifications

To create a time efficient model of the dust environment of a comet relevant for cometary fly-by missions we make several simplifying assumptions. In the following the most important assumptions are listed. The outflow velocity is calculated with an identical approach to the model described in Marschall et al. [2022] and a more detailed description of the underlying assumptions can be found in Zakharov et al. [2021a] and Zakharov et al. [2021b].

- The acceleration zone of the dust is not modelled. It is assumed that the dust particles are ejected at terminal velocity. As described in Divine et al. [1986] the dust particles move along independent ballistic trajectories outside of the acceleration zone. The model is valid in a range of $R > 10R_N$.
- The coma is assumed to follow a cylindrical symmetry, which makes it possible to calculate the trajectories of the dust particles in a two-dimensional grid (see Figure 1).
- The dust particles are assumed to be spherical and homogeneous.
- The gas and dust emission is assumed to be smooth from a spherical nucleus surface.
- It is assumed that the gas flow is independent of the dust (i.e. no back-coupling and no sublimation or re-condensation).

4 Method

Using the listed assumptions we can calculate the trajectory of every simulated particle analytically. Setting the origin of the coordinate system at the nucleus and the emission angle θ as $0°$ at the sub-solar point the position of a particle in two dimensions (see Figure 1) is given by

$$\vec{r} = \begin{pmatrix} x \\ y \end{pmatrix} = \begin{pmatrix} \frac{1}{2}gt^2 - v_0 t\cos(\theta) \\ v_0 t\sin(\theta) \end{pmatrix}, \tag{1}$$

where g is the acceleration the particle experiences due to the solar radiation pressure and v_0 is the terminal outflow velocity. The velocity of a dust particle at a given point in time is

$$\vec{v} = \begin{pmatrix} v_x \\ v_y \end{pmatrix} = \begin{pmatrix} gt - v_0\cos(\theta) \\ v_0\sin(\theta) \end{pmatrix}. \tag{2}$$

Hence, the absolute value of the velocity is

$$|\vec{v}| = \sqrt{g^2t^2 + v^2 - 2gt\cos(\theta)}. \tag{3}$$

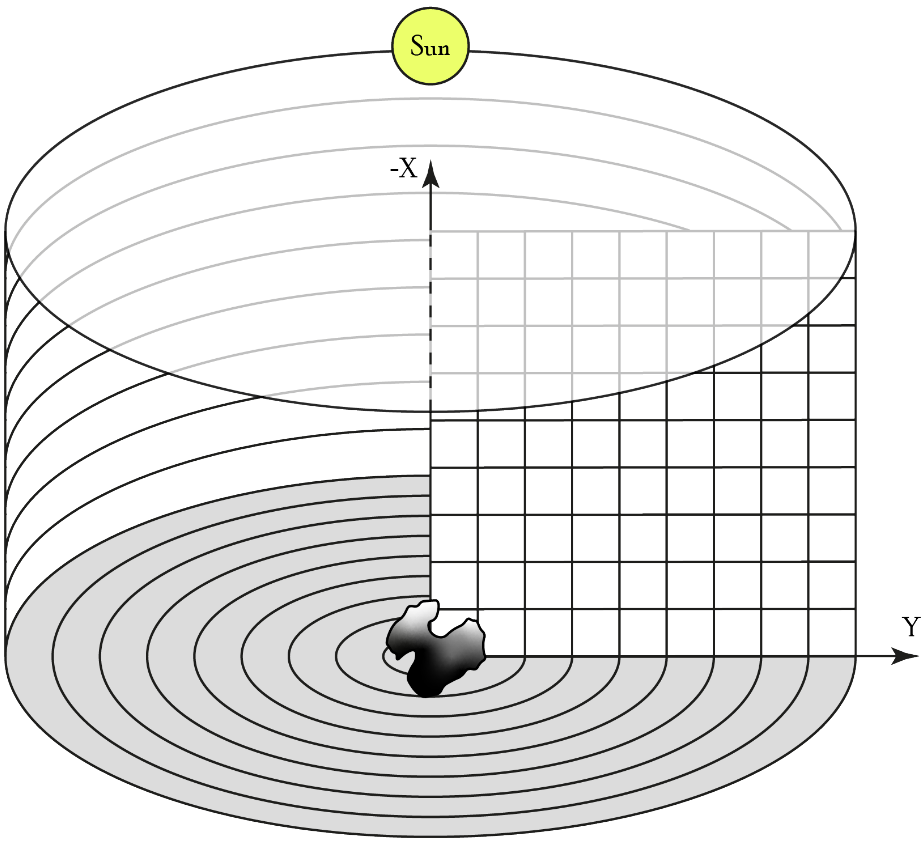

Figure 1: Cylindrical grid used for the model

The acceleration g is

$$g = \frac{GM_{\odot}}{r_h^2}\beta \tag{4}$$

with β being defined as the ratio of the solar radiation pressure force to the solar gravity and r_h being the heliocentric distance in astronomical units. For spherical particles β can be written as

$$\beta = \frac{3L_{\odot}Q_{pr}}{16\pi c GM_{\odot}\rho a}, \tag{5}$$

where $L_{\odot}$ is the solar luminosity at 1 AU, Q_{pr} is the radiation pressure efficiency and ρ is the mass density of the dust particles. The radiation pressure efficiency of a particle is determined by its scattering properties by

$$Q_{pr} = Q_{abs} + Q_{sca}(1 - < \cos p_s >), \tag{6}$$

where the absorption efficiency Q_{abs}, the scattering efficiency Q_{sca} and phase function p_s, required to calculate the asymmetry parameter $< \cos p_s >$, are calculated using Mie scattering theory. A modification of an open source Mie scattering code by Nobuhiro Moteki was used (the theoretical basis can be found in Kerker et al. [1983]). The user can choose between four different materials listed in Table 1. The scattering properties have been pre-computed for 120 size bins from 0.1 microns to 10 cm. For other particle sizes the scattering properties are interpolated.

Material	$\underline{n}$	λ	Reference
Water ice	$1.31 + 0\,i$	600 nm	-
Enstatite	$1.63 + 4.4 \cdot 10^{-4}\,i$	400 nm	Egan and Hilgeman [1975]
Astronomical silicate	$1.81 + 0.1012\,i$	600 nm	Laor and Draine [1993]
Troilite	$1.40 + 1.25\,i$	400 nm	Egan and Hilgeman [1975]

Table 1: List of materials the user can choose from.

The dust dynamics of different sized particles are different because of the size dependency of β. For this reason the dust density of each particle size bin is simulated separately. As the particle size varies over several orders of magnitude logarithmic size bins are used. The size bins are given by

$$\log_{10}(a_i) = \alpha_{max} - \frac{(\alpha_{max} - \alpha_{min}) \cdot i}{N_b}, \tag{7}$$

where $\alpha_{max} = \log_{10}(a_{max})$ and $\alpha_{min} = \log_{10}(a_{min})$ with a_{max} and a_{min} are the largest and smallest considered particle sizes and N_b is the number of size bins. We chose our time step Δt to be

$$\Delta t = \frac{L}{\iota \cdot |\vec{v}|}, \tag{8}$$

where $\iota > 1$ describes approximately the number of points sampled along the trajectory of a test particle per cell. We chose $\iota = 3$.

In a cylindrical grid as illustrated in Figure 1 the cell volume is $V = (2y + 1)\pi L^3$.

Assuming an isotropic outflow velocity there is an analytical solution for the dust density in the coma which is described by the fountain model (for a detailed explanation see Eddington [1910] and Divine et al. [1986]). If the outflow velocity is not isotropic a numerical model is used.

In our numerical model test particles are emitted for equally spaced emission angles. Because the test particles are emitted from a sphere the contribution of a test particle to the dust density needs to be scaled to the corresponding surface area of the sphere. Properly normalized this scaling factor is $k = \frac{1}{2}\pi \sin\theta$.

A potential variation in the production rate due to the rotation of the nucleus is modelled by

$$J(t) = 1 + A\cos\frac{2\pi t}{T}, \tag{9}$$

where T is the rotational period of the nucleus, t is the time of flight of the dust particle and $A \in [0,1]$ is the amplitude of the variation (the corresponding user inputs described in 2.6).

Using N test particles, the contribution of each test particle to the dust number density is

$$\Delta n_d(a) = \frac{1}{2}|\sin\theta|\frac{Q_d(a,\theta)\Delta t}{m(a)NV}J(t). \tag{10}$$

To introduce an angular dependency to the model there are several options to choose from. The options are

- Independent of emission angle:
  $A(\theta) = A_0$
- Cosine-law:
  $A(\theta) = A_0(1 + k\cos\theta)$
  k is the amplitude of cosine (see 2.5).
- Gaussian distribution:
  $A(\theta) = 7.179 \cdot e^{-\frac{16\theta^2}{\pi^2}}$
- Maxwell distribution:
  $A(\theta) = 43.489 \cdot A_0(\theta + \sqrt{2})^2 \cdot e^{-\frac{(\theta+\sqrt{2})^2}{2}}$

All functions have been normalized such that $A_0 = \frac{1}{4\pi}\int_0^{2\pi}\int_0^{\pi} A(\theta)\sin\theta d\theta d\varphi$. The emission angle dependence of the outflow velocity and the dust production rate are tied to each other for consistency.

The outflow velocity is estimated based on an approximation of the numerical solution as described by Marschall et al. [2022]. It is calculated by

$$v_d(a) = \frac{58.903\sqrt{T_N}}{1 + 0.6\sqrt{1.5/Iv}}, \tag{11}$$

with

$$Iv = 4.038 \cdot 10^{-29} \frac{Q_g}{R_N \rho_d a \sqrt{T_N}}, \tag{12}$$

where T_N is the surface temperature of the nucleus, Q_g is the gas production rate in molecules per second (in our case we assume pure H_20 gas with a molecular mass of 18 g/mol), R_N is the nucleus radius and ρ_d is the bulk dust density.

5 $Af\rho$

The quantity $Af\rho$ is used to measure the reflected solar radiation from a cometary dust coma. For a more detailed explanation of the calculation of $Af\rho$ and how it relates to the mass-loss rate of comets see Fink and Rubin [2012]. The user should note, that the relationship between $Af\rho$ and the dust production rate is not well constrained. As shown in Marschall et al. [2022], the dust production rate can be in the range of several orders of magnitude for a given $Af\rho$. The estimation of the dust production rate based on $Af\rho$ should be used with utmost care. To calculate $Af\rho$ we set $\rho = 150$ km. The filling factor f can be calculated by $f = \frac{N\sigma_{geom}}{\pi\rho^2}$, where N is the number of dust particles along the line of sight and σ_{geom} is the geometric cross-section of a single particle. Because the column integration of each grid cell is computationally expensive we only perform the integration for 4 grid cells (In grid coordinates ($\pm\rho$,0) and (0,$\pm\rho$)) scale accordingly. This approach is justified, because the quantity of $Af\rho$ assumes force-free radial outflow. By taking the sum over all size bins we can write $Af\rho$ as

$$Af\rho = 2\pi \sum_a \frac{1}{N_{cell}} N(a) a^2 Q_{sca}(a) p_s(a, \phi), \tag{13}$$

where $N_{cell} = 4$ is the number of grid cells that are used to calculate the filling factor and $N(a)$ is the total number of dust particles of a given size along the columns of all the used grid cells.

Based on the assumption of force-free radial outflow $Af\rho$ can be used to estimate the dust production rate for a given particle size distribution and the corresponding scattering properties. The relationship between the dust production rate and $Af\rho$ is

$$Af\rho = \pi \sum_a a^2 Q_{sca}(a) p_s(a, \phi) \frac{Q_d(a)}{2v_d(a)}. \tag{14}$$

To solve for the global dust production rate we can express the size dependent dust production rate as

$$Q_d(a) = Q_d \cdot \frac{a^{3-\kappa}}{\sum_i a_i^{3-\kappa}}. \tag{15}$$

$$Q_d(a) = Q_d \cdot \frac{\int_{a_1}^{a_2} \tilde{a}^{3-\kappa} d\tilde{a}}{\int_{a_{min}}^{a_{max}} \tilde{a}^{3-\kappa} d\tilde{a}}, \tag{16}$$

where a_1 and a_2 are the size limits of the corresponding size bin. TThis expression implicitly makes use of the assumption that the dust mass density is independent of the particle size.

6 Smoothing

To remove numerical artefacts a two-dimensional Gaussian smoothing with is applied. We set two parameter to control how much smoothing is applied. The parameters are the smoothing radius, which is the maximum distance of two cells to affect the smoothed value of each other and the standard deviation σ of the two-dimensional Gaussian. To achieve high efficiency and accuracy one needs to balance artefacts of the numerical model with artefacts of the smoothing. This balance depends on how many test particles pass through a given grid-cell. Because there are more test particles close to the nucleus less smoothing is required than further out in the coma. To keep the model simple but still account for a variation in the amount of smoothing that is required we divided the coma in four smoothing regions as shown in Table 2. The smoothing parameters are hard-coded based on tests comparing the numerical model to the analytical solution and can not be set by the user.

Distance to nucleus R	Smoothing radius	σ
R < 200 km	40 km	27 km
200 km <= R <2000 km	80 km	46 km
2000 km <= R < 20000 km	180 km	103 km
R >= 20000 km	400 km	200 km

Table 2: Smoothing parameters dependent on the cometocentric distance.

7 Spacecraft trajectory

To get the dust densities and total impact mass along a spacecraft trajectory the user can set a trajectory by the user inputs listed in 2.8. The user gets the dust number density, the flux and the fluence as a function of time for each size bin. In addition, the total impact mass along the trajectory is calculated.

8 Output Files

The software generates two output files for each size bin. The first file contains the grid of the dust densities and the second file contains the information related to the spacecraft trajectory. All the user inputs and all relevant quantities (e.g. the outflow velocities) are stored in two header files. Additionally to all the user inputs the header file for the dust density files contains the position of the nucleus in the grid (only the x-coordinate is given, because the y-coordinate is always 0), the calculated $Af\rho$ and a list of the particle radii, terminal outflow velocities, beta parameters, radiation pressure efficiencies, absorption efficiencies, scattering efficiencies, phase functions and size dependent production rates for each size bin. In the second header file one can find the user inputs corresponding to the trajectory, the impact mass per size bin and the total impact mass. An simple example of how the file containing the dust densities can be read with Python is shown below.

```
import numpy as np

path = "file.dat"
gridsize_x =
gridsize_y =

data = np.fromfile(path, dtype=np.double)
data = np.array(data)
dust_density_grid = data.reshape((gridsize_x, gridsize_y))
```

The second file contains the dust densities, flux and fluence along the spacecraft trajectory and the corresponding time and position of the spacecraft. The format of the file is:

```
Dust density, Flux, Fluence, R, S, time
```

Here the spacecraft coordinates are given in the cometocentric bipolar system (see Divine et al. [1986] for more details). The R-coordinate is the cometocentric distance and the S-coordinate is the same as the x-coordinate. The time is given relative to closest approach.

9 Format of the Scattering Files

The scattering information is saved in a custom format that makes it easy and efficient to read it. If one wants to use their on scattering files it should be in the same format. The files are structured as shown in Table 3.

References

N. Divine, H. Fechtig, T. I. Gombosi, M. S. Hanner, H. U. Keller, S. M. Larson, D. A. Mendis, R. L. Newburn, R. Reinhard, Z. Sekanina, and D. K. Yeomans.

1	Q_{sca}
2	Q_{abs}
3	Q_{pr}
4	$p_s(0^\circ)$
5	$p_s(1^\circ)$
$\vdots$	$\vdots$
184	$p_s(180^\circ)$

Table 3: Structure of the scattering files.

The Comet Halley Dust and Gas Environment. , 43:1, February 1986. doi: 10.1007/BF00175326.

A. S. Eddington. The Envelopes of Comet Morehouse (1908 c). *Monthly Notices of the Royal Astronomical Society*, 70(5):442–458, 03 1910. ISSN 0035-8711. doi: 10.1093/mnras/70.5.442. URL `https://doi.org/10.1093/mnras/70.5.442`.

W G Egan and T Hilgeman. Interstellar medium: Uv complex index of refraction of several candidate materials. *Astron. J., v. 80, no. 8, pp. 587-594*, 8 1975. doi: 10.1086/111782. URL `https://www.osti.gov/biblio/4156980`.

Uwe Fink and Martin Rubin. The calculation of af and mass loss rate for comets. *Icarus*, 221:721, 09 2012. doi: 10.1016/j.icarus.2012.09.001.

M. Kerker, D.-S. Wang, and C. L. Giles. Electromagnetic scattering by magnetic spheres. *J. Opt. Soc. Am.*, 73(6): 765–767, Jun 1983. doi: 10.1364/JOSA.73.000765. URL `https://opg.optica.org/abstract.cfm?URI=josa-73-6-765`.

Ari Laor and Bruce T. Draine. Spectroscopic Constraints on the Properties of Dust in Active Galactic Nuclei. , 402:441, January 1993. doi: 10.1086/172149.

Raphael Marschall, Vladimir Zakharov, Cecilia Tubiana, Michael S. P. Kelley, Carlos Corral van Damme, Colin Snodgrass, Geraint H. Jones, Stavro L. Ivanovski, Frank Postberg, Vincenzo Della Corte, Jean-Baptiste Vincent, Olga Muñoz, Fiorangela La Forgia, Anny-Chantal Levasseur-Regourd, and Comet Interceptor Team. Determining the dust environment of an unknown comet for a spacecraft flyby: The case of ESA's Comet Interceptor mission. , 666:A151, October 2022. doi: 10.1051/0004-6361/202243648.

V.V. Zakharov, A.V. Rodionov, M. Fulle, S.L. Ivanovski, N.Y. Bykov, V. Della Corte, and A. Rotundi. Practical relations for assessments of the gas coma parameters. *Icarus*, 354:114091, 2021a. ISSN 0019-1035. doi: https://doi.org/10.1016/j.icarus.2020.114091. URL `https://www.sciencedirect.com/science/article/pii/S0019103520304371`.

V.V. Zakharov, A. Rotundi, V. Della Corte, M. Fulle, S.L. Ivanovski, A.V. Rodionov, and N.Y. Bykov. On the similarity of dust flows in the inner coma of comets. *Icarus*, 364:114476, 2021b. ISSN 0019-1035. doi: https://doi.org/10.1016/j.icarus.2021.114476. URL https://www.sciencedirect.com/science/article/pii/S0019103521001561.