Full-field modeling of heat transfer in asteroid regolith: Radiative thermal conductivity of polydisperse particulates

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Abstract

Characterizing the surface material of an asteroid is important for understanding its geology and for informing mission decisions, such as the selection of a sample site. Diurnal surface temperature amplitudes are directly related to the thermal properties of the materials on the surface. We describe a numerical model for studying the thermal conductivity of particulate regolith in vacuum. Heat diffusion and surface-to-surface radiation calculations are performed using the finite element (FE) method in three-dimensional meshed geometries of randomly packed spherical particles. We validate the model for test cases where the total solid and radiative conductivity values of particulates with monodisperse particle size frequency distributions (SFDs) are determined at steady-state thermal conditions. Then, we use the model to study the bulk radiative thermal conductivity of particulates with polydisperse, cumulative power-law particle SFDs. We show that for each polydisperse particulate geometry tested, there is a corresponding monodisperse geometry with some effective particle diameter that has an identical radiative thermal conductivity. These effective diameters are found to correspond very well to the Sauter mean particle diameter, which is essentially the surface-area-weighted mean. Next, we show that the thermal conductivity of the particle material can have an important effect on the radiative component of the thermal conductivity of particulates, especially if the particle material conductivity is very low or the spheres are relatively large, owing to non-isothermality in each particle. We provide an empirical correlation to predict the effects of non-isothermality on radiative thermal conductivity in both monodisperse and polydisperse particulates.

Full-field modeling of heat transfer in asteroid regolith: Radiative thermal conductivity of polydisperse particulates 1,2Andrew J. Ryan, 3Daniel Pino Muñoz, 3Marc Bernacki, 1Marco Delbo 1Université Côte d'Azur, Observatoire de la Côte d'Azur, CNRS, Laboratoire Lagrange, Nice, France; 2Now at: Lunar and Planetary Laboratory, University of Arizona, Tucson, AZ, USA. 3Mines ParisTech, PSL Research University, CEMEF - Centre de mise en forme des matériaux, Sophia Antipolis Cedex, France. Corresponding author: Andrew Ryan (ajryan@orex.lpl.arizona.edu) **Key Points:** A new finite element model for analyzing the solid and radiative conductivity of • particulate regoliths is presented. • Non-isothermality in particles with low material thermal conductivity or large sizes can markedly lower the radiative thermal conductivity Particulate size mixtures are shown to have a radiative thermal conductivity that is • equivalent to the Sauter mean particle diameter

47 Abstract

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- radiative conductivity values of particulates with monodisperse particle size frequency
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69 Plain Language Summary

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71 The thermal conductivity of asteroid regolith is related to the properties of the particulate 72 assemblage (e.g. size distribution). Spacecraft missions that measure the surface temperature of 73 asteroids, like OSIRIS-REx at asteroid Bennu, can take advantage of this by relating the 74 observed temperatures to the physical properties of the regolith. We present a 3D model for 75 studying the thermal conductivity of regolith, where heat flow is simulated in randomly packed 76 spheres. We found that for cases where the particle sizes are monodisperse, our model 77 reproduces the thermal conductivity values predicted by simpler theoretical models. However, 78 this is only true if the particles themselves are made of a material that itself has relatively high 79 thermal conductivity, which may not be the case for the regolith on Bennu. We determined the 80 values for a correction factor to account for these cases. Neglecting it could cause one to appreciably underestimate particle sizes on asteroid surfaces, which could pose a risk for sample 81 82 collection. Finally, we found that regoliths with particle size mixtures can have radiative thermal 83 conductivities that are identical to monodisperse regoliths. We found that the surface-area-84 weighted mean particle size of the mixed regoliths is representative of the bulk radiative thermal 85 conductivity.

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87 **1 Introduction**

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Asteroids and airless bodies, such as the Moon, are commonly blanketed in loose and unconsolidated material known as regolith, which preserves a record of the geophysical history of the body (Murdoch et al., 2015). The particle size, maturity, and depth of the regolith layer are thought to vary within the asteroid populations depending on the size, composition, shape, and age

93 of these bodies (Murdoch et al., 2015; and references therein). Regolith physical properties also 94 place important constraints on mission planning, particularly for safety during sample acquisition 95 events. NASA's Origins, Spectral Interpretation, Resource Identification, and Security-Regolith 96 Explorer (OSIRIS-REx, Lauretta et al., 2019) and JAXA's Hayabusa2 (Watanabe et al., 2019) 97 missions are currently studying the surface of carbonaceous asteroids (101955) Bennu and 98 (162173) Ryugu, respectively. The prime objective for both missions is to collect regolith samples 99 and return them to Earth. Infrared emission measurements of the asteroid surface by OSIRIS-100 REx's Thermal Emission Spectrometer (OTES, Christensen et al., 2018) and Visible and InfraRed Spectrometer (OVIRS, Reuter et al., 2018), and by Hayabusa2's Thermal Infrared Imager (TIR, 101 102 Okada et al., 2017), are currently being used to infer the physical properties of the regolith, such 103 as particle size distribution, porosity, and composition. This is possible because the amplitude of 104 diurnal temperature cycling of the regolith is directly related to the thermal inertia of the regolith, 105 which in turn is controlled by the physical characteristics of the regolith.

106 OSIRIS-REx and Hayabusa2 recently revealed that asteroids Bennu and Ryugu are both 107 covered in abundant large boulders with very little fine regolith surface cover, which increases the 108 challenge of sample site selection (Lauretta et al., 2019; DellaGiustina and Emery et al., 2019; 109 Walsh et al., 2019; Sugita et al., 2019; Watanabe et al., 2019). Preliminary infrared telescopic 110 observations of these asteroids were interpreted to represent regolith with particle diameters 111 ranging from a few millimeters to about a centimeter for Bennu (Emery et al., 2014; Müller et al., 112 2017). However, the images of the surfaces of Bennu and Ryugu from both space missions show 113 that this is not case. The mismatch between regolith size predictions and surface imaging observations could be due to unexpectedly low thermal conductivity and density of the solid 114 115 material composing the boulders of these asteroids (Grott et al., 2019), limitations in the models used to interpret thermal infrared observations in term of regolith particle sizes, or a combination 116 of both. In this work, we focus on the latter and seek to improve existing thermophysical models 117 118 for asteroid regoliths.

119 Several theoretical models exist that predict the thermal conductivity of monodisperse 120 particulate media as a function of particle size, packing structure, and physical parameters of the 121 particles themselves, such as their thermal conductivity and emissivity (e.g., van Antwerpen et 122 al., 2012; Gundlach & Blum, 2012, 2013; Sakatani et al., 2017). However, no such models have 123 sought to describe polydisperse particulates, despite the prevalence of particle size mixtures in 124 nature (except for where there are advanced natural sorting mechanisms in place). Furthermore, 125 only some models (e.g., van Antwerpen et al., 2012) have sought to incorporate particulate non-126 isothermality effects, which could be important for regolith on Ryugu and Bennu, particularly if 127 the geologic materials have unusually low densities and thermal conductivities.

128 Experimental studies have provided invaluable data necessary to calibrate theoretical 129 models for particulate thermal conductivity, including some preliminary analyses of polydisperse 130 samples (Sakatani et al., 2017, 2018; Ryan, 2018;). However, such experiments are known to be 131 difficult to perform and can produce results with uncertainties that are difficult to quantify, e.g. 132 due to factors that are difficult to control or know, such as changes in particulate porosity in the 133 vicinity of heat sources/sinks (Presley & Christensen, 1997; Ryan, 2018). This limits the number 134 of experiments that can reasonably be performed and the utility of the results. Furthermore, there 135 is often uncertainty in the physical aspects of the samples being studied, such as the nature of the 136 packing structure, the magnitude of contact deformation between particles, and relevant physical 137 parameters of the particles themselves, such as their thermal conductivity and emissivity, that 138 can complicate the process of relating experimental results to theoretical models. This problem

139 leads us to the methods presented herein, where advanced numerical methods are used to create a

realistic, though idealized, simulation of a thermal conductivity experiment in which physical

parameters related to the "experimental" samples are well controlled and thus known withcertainty.

143 We present a thermophysical model for particulates in which a bed of spherical particles 144 is fully rendered in a three-dimensional finite element (FE) mesh framework. This type of model 145 enables rapid and well-controlled investigations of the fundamental parameters that affect 146 particulate thermal conductivity. In this work, we present validation cases for solid and radiative 147 thermal conduction through ordered and randomly packed monodisperse particulates. Then, we 148 present the findings of a study of the radiative thermal conductivity properties in mixtures that 149 follow power-law particle size frequency distributions (SFDs) commonly observed in boulders 150 and coarse regolith on asteroid surfaces (Bierhaus et al., 2018). Radiative thermal conductivity is selectively studied here because its magnitude tends to greatly exceed that of conduction through 151 152 the solids for coarse particulates (> a few mm diameter, as explained in Section 2: Background 153 and shown in Figure 1). Given the likely abundance of coarse materials on Bennu and Ryugu and 154 the need to identify particle size thresholds below ~ 2 cm for sampling, the study of radiative 155 thermal conductivity in coarse particulates mixtures is of high priority. We pay particular attention in these analyses to the effects of particle non-isothermality, given the initial findings 156 157 by OSIRIS-REx and Hayabusa2 of geologic materials with potentially low thermal conductivity 158 on Bennu and Ryugu (DellaGiustina and Emery et al., 2019; Sugita et al., 2019; Grott et al., 159 2019).

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161 **2 Background**

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163 Two modes of heat transfer exist in particulate media in a vacuum — radiation between 164 particles and conduction through the solids at the contacts between particles (Wesselink, 1948; Watson, 1964; Wechsler et al., 1972; van Antwerpen et al., 2010; De Beer et al., 2018). These 165 are typically represented in terms of their contributions to the bulk thermal conductivity of the 166 167 regolith, where conductivity due to radiative heat transfer is denoted by k_r and conductivity due 168 to the contacts between the particles is denoted by k_s . In the presence of an atmosphere, a third 169 heat conduction term must be considered to account to heat transfer through pore-filling gas. The 170 gas thermal conductivity, k_g , tends to be the dominant heat transfer mechanism on Mars (Presley 171 & Christensen, 1997). Although gas conduction will not be considered in this present work, a 172 proper treatment of thermal conductivity due to radiation and particle contacts is still useful for improving models of regolith thermal conductivity on Mars, Earth, or other bodies with 173 174 appreciable atmospheres.

175 For large, opaque particles, heat transfer by radiation is governed by the Stefan-Boltzmann law, which is influenced by the temperature, emissivity, and distance between 176 177 radiating surfaces. Most theoretical formulations for radiative heat transfer in particulates begin 178 by approximating the particles as a series of parallel, radiating plates separated by some 179 representative distance for radiative transfer. The radiative thermal conductivity (k_r) of such a 180 configuration is proportional to the cube of the local mean temperature (e.g., Wesselink, 1948). 181 The representative distance for radiative transfer is often related to the size of the pore space 182 between particles, which in turn is related to porosity and particle diameter, as is the case in the 183 model for regolith thermal conductivity by Sakatani et al. (2017).

184 The regolith thermal conductivity model by Gundlach and Blum (2012; 2013) uses the 185 mean free path of the photon as the representative distance for radiative transfer. This 186 formulation is based on theory for very small particles (<100 µm diameter), where particle 187 transparency becomes important (Merrill, 1969). As such, it should be used with caution for 188 larger particulates, particularly given that Gundlach and Blum's model predicts a much stronger 189 dependence between radiative thermal conductivity and porosity than most other theoretical 190 models (e.g., Schotte, 1960; Watson, 1964; Breitbach & Barthels, 1980; van Antwerpen et al., 191 2012; Sakatani et al., 2017).

192 A more advanced formulation by van Antwerpen et al. (2012) separately describes the 193 radiative contribution of immediately adjacent spheres (short-range radiation) and nonadjacent 194 spheres that still have some direct line of sight (long-range radiation). They incorporate 195 approximations to describe the view factors—i.e., the proportion of radiation emitted from one 196 surface that reaches another—between spheres for both of their radiative conductivity 197 formulations. Furthermore, they demonstrate that the thermal conductivity of the solid material 198 that composes the spheres can influence the radiative thermal conductivity, building upon work 199 by Breitbach and Barthels (1980) and Singh and Kaviany (1994). In such cases, thermal 200 gradients are present within individual particles, with the consequence being that the radiative 201 thermal conductivity would not increase in proportion to the cube of the temperature but rather at 202 a lower rate. Van Antwerpen et al. (2012) introduce an updated description of a non-isothermal 203 correction factor, f_k , that is related to a dimensionless parameter, Λ_s :

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where k_m is the thermal conductivity of the material that constitutes the particles (the thermal conductivity of a single particle), *D* is particle diameter, σ is the Stefan-Boltzmann constant, and *T* is the mean local temperature. If $1/\Lambda_s$ is greater than approximately 0.04, the particle nonisothermality can have a meaningful, measurable effect (>~1%) on radiative thermal conductivity. Van Antwerpen et al. (2012) provide correlation coefficients to relate Λ_s to the correction factor, *fk* in the direction of heat flow:

 $\Lambda_s = \frac{k_m}{4D\sigma T^3}$

215 (Eq. 2)

$$f_k = a_1 \tan^{-1} \left(a_2 \left(\frac{1}{\Lambda_s} \right)^{a_3} \right) + a_4$$

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218 When emissivity is unity, $a_1 = -0.3966$, $a_2 = 0.7495$, $a_3 = 0.5738$, and $a_4 = 1.0484$. When 219 $1/\Lambda_s < 0.01$, $f_k = 1$. These four correction factor coefficients were determined from numerical 220 simulations of radiative heat transfer between two almost-touching hemispheres, implying that 221 they are accurate for correcting short-range radiation non-isothermality. Van Antwerpen et al. 222 (2012) use the non-isothermal correction factor for both short- and long-range radiative 223 conductivity by simply multiplying each conductivity by f_k but note that more work is needed to 224 verify its validity for long-range radiation. Experimental and theoretical work describing particle 225 thermal conductivity in the context of planetary regoliths has yet to incorporate non-226 isothermality in the radiative thermal conductivity, primarily owing to the normally small size of 227 the particles under consideration (typically <1 mm) and the relatively high thermal conductivity

of geologic materials (e.g., basalt: $\sim 1-2.5$ W m₋₁ K₋₁ (Desai et al., 1974)). Finally, it should be noted that even though the thermophysical properties of a planetary surface are determined in terms of thermal inertia, which is related to the square root of thermal conductivity, the effects of non-isothermality could still considerably affect the estimation of particle size on rubble pile asteroids like Bennu and Ryugu.

233 Having discussed the thermal conductivity of particulates due to radiation (k_r) , we now 234 move our attention to the thermal conduction through the particle-to-particle contacts. The bulk 235 thermal conductivity of particulates due to these contacts (k_s) is directly related to but typically 236 much smaller than the thermal conductivity of the individual particles themselves (denoted here 237 by k_m for *material* conductivity). Although the thermal conductivity of most common geologic 238 materials is relatively high (~ 2 to 4 W m-1 K-1), the flow of heat from one particle to the next is 239 severely hindered by the very small size of the contacts between particles. The size of these 240 contacts and the average number of contacts between particles (the coordination number) thus 241 strongly influence the solid thermal conductivity of particulates. To estimate the size of the 242 contacts, Gundlach and Blum (2013) and Sakatani et al. (2017) use the model for interparticle 243 forces due to adhesion and the resulting Hertzian deformation by Johnson, Kendall, & Roberts 244 (1971) ("JKR theory") to predict the particle contact radii that are used in their models for the 245 thermal conductivity of particulates. The contact radii r_c are typically very small compared with 246 the radii of the particles R_p , with values for the ratio r_c/R_p in the range of 0.0005–0.005 247 (depending on values for particle elastic moduli, surface energy, and gravity). As such, the 248 magnitude of thermal conductivity by means of heat transfer between the particles via their 249 contacts, k_s , is typically several factors or even orders of magnitude smaller than the thermal 250 conductivity of the particle material itself, k_m . Sakatani et al. (2017) have proposed that k_s and k_m 251 are linearly related to each other by the ratio r_c/R_p (Sakatani et al., 2017). Also, they and others 252 (e.g. van Antwerpen et al., 2012) have propose that k_s is linearly related to the mean coordination 253 number. Several model correlations between coordination number and porosity have been 254 proposed (see van Antwerpen et al. (2010) for a review), but more work is needed on this topic 255 to resolve discrepancies between models and to determine the effects of particle sphericity and 256 roughness.

Figure 1 illustrates the relative contributions of radiative thermal conductivity and solid conductivity to the total thermal conductivity of particulates on Bennu, as predicted by the particulate thermal conductivity model by Sakatani et al. (2017). The radiative thermal conductivity increases linearly with particle diameter, whereas solid thermal conductivity only changes modestly (or not at all, if adhesion is neglected). Therefore, the radiative thermal conductivity term comes to dominate for particles larger than a few millimeters in diameter.

263 All existing theoretical models for regolith thermal conductivity assume monodisperse particle SFDs (all particles have the same size). Some experimental work, however, has been 264 conducted to determine whether these models could be used to approximate the thermal 265 266 properties of particulates with polydisperse SFDs. Sakatani et al. (2018) measured the thermal 267 properties of the JSC-1 lunar regolith simulant (maximum diameter <=~1 mm) with a log-normal 268 cumulative particle mass distribution and found a thermal conductivity approximately equivalent 269 to that of the volumetric median particle size ($\sim 100 \ \mu m$). However, it remains to be determined 270 whether this relationship is applicable to other particle size distributions and whether it holds for 271 both radiative and solid conductivity terms.

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275 **Figure 1.** Illustrative example of the predicted ratio of radiative to solid thermal conductivity 276 (i.e. k_r/k_s) in monodisperse particulates on Bennu as a function of particle diameter (indicated next to the lines). Values were calculated with the model from Sakatani et al. (2017), using 277 278 parameters assumed for asteroid Bennu, where particulate material properties are similar to CM 279 chondrite Cold Bokkeveld (Opeil et al., 2010), surface energy is 0.02 J m-2, depth of burial is 1 280 cm. gravity is 75 μ m s₋₂, emissivity is 1.0, and porosity is 0.40. Van Antwerpen et al. (2012) and 281 Gundlach and Blum (2013) models yield comparable predictions when the same or similar input 282 parameters are used.

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286 **3 Methods and Model Validation**

We study the thermal conductivity of particulates in a vacuum within a FE framework where constant heat flux is applied to one side of a three-dimensional, parallelepiped geometry of randomly packed spheres while a constant temperature boundary condition is applied to the opposite side (Figures 2 & 3). Once the model temperatures reach steady state, the thermal conductivity of the particulates can be calculated from the temperature differential between the two opposing geometry boundaries where the flux and fixed temperature boundary conditions have been applied:

 $k = -q \frac{\Delta x}{\Delta T}$

295 296 (Eq. 3)

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299 Or in the case where the contribution of the two plates is removed:

300 301 (Eq. 4)

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$$k = \frac{\Delta x_{total} - \Delta x_{plates}}{\frac{\Delta T}{q} - \frac{\Delta x_{plates}}{k_m}}$$

304 where *q* is applied heat flux along the geometry boundary, Δx_{total} and Δx_{plates} are the

thicknesses of the entire geometry and of the plates (Figure 2), ΔT is the final steady-state

temperature differential across the entire domain (including the end plates), Δx_{total} is the total distance between the outer surfaces of the two plates, Δx_{plates} is the combined thickness of the

two plates, and k_m is the material thermal conductivity used in the simulation, which is the same for the plates as it is for the spheres. All adjacent boundaries are insulated such that the net heat

310 flux occurs only in one direction.

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Figure 2. Cross-sectional illustration of packed sphere and end plate geometry that is used for steady-state thermal conductivity determination (Equation 4). Plate thicknesses are exaggerated and are not to scale. See Figure 3 for an example 3D geometry.

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317 Multiple simulations for a single geometry are typically conducted across a range of 318 temperatures. In this work, the fixed-temperature plates were typically set to temperatures of 319 250, 300, 350, and 400 K. The prescribed flux values (q) were chosen based on the estimated 320 bulk thermal conductivity of the geometry so that a thermal gradient (ΔT) on the order of 15 K 321 would be achieved at steady state. The resulting thermal conductivity that is determined at the 322 end of the simulation is assumed to be representative of the mean temperature of the geometry at 323 the final steady state. If the prescribed heat flux is too high, the thermal gradient at steady state 324 would be very large, which makes it dubious to use the mean temperature to represent the bulk 325 conductivity given the temperature dependence of radiative heat transfer. If the flux is too small, 326 the final temperature gradient value might be so small that precision is lost.

Heat conduction calculations for the tetrahedral domain mesh elements within the threedimensional model geometry are performed using an implicit diffusion equation solver that is part of the CIMLib scientific FE library (Digonnet et al., 2007). Radiative heat transfer between triangular surface mesh elements is calculated following the Stefan-Boltzmann law in the

331 following manner for element *i* of *n* elements:

332 (Eq. 5)

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$$Q_i = \sum_{j=1}^{n} A_i F_{ij} \sigma (T_i^4 - T_j^4)$$

334 where A is the area, F_{ij} is the view factor from element i to j (i.e. the fraction of radiation leaving 335 surface *i* that strikes surface *j*), and σ is the Stefan-Boltzmann constant. This value is added 336 explicitly to the heat diffusion calculations, such that the surface temperatures from the previous 337 time step are used for the calculation in Equation 5. A good discretization of the surface of the 338 particles requires a large number of triangular surface elements. Thus, the number of possible pairs of surface elements that could "see" each other is high and requires an efficient 339 340 computation of the view factors. The Intel Embree high-performance ray-tracing library meets 341 these demands by rapidly tracing rays between all surface elements that share direct line of sight. 342 View factors for all non-obstructed elements are calculated using the single line integration 343 method described by Mitalas & Stephenson (1966) (c.f. Walton, 1986). The surface mesh size is 344 refined such that the precise calculation of partially obstructed view factors between elements is 345 not necessary, given that these types of calculations tend to be slower and less accurate (Walton, 346 2002). Emissivity is assumed to be unity, and as such, multiple reflections are not calculated. 347 Our view factor calculations and explicit radiative heat transfer solver were validated with a 348 geometric configuration with a known analytical solution — two concentric, hollow spheres are 349 assigned fixed-temperature boundary conditions at the inner surface of the inner sphere and at 350 the outer surface of the outer sphere (see Appendix A). The resulting steady-state temperatures of the outside of the inner sphere and the inside of the outer sphere were found to be within 1.5% 351 352 of the analytical solution. The analytical expression for this test case is derived in Appendix A. 353 The geometries used in this study consist of three-dimensional beds of spheres that have

been cropped to the shape of a parallelepiped box. Sphere coordinates are generated with the optimized dropping and rolling method described by Hitti & Bernacki (2013), following userspecified SFDs. Plates are added to the top and bottom of the volume to create uniform surfaces for the heat flux and fixed temperature boundary conditions. The geometries are rendered and meshed using the Netgen automatic three-dimensional tetrahedral mesh generator (Schöberl, 1997) (Figures 3 and 4).

360 We performed a size convergence study with a simple cubic packing structure to determine the optimal representative volume element (i.e. parallelepiped width and height) 361 362 where boundary effects are minimized. Model widths of only four particle diameters produced homogenized thermal conductivity results that were within ~5% of the convergence value for a 363 much wider volume. Similarly, a model thickness of four to five sphere diameters produced 364 365 thermal homogenized conductivity results within $\sim 5\%$ of the convergence value. As such, we conducted all further analyses with model geometries widths and heights of at least four sphere 366 367 diameters. Commonly, we used larger geometries for random packings to capture a larger, more 368 representative sampling of the packing. Most simulations thus contained between 120 and 175 spheres. Typical element counts were 500,000 to 3 million for volumetric (tetrahedral) elements 369 370 and 130,000 to 500,000 surface (triangular) elements. View factor computation times ranged 371 from a few minutes up to about 6 hours. Convergence in each heat flow simulation was typically 372 achieved within 3–24 hours, depending on the number of elements and the number of processors 373 used.

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Figure 3. Meshed monodisperse sphere geometry colorized with final steady-state temperatures

379 from a numerical simulation where a constant heat flux was applied to the bottom boundary plate

and a fixed temperature (250 K) was imposed on the top plate. In this particular case, the spheres

are not touching, so heat transfer between spheres is accomplished solely by radiation. In other

382 conditions, as explained in the text and shown in Figure 4, we generated contact bridges between 383 spheres to study the combined effect of solid and radiative heat transfer in a particulate medium.

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Figure 4. Example mesh refinement in a case where the spheres are touching and the ratio of particle contact neck size r_c to sphere radius $R_p = 0.05$.

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Contacts between spheres can be approximated by adding cylindrical bridges at each contact location with radii equal to the desired contact radius r_c . It is necessary to use a fine mesh in the vicinity of the sphere contacts, given the narrowness of the geometry and the expectation of steep thermal gradients due to thermal constriction resistance (Figure 4). Following the numerical work by De Beer (2014), we use a minimum mesh element size that is approximately $0.2*r_c$. To validate the solid conductivity within our model, we performed a series of tests with

395 ordered packing structures where the size of the contact neck, *rc*, was systematically varied

396 (Figure 5). Our numerical results are in very good agreement with theoretical predictions by Siu 397 & Lee (2000). Simulations with sphere contacts are generally more computationally intensive

398 than those where the spheres are not in contact owing to the increased number of mesh elements.

399 Therefore, although we have demonstrated the utility of this model for studying solid conduction

400 through particulates via sphere-to-sphere contacts, the remainder of this work focuses on heat

401 transfer between non-touching spheres by radiation only.

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407 To study the thermal conductivity of particulates due to radiation only, we reduced the 408 diameter of the spheres by 0.1–0.5% to avoid overlaps. This was beneficial for computation 409 times, as the removal of the contacts between spheres greatly reduced the mesh element count. 410 We performed a sensitivity analysis to determine whether these slight reductions in sphere radius would appreciably affect the radiative thermal conductivity. We found that 1% radius reduction 411 412 lowered the thermal conductivity by <1%. The applied change to sphere radius is thus assumed 413 to be negligible.

414 In Figure 6, we compare the radiative thermal conductivity of a dense random packing of 415 two test cases with monodisperse spheres with 2-mm and 1-cm diameters to theoretical model predictions. The model by Sakatani et al. (2017) predicts the radiative thermal conductivity 416 417 results of the numerical simulations with an accuracy of approximately $\pm 5\%$. Although in these 418 cases their model overpredicted our results for smaller spheres and underpredicted our model for 419 larger spheres, results from other test cases showed no systematic trend with particle diameter. 420 We conclude from these tests that the Sakatani et al. (2017) model can be used to reliably predict 421 the radiative thermal conductivity of a monodisperse sample, which we use to our advantage to 422 compare polydisperse geometries to monodisperse geometries with equivalent radiative thermal 423 conductivity values. 424

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Figure 6. Radiative thermal conductivity results from numerical simulations of two
monodisperse particulate geometries with diameters of 2 mm (upper plot) and 1 cm (lower plot,
also shown in Figure 3). These results are compared to theoretical model predicted values.
Temperatures were taken as the mean temperature from the numerical simulations.

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4 Result for Monodisperse and Polydisperse Particulates

435 To study the radiative thermal conductivity (k_r) of particle size mixtures, we conducted 436 numerical simulations of steady-state heat flow following the methodology described above 437 where the spheres are not touching each other. We analyzed 16 randomly packed polydisperse particulate geometries with particle SFDs following a cumulative power law (Table 1). We used 438 439 five different millimeter- to centimeter-scale particle size ranges, some of which were directly 440 based on the size ranges described in Bierhaus et al. (2018) for tests of the OSIRIS-REx Touch-441 and-Go Sample-Acquisition Mechanism (TAGSAM) tests. These size ranges are relatively 442 narrow due to the possible absence of fines on Itokawa (Bierhaus et al., 2018), which may also 443 true for Bennu and Ryugu. Also, wider size ranges would require larger representative volumes, 444 which could prohibitively increase the number of spheres and thus mesh elements. We generated 445 packings for each size range by using various different cumulative power-law exponent values 446 (e.g., Figure 7). We performed steady-state heat flow simulations at four different temperatures 447 (approximately 250, 300, 350, and 400 K) to determine the radiative thermal conductivity as a 448 function of temperature. We conducted all simulations with a solid material thermal conductivity 449 value k_m of 1.0 W m₋₁ K₋₁. Many of the simulations were recomputed with higher and lower k_m

450 values of 10.0, 0.5, 0.1, and 0.05 W m_{-1} K $_{-1}$ to study the non-isothermality effect (Equations 1 and 2).

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453 Table 1. Particle diameter size ranges used for polydisperse particulate models and the power-

454 law exponent values used for each size range. The second and third row size ranges correspond

455 to the "7c" and "7d" size distributions used by Bierhaus et al. (2018) for OSIRIS-REx TAGSAM

456 sample collection testing. The geometries given in the last row (10–30 cm diameter) are shown

457 in Figure 7.

Particle diameter (mm)		
min	max	Power law exponent values
3.18	12.7	-2.5, -3.0, -3.5
3.18	15.88	-2.5, -3.0, -3.5
3.18	19.05	-2.5, -3.0, -3.5
6.35	19.05	-2.5, -3.0, -3.5
10.0	30.0	-3.0, -4.0, -6.0, -8.0

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460 An example set of results for one packing geometry as a function of temperature and k_m is presented in Figure 8. In the simulations where k_m is high (≥ 1.0 W m⁻¹ K⁻¹), the radiative thermal 461 conductivity scales with the cube of the temperature, as predicted by theory. Lower values of k_m 462 463 cause the radiative thermal conductivity to decrease, particularly for higher temperatures. In 464 extreme cases (e.g., $k_m = 0.05$ W m⁻¹ K⁻¹), the radiative conductivity was found to increase 465 nearly linearly with temperature, rather than with temperature to the third power. These 466 observations are similar to the non-isothermality described by van Antwerpen et al. (2012). Non-467 isothermality may be quantified as the ratio between the numerical radiative thermal conductivity 468 results with non-isothermality $(1/\Lambda_{s} < 0.04)$ and results without non-isothermality $(1/\Lambda_{s} > 0.04)$. 469 For example, we calculated non-isothermality correction factor (f_k) values for the numerical 470 radiative thermal conductivity results in Figure 8 by calculating the ratio between all points on 471 the plot and the solid theoretical curve. The calculated values of f_k from all polydisperse 472 simulations and our monodisperse validation simulations are plotted in Figure 9 against $1/\Lambda_s$ 473 (Equation 1). In the case of the polydisperse geometries, we used the effective particle diameters 474 (described in the next paragraph) to calculate the values of Λ_s in Figure 9.

475 It is illustrative to express the conductivity results for these polydisperse geometries in 476 terms of a monodisperse particle diameter that has the same thermal conductivity. We found that, 477 when non-isothermality is negligible (i.e. $1/\Lambda_s < 0.04$), the radiative thermal conductivity of each 478 polydisperse geometry is equivalent to the radiative thermal conductivity of a monodisperse 479 geometry with some *effective* particle diameter. To determine the effective particle diameter for 480 each polydisperse geometry, we used the Sakatani et al. (2017) model to calculate predicted 481 monodisperse radiative thermal conductivity values. The model input diameter was allowed to 482 vary as a free input parameter, whereas porosity and average coordination number were known from the polydisperse geometries. The determination of effective particle diameter was done 483

484 only with the numerical thermal conductivity simulation solutions that we expected to be 485 unaffected by non-isothermality—i.e., $1/\Lambda_s$ was less than ~0.04. We expect the uncertainty in the 486 determined effective particle sizes to be approximately $\pm 5\%$, on the basis of the goodness of fit 487 between the Sakatani model predictions and our monodisperse numerical test cases. The 488 resulting effective particle diameters are compared to volumetric mean particle size, volumetric 489 median particle size, and the surface-volume mean particle diameter (Sauter mean) of each 490 polydisperse geometry in Figure 10. The Sauter mean diameter, D_{32} , was calculated as the 491 average of the volume-to-surface ratio of *n* particles by: 492 493 (Eq. 6)

$$D_{32} = \frac{\sum_{i=1}^{n} D_i^3}{\sum_{i=1}^{n} D_i^2}$$







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- 500







502 **Figure 7.** Steady-state temperature solution examples for the 10–30 mm diameter particle size 503 range with four different power-law exponent values: -8.0, -6.0, -4.0, and -3.0. The material 504 solid thermal conductivity used in these simulations is $k_m = 10.0$ W m-1 K-1, chosen to minimize

- 505 non-isothermality within the individual spheres.
- 506





508 **Figure 8.** Numerical radiative thermal conductivity results for a mixture of particles having 509 diameters 6.35-19.05 mm with an exponential slope of -2.5 as a function of temperature and 510 solid particle material thermal conductivity k_m . The effective particle diameter for the case where

 $k_m = 10.0 \text{ W m}_{-1} \text{ K}_{-1}$ is well fit by the theoretical model of Sakatani et al. (2017) with an effective

512 particle diameter of 11 mm. It is clear that lowering the value of k_m can substantially reduce the 513 radiative thermal conductivity of the particulates, particularly at higher temperatures. Mean

temperature from the numerical simulations were used to plot the x-axis temperatures here. For

515 most simulations, the range in temperatures (ΔT) between the two plates at steady state was less

516 than 15 K. For simulations with very low values of k_m , ΔT was as high as 30 K.

517



518

519 **Figure 9.** Original non-isothermal correction factor proposed by van Antwerpen et al. (2012) 520 (dashed line), shown with our values for the correction factor from numerical results (points) and

a corresponding fit line (solid gray line). Λ_s values were calculated using the effective particle

522 diameter for each geometry. Both lines are calculated using Equation 2, assuming that $f_k = 1$

523 when the equation produces a value greater than unity (when $1/\Lambda_s < \sim 0.04$). Numerical test

results are shown for all polydisperse geometries in Table 1 and a set of monodisperse validation cases (e.g. Figures 3 and 6) at temperatures ranging from 250-400 K and with k_m values ranging from 0.05-10.0 W m-1 K-1.







Figure 10. Comparison of the effective particle diameter determined from the radiative thermal conductivity numerical results to different expressions of the mean particle diameter for the 16 polydisperse geometries (Table 1). Effective particle diameter of a polydisperse particulate geometry is defined as the diameter of a monodisperse particulate geometry that has the same radiative thermal conductivity.

547 **5 Discussion**

548

549 The new values of f_k versus $1/\Lambda_s$ in Figure 9 provide compelling evidence that an 550 isothermal correction factor correlation exists that is applicable to both monodisperse and 551 polydisperse particulates. We find that the f_k values are well fit by Equations 2 and 3 using the 552 follow coefficient values:

- 553 554 a1= -0.568
- $555 \quad a_2 = 0.912$
- 556 a₃ = 0.765
- 557 a₄ = 1.035
- 558

559 The value of f_k approaches unity as $1/\Lambda_s$ drops to 0.04. Any value of f_k is assumed to be unity 560 when $1/\Lambda_s < \sim 0.04$, as shown in Figure 9. The original correction factor correlation proposed by van Antwerpen et al. (2012) underestimates the effects of non-isothermality that were 561 562 observed in our simulations (Figure 9). As mentioned in Section 2, their correction factor values 563 were determined from a numerical model of only short-range radiation between directly adjacent 564 spheres and had not been validated for long-range radiation. Our correlation accurately accounts 565 for both short- and long-range radiation together and appears to be valid under a wide range of 566 particle SFDs. We are confident that our correlation is not simply recording a bias in our 567 numerical results, given that it is composed of numerical solutions from geometries with multiple 568 different length and width dimensions, temperature differentials, absolute temperatures, mesh 569 sizes, and boundary flux values. However, all geometries tested here are dense random packings 570 of spheres with unit emissivity, whereas the regolith on Bennu, Ryugu, and other airless bodies is 571 surely composed of non-spherical particles, possibly with a much wider range of porosities and 572 non-unit emissivity. We intend to consider non-sphericity, roughness, different packing densities, 573 and lower emissivities in future studies.

574 Our non-isothermality results have important implications for the interpretation of 575 thermal inertia on Bennu and Ryugu. Initial results from OSIRIS-REx and Hayabusa2 indicate 576 that the rocks on both asteroids may have very low thermal conductivities. Recently, Grott et al. (2019) determined that the boulder on the surface of Ryugu has a thermal conductivity in the 577 578 range of 0.06–0.16 W m-1 K-1, based on measurements by the MARA radiometer aboard the 579 Hayabusa2 MASCOT lander. If the particulates that compose the regolith in finer-particulate 580 regions have similarly low thermal conductivity values, the non-isothermal correction factor 581 described here would be necessary to correctly interpret the surface thermal inertia values. As an 582 illustrative example, we performed a particle size inversion using a hypothetical regolith thermal 583 inertia value of 200 J m-2 K-1 s-1/2 for Bennu (Figure 11). This value falls near the low end of 584 thermal inertia values so far determined for Bennu (Rozitis et al., 2019), which could be 585 indicative in some cases of particulate regoliths. To avoid model bias, we used three different 586 models to produce particle size predictions for this thermal inertia value, where the thermal 587 conductivity of the individual particles (k_m) is allowed to vary. We assume that particle density 588 must also vary with k_m due to changes in microporosity within the regolith particles. Following 589 the work by Grott et al. (2019), we use the average results from two models for meteorite 590 thermal conductivity as a function of porosity to determine the regolith particle microporosity 591 that would correspond to each x-axis value of k_m (Henke et al., 2019; Flynn et al., 2019). Density 592 is then calculated by assuming an average CM meteorite grain density (2960 kg m-3, Flynn et al., 593 2018). The predicted particle sizes are shown using the three models with and without the non-

isothermality correction (Equation 2) applied to the radiative thermal conductivity term. For

595 comparison, the thermal conductivity of the Cold Bokkeveld CM2 chondrite meteorite (Opeil et 596 al. 2010) and the boulder on Ryugu (Grott et al., 2019) are included as vertical line and a

al. 2010) and the boulder on Ryugu (Grott et al., 2019) are included as vertical line and a
 vertical, gray bar. Finally, the diurnal skin depth (i.e. the approximate depth at which the

amplitude of the thermal wave is attenuated by a factor of 1/e) for a 200 J m₋₂ K₋₁ s_{-1/2} thermal

599 inertia surface is shown as a thick gray line. The skin depth is calculated by:

600 (Eq. 7)

$$\delta = \frac{TI}{\rho c_p} \sqrt{\frac{P}{\pi}}$$

602 The rotation period, *P*, for Bennu is 15466 seconds (Lauretta et al., 2019), thermal inertia, *TI*, is

assumed at 200 J m⁻² K⁻¹ s^{-1/2}, specific heat, c_p , is 750 J kg⁻¹ K⁻¹ (Biele et al., 2019), and bulk

604 density, ρ , is estimated as a function of k_m , using the average of two models by Henke et al.

605 (2016) and Flynn et al. (2018) (see Methods section in Grott et al., 2019), assuming a grain

density of 2960 kg m-3 (Flynn et al., 2018) and a regolith macroporosity of 0.40.

607



608



611 up the regolith particles (k_m). Three regolith thermal conductivity models are used, both without

and with the use of the non-isothermal correction factor, to make particle size predictions. For

613 simplicity, only one macroporosity (0.40) is considered here. Increasing the assumed porosity

614 would have the effect of further increasing the predicted particle diameters. The predicted diurnal

skin depth is shown as a thick, gray line. Two reference k_m values are displayed with vertical

616 lines/bars: The Cold Bokkeveld (CM2) meteorite (Opeil et al., 2010) and the Ryugu boulder

617 examined by the MARA radiometer data (Grott et al., 2019). Model input values:

618 macroporosity=0.40; specific heat =750 J kg-1 K-1 (a); particle density is a function of thermal

619 conductivity, using the average of two models (b,c) for meteorite thermal conductivity vs

620 microporosity and assuming an average CM grain density=2960 kg m-3 (c); surface

621 energy= 0.032 Jm_{-2} (d); emissivity=1.0; Bennu mid-latitudes surface acceleration= $40 \mu m s_{-2}$ (e);

Poisson's ratio=0.27 (f); Young's Modulus=5.63e9 Pa (f); mean burial depth=10 mm; Sakatani

623 model tunable solid contact conductivity parameter ξ =0.63 (d); tunable radiative conductivity 624 parameter ζ =0.85 (d). References for model inputs: aBiele et al. (2019), bHenke et al. (2016).

624 parameter ζ=0.85 (d). References for model inputs: ^aBiele et al. (2019), ^bHenke et al. (2016), 625 cFlynn et al. (2018), ^dSakatani et al., (2018), ^eScheeres et al. (2019), ^fA.R. Hildebrand (personal

626 communication, 2018), measured values for Tagish Lake simulant.

627

628

629 The diurnal skin depth line in Figure 11 can be considered an approximate upper cutoff 630 for the validity of the particle size determination. This is based on the well-known idea that 631 regoliths composed of particles that that are much larger than the diurnal skin depth are expected 632 to behave thermally like solid rock (e.g. Christensen, 1986). Particle size predictions that exceed 633 the diurnal skin depth should be considered indeterminate, such that the particles could be *any* 634 size larger than the approximate diurnal skin depth. Interestingly, we see in Figure 11 that if the 635 non-isothermality effect is ignored, one might conclude that a thermal inertia of 200 J m-2 K-1 s- $\frac{1}{2}$ is consistent with effective particle diameters in the range of ~10–25 mm, depending on 636 assumptions of k_m , density, and macroporosity. However, once non-isothermality is accounted 637 638 for, the predicted particle size increases markedly as k_m is reduced. If the particles have a k_m 639 value that is similar to the Ryugu boulder from Grott et al. (2019) (grey shaded vertical bar), then 640 one can only conclude that the regolith is predominantly composed of particles larger than ~15 641 mm. It very well could just be boulders or a bedrock. Conversely, if we assume that the regolith 642 particles have a k_m that is equivalent the Cold Bokkeveld meteorite, one could conclude that this 643 thermal inertia observation is consistent with a regolith with an effective particle size near 10 644 mm.

In addition to our findings related to non-isothermality, we have also found that a polydisperse particulate generally has a radiative thermal conductivity that is equivalent to a monodisperse particulates with some effective particle diameter (Figure 8, solid line), at least in the case of particulates that follow cumulative power law SFDs. We also found that the effective particle diameter can be used in Equation 1 to calculate Λ_s for the determination of the nonisothermality correction factor, f_k , for a polydisperse regolith.

651 Figure 10 compares the effective particle diameters for 16 polydisperse geometries to 652 various expressions for the mean and median particle diameter in a particle size mixture. The 653 best correspondence, nearly 1:1, is found with the Sauter mean particle diameter. The Sauter 654 mean diameter may be physically interpreted as the diameter that could be used to produce a 655 monodisperse population of spheres that has the same surface area and the same volume (but not 656 the same number of spheres) as the polydisperse sphere population (Kowalczuk & Drzymala, 2016). In the context of our work, this means that the radiative thermal conductivity of a 657 658 polydisperse population of spheres is the same as the radiative thermal conductivity of a 659 population of monodisperse spheres that has the same total mass (or volume) and same total 660 surface area—suggesting that the total surface area present within a particulate volume is an

661 important control on the radiative thermal conductivity. This is perhaps not surprising, given that 662 heat diffusion through opaque particulates is largely limited by radiative heat transfer between the particle surfaces. If surface area is indeed a control, then replacing the spheres with any other 663 664 particle shape would have the effect of increasing the total surface present within the system (if porosity is kept the same) and thus should decrease the radiative thermal conductivity. This idea 665 is consistent with experimental datasets by Sakatani et al. (2017), in which they found that 666 monodisperse, angular basaltic particles from the JSC-1A lunar simulant had a lower radiative 667 668 thermal conductivity than spherical glass particles with equivalent diameters. Whether this is truly due to changes in surface area or instead to some other factor, such as changes in the length 669 670 scales of the void spaces, is an interesting subject of investigation for a future study.

671 In Figure 10, there appears to also be a nearly 1:1 correspondence between effective particle diameter and volumetric median particle size. This correlation supports experimental 672 results by Sakatani et al. (2018), who found that the thermal conductivity of the JSC-1 lunar 673 674 regolith simulant was equivalent to the volumetric median particle size for both radiative and 675 solid thermal conductivity terms. However, the particle diameters deviate from this trendline in 676 Figure 10 by up to $\pm 15\%$. As such, thermal inertia measurements of a regolith with an unknown 677 SFD could be used to estimate the volumetric median particle size of the regolith to within about 678 $\pm 15\%$ of the true value. One could also use thermal data to estimate the Sauter mean particle size 679 with a higher degree of accuracy, but the volumetric median particle size is perhaps a more 680 useful metric because of its more common use in statistical reports.

681 Although these findings related to regolith particle SFDs might aid us in interpreting regolith properties from thermal inertia, we must again point out the importance of the 682 683 relationship between regolith particle size and diurnal skin depth, particularly for analyses on fast rotators with apparently low thermal conductivity boulders like Bennu and Ryugu. If the 684 685 effective particle size in some region is larger than the diurnal skin depth, the apparent thermal 686 inertia is expected to be that of the solid rock, thus precluding particle size determination from 687 thermal data. As seen in Figure 11, even the lower end of the thermal inertia values on Bennu 688 $(200 \text{ J} \text{ m}_{-2} \text{ K}_{-1} \text{ s}_{-1/2})$ corresponds to particle size predictions that approach or exceed this cutoff. 689 Although this complicates or even prevents the interpretation of regolith thermal inertia in terms 690 of particle size, it might present an opportunity to predict the thermal properties of the individual 691 regolith particles: The OSIRIS-REx spacecraft will obtain very high-resolution photos and 692 (ideally) ride-along OTES and OVIRS spectra of selected sample site. Should the site contain 693 abundant fine-particulate regolith, the regolith particle SFD, particle shape, and packing 694 configuration could be constrained from these data, providing a valuable ground truth for thermal 695 models. An analysis like the one shown in Figure 11 could be repeated with constraints on the 696 effective particle size in order to estimate the value of k_m . If k_m is low, then perhaps the regolith 697 particles have a high degree of microporosity and are derived from the low density/conductivity 698 boulders. Conversely, if *k_m* is high—perhaps even higher than the surrounding boulders—then 699 this could indicate that the regolith particles are stronger clasts weathered out of a weaker, lower 700 density/conductivity boulder matrix. Either scenario would provide interesting information 701 regarding the nature of Bennu's boulders and regolith formation processes.

702703 6 Conclusions

704

In this work, we build upon the fundamental knowledge of particulate regolith thermal
 properties in an effort to improve our ability to infer the physical properties (namely particle size

distribution) of regolith from remote thermal measurements. This work was motivated by the
ongoing OSIRIS-REx mission at asteroid Bennu. Radiative thermal conductivity was chosen as
the focus here owing to the dominance of the radiative heat transfer (relative to heat conduction
through the contacts between particles) for coarse, centimeter-scale regolith, which is the
material of interest for sampling on Bennu.

712 We presented a new thermophysical model for asteroid regolith where the individual 713 regolith particles are represented as randomly packed spheres in a FE mesh framework. Heat 714 conduction and surface-to-surface radiation are modeled in a steady-state configuration to 715 determine the bulk conductivity properties of the particulates. With this model, we determined 716 the radiative thermal conductivity of a series of polydisperse particle geometries with cumulative 717 power-law SFDs. We found that the thermal conductivity of the particulate material can have a 718 very strong influence on the radiative thermal conductivity, particularly when material thermal 719 conductivity (k_m) is very low, the temperature is high, and/or particles are large, owing to non-720 isothermality within individual particles (Figure 8). When this non-isothermality is negligible, 721 the radiative thermal conductivity of polydisperse geometries scales normally with the cube of 722 the temperature, as is also the case for monodisperse particulates. When non-isothermality is 723 substantive, the radiative thermal conductivity has a weaker temperature dependence. The 724 magnitude of non-isothermality for polydisperse and monodisperse particulates is larger than 725 previously predicted, and new correlation coefficients ($a_1 = -0.568$, $a_2 = 0.912$, $a_3 = 0.765$, $a_4 =$ 726 1.035) were provided for a correction factor (Equation 2) for the radiative thermal conductivity. 727 This correction factor can be applied to any model for regolith thermal conductivity (e.g. 728 Sakatani et al., 2017; Gundlach and Blum, 2013) by multiplying the model-predicted radiative 729 thermal conductivity term by f_k . If the regolith particles on Bennu have very low thermal 730 conductivity, particle predictions from thermal inertia could be notably underestimated if non-731 isothermality is not taken into account in the regolith thermal conductivity model.

732 Finally, we found that the radiative thermal conductivity for each polydisperse simulation 733 is identical to that of a monodisperse simulation with some effective particle diameter. A 1:1 734 correspondence exists between the effective particle diameter determined for the numerical 735 results for each polydisperse geometry and the Sauter mean particle diameter (Figure 10). We 736 conclude that amount of surface area per unit mass and volume within a particulate geometry is 737 closely related to the total radiative conductivity, leading to the prediction that non-spherical 738 particles should have lower radiative thermal conductivity values. The effective particle 739 diameters of the mixtures also correspond within $\pm 15\%$ to the volumetric median particle 740 diameter, enabling a convenient means of interpreting thermophysical data on the regolith of 741 asteroid Bennu and other airless bodies, particularly when ancillary information about the 742 regolith such as cumulative power-law slope and maximum particle size can be gained from 743 image data.

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- 745

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747

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758

759 **Appendix A**

760

761 For the radiation validation test, we define a steady-state configuration with two 762 concentric spherical shells with surface emissivity values of unity. We number the four surfaces 763 as 1–4, starting from the inner surface of the inner spherical shell (Figure A1). Fixed temperatures are defined at surfaces 1 and 4, while surfaces 2 and 3 exchange energy via 764 radiation. Once final steady state is achieved, the final temperatures of surfaces 2 and 3 are 765 related to the net energy transfer between surfaces 2 and 3 by: 766

767

 $Q = A_2 \sigma f_{2-3} (T_2^4 - T_3^4)$ (1)

770 where Q is energy transfer in watts, A_2 is the area of surface 2, f_{2-3} is the view factor or

configuration factor for surface 2 to surface 3, which in this case is equal to one, σ is the Stefan-771

772 Boltzmann constant, and T is the temperature of the surface denoted by the subscript.







775 Figure A1. Hollow spheres radiation validation case. The four surfaces referenced in the text are 776 labeled. 777

778 To describe steady-state heat conduction through the spherical shells, we start with the 779 one-dimensional form of the heat equation in spherical coordinates: 780

780
781
$$\frac{1}{r^2} \frac{d}{dt} \left(r^2 \frac{dT}{dr} \right) = 0$$
 (2)

782

783 The first integral gives:

784

$$785 r^2 \frac{dT}{dr} = C_a (3)$$

787 where C_a is in integration constant. From Fourier's Law:

788 789

$$Q = -kA\frac{dT}{dr}$$

790

791 we determine C_a : 792

 $C_a = \frac{-Qr^2}{kA}$

Taking the second integral of the heat equation (Equation 2) gives:

796 797

798

$$T(r) = -\frac{C_a}{r} + C_b \tag{6}$$

For the case of the inner spherical shell, we can evaluate this equation at r_1 and r_2 to determine the value of C_b :

(4)

(5)

801

802	$T_1 = \frac{-C_a}{r_1} + C_b$	
803	$T_2 = \frac{-\bar{C}_a}{r_2} + C_b$	
804	$C_b = T_1 + \frac{c_a}{r_1} = T_2 + \frac{c_a}{r_2}$	(7)
805		
806	We can substitute this into Equation	6 to find:
807	$T(r) = T_1 + C_a \left(\frac{1}{r_1} - \frac{1}{r}\right)$	(8)
808		
809	Evaluating at $r = r_2$ provides an expr	ession for <i>T</i> ₂ :
810		
811	$T_2 = T_1 - \frac{Qr_2^2}{kA_2} \left(\frac{1}{r_1} - \frac{1}{r_2}\right)$	(9)
812		
813	Similarly, an expression for T ₃ is fou	nd to be:
814		
815	$T_3 = T_4 - \frac{Qr_3^2}{kA_3} \left(\frac{1}{r_4} - \frac{1}{r_3}\right)$	(10)

816
817 Substituting Equation 9 and 10 into Equation 1 gives us the final expression for net heat transfer
818 in the system:

819
$$Q = A_2 \sigma \left[\left(T_1 - \frac{Qr_2^2}{kA_2} \left(\frac{1}{r_1} - \frac{1}{r_2} \right) \right)^4 - \left(T_4 - \frac{Qr_3^2}{kA_3} \left(\frac{1}{r_4} - \frac{1}{r_3} \right) \right)^4 \right]$$
(11)
820

820

Equation 11 may be solved for Q numerically. In our work, we used the *fsolve()* function within the SciPy Python library. Once Q is found, the values of T_2 and T_3 are found from Equations 9 and 10 and can be compared to the results of the numerical test when steady state is achieved.

824

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