Infrared emissivity of icy surfaces

Sensitivity to regolith properties and water-ice contaminants

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ABSTRACT

Context. Most analyses of the infrared emission of Saturn’s rings and icy satellites have considered pure water ice as the constituent of regolith and particle surfaces. Visual and near-infrared observations have shown, however, that darkening and reddening contaminants are present at a fraction level of a few percent. In the spectral domain 10–2000 cm$^{-1}$, water ice becomes transparent in a few windows, which in particular causes the roll-off of emissivity of icy surfaces that is observed below 50 cm$^{-1}$. Their emissivity there may be affected by these contaminants.

Aims. We present a quantitative global sensitivity analysis of a hybrid Mie-Hapke model to evaluate the influence of regolith properties and contaminant fraction on the infrared emissivity of icy rings or moons over this spectral range.

Methods. A hybrid Mie–Hapke model of the hemispherical emissivity $\varepsilon(\omega)$ was made, including various diffraction correction and mixing types with tholins or amorphous carbon grains, or grain size distributions and some anisotropy in emission. A Sobol global sensitivity analysis provided quantitative levels of importance for these factors versus wave number $\omega$.

Results. Given the a priori uncertainties, the most important factor acting on $\varepsilon(\omega)$ remains the size distribution of regolith grains and the average anisotropy factor $\xi$. For $\omega > 50$ cm$^{-1}$, $\xi$, the power-law index $p$ and the minimum $a_{\text{min}}$ of the size distribution are most influential. In windows of water-ice transparency (10–50, 300–600, and 900–1300 cm$^{-1}$), the emissivity is also sensitive, but to a lesser extent, to the maximum grain size $a_{\text{max}}$ and the fraction $f$ of contaminants, if mixed at the molecular level.

Conclusions. This model provides a self-consistent tool for interpreting multi-modal observations of the thermal emission from icy surfaces. It also offers interesting insights into recent mid-infrared observations of Saturn’s rings and Jupiter’s moon Ganymede by the JWST-MIRI instrument.

Key words. radiative transfer – scattering – planets and satellites: rings – planets and satellites: surfaces

1. Introduction

While the Voyager Infrared Interferometer Spectrometer and Radiometer (IRIS) paved the way for thermal exploration of the outer Solar System in the spectral range 1.4–170 μm, the Cassini Composite Infrared Spectrometer (CIRS) opened up a new field for studying the thermal properties of Saturn’s rings and the surface of icy moons through its still unique broad spectral coverage from 7 to 1000 μm, which made it possible to observe most of their spectrum and wavelength of maximum thermal emission (Flasar et al. 2004).

The brightness temperature of Saturn’s rings has been known for a long time to dramatically decrease by tens of kelvins in between 20 μm and millimetre wavelengths (Esposito et al. 1984). The focal plane FP1 of CIRS was the first to fully cover the spectral region 16.7–1000 μm (10–600 cm$^{-1}$) and accurately described this decrease for wave numbers $\omega_n < 50$ cm$^{-1}$, identified as a roll-off in emissivity (Flasar et al. 2004; Spilker et al. 2005). It was indeed expected to result from the increasing transparency of water ice in this range and to depend on the size distribution of ring particles or of regolith grains with which they might be covered. Assuming ring particles are made of pure water ice, Spilker et al. (2005) studied the spectra of the lit side of the three main rings, A, B, and C, acquired in 2004, early in the mission. All exhibited similar roll-offs, and a simple model of emissivity, assuming regolith-free ring particles following a power-law size distribution, was shown to reasonably reproduce the observed spectra, and no exact adjustment was proposed. Morishima et al. (2012) analysed all FP1 spectra obtained with the lowest spectral resolution (15.5 cm$^{-1}$) before the equinox in 2010 and showing ring temperatures above 70 K in order to reject noisier spectra. Inverting a diffraction-corrected hybrid Mie-Hapke emissivity model of ring particles covered with a regolith of pure water-ice grains with these data, they found the emissivity to depend on temperature, most probably reflecting that grains of various sizes have different temperatures depending on illumination and viewing angles. The size distribution of regolith grains was found to be broad, ranging from 1 μm to 1–10 cm, with a power-law index of $p \sim 3$, almost similar and independent of temperature in the two main thickest A and B rings.

CIRS observations of Saturn’s icy moons have also mostly been analysed assuming that their surface emissivity is equal or close to unity. The aim was then to determine the space-time distribution of surface temperatures to derive maps of the regolith thermal inertia. The discovery of thermal anomalies on the surface of icy moons has certainly made an essential contribution to understanding the differential effects of space weathering between their leading and trailing hemispheres (Howett et al. 2011, 2012, 2018; Paranicas et al. 2014; Nordheim et al. 2017). Carvano et al. (2007) provided the only but qualitative study of the emissivity of Phoebe, Iapetus, Enceladus, Tethys, and

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Hyperion in the range 50–400 cm\(^{-1}\), that is, above the roll-off region. The lack of spectral signatures in the emissivity of these moons in the dataset available at this early time in the mission was interpreted as essentially due to the very high porosity (>95%) of clumps of small grains that may cover the surface. In the case of Tethys, an intimate mixture of water ice with amorphous carbon (AmC) could also suppress spectral features if ice grains are larger than contaminant grains, or if the fraction of AmC were at least 75%. Nor did Howett et al. (2016) detect any spectral signature in Rhea’s spectra captured in 2013 and 2015 flybys in a similar spectral range.

It has long been known that crystalline water ice is the main component of Saturn’s rings and the surfaces of the icy moons. Visible and near-infrared (NIR) ring spectra could be satisfactorily reproduced by a mixture of regolith grains with typical sizes from tens of micrometres to millimetres, the water ice being slightly contaminated (a few percent) by still-debated tholins (Th) and AmC or silicate inclusions to reproduce observed spectral reddening and darkening, respectively (Poulet et al. 2003; Cuzzi et al. 2018). Low absorption by CO\(_2\) has also been observed for some of these moons (Clark et al. 2008; Filacchione et al. 2022).

Finally, the analysis of the huge CIRS dataset on Saturn’s rings and moons is still incomplete, both in terms of seasonal effects over the 13 yr that the mission lasted and on spectral behaviours, in particular, that of emissivities (Spilker et al. 2018; Howett et al. 2018). It is still not known how much the emissivity varies in the spectral range of FP1 due to contaminants, in particular, in the spectral regions where water ice becomes transparent, and how this may modify the observed thermal emission and the retrieved temperatures. Other instruments have taken over from Earth orbit to observe the thermal emission from icy worlds in spectral domains related to that of CIRS. The Atacama Large Millimeter/submillimeter Array (ALMA) within its receiver bands 7 to 10 can explore the sub-millimeter range down to 320 \(\mu\)m (950 GHz), that is, in between 10 and 32 \(\mu\)m, and the Mid-Infrared Instrument (MIRI) of the James Webb Space Telescope (JWST) can probe their thermal emission in between 4.9 and 28 \(\mu\)m (357–2040 cm\(^{-1}\)). Upcoming space instruments will also target the Galilean satellites, for instance the Submillimetre Wave Instrument (SWI) on board the Jupiter ICy moons Explorer (JUICE) around 520 \(\mu\)m (17.7–21 cm\(^{-1}\)) and 250 \(\mu\)m (36–42 cm\(^{-1}\)), or the Europa Thermal Emission Imaging System (E-THEMIS) on board Europa-Clipper in the range 7–80 \(\mu\)m (125–1429 cm\(^{-1}\); Christensen et al. 2024). These instruments will therefore also explore these spectral regions where water ice can be transparent and the emissivity is sensitive to both the presence of contaminants and the size distribution of the regolith grains.

In the present study, we estimate quantitatively how much the hemispherical emissivity of a regolith covering ring particles or surface of moons is sensitive, in the wavelength range 5–1000 \(\mu\)m (10–2000 cm\(^{-1}\)), to the size distribution of grains, the type of contaminant, its fraction, and how it is mixed with water ice. The influence of temperature on the optical properties of water ice is also considered. In section 2, a hybrid Mie-Hapke model for regolith hemispherical emissivity is proposed that includes these factors together with the diffraction correction of Mie calculations and an asymmetry factor of the regolith. A global sensitivity analysis yields quantitative estimates of the importance of these factors, which may be used to reduce their number depending on the spectral range of the data on which the model is inverted. Its results are presented and discussed in sect. 3.

2. Mie-Hapke hybrid model

Mie-Hapke hybrid models for regoliths couple the formalism developed by Hapke (2012) to estimate their reflectance and emittance based on the scattering and absorption efficiencies of spherical grains provided by the Mie theory. These models require knowledge of the optical properties such as the complex refractive index or dielectric constant of the materials involved and must include a correction for the independent scattering hypothesis of Mie’s theory to be suitable for the closely packed medium of regoliths.

2.1. Composition of grains

Within Saturn’s magnetosphere, which is bombarded by plasma and highly energetic particles, the surface chemistry of rings and icy moons is almost certainly complex. Radiolysis and photolysis may indeed lead to a mixture that is rich in various icy components, such as nitrogen oxides (Delitsky & Lane 2002). We limit ourselves here to a mixture of water ice and contaminants capable of reddening and darkening the spectrum, such as the proposed Th and AmC. A more complete sensitivity analysis would require refractive indices of complex icy mixtures on the wide spectral range of FP1, which are not available.

2.1.1. Water ice

Several authors have produced measurements of the complex refractive index \(n = n_\text{i} + in_\text{r}\) of water ice at low temperatures between 10 and 140 K, very few of which cover the full spectral range 10–2000 cm\(^{-1}\) (Fig. 1). In mid- and far-infrared domains, the dominant absorption mechanisms are bending mode at 6 \(\mu\)m (1666 cm\(^{-1}\)), molecular hindered rotation at 12 \(\mu\)m (833 cm\(^{-1}\)), and lattice vibrations at 45 and 65 \(\mu\)m (222 and 154 cm\(^{-1}\)), which translate into a high imaginary part \(n_\text{r}\) of the refractive index (Fig. 1 bottom). In these specific ranges, the real part \(n_\text{i}\) oscillates between 1 and 2. At sub-millimetre wavelengths, about the roll-off of \(n_\text{i}\) at (below 50 \(\mu\)m), \(n_\text{i}\) is about constant and ice becomes transparent (Warren & Brandt 2008; Warren 2019, Fig. 1 top). The optical properties depend on the temperature and phase of the ice, either crystalline (Ih) or amorphous (Am), the latter irreversibly transforming into the former at temperatures between 125 and 150 K (e.g. Jenniskens & Blake 1996).

The optical constants for crystalline water ice that have long been the most frequently used result from a compilation of measurements by Warren (1984), covering the entire range from UV to mm, and updated for a temperature of 266 K (Warren & Brandt 2008), that is, well above the temperatures of interest here (Fig. 1). Hudgins et al. (1993) produced measurements at 10, 100, and 140 K for water ice from 50 to 4000 cm\(^{-1}\) and reported an apparent phase transition between 100 and 140 K. They made available additional data at intermediate temperatures (40, 80 and 120 K) from 500 to 4000 cm\(^{-1}\). Some divergence in the range 400–600 cm\(^{-1}\) can be seen between these data that corresponds to a change in detectors and a knitting that operates for 10, 100, and 140K at the junction of spectra recorded both in the mid- and far-infrared. The estimates above 455 cm\(^{-1}\) for amorphous ice by Mastrapa et al. (2009) are consistent with Hudgins et al. (1993) for comparable temperatures, but remain of marginal spectral coverage. In the most absorptive region (80–300 cm\(^{-1}\)), the optical constants by Curtis et al. (2005) are comparable to those of Hudgins et al. (1993). Elsewhere, they differ significantly. \(n_\text{i}\) estimated by Hudgins et al. (1993) appears to be either smaller or larger in between 300 and 600 cm\(^{-1}\), and noisier below...
Fig. 1. Complex refractive index of water ice, either crystalline (Ih) or amorphous (Am), as proposed by various authors at different temperatures. (top) Real part $n_r$ and (bottom) imaginary part $n_k$. Legends correspond to authors $T$ (K) ice phase with authors C05 (Curtis et al. 2005), M83 (Mishima et al. 1983), H93 (Hudgins et al. 1993), M09 (Mastrapa et al. 2009), and W08 (Warren & Brandt 2008).

100 cm$^{-1}$. They are consistent above 500 cm$^{-1}$ and at temperatures of 40, 80, and 120 K. For both sets of measurements, $n_k$ always appears to increase slightly with decreasing temperature.

Mätzler et al. (2006) summarized experimental and theoretical work on the dielectric properties of Ih ice between 1 MHz and 1 THz ($\geq 300$ µm, $\leq 33$ cm$^{-1}$), in particular, that of Hufford (1991). The latter formulated the frequency and temperature variations of the dielectric constant from measurements and the theoretical work by Mishima et al. (1983) for temperatures in between 80 and 202 K. We have used this synthesis to deduce the dependence of the indices $n_r$ and $n_k$ on wave number between 10 and 33 cm$^{-1}$ and temperature. $n_k$ can be considered as constant with temperature, while $n_r$ (Fig. 1, bottom) is significantly impacted by temperature. This same formalism at millimetre wavelengths was included by de Kleer et al. (2021) in their thermal model to analyse ALMA observations of Ganymede. The emissivity was calculated from the complex dielectric constant, which depends on porosity and on a meteoritic dust fraction of 20% mixed with ice at the molecular scale, and on temperature. It was found to be $0.78 \pm 0.04$ at 343 GHz (0.87 mm).

As the crystalline phase is observed at the very surface, we chose, just like Morishima et al. (2012), to merge the Curtis et al. (2005) data at 136 K to the sub-millimetre model as described above, through a cubic-spline extrapolation in between 33 and 50 cm$^{-1}$. The sub-millimetre model for $n_k(w, T_0)$ can be calculated for any ice temperature $T_0$ (Fig. 2, bottom). Between 566 and 2000 cm$^{-1}$, Hudgins et al. (1993) data at 120 K for Am ice phase were chosen, after being smoothed to remove some noise in the transparency window near 9.5 µm (1050 cm$^{-1}$). These data are indeed very close to the Curtis et al. (2005) measurements at 136 K for the Ih phase at 530 cm$^{-1}$, and they are almost identical above 700 cm$^{-1}$ to the Ih phase at 140K. This merging constitutes the Ih-$T_0$ optical properties used in the following (Fig. 2). This illustrates the difficulty of finding a complex refractive index for the Ih ice phase versus temperature over the full range 10–2000 cm$^{-1}$ in order to conduct a sensitivity analysis of emissivity versus temperature. The sub-millimetre range, about the roll-off ($\leq 33$ cm$^{-1}$), is the only range where this can be studied because it has been modelled. Therefore, no temperature dependence of optical properties was considered above 33 cm$^{-1}$.

2.1.2. Contaminants

Poulet et al. (2003) adjusted a B ring spectrum in the NIR domain with 10-to-1300 µm sized grains of water ice with 0.74% intra-particle Th inclusions mixed with 2.3% of 10 µm sized AmC grains. Filacchione et al. (2012) also selected an intra-particle mixture of ice with a Th fraction lower than 0.5% to model NIR spectra of Mimas, Enceladus, Dione, Tethys, and
Rhea obtained by the Visual and Infrared Mapping Spectrometer onboard Cassini, which they combined with an additional intimate (volumic) mixture of AmC grains to reproduce the reddening and darkening of their spectrum. The NIR spectra of Mimas yield a satisfactory fit with the Hapke theory with 0.1% of Th and 2% of AmC inclusions (Filacchione et al. 2012). Potential contaminants such as these were therefore chosen for this study.

The optical constants of AmC were taken from Preibisch et al. (1993). They are consistent with many other estimates (Zubko et al. 1996). The optical constants for Th originate from Khare et al. (1984) as they remain those that cover our spectral range of interest (Brassé et al. 2015). Both contaminants exhibit significantly different optical properties, but no significant spectral features in the region of interest except for Th at about 6 μm (1666 cm⁻¹; Fig. 2). They are more absorbent than water ice. The effect of mixing water ice at the molecular scale with 1% of Th increases the absorption, but does not alter the real part of the refractive index. The effect is mostly significant in the region of the roll-off and is slightly lower than the mixing effect with 3% of AmC (Fig. 2). The sensitivity to the contaminant fraction will have to be observed in areas in which water ice is relatively transparent, that is to say, in the ranges 10–50 cm⁻¹, 300–600 cm⁻¹, and 900–1300 cm⁻¹. Other types of mixtures will also be considered to quantify the sensitivity of emissivity to the fraction of contaminants (Sect. 2.4).

2.2. Hemispherical emissivity of a regolith

Hapke (2012) proposed the model for isotropic multiple scattering approximation (IMSA) for the hemispherical emissivity $\varepsilon_h(w_n, a)$ of a regolith of grains with size $a$. In case of isotropic scattering, it is written at wave number $w_n$ as

$$
\varepsilon_h(w_n, a) \sim \frac{2\gamma(w_n, a)}{1 + \gamma(w_n, a)} \left(1 + \frac{r_0(w_n, a)}{6}\right),
$$

where

$$
r_0(w_n, a) = 1 - \gamma(w_n, a),
$$

and

$$
\gamma(w_n, a) = \sqrt{1 - \omega_0(w_n, a)}
$$
as a function of the single-scattering albedo of the grain $\omega_0(w_n, a)$, provided possibly by Mie’s theory. The hemispherical reflectance is approximated as follows:

$$
r_x(w_n, a) \sim 1 - \varepsilon_x(w_n, a) - r_0(w_n, a) \left(1 - \frac{\gamma(w_n, a)}{3(1 + \gamma(w_n, a))}\right).
$$

2.3. Diffraction-corrected Mie scattering albedos

The estimation of single-scattering albedos $\omega_0(w_n, a)$ by Mie’s theory includes the diffraction pattern: Grains larger than the wavelength (with a size parameter $x = 2\pi a/\lambda$ greater than a few units) have an important asymmetry factor $\xi_a = <\cos \theta> \sim 1$, a single-scattering albedo $\omega_0(w_n, a) \sim 0.5$ because their scattering and extinction efficiencies are $Q_s \sim 1$ and $Q_m \sim 2$, respectively (Fig. 3, top). Within a close-packed medium, diffraction peaks of grains interfere, so that their scattering efficiency and the asymmetry factor of their phase function should differ from Mie’s predictions. According to Wald (1994), independent scattering in regolith may be approached for transparent large particles when the scattering lobe and diffraction peak coincide. He proposed a diffraction-corrected single-scattering albedo, which is valid for the mid-infrared domain (2–14 μm) and absorbing snow particles much larger than the wavelength, that is, $\geq 50$μm in their case. García-Santos et al. (2016) reviewed efforts made in Earth science to validate compactness correction methods in emissivity models of snow and mineral surfaces in the spectral range 8–14 μm. The Mie-Hapke hybrid model corrected for diffraction with various methods (static structure factor; Wald (1994) and delta-Eddington (see below) corrections) was tested on emissivity measurements of quartz and gypsum samples, with grain sizes ranging from 15-to-277 μm, and against another model. The Hapke model appeared to perform best with the delta-Eddington correction for sizes $a > 75$ μm. For smaller grain sizes, the correction according to Wald (1994) gave better results.

Carvano et al. (2007) chose not to include diffraction correction in their model, following results from Moersch & Christensen (1995) established on quartz regoliths in the spectral range of 400–1400 cm⁻¹ (7.25 μm) with grain sizes smaller than 250 μm. Morishima et al. (2012) chose the delta-Eddington approximation ($\delta$-Edd) proposed by Joseph et al. (1976) to estimate the single-scattering albedo $\omega_{0,\delta}$ after diffraction correction,

$$
\omega_{0,\delta}(w_n, a) = \frac{1 - \xi_a^2}{1 - \xi_a^2 - \omega_0} \omega_0
$$

where $\xi_a \equiv \xi(w_n, a)$ is the asymmetry factor, and $\omega_0 \equiv \omega_{\text{Mic}}(w_n, a)$ for a grain of size $a$ as calculated with Mie’s theory. They mentioned that their final results might depend on the diffraction correction method.

For this study, the equivalent slab approximation (esa) as developed by Hapke (2012) is proposed for comparison. It estimates for high $x$ values the diffraction-corrected single-scattering albedo $\omega_{0,esa}$ by calculating the non-diffacted component of the scattered light $q_s = Q_s - Q_a$ and by assuming the extinction efficiency $Q_a = 1$. This approximation was implemented here as the esa diffraction correction, so that

$$
\omega_{0,esa}(w_n, x \geq x_0) \equiv \frac{Q_s}{Q_e} \text{ and } \omega_{\text{Mic}}(w_n, x < x_0) \equiv \omega_{\text{Mic}}(w_n, a),
$$

where $x_0 = 2πa/λ_0$ corresponds to the minimum wave number $w_0$ at which $\omega_{0,esa} < \omega_{\text{Mic}}$ with $\omega_{\text{Mic}} > 0.45$ (Fig. 3, top). Mie calculations were performed with the PyMieScatt Python library (Smulkin et al. 2018). The albedos and hemispherical emissivities were calculated for 41 sizes ranging between 1 μm and 5 cm (Fig. 3). Above this size, $\varepsilon_h(w_n, a)$ is nearly constant in wave number and size. For micrometre-sized grains, all models provide the same results as long as the size parameter $x < 0.2$, corresponding to the Rayleigh regime. For $a = 10$ μm, the diffraction correction methods differ significantly above 300 cm⁻¹ as water ice becomes less absorbing and $x$ becomes large (Fig. 3, bottom and Fig. 2). Above $a = 100$ μm, the effects of diffraction corrections are clearly visible, with $\omega_0$ well below 0.5 for the high values of $x$, above 100 cm⁻¹ ($x$ scales with $w_n$).

As the grain size grows, this is even truer at lower wave numbers. The roll-off in emissivity is well reproduced at $w_n \sim 50$ cm⁻¹ for grain sizes ranging from $a = 100$ μm to a few millimetres (Fig. 3).
Fig. 3. Single-scattering albedo and hemispherical emissivity as a function of grain size and wave number or wavelength. (top) Single-scattering albedo $\omega(w_n, a)$ of a grain with size $a$ (bottom) hemispherical emissivity $\varepsilon_h(w_n, a)$ of regolith covered with these grains made of pure crystalline water ice Ih90. Calculations with the Mie theory (dotted line) or after diffraction corrections such as delta-Eddington (dash-dotted line) or equivalent slab approximation (solid line) are displayed. (Left) $10$–$700$ cm$^{-1}$ range and (right) $5$–$14.3$ cm$^{-1}$ range (or $700$–$2000$ cm$^{-1}$).

2.4. Mixing with contaminants and the effect of the size distribution

Filacchione et al. (2012) studied the absorption bands of water ice at 1.5 and 2.0 μm in spectra of the B ring, from which they derived grain sizes ranging between 40 μm and 0.3-to-0.6 cm, assuming pure water ice. Poulet et al. (2003) adjusted a B ring spectrum with 10-to-1300 μm sized grains of water ice with intra-particle inclusions of 0.7% of Th intimately mixed with 2% of 10 μm sized AmC grains. Grain sizes of 1 μm to 5 cm were therefore considered hereafter together with mono- or poly-dispersed power-law size distributions. As often in NIR reflectance spectral modelling, the effect of any size distribution has been little explored for icy bodies in the thermal infrared, except for Morishima et al. (2012).

Three different types of mixture of water ice with contaminants were considered here: at the molecular level, the intra-particle mixture, secondly as an aerial mixing, and finally as an intimate (volumic) mixture with the same (distribution of the) grain size. The resulting emissivity for an intra-particle mixture was calculated by coupling the optical constants of water ice and the contaminants at a volume fraction $f$ with the Maxwell-Garnett effective medium theory and following Eqs. (1)–(3). The hemispherical emissivity of an aerial mixture of a contaminant covering a fractional area $f$ within the field of view reads

$$\varepsilon_h(w_n, a_i, a_p) = (1-f)\varepsilon_{h,i}(w_n, a_i) + f\varepsilon_{h,p}(w_n, a_p),$$

where $\varepsilon_{h,i}(w_n)$ and $\varepsilon_{h,p}(w_n)$ are the hemispherical emissivities of the icy and contaminant areas, respectively, either made of the same size or not. In the case of an intimate mixture with a volume fraction $f$ and scattering or extinction efficiencies $Q_{e,i}$, $Q_{s,i}$, or $Q_{e,p}$, and $Q_{s,p}$ for the icy or the contaminant populations, respectively, the total single-scattering albedo is

$$\omega_h(w_n, a_i, a_p) = \frac{(1-f)\pi a_i^2 Q_{e,i}(w_n, a_i) + f\pi a_p^2 Q_{e,p}(w_n, a_p)}{(1-f)\pi a_i^2 Q_{s,i}(w_n, a_i) + f\pi a_p^2 Q_{s,p}(w_n, a_p)}$$

where $a_i$ and $a_p$ are their grain sizes, respectively.

Figure 4 displays the hemispherical emissivities of regolith with grain sizes ranging over three orders of magnitudes as a function of contaminant fraction and mixing type when $a_i = a_p = a$ in the case of esa diffraction correction. The results are comparable with the $\delta$-Edd correction. Grains of 10 micrometres have a high emissivity below 300 cm$^{-1}$ (Fig. 4, top left). Above this, $\varepsilon_h$ decreases and appears to be mainly dependent on the AmC fraction of 5% when intra-mixed or, to a lower extent, if intimately mixed (vol). It is almost insensitive to contaminants for an aerial mixing at this fraction level. The impact of 1% Th mixing is negligible. For grains that are ten times as large (100 μm, Fig. 4, middle left), the roll-off in emissivity below 50 cm$^{-1}$
shows significant variation with mixing type (intra or vol) in the case of AmC at 5% fraction. Aerial mixing remains of low impact, just like any type with 1% Th. AmC remains influential above 300 cm\(^{-1}\). For larger grains (Fig. 4, bottom left), the impact of contaminants is restricted to the roll-off region and the 9.5 µm transparency (Fig. 4, bottom right) only for a few percent of intra-mixed contaminants. The hemispherical emissivity is then constant above 40 or 50 cm\(^{-1}\) (geometrical optics regime). The contamination by a maximum fraction of 1% Th appears to be comparatively negligible for the hemispherical emissivity of water ice in the roll-off region.

For a power-law size distribution of grains following \(n(a) da = n_0 a^{-p} da\) with minimum and maximum sizes \(a_{\text{min}}\) and \(a_{\text{max}}\), the scattering albedo of the size distribution reads

\[
\omega_{\text{sca,al}}(w_n) = \frac{\int_{a_{\text{min}}}^{a_{\text{max}}} \pi a^{2-p} Q_{\text{sca}}(w_n, a) da}{\int_{a_{\text{min}}}^{a_{\text{max}}} \pi a^{2-p} Q_{\text{ext}}(w_n, a) da} = \frac{Q_{\text{sca,al}}(w_n)}{Q_{\text{ext,al}}(w_n)}. \tag{9}
\]

Figure 5 illustrates the dependence of \(\epsilon_h(w_n)\) on \(p\), \(a_{\text{min}}\), and \(a_{\text{max}}\) in the case of an intra-mixture. For a steep slope \(p=3\), \(\epsilon_h(w_n)\) is more sensitive to the minimum grain size \(a_{\text{min}}\) than to \(a_{\text{max}}\) in the roll-off region (Fig. 5, left). Other transparency regions (300–600 cm\(^{-1}\) and 7–11 µm) are equally sensitive to both extreme sizes. For \(p = 2\), \(\epsilon_h(w_n, a)\) is insensitive to sub-millimetre \(a_{\text{min}}\) sizes, but strongly affected by the choice of maximum size \(a_{\text{max}}\) within the roll-off region, where this size is comparable to the wavelength. In the case of δ-Edd diffraction correction, the impact of \(a_{\text{max}}\) is higher in the roll-off region as the emissivity variation with large grain sizes is higher in this case (Fig. 3). Finally, in the case of an intimate mixture, the scattering albedo is defined according to

\[
\omega_{\text{sca,al}}(w_n) = \frac{(1-f)Q_{\text{sca,al}}(w_n) + f Q_{\text{sca,al}}(w_n)}{(1-f)Q_{\text{ext,al}}(w_n) + f Q_{\text{ext,al}}(w_n)}, \tag{10}
\]

2.5. Average asymmetry factor

Finally, in the case of anisotropic and multiple scattering within the regolith and for hemispherically averaged quantities, the solution of radiative transfer equations can be approximated by applying the similarity principle, which consists of replacing \(\omega_0\) by

\[
\omega'_\text{ext}(w_n) = \frac{1 - \xi}{1 - \xi \omega_0(w_n)} - \omega_0(w_n), \tag{11}
\]

where \(\xi\) is the regolith average asymmetry factor (Hapke 2012). The hemispherical emissivity \(\epsilon'_\text{h}(w_n)\) can be deduced with equations Eqs. (1)–(3) and Eq. (11). If \(\xi < 0\), the regolith is more retro-diffusive and therefore less emissive, and if \(\xi > 0\), \(\epsilon'_\text{h}(w_n)\) will increase compared to the isotropic case (Fig. 6). With \(\xi\) varying from –0.6 to 0.6, \(\epsilon'_\text{h}(w_n)\) may vary by about ±0.1–0.2.

3. Global sensitivity analysis and discussion

Given the many factors of the model (Table 1), their a priori uncertainties, and their potential interactions on the value of \(\epsilon'_\text{h}(w_n)\), a global sensitivity analysis was carried out to quantitatively determine their importance at any wave number with a view to reducing their number (and simplify the model) before the data analysis. This analysis was conducted with the Sobol view to reducing their number (and simplify the model) before the data analysis.
Fig. 5. Hemispherical emissivity $\varepsilon_h(w_n,a)$ as a function of $p=2$ (dashed line) or $p=3$ (solid line) and (top) $a_{\text{min}}$ or (bottom) $a_{\text{max}}$. The grain composition is water ice Ih90, intra-mixed with 5% AmC. esa diffraction correction is assumed. (Left) 10–700 cm$^{-1}$ range and (right) 5–14.3 µm range (700–2000 cm$^{-1}$).

Fig. 6. Hemispherical emissivity $\varepsilon^*_h(w_n)$ as a function of average asymmetry factor $\xi$ for a size distribution of gains with $a_{\text{min}} = 1$ µm , $a_{\text{max}} = 5$ mm, and $p=2$ (dashed line) or $p=3$ (solid line). The grain composition is water ice Ih90 with intra-mixing of 5% AmC. esa diffraction correction is used.

Method (Sobol 2001; Saltelli et al. 2010) of the SAlib library$^1$. It quantifies how the total variance on $\varepsilon^*_h(w_n)$ (the model output) at a given wave number can be apportioned to input factors uncertainties. It provides two coefficients for a factor $X_i$, the first-order sensitivity $S_i(w_n)$, and the total effect sensitivity $ST_i(w_n)$. $S_i(w_n)$ scales the expected relative reduction of the output variance that would be achieved if the factor were fixed. $ST_i(w_n)$ is the expected relative variance of $\varepsilon^*_h(w_n)$ that would be left if all factors but $X_i$ could be fixed. $ST_i(w_n) \sim 0$ is a necessary and sufficient condition for factor to be non-influential while $S_i(w_n) \sim 0$ is not. In the case of non-linear models, the factors may have small main effects and large interactions with other factors, so that $S_i(w_n)$ is small and $ST_i(w_n)$ is large. This was observed in some cases, in particular, for models assuming a single grain size. In order to decide which factors are ultimately relatively insignificant for the model we present, the total sensitivity coefficient $ST_i(w_n)$ was therefore chosen.

3.1. Sensitivity versus mixing type and diffraction correction

Figure 7 displays the total effects in the case of intra-mixture with an AmC contaminant. In the case of a mono-dispersed size distribution (Fig. 7, top), the grain size $a$ is the most important factor, except in the region of strong ice absorption, where the average asymmetry factor $\xi$ has a similar impact. Both fraction $f$ and temperature $T_0$ are negligible, $<0.05$ in the roll-off region for $f$ and $<0.001$ for $T_0$. $f$ might be conserved if noise is limited in the FIR or in transparency windows. The impact of $\xi$ is more extended spectrally if diffraction is not corrected for (Mie). In the case of a power-law size distribution (Fig. 7, bottom), $T_0$ remains of the lowest and negligible importance. In the roll-off region, all factors $a_{\text{min}}$, $a_{\text{max}}$, $p$, $\xi$, and $f$ have comparable influence. Above 50 cm$^{-1}$, the variance is mainly sensitive to $\xi$ in the ice absorption regions and to $p$ and $a_{\text{min}}$ elsewhere. The analysis shows that $p$ and $a_{\text{min}}$ interact above 50 cm$^{-1}$ as their $S_i(w_n)$ are twice as low as their $ST_i(w_n)$. If the a priori knowledge of the factors are those set out, $T_0$ can be dropped (i.e. fixed to some value). In the case of a power-law size distribution, all factors are influential in some specific spectral regions and should be conserved if the

Table 1. Model factors and hyper-parameters with their a priori range of uncertainty or discrete set of values.

<table>
<thead>
<tr>
<th>Factor $X_i$</th>
<th>Symbol</th>
<th>[range], step</th>
</tr>
</thead>
<tbody>
<tr>
<td>Far-infrared temperature (K)</td>
<td>$T_0$</td>
<td>[50, 90], 10</td>
</tr>
<tr>
<td>Mixing fraction (%)</td>
<td>$f$</td>
<td>[1, 7], 1</td>
</tr>
<tr>
<td>Average asymmetry factor</td>
<td>$\xi$</td>
<td>[-0.6, 0.6], any</td>
</tr>
<tr>
<td>Size distribution $n(a)da = n_0 a^{-p}da$</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Power-law index</td>
<td>$p$</td>
<td>[1.4, 3.4], any</td>
</tr>
<tr>
<td>Minimum size ($\mu$m)</td>
<td>$a_{\text{min}}$</td>
<td>[1, 1000], 9 sizes/decade</td>
</tr>
<tr>
<td>Maximum size (mm)</td>
<td>$a_{\text{max}}$</td>
<td>[1, 50], 9 sizes/decade</td>
</tr>
<tr>
<td>Single size for intra or aerial, vol mixtures</td>
<td>$a, {a_i, a_p}$</td>
<td>[1 $\mu$m, 5 cm], 9 sizes per decade</td>
</tr>
<tr>
<td>Hyper-parameters</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Main material</td>
<td>Ih</td>
<td>crystalline water ice</td>
</tr>
<tr>
<td>Contaminants</td>
<td>AmC, Th</td>
<td>amorphous carbon, tholins</td>
</tr>
<tr>
<td>Mixing type</td>
<td>intra/aerial/vol</td>
<td>Intra-particle, aerial, intimate</td>
</tr>
<tr>
<td>Diffraction correction</td>
<td>None/$\delta$-Edd/esa</td>
<td>Mie, $\delta$-Eddington, equivalent slab approximation</td>
</tr>
</tbody>
</table>

Fig. 7. Total effect sensitivities $S T_i$ in the case of an intra-mixture with AmC contaminant and Mie (dotted line), $\delta$-Edd (dash-dotted line) or esa (solid line) diffraction correction methods and (top) mono-dispersed (bottom) power-law size distributions. The dashed line marks the 3% level.

Fig. 8. Total effect sensitivities $S T_i$ in the case of contamination with an AmC mixture, either intra (dotted line), aerial (dashed line), or volumic (solid line) mixing for (top) mono-dispersed (bottom) power-law size distributions. The esa diffraction correction is used here.

Data inversion is conducted over the whole range. Some may be dropped (fixed), depending on the region of fit. The results do not change in the case of Th contamination, but in the case of a sub-percent fraction, the impact of $f$ will be even smaller in the roll-off region. The behaviour changes little between the esa or $\delta$-Edd diffraction correction methods, as expected.

These same coefficients are shown versus type of mixing in Fig. 8. In the case of a single grain size (Fig. 8 top), the size $a$ is dominant on the variance regardless of the mixing type. The
aerial mixture is equivalent to the intra-mixture with a dominant size of pure icy \((a_1)\) grains; the size of pure AmC grains \((a_0)\) is unimportant. \(ST(\alpha_0) < 0.01\). With vol mixing, the size of pure AmC grains \((a_0)\) cannot be dropped. For all mixing types, the asymmetry factor \(\xi\) keeps its maximum influence in the most absorbing region \((100–300 \text{ cm}^{-1}, 700–900 \text{ cm}^{-1}, \text{ and about } 1660 \text{ cm}^{-1})\). The \(ST_i\) for \(f\) is largest in the roll-off region, but stays \(<0.01\) for both aerial and intimate mixtures. For \(T_0, ST_i < 0.001\) for intra-mixture and \(<0.01\) for both the aerial and intimate mixtures. In the case of a power-law size distribution (Fig. 8 bottom), the sensitivity to factors does not vary much with mixing type, but it does vary in the roll-off region. We note that the impact of \(f\) is relatively stronger within the absorption regions in case of aerial and vol mixture compared to intra-mixture, which is greater in transparency windows. The coefficients for aerial and vol mixing can hardly be distinguished. The overall behaviour remains that \(a_{\text{min}}, a_{\text{max}}, p, \text{ and } \xi\) are of somewhat equally important in the roll-off region and in the \(900–1100 \text{ cm}^{-1}\) range, whereas \(a_{\text{min}}, p, \text{ and } \xi\) are most influential above \(50 \text{ cm}^{-1}\).

### 3.2. Discussion

The global sensitivity analysis shows that given their a priori range of uncertainties (Table 1), the most important factors acting on the hemispherical emissivity \(E_{\text{h}}(\omega_i)\) remain the size distribution of regolith grains and the way in which regolith scatters around infrared light, translating into the average asymmetry factor \(\xi\) and the diffraction correction method (Fig. 8). The factor \(\xi\) may be best constrained where the effect of sizes is minimum, that is, in the ice absorption regions. Regardless of the mixing type, the index \(p\) or minimum size \(a_{\text{min}}\) may be constrained over the spectral range above \(50 \text{ cm}^{-1}\), where ice is less absorbing. In the case of a mono-dispersed size distribution, the constrained size will be that of the intra-mixed grains, while the size of contaminants may be constrained from spectral observations above \(100 \text{ cm}^{-1}\) if vol mixing is assumed (Fig. 8 top). The hemispherical emissivity \(E_{\text{h}}(\omega_i)\) in the region of the roll-off is sensitive to other factors for a poly-dispersed size distribution. It may be possible to constrain \(a_{\text{max}}\) and perhaps \(f\) in the case of intra-mixing if observations at larger wave-numbers \((> 50 \text{ cm}^{-1})\) are also available to constrain \(\xi, p, \text{ and } a_{\text{min}}\). This also requires a good spectral resolution and signal-to-noise ratio in this region.

Initial comparisons of this model with Cassini-CIRS or more recent JWST-MIRI observations are promising for constraining the properties of icy regoliths, regardless of whether they are contaminated. From CIRS spectra of the outer B ring, Morishima et al. (2012) derived \(p = 2.9^{+0.2}_{-0.4}\) and no strong constraint on \(a_{\text{max}} = 3.2^{+0.7}_{-0.5} \text{ cm}\), assuming \(a_{\text{min}} = 1 \mu\text{m}\), pure water ice, a \(\delta\)-Edd diffraction correction, no asymmetry factor, and two populations of grains, cold and warm. For their study, however, they favoured a good S/N at the cost of a good spectral resolution on the roll-off region, that is, \(15.5 \text{ cm}^{-1}\) over this \(40 \text{ cm}^{-1}\) wide region. We are currently studying a set of CIRS spectra of the B ring with our model. Figure 9 displays as an example a few occurrences of this model, including contaminants that are intra-mixed together with two observations of the emissivity \(E_F\) of the thickest part of the unlit B ring by CIRS-FP1. This emissivity within the field of view results from \(E_F = I(\omega_i)/B(\omega_i, T_F)\), where \(I(\omega_i)\) is the observed spectrum, \(\beta = 1\), and \(B(\omega_i, T_F)\) the Planck function for the single fitted temperature \(T_F\). The modelled population follows a power-law size distribution with \(p = 2.8, a_{\text{max}} = 5 \text{ cm}, \text{ and } a_{\text{min}} = 1 \mu\text{m}\) with an average asymmetry factor \(\xi\) = 0. It is observed that the contaminant and mixing type both affect the roll-off slope.

![Fig. 9. Modelled hemispherical emissivity \(E_h\) of a regolith of grains following a power-law size distribution with \(p = 2.8, a_{\text{max}} = 5 \text{ cm}, \text{ and } a_{\text{min}} = 1 \mu\text{m}\). Water ice is crystalline (Ih90) and contaminants are AmC or Th, intra-mixed with fraction \(f\). Two estimates of the emissivity \(E_F\) of the unlit B ring with the CIRS instrument on April 5, 2017, are displayed (blue dots, see text for details). Both esa (solid line) and \(\delta\)-Edd (dash-dotted line) diffraction corrections are shown, assuming \(\xi = 0\).](https://www.nrel.gov/grid/solar-resource/spectra-asm-e490.html)
may be combined: either a spectrally constant emissivity < Fig. 14), for which they proposed three possible origins that wavelength by more than 10 K in between 7 and 11 µm (their Fig. 13) can then be reproduced reasonably well for these regoliths on particles. The solar contribution is plotted for both contaminants in the case of n = 1 mm (dotted line).

**Fig. 10.** Model of the mid-infrared brightness of the optically thick B ring of Saturn. (top) Hemispherical emissivity of a regolith of grains following a power-law size distribution with p = 2.8, a_{min} = 5 cm, and a_{max} = 1 µm (solid line) or a_{max} = 1 mm (dashed line). Water ice is crystalline (ih90), and contaminants (AmC or Th) are intra-mixed with a fraction f. The esa diffraction correction is used here and δ = 0. (bottom) Corresponding modelled brightness temperatures T_b(K) of these regoliths on particles. The solar contribution is plotted for both contaminants in the case of n = 1 mm (dotted line).

local hour angle on the rings, and of the fraction of contaminants that modulate the radiative balance. A peak can be observed near λ = 9.5 µm. It results from the drop in emissivity observed in figure 10, top, which corresponds to a local peak in the hemispherical reflectance r_s, and therefore, to a peak in the solar contribution, which is still detectable above the thermal emission (with a nearly constant brightness temperature). The shape of this peak is highly dependent on the size distribution, the contaminant, its fraction, and the diffraction correction applied (not shown). In the case of pure ice, the thermal contribution is much smaller with an equilibrium temperature ~ 66 K because solar light is only weakly absorbed in the visible domain. The peak is absent in the case of intra-mixed AmC at the 3% level. It has been detected by Hedman et al. (2024). With this simple model, the spectral shape and range of the brightness temperatures observed by Hedman et al. (2024) (reported in the bottom panel of their figure 13) can then be reproduced reasonably well with a filling factor β = 0.95 with the addition of contaminants and current estimates of the size distribution of regolith grains (Morishima et al. 2012). As expected from the global sensitivity analysis, this spectral region may bring complementary information on the regolith properties and composition. This would deserve a quantitative adjustment.

Bockelée-Morvan et al. (2024) targeted the leading and trailing hemispheres of Ganymede with the JWST-MIRI instrument in this same spectral region. They observed a remarkable quasi-linear decrease in the brightness temperature with increasing wavelength by more than 10 K in between 7 and 11 µm (their Fig. 14), for which they proposed three possible origins that may be combined: either a spectrally constant emissivity <1, a decreasing spectral emissivity versus wavelength, or a variety of surface temperature mixing in the PSF. The brightness temperature estimated with our model, including both solar and thermal contributions and assuming the regolith in thermal equilibrium at a solar distance of 4.96 AU (i.e. replacing μ_0 by 1/4 in Eq. (12)), may exhibit a steep slope with increasing wavelength for sub-millimetre grains (Fig. 11). It is shown here for the case of intra-mixed AmC with f = 3%. The size of regolith grains and the nature of the diffraction correction significantly affect the slope of T_b and its linearity in this spectral region. As in the previous case of Saturn’s rings, the slope of T_b depends on the temperature, that is, on the energy balance and thermal history, and on the contaminant mixing in the water ice. Therefore, a convolution of this model with a terrain model and a thermal model remains essential to take into account the surface temperature heterogeneity over the observed hemisphere and to interpret these observations. The influence of the two contaminants (AmC or Th) at the level of a few percent does not yield significant variations in the slope, but their fraction is more influential for λ < 6 µm or λ > 10 µm.

**Fig. 11.** Modelled brightness temperature T_b (K) of a regolith of grains with a given size of 10 µm (solid line), 50 µm (dashed line), or 500 µm (dotted line) at equilibrium temperature at a Jupiter distance of 4.96 AU in the wavelength range of the JWST-MIRI instrument. The grains are composed of pure crystalline ice (ih90) with intra-mixed AmC with a fraction f = 3%. The esa (black) or δ-Edd (red) diffraction corrections are used here, and δ = 0. The solar contribution (orange) is plotted for all sizes in the case of an esa diffraction correction.

4. Conclusions

A hybrid Mie-Hapke model for the hemispherical emissivity of an icy regolith contaminated with either amorphous carbon or tholins along with various types of mixing was proposed here. It can be coupled with two diffraction-correction methods and various types of size distributions, and it includes the average asymmetry factor of the regolith. A global sensitivity analysis quantified the importance of these factors on the variance of its hemispherical emissivity versus wave number. We plan to analyse a wider dataset of the CIRS instrument with this model, for either rings or moons, to complement existing studies, including the consideration of lightly contaminated water ice or seasonal phenomena. This model provides a self-consistent tool for interpreting multi-modal observations of the thermal emission from icy surfaces. It offers interesting insights into recent mid-infrared
observations of Saturn’s rings and the Galilean moon Ganymede by the JWST-MIRI instrument.

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