# Approximating 3D Models of Planetary Evolution in 2D: A Comparison of Different Geometries

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# Abstract

Regardless of the steady increase of computing power during the last decades, 3D numerical models continue to be used in specific setups to investigate the thermochemical convection of planetary interiors, while the use of 2D geometries is still favored in most exploratory studies involving a broad range of parameters. The 2D cylindrical and the more recent 2D spherical annulus geometries are predominantly used in this context, but the extent to how well they reproduce the 3D spherical shell in comparison to each other, and in which setup, has not yet been extensively studied. Here we performed a thorough and systematic study in order to assess which 2D geometry reproduces best the 3D one. In a first set of models, we investigated the effects of the geometry on thermal convection in steady-state setups while varying a broad range of parameters. Additional thermal evolution models of three terrestrial bodies, respectively Mercury, the Moon, and Mars, which have different interior structures, were used to compare the 2D and 3D geometries. Our study shows that the spherical annulus geometry improves results compared to cylindrical geometry when reproducing 3D models. Our results can be used to determine for which setup acceptable differences are expected when using a 2D instead of a 3D geometry.

# Approximating 3D Models of Planetary Evolution in 2D: A Comparison of Different Geometries

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# 5 Key Points:

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6	• Interior dynamics models using the 2D spherical annulus geometry match the re-
7	sults of a 3D spherical shell better than the 2D cylinder.
8	• The difference between 2D and 3D geometries decreases when models are heated
9	from below by the core and from within by radioactive elements.
10	• The spherical annulus shows negligible differences to 3D for the thermal evolution
11	of Mercury and the Moon, and acceptable values for Mars.

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# 12 Abstract

Regardless of the steady increase of computing power during the last decades, 3D nu-13 merical models continue to be used in specific setups to investigate the thermochemi-14 cal convection of planetary interiors, while the use of 2D geometries is still favored in most 15 exploratory studies involving a broad range of parameters. The 2D cylindrical and the 16 more recent 2D spherical annulus geometries are predominantly used in this context, but 17 the extent to how well they reproduce the 3D spherical shell in comparison to each other, 18 and in which setup, has not yet been extensively studied. Here we performed a thorough 19 and systematic study in order to assess which 2D geometry reproduces best the 3D one. 20 In a first set of models, we investigated the effects of the geometry on thermal convec-21 tion in steady-state setups while varying a broad range of parameters. Additional ther-22 mal evolution models of three terrestrial bodies, respectively Mercury, the Moon, and 23 Mars, which have different interior structures, were used to compare the 2D and 3D ge-24 ometries. Our study shows that the spherical annulus geometry improves results com-25 pared to cylindrical geometry when reproducing 3D models. Our results can be used to 26 determine for which setup acceptable differences are expected when using a 2D instead 27 of a 3D geometry. 28

# <sup>29</sup> Plain Language Summary

In geodynamic modeling, numerical models are used in order to investigate how 30 31 the interior of a terrestrial planet evolves from the earliest stage, after the planetary formation, up to present day. The mathematical equations that are used to model the phys-32 ical processes in the interior of rocky planets are discretized and solved using geomet-33 ric meshes. The most commonly used geometries are the 3D spherical shell, the 2D cylin-34 der, and the 2D spherical annulus. While being the most accurate and realistic, the 3D 35 geometry is expensive in terms of computing power and time of execution. On the other 36 hand, 2D geometries provide a reduced accuracy but are computationally faster. Here 37 we perform an extensive comparison between 2D and 3D geometries in scenarios of in-38 creasing complexity. The 2D spherical annulus geometry shows much closer results to 39 the 3D spherical shell when compared to the 2D cylinder and should be considered in 40 2D modeling studies. 41

# 42 **1** Introduction

Geodynamic modeling is a powerful approach to investigate the dynamics of the 43 mantle and lithosphere of terrestrial planets and to explore the evolution of their inte-44 rior that is not directly observable. Such models vary in their complexity and often em-45 ploy different geometries to investigate physical processes such as mantle melting and 46 cooling, and the generation of a magnetic field. When using these models to interpret 47 specific observations of the Earth and other planets, care must be taken in particular for 48 the choice of geometry (see Noack & Tosi, 2012, for an overview of geometries), as this 49 may significantly impact quantities such as the mantle temperature, the convection ve-50 locity, and the heat flux of the simulations. 51

The role of two-dimensional geometry studies in the field of thermochemical man-52 tle convection modeling is still predominant despite an ever-increasing computing power. 53 Although the formulation of 3D grids has seen improvements in previous years with the 54 Yin-Yang grid (Kageyama & Sato, 2004) and the spiral grid (Hüttig & Stemmer, 2008a) 55 among others; simulations with a full spherical shell geometry remain highly expensive 56 in terms of computational power, hence making them inappropriate to study broad ranges 57 of parameters or conduct large exploratory studies. As an alternative, geometrical ana-58 logues to the 3D spherical shell have been extensively used, namely the 2D spherical axi-59 symmetric (van Keken & Yuen, 1995) and the more popular cylindrical geometry (Jarvis, 60 1993). The 2D axi-symmetric geometry has been used in earlier studies of mantle con-61

vection (e.g., van Keken & Yuen, 1995; Jarvis et al., 1995), but in addition to the arti-62 ficial boundaries formed by the poles which trap down- and up-wellings, an asymmetry 63 between the polar and the equatorial regions exists (van Keken, 2001). The cylindrical 64 geometry on the other hand, while resolving the problems of the artificial boundaries at 65 the poles imposed by the axi-symmetric geometry, still exhibits an important drawback. 66 The ratio of the two surfaces (the planetary surface and the core surface) is different in 67 the cylindrical geometry compared to the spherical shell. This leads to a mismatch in 68 heat flux values between these geometries, as the heat flux of the core mantle boundary 69 (CMB) is underestimated and the surface heat flux is overestimated when comparing to 70 a spherical shell with the same ratio between the core and planet radius (i.e., radius ra-71 tio). 72

In order to mitigate this problem, van Keken (2001) introduced a re-scaling of the 73 2D cylindrical geometry such that the ratio of outer and inner areas of the cylinder matches 74 the ratio obtained for the spherical shell. This scaling, however, while correcting the sur-75 face ratio discrepancy of the cylinder, still uses the volume of a cylinder. Additionally, 76 this re-scaling creates an artificially smaller core, which in turn modifies the convection 77 pattern in the mantle, leading for example to a crowding of the plumes near the CMB, 78 a behavior that would not be observed in a 3D spherical shell, when using the original, 79 non-scaled radii. 80

To overcome this major drawback of the cylindrical geometry, another 2D geom-81 etry called "spherical annulus" has been proposed by Hernlund and Tackley (2008). This 82 geometry effectively uses a second degree of curvature and considers the same surfaces 83 and volumes as the 3D geometry. Since no re-scaling is necessary for this geometry, it 84 keeps the same radius ratio as the 3D one. In the study of Hernlund and Tackley (2008), 85 the spherical annulus showed promising results to approximate the 3D spherical geom-86 etry with mean temperature and Nusselt number well reproduced for steady-state ther-87 mal convection calculations. While these results a highly valuable, there are only for the 88 case of an Earth-like radius ratio and only consider thermal convection simulations in 89 the Boussinesq approximation. 90

More recently, Guerrero et al. (2018) performed a more extensive study with the spherical annulus for stagnant lid convection models and compared the temperature distribution between the spherical annulus and the spherical shell. However, an extensive study investigating the ability of the 2D spherical annulus to reproduce results obtained in a 3D spherical shell and a systematic comparison with the 2D cylinder for various setups has never been conducted so far.

In this study, we present simulations of thermal convection in the 2D spherical an-97 nulus and compare the results to the 2D cylinder and the 3D spherical shell. In a first part we focus on simple steady-state convection models using the Boussinesq approxi-99 mation. We vary the Rayleigh number, the radius ratio, and the heating mode for iso-100 viscous cases and run additional temperature-dependent viscosity models to determine 101 which of the two 2D geometries (i.e., cylinder or spherical annulus) is able to best re-102 produce the 3D results. The set of equations that were used for this comparison are de-103 scribed in Section 2.1, the grid geometries are displayed in Section 2.2, and a descrip-104 tion of the cases investigated here is available in Section 2.3. A detailed analysis of the 105 results is presented in Section 2.4. 106

In a second step, we run more complex simulations of thermal evolution with the same geometries in three separate scenarios. We use Moon-like, Mars-like, and Mercurylike thermal evolution models to investigate how well the 2D spherical annulus reproduces the results of the 3D spherical shell geometry. The three planetary bodies were chosen since they cover a wide range of interior structures and they are all thought to have been in a stagnant lid regime over their entire thermal history, which makes them comparable in terms of their tectonic regime (Breuer & Moore, 2015). In Section 3.1 we

list the equations used for the thermal evolution models. A description of the employed 114 parameters and setup of the models is given in Section 3.2. The results are described in 115 Section 3.3. A discussion of the steady-state and thermal evolution models is presented 116 in Section 4, followed by conclusions in Section 5. 117

#### 2 Steady-state mantle convection 118

In a first set of calculations we focus on the comparison between steady-state cal-119 culations in 2D and 3D geometries. For this purpose we test a large number of param-120 eter combinations for isoviscous models and temperature-dependent viscosity. 121

#### 2.1 Mathematical model 122

Fully dynamical models of mantle convection allow us to investigate the spatial and 123 temporal evolution of mantle flow. These models solve the conservation equations of mass, 124 momentum, and energy. Here, the conservation equations are scaled using the mantle 125 thickness D as length scale, the temperature drop across the mantle  $\Delta T$  as temperature 126 scale and the thermal diffusivity  $\kappa$  as time scale. A Table listing the scaling factors is 127 available in the Supplementary Information, SI (Table S1). By assuming a Newtonian 128 rheology, an infinite Prandtl number, and considering the Boussinesq approximation (Schubert 129 et al., 2001; van Zelst et al., 2022), the non-dimensional conservation equations read: 130

$$\mathbf{u} = 0, \tag{1}$$

$$\nabla \cdot \mathbf{u} = 0, \qquad (1)$$
$$\nabla \cdot \left( \eta \left( \nabla \mathbf{u} + (\nabla \mathbf{u})^T \right) \right) + RaT \mathbf{e}_r - \nabla P = 0, \qquad (2)$$

$$\frac{DT}{Dt} - \nabla^2 T - H = 0. ag{3}$$

In Equations 1 – 3, **u** is the velocity vector,  $\eta$  is the viscosity, T is the temperature, 131  $\mathbf{e}_r$  is the radial unit vector, P is the dynamic pressure, and t is the time. 132

The parameter Ra denotes the thermal Rayleigh number, a non-dimensional num-133 ber, which controls the vigor of the convection in the mantle. H is the internal heating 134 rate of the mantle that is given by  $\frac{Ra_Q}{Ra}$ , where  $Ra_Q$  denotes the Rayleigh number as-135 sociated with internal heating. The Rayleigh numbers Ra and  $Ra_Q$  read: 136

$$Ra = \frac{\rho_{ref}g_{ref}\alpha_{ref}\Delta TD^3}{\kappa_{ref}\eta_{ref}}, \quad RaQ = \frac{\rho_{ref}^2g_{ref}\alpha_{ref}HD^5}{\kappa_{ref}\eta_{ref}k_{ref}}, \tag{4}$$

where  $\rho_{ref}$  is the reference density,  $g_{ref}$  is the reference gravitational acceleration,  $\alpha_{ref}$ 137 is the reference thermal expansivity,  $\kappa_{ref}$  is the reference thermal diffusivity,  $\eta_{ref}$  is the 138 reference viscosity,  $k_{ref}$  is the reference thermal conductivity, and H is the internal heat-139 ing rate in W/kg. 140

For the steady-state models, we use a constant or temperature-dependent viscos-141 ity that follows the Frank-Kamenetskii approximation (Frank-Kamenetskii, 1969), which 142 is a linearized form of the Arrhenius law: 143

$$\eta(T) = \exp(\Delta \eta_T (T_{ref} - T)), \tag{5}$$

The parameter  $\Delta \eta_T$  is the viscosity contrast due to temperature and  $T_{ref}$  is the 144 reference temperature at which a non-dimensional viscosity equal to 1 is attained. For 145 the thermal evolution simulations presented further in this study, we use another parametriza-146 tion of the viscosity (Eq. 9), which is discussed more in-depth in the Section 3.1. 147



Figure 1: Representation of a cell of the spherical annulus geometry, in red, its effective volume. The cylindrical geometry is represented in blue, on the equatorial plane. The red area represented corresponds to the intersection of the spherical annulus cell with the equatorial plane. When looking at the grid from a polar point of view, its visualization becomes thus indistinguishable from the cylindrical cell.

# <sup>148</sup> 2.2 Grid geometries

We use the numerical code Gaia (Hüttig & Stemmer, 2008a, 2008b; Hüttig et al., 149 2013) to model the mantle convection in the interior of rocky planets. Gaia solves the 150 conservation equations (Eq. 1-3) in their dimensionless form in 2D and 3D geometries. 151 For the 2D geometry, we use both the classical cylindrical geometry (van Keken, 2001) 152 and the spherical annulus geometry following the approach of Hernlund and Tackley (2008). 153 In the 2D cylindrical geometry, the areas and volumes of the grid cells are typically for-154 mulated using the equations for a cylinder; however, what makes the particularity of the 155 spherical annulus geometry, is the addition of a virtual thickness to the cylindrical ge-156 ometry which varies with the radius r. Thus the spherical annulus has a second degree 157 of curvature, and uses an effective 3-dimensional formulation for the areas and volumes, 158 as represented on Figure 1 (a more detailed description of the spherical annulus geom-159 etry is available in Section S3 of the SI). 160

The 2D cylindrical geometry is scaled according to the scaling introduced by van Keken (2001), where the inner and outer radii of the cylinder grid (i.e., the core radius and the planetary radius, respectively) are changed such that the ratio between the outer and inner areas of the cylinder matches the ratio obtained in a 3D spherical shell geometry. The equations used to correct the inner and outer radii of the cylinder are the fol166 lowing:

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$$\frac{r_{oc}}{r_{ic}} = \frac{r_{os}^2}{r_{is}^2}, \qquad r_{oc} - r_{ic} = r_{os} - r_{is}, \qquad (6)$$

where  $r_{ic}$  and  $r_{oc}$  are the inner and the outer radius of the cylinder, respectively. The inner and outer radii of the spherical shell are denoted by  $r_{is}$  and  $r_{os}$ , respectively. In the following, we will refer to this type of geometry that considers the rescaling of the inner and outer radii as the "scaled cylinder geometry".

# 2.3 Case definition

In the first part of this study, we performed steady-state simulations in order to 172 investigate the effects of the ratio of the inner to outer radius and of heating modes on 173 the results obtained with the 2D cylindrical, 2D spherical annulus, and 3D spherical shell 174 geometry. Our aim is to compare 2D and 3D geometries and determine for which sce-175 narios does the 2D spherical annulus give closer results to the 3D compared to the 2D 176 cylinder. To this end, we use models heated from below (purely bottom-heated), from 177 within (purely internally-heated), and from both below and within (mixed heated). We 178 use an initial random perturbation of the temperature field with an amplitude of 5%, 179 vary the Rayleigh number Ra of our simulations from  $10^4$  up to  $10^8$ , and the radius ra-180 tio f from 0.2 to 0.8 for our isoviscous setup. 181

For the 2D geometries, we use between  $1.1 \times 10^4$  and  $6.7 \times 10^4$  grid points for low Rayleigh number simulations and between  $4.8 \times 10^4$  and  $4.1 \times 10^5$  for simulations with a Rayleigh number higher than  $10^6$ . For the 3D geometries, we use between  $2.04 \times 10^6$ and  $2.94 \times 10^6$  grid points. A more in depth description of each grid and its associated lateral and radial resolution is available in the SI. A short comparison of our results to the ones of Hernlund and Tackley (2008) for isoviscous steady-state cases is presented in Section S4 of the SI.

Each mesh has a prescribed temperature and free-slip velocity as boundary conditions. The temperature of the upper boundary  $T_{surf}$  is set to zero, while the one of the lower boundary is set to one for the bottom heated and mixed heated cases. For the purely internally heated cases we use a zero heat flux at the core-mantle boundary.

The simulations are ran until a statistical steady-state is reached. Then, output quantities such as the average temperature, root-mean-square velocity, and top temperature gradient are computed using an average over the last 10% of the simulation. While for purely steady-state models this is the same as taking the last output, for quasi steadystate time-dependent or periodic models this ensures to retrieve representative average values. The top temperature gradient here is the temperature gradient at the top of the domain, calculated between the last two shells of the grid.

An additional, more complex set of simulations includes the effect of the temper-200 ature dependence of the viscosity, and leads to the formation of a stagnant lid at the top 201 of the convecting domain. These simulation represent simplified Moon-like (f = 0.2), 202 Mars-like (f = 0.5), and Mercury-like (f = 0.8) scenarios. We use here thermal and 203 radiogenic Ra numbers with values similar to those expected for planetary mantles, i.e., 204  $Ra = 5 \times 10^6$  and  $Ra_Q = 5 \times 10^7$  (see values of Ra and  $Ra_Q$  in Table 1). We use the 205 Frank Kamenetskii parametrization for the viscosity (Eq. 5) and set a viscosity contrast 206  $\Delta \eta_T$  to 10<sup>8</sup> at a reference temperature  $T_{ref}$  of 0.5 to ensure that we are in a stagnant 207 lid convection regime. In this setup, the total number of nodes used for the 2D grids lies 208 between  $4.8 \times 10^4$  and  $2.8 \times 10^5$ ; while for the 3D simulations, the total number of nodes 209 is  $2.9 \times 10^6$ . 210

In total, we run 180 isoviscous simulations and 36 temperature-dependent viscosity cases. All parameters and the grid resolutions for these steady-state simulations are listed in Table S2 in the SI.

# 214 **2.4 Results**

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## 2.4.1 Isoviscous convection

For the first set, consisting of isoviscous simulations, we provide a thorough and systematic comparison between the 3D spherical grid and the two 2D geometries, namely the spherical annulus and the cylindrical geometry. A summary of the comparison is shown in Figure 2.

Here, the analysis of the 180 simulations has been summarized into three subplots 220 one for each heating mode. Each subplot contains two rows showing for each the annu-221 lus geometry (first row) and the scaled cylindrical geometry (second row), respectively, 222 the relative error to the 3D results. The computation details of the relative error can be 223 found in the SI (Section S5) along with tables containing the values for each simulation 224 in CSV format. Figure 2 shows that the mean domain temperature of the 3D geome-225 try is more accurately reproduced by the spherical annulus geometry than by the cylin-226 drical one in every heating mode, up to values of  $Ra = 10^7$ . This difference is even more 227 noticeable in the low radius ratiosetups (i.e., f = 0.2 and 0.4), which can be seen for 228 the purely bottom heated and mixed heated scenarios. We also see for the purely inter-229 nal heated cases and high Rayleigh number cases (i.e.,  $Ra = 10^7$  and  $Ra = 10^8$ ) that 230 this difference is even more dramatic with an overestimation of the temperature in the 231 cylindrical geometry by up to  $\sim 20\%$  for the small a radius ratio (i.e., f = 2) and re-232 duces to only a few percent in the spherical annulus. 233

In the case of the root mean square velocity, we see a general increase of the ac-234 curacy with the spherical annulus geometry, however this increase is less pronounced than 235 what is observed for the mean temperature. We see a slightly better match for the purely 236 bottom heated and mixed heated setups, where simulations with  $Ra < 10^7$  go from be-237 ing slightly underestimated by the cylinder to slightly overestimated by the annulus. How-238 ever, the cases with  $Ra > 10^7$  show a net improvement, with an underestimation de-239 creasing for all the cases with a radius ratio higher than 0.2. For the setup with a purely 240 internal heating, however, almost no improvement is visible, with the notable exception 241 of the simulation with a  $Ra = 10^8$  and a radius ratio of 0.2 being overestimated by  $\sim$ 242 40% in the case of the cylinder, which turns to be overestimated only by  $\sim 20\%$  in the 243 case of the spherical annulus. 244

In comparison to the cylinder, the spherical annulus, gives less conclusive results 245 for the top temperature gradient. We can see an improvement in case of small radius ra-246 tios (i.e., f = 0.2) with either purely internal heating or mixed heating, or in the case 247 of high Rayleigh numbers (i.e.,  $Ra \ge 10^7$ ) for purely internal heated cases. Otherwise, 248 for the majority of the setups and heating modes, the spherical annulus does not show 249 significant improvement in reproducing the 3D values compared to the scaled cylindri-250 cal geometry. A comparison of the temperature gradient at the top of the mantle shows 251 that the spherical annulus is hardly able to reproduce the 3D values more accurately than 252 the scaled cylindrical geometry, with the notable exception of low radius ratios of around 253 f = 0.2. 254

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# 2.4.2 Stagnant lid convection

In the second part of the steady-state simulations, we modeled stagnant lid convection while varying the heating mode, the radius ratio, and the geometry in order to study the accuracy of the spherical annulus geometry (see SI, Table S2). In this type of setup, where the viscosity is strongly dependent on temperature, the convection is expected to operate in a stagnant lid regime. This rigid layer that forms at the top of the domain restricts convective heat transfer to the deep interior.

The results are summarized in Figure 3, where we report the relative error of the 263 2D cylindrical, 2D scaled cylindrical, and 2D spherical annulus geometry to the 3D spher-264 ical shell. Here we inspect the mean temperature, the root mean square velocity, the top



Figure 2: Averaged computed relative error to the 3D geometry with 3 different heating modes, i.e., purely basal heated (top row), purely internal heated (middle row), or mixed heated (bottom row) for steady-state isoviscous convection simulations. For each heating mode the first line of plots shows the relative errors for the spherical annulus and the second line represents the scaled cylinder. The thermal Rayleigh number and internal Rayleigh number vary from  $10^4$  to  $10^8$  and the radius ratio from 0.2 to 0.8. The radius ratio indicated on the plot is the one corresponding to the reference 3D simulations. In the case of the cylinder, the radius ratio is scaled, thus a 0.2 radius ratio becomes 0.04 following the scaling formula from van Keken (2001) (eq. 6). For columns from left to right, relative error of the mean temperature, of the v<sub>rms</sub>, and of the top temperature gradient are shown. temperature gradient, and the stagnant lid thickness. For each simulation we use a Raof  $10 \times 10^6$  and  $Ra_O$  of  $10 \times 10^7$ .

In Figure 3, when considering purely basal heating, we see that the spherical an-267 nulus is overall better at reproducing the 3D values compared to the scaled and non-scaled 268 cylinder. The highest discrepancy is observed for the radius ratio f = 0.2, with > 50%269 of overestimation on average for the 2D geometries. For the spherical annulus, the mean 270 temperature matches best the one of the 3D spherical shell when the radius ratio increases, 271 an effect also seen for the  $v_{\rm rms}$ . The top temperature gradient does not follow this pat-272 273 tern, however, while the stagnant lid error is the lowest for f = 0.5. The highest difference to the 3D for the low radius ratio setups (f = 0.2) in the purely bottom heated 274 setup that we found in our models is in agreement with Guerrero et al. (2018). The study 275 by Guerrero et al. (2018) considered stagnant lid convection with only basal heating, and 276 observed that for small radius ratio setups, the spherical annulus would systematically 277 show a hotter temperature when compared to the 3D. This behavior is indeed confirmed 278 by our simulations, where we can observe that the different geometry of plumes between 279 the spherical annulus and the spherical shell create considerable differences in temper-280 ature in the low radius ratio and bottom heated simulations. Plumes in a 2D geometry 281 are rather sheet-like than column-like as they are in a 3D geometry. This leads to a warmer 282 temperature in the 2D geometries compared to the 3D as being the consequence of a topo-283 logical difference between flows in a spherical shell and spherical annulus, as explained 284 by Guerrero et al. (2018). Moreover, this difference is strongly accentuated for low ra-285 dius ratios, where the number of plumes is small and such geometrical effects significantly 286 affect the results. For a better illustration of this behavior we refer the reader to Fig-287 ure S5 of the SI. The increase of temperature differences with increasing f was also ob-288 served by Guerrero et al. (2018) and is confirmed by our results. 289

In the case of a purely internally heated case, we see that the annulus fares remark-290 ably better than the cylindrical geometries and that the average relative error of the mean 291 temperature, the  $v_{\rm rms}$ , and top temperature gradient diminish as the radius ratio decreases. 292 The highest radius ratio (i.e., f = 0.8) shows here the highest discrepancy between 2D 293 and 3D, with more than 50% and 20% of overestimation for the  $v_{rms}$  and the top tem-294 perature gradient respectively, while the stagnant lid is underestimated on average by 295 15%. When taking a closer look at the simulations, it appears that, the internal heat-296 ing simulations in 2D have a tendency to require more convective strength in order to 297 transport the same amount of heat in the domain compared to a 3D simulation, as al-298 ready shown in Hernlund and Tackley (2008). This peculiarity when investigating the 299 temperature and velocity distribution will apparently create a larger amount of down-300 wellings in the case of a 3D model for a given internal heating rate when compared to 301 a 2D one. This can be seen on the Figure S7 of the SI. 302

For cases heated both from below and from within (i.e., mixed heated cases), the spherical annulus is showing the best results for the mean temperature, the top temperature gradient, and the stagnant lid thickness when the radius ratio is the lowest (i.e., f = 0.2). For the highest radius ratio considered here (i.e., f = 0.8), the results obtained with the spherical annulus and the cylinder geometries show similar errors, with the exception of  $v_{rms}$  that seems to be best reproduced by the scaled cylinder geometry.

When combining purely basal heating with internal heating, the main discrepancy previously arising from the low radius ratio and purely basal heated simulations seems to be mitigated by the addition of internal heating. The difference in the temperature distribution between the spherical annulus and the spherical shell tends to disappear (see Figure S7 of the SI).

In summary, for the stagnant lid cases presented here, the mean temperature is overall better reproduced by the spherical annulus independently of the radius ratio or heating mode. Additionally, in the intermediate to low radius ratio simulations ( $f \le 0.5$ ), the spherical annulus can also reproduce the 3D velocities, the top temperature gradient, and the stagnant lid better than the cylinder geometry.



Figure 3: Averaged computed relative error to the 3D geometry with 3 different heating modes (i.e., purely basal heated, purely internal heated, and mixed heated) for steady-state convection simulations with a temperature dependent viscosity. The mean temperature of the domain, the root mean square velocity, the temperature gradient at the top of the domain, and the stagnant lid thickness are compared here. For each subplot analyzing the relative error in a given heating mode, every column represents a different geometry, namely the 2D cylinder, the 2D scaled cylinder, and the 2D spherical annulus. The thermal Rayleigh number is  $5 \times 10^6$ , the internal Rayleigh number is  $5 \times 10^7$ , and the investigated radius ratios are 0.2, 0.5, and 0.8.

# 320 **3** Thermal evolution models

In this part we compare the 2D and 3D geometries in a more complex set-up, by using thermal evolution models in a stagnant lid regime. Compared to the previously discussed steady-state calculations, these models illustrate which of the 2D geometries can best reproduce the 3D results when mantle and core cooling are considered.

# 325 **3.1 Mathematical model**

For the thermal evolution models we use the Extended Boussinesq Approximation (EBA) (Schubert et al., 2001) to account for adiabatic heating and cooling. The energy equation (Eq. 3) becomes:

$$\frac{DT}{Dt} - \nabla \cdot (k\nabla T) - Di\alpha (T + T_{surf})\mathbf{u}_r - \frac{Di}{Ra}\Phi - H = 0, \tag{7}$$

where  $\mathbf{u}_r$  is the radial component of the velocity vector,  $T_{surf}$  is the surface temperature,  $\alpha$  is the thermal expansivity, and  $\Phi$  is the viscous dissipation given by  $\Phi = \tau$ :  $\dot{\varepsilon}/2$ , where  $\tau$  is the deviatoric stress tensor and  $\dot{\varepsilon}$  the strain rate tensor. The dissipation number Di is defined as follows:

$$Di = \frac{\alpha_{ref} g_{ref} D}{c_p},\tag{8}$$

where  $c_p$  is the mantle heat capacity.

In the thermal evolution models, we consider a temperature and pressure dependent viscosity that follows the Arrehnius law of diffusion creep. The non-dimensional equation for viscosity reads (Roberts & Zhong, 2006):

$$\eta(T,z) = exp\left(\frac{E+zV}{T+T_{surf}} - \frac{E+z_{ref}V}{T_{ref}+T_{surf}}\right),\tag{9}$$

where E and V are the activation energy and the activation volume respectively (Karato & Wu, 1993; Hirth & Kohlstedt, 2003).  $T_{ref}$  and  $z_{ref}$  are the reference temperature and depth, respectively, at which the reference viscosity is attained. The non-dimensional  $T_{ref}$ and  $z_{ref}$  values correspond to a dimensional reference temperature of 1600 K and a dimensional reference pressure of 3 GPa, respectively.

The temperature of the lower boundary  $T_{CMB}$  evolves following a 1-D energy balance, assuming a core with constant density and heat capacity (Stevenson et al., 1983):

$$c_c \rho_c V_c \frac{dT_{CMB}}{dt} = -q_c A_c, \tag{10}$$

where  $c_c$  is the heat capacity of the core,  $\rho_c$  is the core density,  $V_c$  is the core volume,  $q_c$  is the heat flux at the core-mantle boundary (CMB), and  $A_c$  is the core surface area. Here we do not consider core crystallization.

As appropriate for thermal evolution models, we take into account the decay of the heat producing elements (i.e.,  $Ur^{238}$ ,  $Ur^{235}$ ,  $Th^{232}$ , and  $K^{40}$ ). The amount of radioactive heat sources is calculated using the concentrations listed in Table 1.

In thermal evolution models we consider the effect of a 50 km laterally homogeneous crust. This crust is enriched in radiogenic elements while the mantle is depleted according to the following mass balance:

$$M_{tot} \cdot Q_{tot} = M_{mantle} \cdot Q_{mantle} + M_{crust} \cdot Q_{crust}, \tag{11}$$

where M is the mass and Q is the heating rate. This setup also considers the blanketing effect of the crust by using a lower thermal conductivity k in the crust compared to the mantle.

# **356 3.2** Case definition

We test three scenarios for the thermal evolution of a Mars-like, the Moon-like, and Mercury-like planet. We model the entire evolution of these planets to determine the variations over time of several key output quantities. These three planetary bodies were chosen because of their different interior structures. In the Mars-like case, the radius ratio between core and planetary radius is f = 0.544. The Moon- and Mercury-like scenarios represent two end-members in terms of their radius ratios, with f = 0.224 and f =0.828, respectively.

In the case of the 2D grids, we use a radial resolution of  $\sim 10$  km for Mars- and Moon-like cases, and a  $\sim 5$  km radial resolution for the thin mantle of Mercury. In the case of the 3D grids, the radial resolution lies between 22 and 9 km, and we use a lateral resolution of 40962 points per shell. A more detailed list of the resolution for every grid is available in Table S2 of the SI.

In the cylindrical geometry, we use both the classical cylinder and the rescaling of van Keken (2001) as done previously in the stagnant lid steady-state simulations. It is worth to note that for the peculiar Moon-like interior structure, the scaling of the respective radii leads to a radius ratio f = 0.0503. Since this is an extreme case, we test whether the rescaling of the cylinder geometry is appropriate for such interior structures in a thermal evolution scenario.

It is important to note here that for each planet we use different Rayleigh num-375 bers (i.e., Ra and  $Ra_Q$ ). These are calculated self-consistently using the mantle thick-376 ness, internal heat sources, and temperature difference accross the mantle specific for each 377 planet. The parameters are listed in Table 1. While for Mars- and Moon-like simulations 378 we use a reference viscosity of  $10^{21}$  Pas, for the Mercury-like case we perform additional 379 tests with a reference viscosity that is lower by two orders of magnitude (i.e.,  $10^{19}$  Pas). 380 Since the thin Mercurian mantle typically leads to a conductive state after a few Gyr 381 of evolution, by using a lower reference viscosity we test additional scenarios, in which 382 convection can be sustained over most of the evolution. The results for Mercury with 383  $\eta_{ref} = 10^{21}$  Pas and  $10^{19}$  Pas are also compared between the 3D spherical shell and 384 the 2D geometries. 385

In all our simulations we consider the presence of a primordial crust with a thick-386 ness of 50 km, which is enriched in radiogenic elements compared to the bulk heat sources 387 of the planet by a factor of 2 and has a two times lower thermal conductivity than the 388 mantle (see Table 1). While being a representative value for the enrichment of the Mer-389 curian crust (Tosi, Grott, et al., 2013), for the two other scenario it allows to increase 390 the complexity of the simulation without having a thermal evolution dominated by the 391 enrichment of the crust. A second set of thermal evolution models neglecting the effects 392 of the crust is listed in Section S7 of the SI. 393

# 3.3 Results

394

In the following, we present the results obtained for the thermal history of Mars, the Moon, and Mercury for all geometries. Similar to the steady-state calculations, we show in Figure 3 the difference of the 2D cylinder, 2D scaled cylinder, and 2D spherical annulus to the 3D results after 4.5 Gyr of evolution (i.e., at present day). In addition to the error shown in percent, we also list the difference between the dimensional values for mean temperature, CMB temperature, root mean square velocity, lid thickness, as well as surface and CMB heat fluxes (Figure 4).

Figure 5 shows the entire evolution over 4.5 Gyr of the output quantities of interest for all four geometries (2D cylinder, 2D scaled cylinder, 2D spherical annulus, and 3D spherical shell) for a Mars-like geometry. Our results show clearly that in the case of a Mars-like geometry, the values obtained during the entire thermal evolution with



Thermal evolution cases

Figure 4: Relative error to the 3D in the case of thermal evolution simulations. In each panel we vary the planet on the y axis and on the x axis we vary the geometry. We investigate the relative error for: the mean temperature (a), the CMB temperature (b), the root mean square velocity (c), the stagnant lid thickness (d), the surface heat flux (e), and the CMB heat flux (f). A color in the blue indicates an underestimation of the results obtained in the 3D geometry whereas a color in the red indicates an overestimation. 2D Cyl stands for non-scaled 2D cylindrical geometry, 2D Sca Cyl is 2D cylindrical geometry. Each panel shows the relative error in % to the 3D and the absolute error in dimensional unit.

Symbol	Description (Unit)	Mars	Moon	Mercury
$R_p$	Planetary radius (km)	3400	1740	2440
$\dot{R_c}$	Core radius (km)	1850	390	2020
D	Mantle thickness (km)	1550	1350	420
f	Radius ratio (-)	0.544	0.224	0.827
$T_{surf}$	Surface temperature (K)	220	250	440
$T_{CMB}$	CMB temperature (K)	2000	2000	2000
$T_{ref}$	Reference temperature (K)	1600	1600	1600
$\Delta T$	Temperature contrast across the mantle (K)	1780	1750	1560
g	Gravitational acceleration $(m.s^{-2})$	3.7	1.6	3.7
$\eta_{ref}$	Reference viscosity $(Pas)$	$10^{21}$	$10^{21}$	$10^{21}$
$\kappa$	Thermal diffusivity $(m^2/s)$	$1 \times 10^{-6}$	$1.06 \times 10^{-6}$	$1.04 \times 10^{-6}$
$\alpha$	Thermal expansivity $(K^{-1})$	$2.50 \times 10^{-5}$	$2.50 \times 10^{-5}$	$2.50 \times 10^{-5}$
Ra	Rayleigh number(-)	$2.14 \times 10^6$	$5.35 \times 10^5$	$3.49 \times 10^4$
RaQ	Internal heating Rayleigh number (-)	$5.91  imes 10^7$	$8.70  imes 10^6$	$8.00  imes 10^4$
$\rho_{core}$	Core density $(kg/m^3)$	6000	7500	6980
$\rho_{mantle}$	Mantle density $(kg/m^3)$	3500	3300	3380
$\rho_{crust}$	Crust density $(kg/m^3)$	2900	2700	2900
$c_{p,m}$	Mantle heat capacity $(kgK)$	1142	1142	1142
$c_{p,c}$	Core heat capacity $(kgK)$	850	850	850
$\tilde{V}$	Activation volume $(m^3/mol)$	$6.00 \times 10^{-6}$	$6.00 \times 10^{-6}$	$6.00 \times 10^{-6}$
E	Activation energy $(J/mol)$	$3.00 \times 10^5$	$3.00 \times 10^5$	$3.00 \times 10^5$
$k_m$	Mantle thermal conductivity $(Wm^{-1}K^{-1})$	4	4	4
$k_{cr}$	Crust thermal conductivity $(Wm^{-1}K^{-1})$	3	2	3
$D_{crust}$	Primordial crust thickness (km)	50	50	50
	Heat source concentration	(Taylor, 2013)	(Taylor, 1982)	(Padovan et al., 2017)
$C_U$	Uranium concentration (ppb)	16	33	7
$C_{Th}$	Thorium concentration (ppb)	58	125	29
$C_K$	Potassium concentration (ppm)	309	83	550

Table 1: Parameters for thermal evolution calculations for Mars, Moon, and Mercury. Note that the non-dimensional radii are rescaled according to Eq. 6 for the scaled cylinder geometry.

a 3D geometry are more closely reproduced by the spherical annulus than the cylinder, 406 irrespective of whether it is scaled or not. It is to note that the spherical annulus geom-407 etry is reproducing especially well the evolution of the mean and core-mantle boundary 408 temperatures (see Figure 4 for the actual present-day error), while the velocities are sys-409 tematically overestimated by the 2D geometries (27.7%) for the spherical annulus and 29.6%410 for the rescaled cylinder). This directly affects the calculation of the stagnant lid thick-411 ness, and thus underestimates it by 6.2% for the annulus and 8.1% for the rescaled cylin-412 der. When trying to reproduce the heat fluxes at present day, the spherical annulus is 413 somewhat better than the scaled cylinder, with an approximated underestimation of the 414 CMB heat flux by 22% compared to 28% for the scaled cylinder, while the surface heat 415 flux will be overestimated by 6% and 8% for the annulus and the scaled cylinder, respec-416 tively. While we focus in this part mostly on present-day values, when examining the 417 entire thermal evolution of the planet we observe in the early and middle stages (between 418 1 and 3 Gyr) a relative error even larger as the one observed at present day, as seen on 419 Figure 5c and e. The Mars-like setup is the most challenging setup to reproduce for the 420 spherical annulus, and although exhibiting relatively low errors, it still shows the high-421 est discrepancies between the thermal evolution cases with different interior structures. 422 The overestimation of the mean temperature, mean velocity, surface heat flow, and un-423 derestimation of the stagnant lid thickness can be linked directly to the mixed heated, 424 temperature-dependent viscosity simulation with a radius ratio of 0.5, which shows the 425 same type of relative error (see Figure 3) 426



Figure 5: Timeseries of a Mars-like case with an initial crust of 50 km and with 4 different geometries (2D non-scaled cylindrical, 2D cylindrical, 2D spherical annulus and 3D spherical shell). The values shown here are the mean temperature (a), the core-mantle boundary temperature (b), the surface heat flux (c), the core-mantle boundary heat flux (d), the averaged root mean square velocity of the domain (e), and the lid thickness (f) from 4.5 Gyr ago to present day, respectively. The shaded areas show the min.-max. variations during the evolution. The non-scaled cylinder has been added to show the effect of the rescaling introduced by van Keken (2001).

In the case of a Moon-like setup (Figure 6) the differences between the spherical 427 annulus and the cylinder are typically larger than in the Mars-like case. However the dif-428 ference between the spherical annulus and the 3D is significantly lower in the case of the 429 mean temperature, the stagnant lid thickness and the surface heat flow; as can be seen 430 on Figures 6a, c, and f. The temperatures through time are very well reproduced by the 431 spherical annulus (less than 2% of error compared to more than 12% for the cylindri-432 cal geometries). Similarly, the surface heat flux and the stagnant-lid thickness show a 433 good match between the spherical annulus and the 3D geometries (see Table S5 of the 434 SI). Concerning the cylindrical geometries, the effects of the rescaling are plainly visi-435 ble on the overall temperatures and heat fluxes evolution. As van Keken (2001) showed, 436 the cylinder tends to overestimate the relative importance of the CMB radius compared 437 to planetary radius and requires a rescaling of the radii. However, for the very low aspect-438 ratio of the lunar mantle, even when the rescaling is applied the results are still largely 439 different compared to a 3D spherical shell geometry. A better approximation of the 3D 440 results is obtained by the spherical annulus, where such rescaling is not needed. We see 441 that the CMB heat flux stays at around -1.86 mW m<sup>-2</sup> even at present day, meaning that 442 the core is actively heated by the mantle, although in the other geometries the core is 443 already cooling (see Figure 6b and d), a behavior which is also seen for Mars with the 444 non-scaled cylindrical geometry. Similar to what has been seen previously for the low 445 aspect-ratio cases with temperature-dependent viscosity combining basal heating and 446 internal heating (see Figure 3), the scaled and non-scaled cylindrical geometries show 447 large disagreements in all studied metrics. Nevertheless, even in the spherical annulus, 448 the mean velocity and the CMB heat flux present the largest errors among the investi-449 gated quantities. 450

In Figure 7, we show the results of the thermal evolution for a Mercury-like setup. 451 Here we used two sets of simulations in order to illustrate the case of a initially weakly 452 convecting mantle with a reference viscosity set as  $\eta_{ref} = 10^{21}$  Pas resulting in a Rayleigh 453 number of  $Ra = 3.49 \times 10^4$ ; and the case of a mantle presenting a stronger initial con-454 vection with a reference viscosity lowered by two orders of magnitude, thus increasing 455 the Rayleigh number to  $Ra = 3.49 \times 10^6$ . Here again the global trend previously seen 456 for Mars and the Moon emerges. As shown in figure 4, the spherical annulus geometry 457 again reproduces best the 3D results with an approximate error of less than 1%, with 458 a notable exception for the velocities, which are highly overestimated (more than 90%459 of relative error). The very high relative error of the  $v_{rms}$  is explained by the present-460 day state of the Mercurian mantle. In our simulations, a Mercury-like planet falls into 461 a quasi-conductive state after a couple of Gyr of evolution irrespective of the geometry 462 (Figure 7), which in turn gives very low absolute  $v_{rms}$  values. Yet the absolute differ-463 ence of velocity between the geometry is very small (less than  $1 \times 10^3$  cm/year). De-464 spite these high relative error values in the velocities, the stagnant lid thickness is, how-465 ever, quite well reproduced by the 2D geometries, giving a maximum relative error of 466 19 km (or an underestimation of 6.5%). 467

# 468 4 Discussion

Our results show that the spherical annulus can reproduce the 3D spherical shell
geometry better than the cylindrical geometry, consistent with previous studies by Hernlund
and Tackley (2008). Our systematic study, using simulations of increasing complexity,
shows for the first time in great detail the difference in using a 2D geometry instead of
a more realistic 3D spherical shell domain when modeling thermal convection in planetary mantles.

When using the cylindrical geometry, whether scaled or not, the results show substantial differences to the 3D geometry results in steady-state and thermal evolution simulations. The necessity of choosing between a scaled and a non-scaled cylinder in modeling geodynamic processes inevitably results in a trade-off between an accurate repre-



Figure 6: Timeseries of a Moon-like case with an initial crust of 50 km and with 4 different geometries (2D non-scaled cylindrical, 2D scaled cylindrical, 2D non-scaled cylindrical, 2D spherical annulus and 3D spherical shell). For a description off the values investigated, see Figure 5.



Figure 7: Timeseries of a Mercury-like case with an initial crust of 50 km, with 4 different geometries and 2 different reference viscosities. For a description off the values investigated, see Figure 5. The dotted lines represent simulations with a reference viscosity of  $\eta_{ref}=10^{19}$  Pa s while the solid lines represent the cases with a reference viscosity of  $\eta_{ref}=10^{21}$  Pa s. The maximum and minimum of the output quantities are not displayed here, since these variations are negligible.

sentation of the deep interior structures in the case of the non-scaled cylinder, especially
important when studying thermochemical structures (Stegman et al., 2003; Nakagawa
& Tackley, 2004; Yu et al., 2019; Kameyama, 2022), and a correct representation of the
heat fluxes as well as root mean square velocity in the domain (Deschamps et al., 2010;
Mulyukova et al., 2015) for the scaled one. To circumvent these inaccuracies, the systematic use of the spherical annulus in reproducing thermochemical convection in 3D is
thus strongly recommended.

In the case of steady-state simulations, we showed that the spherical annulus has the largest error in the high radius ratio scenarios (i.e, f = 0.6 and 0.8). The efficiency of the spherical annulus in reducing the error to the 3D (compared to the results of the scaled cylinder) is most visible in the case of a low radius ratio configuration (i.e., f =0.2), while nonetheless displaying large discrepancies in the mean temperature in the case of bottom heated and temperature-dependent setups, as also seen by Guerrero et al. (2018).

Concerning the heating modes, as reported by Hernlund and Tackley (2008), the 492 purely internally heated cases show the largest difference between the 2D and 3D geome-493 tries, while the mixed heating cases (bottom and internal heating) tends to be the heat-494 ing mode for which the spherical annulus exhibits the smallest errors in comparison to 495 the spherical shell, as the difference in the temperature distribution between the spher-496 ical annulus and the spherical shell tends to disappear (see Figure S6 of the SI). This 497 particularity becomes quite useful when trying to model more realistic processes such as thermal evolution models of terrestrial planets, as the silicate mantles of planets will 499 invariably show heating induced by both the presence of radiogenic elements in the man-500 tle and by the core. The smaller error between the 2D spherical annulus and 3D spher-501 ical shell observed in mixed heated cases makes the spherical annulus an acceptable al-502 ternative to model more complex scenario (Figure 4), for which a 3D geometry is too ex-503 pensive. The trend of the relative error in the steady-state stagnant lid simulations with 504 mixed heating is also observed in the case of thermal evolution models: the errors in the 505 surface heat flux and stagnant lid thickness increase with increasing radius ratio (cf. the 506 errors obtained for the Moon and Mars in Figure 4). However in the case of Mercury, 507 while the steady-state simulations would predict the largest errors, the low Rayleigh num-508 ber in thermal evolution models and the transition to a conductive state during the ther-509 mal evolution strongly reduce the discrepancy between 2D and 3D geometries. 510

The results presented here show that the spherical annulus is to be preferred to the 511 cylindrical geometry, whether for steady-state simulations or thermal evolution simula-512 tions. However, in the case of the thermal evolution simulations one should question whether 513 this geometry is sufficient to approximate the 3D spherical shell. Some observables such 514 as the heat flux, the mechanical thickness of the lithosphere and the crust produced by 515 partial melting of the mantle are used to evaluate the thermochemical evolution of a planet. 516 But an important question is whether the 2D spherical annulus is accurate enough to 517 reproduce the results of a 3D spherical shell for the above mentioned quantities, and which 518 of these observables can be affected the most. 519

Additional post-processing has thus been conducted in order to better character-520 ize the differences of more complex processes in the spherical annulus compared to the 521 spherical shell. We exclude from this comparison the cylindrical geometry given its lack 522 of accuracy in reproducing 3D. Moreover, the areas and volumes in the 2D cylindrical 523 geometry are truly 2D and thus difficult to compare to the 3D spherical shell. Melting 524 in the mantle, the thickness of the mechanical lithosphere, and heat fluxes are shown in 525 Figure 8 as a function of time. For the calculation of the mechanical lithosphere thick-526 ness, we follow the approach of Grott and Breuer (2008). The calculations involving par-527 tial melting of the mantle are highly simplified and do not include the effects of latent 528 heat or mantle depletion. While the quantities presented in Figure 8 are based on sim-529 ple post-processing of the thermal evolution results, they are meant to provide first or-530 der implications for the thermal evolution modeling with 2D and 3D geometries (for ad-531 ditional information concerning the post processing, see S11, S12). 532

When reproducing 3D simulations, the spherical annulus is well suited to replicate melting, mechanical thickness and heat fluxes. In particular the heat fluxes, and especially the CMB heat flux (Figure 8g, h, i) are especially well reproduced in terms of values and trend of evolution. The largest errors were observed for a Mars-like structure with an overestimation of less than 1.5 mW m<sup>-2</sup> compared to the 3D for the surface heat flux and an almost identical CMB heat flux (less than 1 mW m<sup>-2</sup> lower values compared to the 3D case).

The mechanical thickness for a Moon-like interior structure will be underestimated 540 on average by 5% for the spherical annulus, while the amount of melting will be over-541 estimated by 10% as in the case of Mercury. Since the computation of the amount of par-542 tial melting in the mantle through time relies on the temperature profile of the simula-543 tion, it is not surprising to see on one hand the underestimation of the mechanical thick-544 ness and on the other hand a systematic overestimation of partial melting by the spher-545 ical annulus compared to the 3D. The main reason explaining these differences is that 546 the spherical annulus will consistently overestimate the overall mantle temperature, lead-547 ing to a hotter temperature profile, thus directly affecting the degree of melting and the 548 thickness of the mechanical lithosphere. 549

In the case of a Mars-like structure (Figure 8b, e) the differences between 2D and 550 3D are larger, in particular in the case of partial melting, which the annulus will over-551 estimate by a maximum of 30% at around 1.5 Gyr. The mechanical thickness will be un-552 derestimated on average by 10 %. In particular the differences in partial melting could 553 lead to an overestimation of the crustal thickness in the 2D spherical annulus geometry. 554 This in turn could lead to more crustal production due to a mechanism called "crustal 555 blanketing" (e.g., Schumacher & Breuer, 2006), in which the reduced thermal conduc-556 tivity of the crust will prevent efficient cooling of the mantle. A higher crustal produc-557 tion rate could then lead to a stronger depletion of the mantle in crustal components and 558 volatile elements. Hence, care should be taken when the spherical annulus geometry is 559 employed to study partial melting and subsequent crust production or degassing in par-560 ticular for planets with an intermediate radius ratio, like Mars or Venus. These processes 561 and the differences between 2D and 3D geometries for such scenarios need to be quan-562 tified in future studies. 563



Figure 8: Timeseries of the three scenario investigated (from left to right; the Moon, Mars and Mercury). First row shows the fraction of molten mantle (in %) at a given time in the evolution for each planet, second row shows the mechanical thickness of the lithosphere (in km) during the evolution, and the third row shows the CMB and surface heat fluxes (in mW m<sup>-2</sup>). Since the cylindrical geometry shows the largest difference to the 3D, it was not included in this comparison. All the equations used in order to compute these quantities are described in the SI.

# 564 5 Conclusions

The main goal of this study is to provide a systematic comparison between different geometries in order to determine how accurate can 2D geometries reproduce 3D results. To this end, we investigated (scaled and non-scaled) 2D cylinder, 2D spherical annulus, and 3D spherical shell geometries in a series of scenarios. We started with isoviscous steady-state models, included the effects of a temperature dependent viscosity, and finally tested the different geometries for thermal evolution setups. Our main findings are the following:

5721. While it is obvious that a 3D geometry should be preferred over a 2D one, due to573the high computational cost, this may not always be feasible. Applying models574with different complexities, we demonstrated that the 2D spherical annulus ge-575ometry is able to reproduce the 3D models much better than the 2D cylinder, in576particular for the low radius ratio setups. The latter is also clearly seen when mod-577eling the thermal evolution of the Moon.

578	2.	For steady-state scenarios, our models show that the 2D geometries will mostly
579		overestimate the mean temperature compared to 3D, a result largely explained
580		by the geometry of mantle plumes (i.e., sheet-like in 2D vs. columnar-like in 3D).
581		This discrepancy decreases with an increasing Rayleigh number but is more ac-
582		centuated for low-radius ratio cases, a result already observed by Guerrero et al.
583		(2018). The differences in temperature between the 2D and 3D geometries decreases
584		for mixed heated cases (i.e., heated both from below and from within). This is es-
585		pecially true in the case of the spherical annulus, since the spherical annulus is a
586		geometry which uses the same cell volumes as a 3D spherical shell.
587	3.	We find that for intermediate ratios of the inner to outer radius (e.g., Mars-like
588		thermal evolution case), the differences in the results for the 2D and 3D geome-
589		tries are larger than for extreme radius ratios. In contrast to the temperature-dependent
590		steady-state cases, where the difference in surface heat flux and stagnant lid thick-
591		ness between 2D geometries and 3D geometries is largest for high radius ratios,
592		the difference obtained for Mercury-like evolution parameters is minimal. This is

due to the low Rayleigh number of Mercury that leads to the transition to a conductive state during its thermal history.

593

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4. Care needs to be taken when studying melting processes with the spherical annulus in thermal evolution setups with intermediate radius ratios (e.g., Mars and Venus), as this geometry might overestimate crustal production by up to 30% compared to a 3D simulation leading to a different thermal history of the interior.

Future studies need to test the accuracy of the 2D spherical annulus in reproducing the 3D spherical shell geometry in more complex scenarios considering variable thermal conductivity and expansivity (Tosi, Yuen, et al., 2013), chemical buoyancy (Nakagawa et al., 2010), as well as partial melting of the mantle and its influence on thermal evolution.

# <sup>604</sup> Data Availability Statement

<sup>605</sup> Supplementary datasets containing all values shown in tables and figures are available <sup>606</sup> upon request on Zenodo : https://doi.org/10.5281/zenodo.8047757

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# Approximating 3D Models of Planetary Evolution in 2D: A Comparison of Different Geometries

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# 5 Key Points:

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6	• Interior dynamics models using the 2D spherical annulus geometry match the re-
7	sults of a 3D spherical shell better than the 2D cylinder.
8	• The difference between 2D and 3D geometries decreases when models are heated
9	from below by the core and from within by radioactive elements.
10	• The spherical annulus shows negligible differences to 3D for the thermal evolution
11	of Mercury and the Moon, and acceptable values for Mars.

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# 12 Abstract

Regardless of the steady increase of computing power during the last decades, 3D nu-13 merical models continue to be used in specific setups to investigate the thermochemi-14 cal convection of planetary interiors, while the use of 2D geometries is still favored in most 15 exploratory studies involving a broad range of parameters. The 2D cylindrical and the 16 more recent 2D spherical annulus geometries are predominantly used in this context, but 17 the extent to how well they reproduce the 3D spherical shell in comparison to each other, 18 and in which setup, has not yet been extensively studied. Here we performed a thorough 19 and systematic study in order to assess which 2D geometry reproduces best the 3D one. 20 In a first set of models, we investigated the effects of the geometry on thermal convec-21 tion in steady-state setups while varying a broad range of parameters. Additional ther-22 mal evolution models of three terrestrial bodies, respectively Mercury, the Moon, and 23 Mars, which have different interior structures, were used to compare the 2D and 3D ge-24 ometries. Our study shows that the spherical annulus geometry improves results com-25 pared to cylindrical geometry when reproducing 3D models. Our results can be used to 26 determine for which setup acceptable differences are expected when using a 2D instead 27 of a 3D geometry. 28

# <sup>29</sup> Plain Language Summary

In geodynamic modeling, numerical models are used in order to investigate how 30 31 the interior of a terrestrial planet evolves from the earliest stage, after the planetary formation, up to present day. The mathematical equations that are used to model the phys-32 ical processes in the interior of rocky planets are discretized and solved using geomet-33 ric meshes. The most commonly used geometries are the 3D spherical shell, the 2D cylin-34 der, and the 2D spherical annulus. While being the most accurate and realistic, the 3D 35 geometry is expensive in terms of computing power and time of execution. On the other 36 hand, 2D geometries provide a reduced accuracy but are computationally faster. Here 37 we perform an extensive comparison between 2D and 3D geometries in scenarios of in-38 creasing complexity. The 2D spherical annulus geometry shows much closer results to 39 the 3D spherical shell when compared to the 2D cylinder and should be considered in 40 2D modeling studies. 41

# 42 **1** Introduction

Geodynamic modeling is a powerful approach to investigate the dynamics of the 43 mantle and lithosphere of terrestrial planets and to explore the evolution of their inte-44 rior that is not directly observable. Such models vary in their complexity and often em-45 ploy different geometries to investigate physical processes such as mantle melting and 46 cooling, and the generation of a magnetic field. When using these models to interpret 47 specific observations of the Earth and other planets, care must be taken in particular for 48 the choice of geometry (see Noack & Tosi, 2012, for an overview of geometries), as this 49 may significantly impact quantities such as the mantle temperature, the convection ve-50 locity, and the heat flux of the simulations. 51

The role of two-dimensional geometry studies in the field of thermochemical man-52 tle convection modeling is still predominant despite an ever-increasing computing power. 53 Although the formulation of 3D grids has seen improvements in previous years with the 54 Yin-Yang grid (Kageyama & Sato, 2004) and the spiral grid (Hüttig & Stemmer, 2008a) 55 among others; simulations with a full spherical shell geometry remain highly expensive 56 in terms of computational power, hence making them inappropriate to study broad ranges 57 of parameters or conduct large exploratory studies. As an alternative, geometrical ana-58 logues to the 3D spherical shell have been extensively used, namely the 2D spherical axi-59 symmetric (van Keken & Yuen, 1995) and the more popular cylindrical geometry (Jarvis, 60 1993). The 2D axi-symmetric geometry has been used in earlier studies of mantle con-61

vection (e.g., van Keken & Yuen, 1995; Jarvis et al., 1995), but in addition to the arti-62 ficial boundaries formed by the poles which trap down- and up-wellings, an asymmetry 63 between the polar and the equatorial regions exists (van Keken, 2001). The cylindrical 64 geometry on the other hand, while resolving the problems of the artificial boundaries at 65 the poles imposed by the axi-symmetric geometry, still exhibits an important drawback. 66 The ratio of the two surfaces (the planetary surface and the core surface) is different in 67 the cylindrical geometry compared to the spherical shell. This leads to a mismatch in 68 heat flux values between these geometries, as the heat flux of the core mantle boundary 69 (CMB) is underestimated and the surface heat flux is overestimated when comparing to 70 a spherical shell with the same ratio between the core and planet radius (i.e., radius ra-71 tio). 72

In order to mitigate this problem, van Keken (2001) introduced a re-scaling of the 73 2D cylindrical geometry such that the ratio of outer and inner areas of the cylinder matches 74 the ratio obtained for the spherical shell. This scaling, however, while correcting the sur-75 face ratio discrepancy of the cylinder, still uses the volume of a cylinder. Additionally, 76 this re-scaling creates an artificially smaller core, which in turn modifies the convection 77 pattern in the mantle, leading for example to a crowding of the plumes near the CMB, 78 a behavior that would not be observed in a 3D spherical shell, when using the original, 79 non-scaled radii. 80

To overcome this major drawback of the cylindrical geometry, another 2D geom-81 etry called "spherical annulus" has been proposed by Hernlund and Tackley (2008). This 82 geometry effectively uses a second degree of curvature and considers the same surfaces 83 and volumes as the 3D geometry. Since no re-scaling is necessary for this geometry, it 84 keeps the same radius ratio as the 3D one. In the study of Hernlund and Tackley (2008), 85 the spherical annulus showed promising results to approximate the 3D spherical geom-86 etry with mean temperature and Nusselt number well reproduced for steady-state ther-87 mal convection calculations. While these results a highly valuable, there are only for the 88 case of an Earth-like radius ratio and only consider thermal convection simulations in 89 the Boussinesq approximation. 90

More recently, Guerrero et al. (2018) performed a more extensive study with the spherical annulus for stagnant lid convection models and compared the temperature distribution between the spherical annulus and the spherical shell. However, an extensive study investigating the ability of the 2D spherical annulus to reproduce results obtained in a 3D spherical shell and a systematic comparison with the 2D cylinder for various setups has never been conducted so far.

In this study, we present simulations of thermal convection in the 2D spherical an-97 nulus and compare the results to the 2D cylinder and the 3D spherical shell. In a first part we focus on simple steady-state convection models using the Boussinesq approxi-99 mation. We vary the Rayleigh number, the radius ratio, and the heating mode for iso-100 viscous cases and run additional temperature-dependent viscosity models to determine 101 which of the two 2D geometries (i.e., cylinder or spherical annulus) is able to best re-102 produce the 3D results. The set of equations that were used for this comparison are de-103 scribed in Section 2.1, the grid geometries are displayed in Section 2.2, and a descrip-104 tion of the cases investigated here is available in Section 2.3. A detailed analysis of the 105 results is presented in Section 2.4. 106

In a second step, we run more complex simulations of thermal evolution with the same geometries in three separate scenarios. We use Moon-like, Mars-like, and Mercurylike thermal evolution models to investigate how well the 2D spherical annulus reproduces the results of the 3D spherical shell geometry. The three planetary bodies were chosen since they cover a wide range of interior structures and they are all thought to have been in a stagnant lid regime over their entire thermal history, which makes them comparable in terms of their tectonic regime (Breuer & Moore, 2015). In Section 3.1 we

list the equations used for the thermal evolution models. A description of the employed 114 parameters and setup of the models is given in Section 3.2. The results are described in 115 Section 3.3. A discussion of the steady-state and thermal evolution models is presented 116 in Section 4, followed by conclusions in Section 5. 117

#### 2 Steady-state mantle convection 118

In a first set of calculations we focus on the comparison between steady-state cal-119 culations in 2D and 3D geometries. For this purpose we test a large number of param-120 eter combinations for isoviscous models and temperature-dependent viscosity. 121

#### 2.1 Mathematical model 122

Fully dynamical models of mantle convection allow us to investigate the spatial and 123 temporal evolution of mantle flow. These models solve the conservation equations of mass, 124 momentum, and energy. Here, the conservation equations are scaled using the mantle 125 thickness D as length scale, the temperature drop across the mantle  $\Delta T$  as temperature 126 scale and the thermal diffusivity  $\kappa$  as time scale. A Table listing the scaling factors is 127 available in the Supplementary Information, SI (Table S1). By assuming a Newtonian 128 rheology, an infinite Prandtl number, and considering the Boussinesq approximation (Schubert 129 et al., 2001; van Zelst et al., 2022), the non-dimensional conservation equations read: 130

$$\mathbf{u} = 0, \tag{1}$$

$$\nabla \cdot \mathbf{u} = 0, \qquad (1)$$
$$\nabla \cdot \left( \eta \left( \nabla \mathbf{u} + (\nabla \mathbf{u})^T \right) \right) + RaT \mathbf{e}_r - \nabla P = 0, \qquad (2)$$

$$\frac{DT}{Dt} - \nabla^2 T - H = 0. ag{3}$$

In Equations 1 – 3, **u** is the velocity vector,  $\eta$  is the viscosity, T is the temperature, 131  $\mathbf{e}_r$  is the radial unit vector, P is the dynamic pressure, and t is the time. 132

The parameter Ra denotes the thermal Rayleigh number, a non-dimensional num-133 ber, which controls the vigor of the convection in the mantle. H is the internal heating 134 rate of the mantle that is given by  $\frac{Ra_Q}{Ra}$ , where  $Ra_Q$  denotes the Rayleigh number as-135 sociated with internal heating. The Rayleigh numbers Ra and  $Ra_Q$  read: 136

$$Ra = \frac{\rho_{ref}g_{ref}\alpha_{ref}\Delta TD^3}{\kappa_{ref}\eta_{ref}}, \quad RaQ = \frac{\rho_{ref}^2g_{ref}\alpha_{ref}HD^5}{\kappa_{ref}\eta_{ref}k_{ref}}, \tag{4}$$

where  $\rho_{ref}$  is the reference density,  $g_{ref}$  is the reference gravitational acceleration,  $\alpha_{ref}$ 137 is the reference thermal expansivity,  $\kappa_{ref}$  is the reference thermal diffusivity,  $\eta_{ref}$  is the 138 reference viscosity,  $k_{ref}$  is the reference thermal conductivity, and H is the internal heat-139 ing rate in W/kg. 140

For the steady-state models, we use a constant or temperature-dependent viscos-141 ity that follows the Frank-Kamenetskii approximation (Frank-Kamenetskii, 1969), which 142 is a linearized form of the Arrhenius law: 143

$$\eta(T) = \exp(\Delta \eta_T (T_{ref} - T)), \tag{5}$$

The parameter  $\Delta \eta_T$  is the viscosity contrast due to temperature and  $T_{ref}$  is the 144 reference temperature at which a non-dimensional viscosity equal to 1 is attained. For 145 the thermal evolution simulations presented further in this study, we use another parametriza-146 tion of the viscosity (Eq. 9), which is discussed more in-depth in the Section 3.1. 147



Figure 1: Representation of a cell of the spherical annulus geometry, in red, its effective volume. The cylindrical geometry is represented in blue, on the equatorial plane. The red area represented corresponds to the intersection of the spherical annulus cell with the equatorial plane. When looking at the grid from a polar point of view, its visualization becomes thus indistinguishable from the cylindrical cell.

# <sup>148</sup> 2.2 Grid geometries

We use the numerical code Gaia (Hüttig & Stemmer, 2008a, 2008b; Hüttig et al., 149 2013) to model the mantle convection in the interior of rocky planets. Gaia solves the 150 conservation equations (Eq. 1-3) in their dimensionless form in 2D and 3D geometries. 151 For the 2D geometry, we use both the classical cylindrical geometry (van Keken, 2001) 152 and the spherical annulus geometry following the approach of Hernlund and Tackley (2008). 153 In the 2D cylindrical geometry, the areas and volumes of the grid cells are typically for-154 mulated using the equations for a cylinder; however, what makes the particularity of the 155 spherical annulus geometry, is the addition of a virtual thickness to the cylindrical ge-156 ometry which varies with the radius r. Thus the spherical annulus has a second degree 157 of curvature, and uses an effective 3-dimensional formulation for the areas and volumes, 158 as represented on Figure 1 (a more detailed description of the spherical annulus geom-159 etry is available in Section S3 of the SI). 160

The 2D cylindrical geometry is scaled according to the scaling introduced by van Keken (2001), where the inner and outer radii of the cylinder grid (i.e., the core radius and the planetary radius, respectively) are changed such that the ratio between the outer and inner areas of the cylinder matches the ratio obtained in a 3D spherical shell geometry. The equations used to correct the inner and outer radii of the cylinder are the fol166 lowing:

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$$\frac{r_{oc}}{r_{ic}} = \frac{r_{os}^2}{r_{is}^2}, \qquad r_{oc} - r_{ic} = r_{os} - r_{is}, \qquad (6)$$

where  $r_{ic}$  and  $r_{oc}$  are the inner and the outer radius of the cylinder, respectively. The inner and outer radii of the spherical shell are denoted by  $r_{is}$  and  $r_{os}$ , respectively. In the following, we will refer to this type of geometry that considers the rescaling of the inner and outer radii as the "scaled cylinder geometry".

# 2.3 Case definition

In the first part of this study, we performed steady-state simulations in order to 172 investigate the effects of the ratio of the inner to outer radius and of heating modes on 173 the results obtained with the 2D cylindrical, 2D spherical annulus, and 3D spherical shell 174 geometry. Our aim is to compare 2D and 3D geometries and determine for which sce-175 narios does the 2D spherical annulus give closer results to the 3D compared to the 2D 176 cylinder. To this end, we use models heated from below (purely bottom-heated), from 177 within (purely internally-heated), and from both below and within (mixed heated). We 178 use an initial random perturbation of the temperature field with an amplitude of 5%, 179 vary the Rayleigh number Ra of our simulations from  $10^4$  up to  $10^8$ , and the radius ra-180 tio f from 0.2 to 0.8 for our isoviscous setup. 181

For the 2D geometries, we use between  $1.1 \times 10^4$  and  $6.7 \times 10^4$  grid points for low Rayleigh number simulations and between  $4.8 \times 10^4$  and  $4.1 \times 10^5$  for simulations with a Rayleigh number higher than  $10^6$ . For the 3D geometries, we use between  $2.04 \times 10^6$ and  $2.94 \times 10^6$  grid points. A more in depth description of each grid and its associated lateral and radial resolution is available in the SI. A short comparison of our results to the ones of Hernlund and Tackley (2008) for isoviscous steady-state cases is presented in Section S4 of the SI.

Each mesh has a prescribed temperature and free-slip velocity as boundary conditions. The temperature of the upper boundary  $T_{surf}$  is set to zero, while the one of the lower boundary is set to one for the bottom heated and mixed heated cases. For the purely internally heated cases we use a zero heat flux at the core-mantle boundary.

The simulations are ran until a statistical steady-state is reached. Then, output quantities such as the average temperature, root-mean-square velocity, and top temperature gradient are computed using an average over the last 10% of the simulation. While for purely steady-state models this is the same as taking the last output, for quasi steadystate time-dependent or periodic models this ensures to retrieve representative average values. The top temperature gradient here is the temperature gradient at the top of the domain, calculated between the last two shells of the grid.

An additional, more complex set of simulations includes the effect of the temper-200 ature dependence of the viscosity, and leads to the formation of a stagnant lid at the top 201 of the convecting domain. These simulation represent simplified Moon-like (f = 0.2), 202 Mars-like (f = 0.5), and Mercury-like (f = 0.8) scenarios. We use here thermal and 203 radiogenic Ra numbers with values similar to those expected for planetary mantles, i.e., 204  $Ra = 5 \times 10^6$  and  $Ra_Q = 5 \times 10^7$  (see values of Ra and  $Ra_Q$  in Table 1). We use the 205 Frank Kamenetskii parametrization for the viscosity (Eq. 5) and set a viscosity contrast 206  $\Delta \eta_T$  to 10<sup>8</sup> at a reference temperature  $T_{ref}$  of 0.5 to ensure that we are in a stagnant 207 lid convection regime. In this setup, the total number of nodes used for the 2D grids lies 208 between  $4.8 \times 10^4$  and  $2.8 \times 10^5$ ; while for the 3D simulations, the total number of nodes 209 is  $2.9 \times 10^6$ . 210

In total, we run 180 isoviscous simulations and 36 temperature-dependent viscosity cases. All parameters and the grid resolutions for these steady-state simulations are listed in Table S2 in the SI.

# 214 **2.4 Results**

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## 2.4.1 Isoviscous convection

For the first set, consisting of isoviscous simulations, we provide a thorough and systematic comparison between the 3D spherical grid and the two 2D geometries, namely the spherical annulus and the cylindrical geometry. A summary of the comparison is shown in Figure 2.

Here, the analysis of the 180 simulations has been summarized into three subplots 220 one for each heating mode. Each subplot contains two rows showing for each the annu-221 lus geometry (first row) and the scaled cylindrical geometry (second row), respectively, 222 the relative error to the 3D results. The computation details of the relative error can be 223 found in the SI (Section S5) along with tables containing the values for each simulation 224 in CSV format. Figure 2 shows that the mean domain temperature of the 3D geome-225 try is more accurately reproduced by the spherical annulus geometry than by the cylin-226 drical one in every heating mode, up to values of  $Ra = 10^7$ . This difference is even more 227 noticeable in the low radius ratiosetups (i.e., f = 0.2 and 0.4), which can be seen for 228 the purely bottom heated and mixed heated scenarios. We also see for the purely inter-229 nal heated cases and high Rayleigh number cases (i.e.,  $Ra = 10^7$  and  $Ra = 10^8$ ) that 230 this difference is even more dramatic with an overestimation of the temperature in the 231 cylindrical geometry by up to  $\sim 20\%$  for the small a radius ratio (i.e., f = 2) and re-232 duces to only a few percent in the spherical annulus. 233

In the case of the root mean square velocity, we see a general increase of the ac-234 curacy with the spherical annulus geometry, however this increase is less pronounced than 235 what is observed for the mean temperature. We see a slightly better match for the purely 236 bottom heated and mixed heated setups, where simulations with  $Ra < 10^7$  go from be-237 ing slightly underestimated by the cylinder to slightly overestimated by the annulus. How-238 ever, the cases with  $Ra > 10^7$  show a net improvement, with an underestimation de-239 creasing for all the cases with a radius ratio higher than 0.2. For the setup with a purely 240 internal heating, however, almost no improvement is visible, with the notable exception 241 of the simulation with a  $Ra = 10^8$  and a radius ratio of 0.2 being overestimated by  $\sim$ 242 40% in the case of the cylinder, which turns to be overestimated only by  $\sim 20\%$  in the 243 case of the spherical annulus. 244

In comparison to the cylinder, the spherical annulus, gives less conclusive results 245 for the top temperature gradient. We can see an improvement in case of small radius ra-246 tios (i.e., f = 0.2) with either purely internal heating or mixed heating, or in the case 247 of high Rayleigh numbers (i.e.,  $Ra \ge 10^7$ ) for purely internal heated cases. Otherwise, 248 for the majority of the setups and heating modes, the spherical annulus does not show 249 significant improvement in reproducing the 3D values compared to the scaled cylindri-250 cal geometry. A comparison of the temperature gradient at the top of the mantle shows 251 that the spherical annulus is hardly able to reproduce the 3D values more accurately than 252 the scaled cylindrical geometry, with the notable exception of low radius ratios of around 253 f = 0.2. 254

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# 2.4.2 Stagnant lid convection

In the second part of the steady-state simulations, we modeled stagnant lid convection while varying the heating mode, the radius ratio, and the geometry in order to study the accuracy of the spherical annulus geometry (see SI, Table S2). In this type of setup, where the viscosity is strongly dependent on temperature, the convection is expected to operate in a stagnant lid regime. This rigid layer that forms at the top of the domain restricts convective heat transfer to the deep interior.

The results are summarized in Figure 3, where we report the relative error of the 263 2D cylindrical, 2D scaled cylindrical, and 2D spherical annulus geometry to the 3D spher-264 ical shell. Here we inspect the mean temperature, the root mean square velocity, the top



Figure 2: Averaged computed relative error to the 3D geometry with 3 different heating modes, i.e., purely basal heated (top row), purely internal heated (middle row), or mixed heated (bottom row) for steady-state isoviscous convection simulations. For each heating mode the first line of plots shows the relative errors for the spherical annulus and the second line represents the scaled cylinder. The thermal Rayleigh number and internal Rayleigh number vary from  $10^4$  to  $10^8$  and the radius ratio from 0.2 to 0.8. The radius ratio indicated on the plot is the one corresponding to the reference 3D simulations. In the case of the cylinder, the radius ratio is scaled, thus a 0.2 radius ratio becomes 0.04 following the scaling formula from van Keken (2001) (eq. 6). For columns from left to right, relative error of the mean temperature, of the v<sub>rms</sub>, and of the top temperature gradient are shown. temperature gradient, and the stagnant lid thickness. For each simulation we use a Raof  $10 \times 10^6$  and  $Ra_O$  of  $10 \times 10^7$ .

In Figure 3, when considering purely basal heating, we see that the spherical an-267 nulus is overall better at reproducing the 3D values compared to the scaled and non-scaled 268 cylinder. The highest discrepancy is observed for the radius ratio f = 0.2, with > 50%269 of overestimation on average for the 2D geometries. For the spherical annulus, the mean 270 temperature matches best the one of the 3D spherical shell when the radius ratio increases, 271 an effect also seen for the  $v_{\rm rms}$ . The top temperature gradient does not follow this pat-272 273 tern, however, while the stagnant lid error is the lowest for f = 0.5. The highest difference to the 3D for the low radius ratio setups (f = 0.2) in the purely bottom heated 274 setup that we found in our models is in agreement with Guerrero et al. (2018). The study 275 by Guerrero et al. (2018) considered stagnant lid convection with only basal heating, and 276 observed that for small radius ratio setups, the spherical annulus would systematically 277 show a hotter temperature when compared to the 3D. This behavior is indeed confirmed 278 by our simulations, where we can observe that the different geometry of plumes between 279 the spherical annulus and the spherical shell create considerable differences in temper-280 ature in the low radius ratio and bottom heated simulations. Plumes in a 2D geometry 281 are rather sheet-like than column-like as they are in a 3D geometry. This leads to a warmer 282 temperature in the 2D geometries compared to the 3D as being the consequence of a topo-283 logical difference between flows in a spherical shell and spherical annulus, as explained 284 by Guerrero et al. (2018). Moreover, this difference is strongly accentuated for low ra-285 dius ratios, where the number of plumes is small and such geometrical effects significantly 286 affect the results. For a better illustration of this behavior we refer the reader to Fig-287 ure S5 of the SI. The increase of temperature differences with increasing f was also ob-288 served by Guerrero et al. (2018) and is confirmed by our results. 289

In the case of a purely internally heated case, we see that the annulus fares remark-290 ably better than the cylindrical geometries and that the average relative error of the mean 291 temperature, the  $v_{\rm rms}$ , and top temperature gradient diminish as the radius ratio decreases. 292 The highest radius ratio (i.e., f = 0.8) shows here the highest discrepancy between 2D 293 and 3D, with more than 50% and 20% of overestimation for the  $v_{rms}$  and the top tem-294 perature gradient respectively, while the stagnant lid is underestimated on average by 295 15%. When taking a closer look at the simulations, it appears that, the internal heat-296 ing simulations in 2D have a tendency to require more convective strength in order to 297 transport the same amount of heat in the domain compared to a 3D simulation, as al-298 ready shown in Hernlund and Tackley (2008). This peculiarity when investigating the 299 temperature and velocity distribution will apparently create a larger amount of down-300 wellings in the case of a 3D model for a given internal heating rate when compared to 301 a 2D one. This can be seen on the Figure S7 of the SI. 302

For cases heated both from below and from within (i.e., mixed heated cases), the spherical annulus is showing the best results for the mean temperature, the top temperature gradient, and the stagnant lid thickness when the radius ratio is the lowest (i.e., f = 0.2). For the highest radius ratio considered here (i.e., f = 0.8), the results obtained with the spherical annulus and the cylinder geometries show similar errors, with the exception of  $v_{rms}$  that seems to be best reproduced by the scaled cylinder geometry.

When combining purely basal heating with internal heating, the main discrepancy previously arising from the low radius ratio and purely basal heated simulations seems to be mitigated by the addition of internal heating. The difference in the temperature distribution between the spherical annulus and the spherical shell tends to disappear (see Figure S7 of the SI).

In summary, for the stagnant lid cases presented here, the mean temperature is overall better reproduced by the spherical annulus independently of the radius ratio or heating mode. Additionally, in the intermediate to low radius ratio simulations ( $f \le 0.5$ ), the spherical annulus can also reproduce the 3D velocities, the top temperature gradient, and the stagnant lid better than the cylinder geometry.



Figure 3: Averaged computed relative error to the 3D geometry with 3 different heating modes (i.e., purely basal heated, purely internal heated, and mixed heated) for steady-state convection simulations with a temperature dependent viscosity. The mean temperature of the domain, the root mean square velocity, the temperature gradient at the top of the domain, and the stagnant lid thickness are compared here. For each subplot analyzing the relative error in a given heating mode, every column represents a different geometry, namely the 2D cylinder, the 2D scaled cylinder, and the 2D spherical annulus. The thermal Rayleigh number is  $5 \times 10^6$ , the internal Rayleigh number is  $5 \times 10^7$ , and the investigated radius ratios are 0.2, 0.5, and 0.8.

# 320 **3** Thermal evolution models

In this part we compare the 2D and 3D geometries in a more complex set-up, by using thermal evolution models in a stagnant lid regime. Compared to the previously discussed steady-state calculations, these models illustrate which of the 2D geometries can best reproduce the 3D results when mantle and core cooling are considered.

# 325 **3.1 Mathematical model**

For the thermal evolution models we use the Extended Boussinesq Approximation (EBA) (Schubert et al., 2001) to account for adiabatic heating and cooling. The energy equation (Eq. 3) becomes:

$$\frac{DT}{Dt} - \nabla \cdot (k\nabla T) - Di\alpha (T + T_{surf})\mathbf{u}_r - \frac{Di}{Ra}\Phi - H = 0, \tag{7}$$

where  $\mathbf{u}_r$  is the radial component of the velocity vector,  $T_{surf}$  is the surface temperature,  $\alpha$  is the thermal expansivity, and  $\Phi$  is the viscous dissipation given by  $\Phi = \tau$ :  $\dot{\varepsilon}/2$ , where  $\tau$  is the deviatoric stress tensor and  $\dot{\varepsilon}$  the strain rate tensor. The dissipation number Di is defined as follows:

$$Di = \frac{\alpha_{ref} g_{ref} D}{c_p},\tag{8}$$

where  $c_p$  is the mantle heat capacity.

In the thermal evolution models, we consider a temperature and pressure dependent viscosity that follows the Arrehnius law of diffusion creep. The non-dimensional equation for viscosity reads (Roberts & Zhong, 2006):

$$\eta(T,z) = exp\left(\frac{E+zV}{T+T_{surf}} - \frac{E+z_{ref}V}{T_{ref}+T_{surf}}\right),\tag{9}$$

where E and V are the activation energy and the activation volume respectively (Karato & Wu, 1993; Hirth & Kohlstedt, 2003).  $T_{ref}$  and  $z_{ref}$  are the reference temperature and depth, respectively, at which the reference viscosity is attained. The non-dimensional  $T_{ref}$ and  $z_{ref}$  values correspond to a dimensional reference temperature of 1600 K and a dimensional reference pressure of 3 GPa, respectively.

The temperature of the lower boundary  $T_{CMB}$  evolves following a 1-D energy balance, assuming a core with constant density and heat capacity (Stevenson et al., 1983):

$$c_c \rho_c V_c \frac{dT_{CMB}}{dt} = -q_c A_c, \tag{10}$$

where  $c_c$  is the heat capacity of the core,  $\rho_c$  is the core density,  $V_c$  is the core volume,  $q_c$  is the heat flux at the core-mantle boundary (CMB), and  $A_c$  is the core surface area. Here we do not consider core crystallization.

As appropriate for thermal evolution models, we take into account the decay of the heat producing elements (i.e.,  $Ur^{238}$ ,  $Ur^{235}$ ,  $Th^{232}$ , and  $K^{40}$ ). The amount of radioactive heat sources is calculated using the concentrations listed in Table 1.

In thermal evolution models we consider the effect of a 50 km laterally homogeneous crust. This crust is enriched in radiogenic elements while the mantle is depleted according to the following mass balance:

$$M_{tot} \cdot Q_{tot} = M_{mantle} \cdot Q_{mantle} + M_{crust} \cdot Q_{crust}, \tag{11}$$

where M is the mass and Q is the heating rate. This setup also considers the blanketing effect of the crust by using a lower thermal conductivity k in the crust compared to the mantle.

# **356 3.2** Case definition

We test three scenarios for the thermal evolution of a Mars-like, the Moon-like, and Mercury-like planet. We model the entire evolution of these planets to determine the variations over time of several key output quantities. These three planetary bodies were chosen because of their different interior structures. In the Mars-like case, the radius ratio between core and planetary radius is f = 0.544. The Moon- and Mercury-like scenarios represent two end-members in terms of their radius ratios, with f = 0.224 and f =0.828, respectively.

In the case of the 2D grids, we use a radial resolution of  $\sim 10$  km for Mars- and Moon-like cases, and a  $\sim 5$  km radial resolution for the thin mantle of Mercury. In the case of the 3D grids, the radial resolution lies between 22 and 9 km, and we use a lateral resolution of 40962 points per shell. A more detailed list of the resolution for every grid is available in Table S2 of the SI.

In the cylindrical geometry, we use both the classical cylinder and the rescaling of van Keken (2001) as done previously in the stagnant lid steady-state simulations. It is worth to note that for the peculiar Moon-like interior structure, the scaling of the respective radii leads to a radius ratio f = 0.0503. Since this is an extreme case, we test whether the rescaling of the cylinder geometry is appropriate for such interior structures in a thermal evolution scenario.

It is important to note here that for each planet we use different Rayleigh num-375 bers (i.e., Ra and  $Ra_Q$ ). These are calculated self-consistently using the mantle thick-376 ness, internal heat sources, and temperature difference accross the mantle specific for each 377 planet. The parameters are listed in Table 1. While for Mars- and Moon-like simulations 378 we use a reference viscosity of  $10^{21}$  Pas, for the Mercury-like case we perform additional 379 tests with a reference viscosity that is lower by two orders of magnitude (i.e.,  $10^{19}$  Pas). 380 Since the thin Mercurian mantle typically leads to a conductive state after a few Gyr 381 of evolution, by using a lower reference viscosity we test additional scenarios, in which 382 convection can be sustained over most of the evolution. The results for Mercury with 383  $\eta_{ref} = 10^{21}$  Pas and  $10^{19}$  Pas are also compared between the 3D spherical shell and 384 the 2D geometries. 385

In all our simulations we consider the presence of a primordial crust with a thick-386 ness of 50 km, which is enriched in radiogenic elements compared to the bulk heat sources 387 of the planet by a factor of 2 and has a two times lower thermal conductivity than the 388 mantle (see Table 1). While being a representative value for the enrichment of the Mer-389 curian crust (Tosi, Grott, et al., 2013), for the two other scenario it allows to increase 390 the complexity of the simulation without having a thermal evolution dominated by the 391 enrichment of the crust. A second set of thermal evolution models neglecting the effects 392 of the crust is listed in Section S7 of the SI. 393

# 3.3 Results

394

In the following, we present the results obtained for the thermal history of Mars, the Moon, and Mercury for all geometries. Similar to the steady-state calculations, we show in Figure 3 the difference of the 2D cylinder, 2D scaled cylinder, and 2D spherical annulus to the 3D results after 4.5 Gyr of evolution (i.e., at present day). In addition to the error shown in percent, we also list the difference between the dimensional values for mean temperature, CMB temperature, root mean square velocity, lid thickness, as well as surface and CMB heat fluxes (Figure 4).

Figure 5 shows the entire evolution over 4.5 Gyr of the output quantities of interest for all four geometries (2D cylinder, 2D scaled cylinder, 2D spherical annulus, and 3D spherical shell) for a Mars-like geometry. Our results show clearly that in the case of a Mars-like geometry, the values obtained during the entire thermal evolution with



Thermal evolution cases

Figure 4: Relative error to the 3D in the case of thermal evolution simulations. In each panel we vary the planet on the y axis and on the x axis we vary the geometry. We investigate the relative error for: the mean temperature (a), the CMB temperature (b), the root mean square velocity (c), the stagnant lid thickness (d), the surface heat flux (e), and the CMB heat flux (f). A color in the blue indicates an underestimation of the results obtained in the 3D geometry whereas a color in the red indicates an overestimation. 2D Cyl stands for non-scaled 2D cylindrical geometry, 2D Sca Cyl is 2D cylindrical geometry. Each panel shows the relative error in % to the 3D and the absolute error in dimensional unit.

Symbol	Description (Unit)	Mars	Moon	Mercury
$R_p$	Planetary radius (km)	3400	1740	2440
$\dot{R_c}$	Core radius (km)	1850	390	2020
D	Mantle thickness (km)	1550	1350	420
f	Radius ratio (-)	0.544	0.224	0.827
$T_{surf}$	Surface temperature (K)	220	250	440
$T_{CMB}$	CMB temperature (K)	2000	2000	2000
$T_{ref}$	Reference temperature (K)	1600	1600	1600
$\Delta T$	Temperature contrast across the mantle (K)	1780	1750	1560
g	Gravitational acceleration $(m.s^{-2})$	3.7	1.6	3.7
$\eta_{ref}$	Reference viscosity $(Pas)$	$10^{21}$	$10^{21}$	$10^{21}$
$\kappa$	Thermal diffusivity $(m^2/s)$	$1 \times 10^{-6}$	$1.06 \times 10^{-6}$	$1.04 \times 10^{-6}$
$\alpha$	Thermal expansivity $(K^{-1})$	$2.50 \times 10^{-5}$	$2.50 \times 10^{-5}$	$2.50 \times 10^{-5}$
Ra	Rayleigh number(-)	$2.14 \times 10^6$	$5.35 \times 10^5$	$3.49 \times 10^4$
RaQ	Internal heating Rayleigh number (-)	$5.91  imes 10^7$	$8.70  imes 10^6$	$8.00  imes 10^4$
$\rho_{core}$	Core density $(kg/m^3)$	6000	7500	6980
$\rho_{mantle}$	Mantle density $(kg/m^3)$	3500	3300	3380
$\rho_{crust}$	Crust density $(kg/m^3)$	2900	2700	2900
$c_{p,m}$	Mantle heat capacity $(kgK)$	1142	1142	1142
$c_{p,c}$	Core heat capacity $(kgK)$	850	850	850
$\tilde{V}$	Activation volume $(m^3/mol)$	$6.00 \times 10^{-6}$	$6.00 \times 10^{-6}$	$6.00 \times 10^{-6}$
E	Activation energy $(J/mol)$	$3.00 \times 10^5$	$3.00 \times 10^5$	$3.00 \times 10^5$
$k_m$	Mantle thermal conductivity $(Wm^{-1}K^{-1})$	4	4	4
$k_{cr}$	Crust thermal conductivity $(Wm^{-1}K^{-1})$	3	2	3
$D_{crust}$	Primordial crust thickness (km)	50	50	50
	Heat source concentration	(Taylor, 2013)	(Taylor, 1982)	(Padovan et al., 2017)
$C_U$	Uranium concentration (ppb)	16	33	7
$C_{Th}$	Thorium concentration (ppb)	58	125	29
$C_K$	Potassium concentration (ppm)	309	83	550

Table 1: Parameters for thermal evolution calculations for Mars, Moon, and Mercury. Note that the non-dimensional radii are rescaled according to Eq. 6 for the scaled cylinder geometry.

a 3D geometry are more closely reproduced by the spherical annulus than the cylinder, 406 irrespective of whether it is scaled or not. It is to note that the spherical annulus geom-407 etry is reproducing especially well the evolution of the mean and core-mantle boundary 408 temperatures (see Figure 4 for the actual present-day error), while the velocities are sys-409 tematically overestimated by the 2D geometries (27.7%) for the spherical annulus and 29.6%410 for the rescaled cylinder). This directly affects the calculation of the stagnant lid thick-411 ness, and thus underestimates it by 6.2% for the annulus and 8.1% for the rescaled cylin-412 der. When trying to reproduce the heat fluxes at present day, the spherical annulus is 413 somewhat better than the scaled cylinder, with an approximated underestimation of the 414 CMB heat flux by 22% compared to 28% for the scaled cylinder, while the surface heat 415 flux will be overestimated by 6% and 8% for the annulus and the scaled cylinder, respec-416 tively. While we focus in this part mostly on present-day values, when examining the 417 entire thermal evolution of the planet we observe in the early and middle stages (between 418 1 and 3 Gyr) a relative error even larger as the one observed at present day, as seen on 419 Figure 5c and e. The Mars-like setup is the most challenging setup to reproduce for the 420 spherical annulus, and although exhibiting relatively low errors, it still shows the high-421 est discrepancies between the thermal evolution cases with different interior structures. 422 The overestimation of the mean temperature, mean velocity, surface heat flow, and un-423 derestimation of the stagnant lid thickness can be linked directly to the mixed heated, 424 temperature-dependent viscosity simulation with a radius ratio of 0.5, which shows the 425 same type of relative error (see Figure 3) 426



Figure 5: Timeseries of a Mars-like case with an initial crust of 50 km and with 4 different geometries (2D non-scaled cylindrical, 2D cylindrical, 2D spherical annulus and 3D spherical shell). The values shown here are the mean temperature (a), the core-mantle boundary temperature (b), the surface heat flux (c), the core-mantle boundary heat flux (d), the averaged root mean square velocity of the domain (e), and the lid thickness (f) from 4.5 Gyr ago to present day, respectively. The shaded areas show the min.-max. variations during the evolution. The non-scaled cylinder has been added to show the effect of the rescaling introduced by van Keken (2001).

In the case of a Moon-like setup (Figure 6) the differences between the spherical 427 annulus and the cylinder are typically larger than in the Mars-like case. However the dif-428 ference between the spherical annulus and the 3D is significantly lower in the case of the 429 mean temperature, the stagnant lid thickness and the surface heat flow; as can be seen 430 on Figures 6a, c, and f. The temperatures through time are very well reproduced by the 431 spherical annulus (less than 2% of error compared to more than 12% for the cylindri-432 cal geometries). Similarly, the surface heat flux and the stagnant-lid thickness show a 433 good match between the spherical annulus and the 3D geometries (see Table S5 of the 434 SI). Concerning the cylindrical geometries, the effects of the rescaling are plainly visi-435 ble on the overall temperatures and heat fluxes evolution. As van Keken (2001) showed, 436 the cylinder tends to overestimate the relative importance of the CMB radius compared 437 to planetary radius and requires a rescaling of the radii. However, for the very low aspect-438 ratio of the lunar mantle, even when the rescaling is applied the results are still largely 439 different compared to a 3D spherical shell geometry. A better approximation of the 3D 440 results is obtained by the spherical annulus, where such rescaling is not needed. We see 441 that the CMB heat flux stays at around -1.86 mW m<sup>-2</sup> even at present day, meaning that 442 the core is actively heated by the mantle, although in the other geometries the core is 443 already cooling (see Figure 6b and d), a behavior which is also seen for Mars with the 444 non-scaled cylindrical geometry. Similar to what has been seen previously for the low 445 aspect-ratio cases with temperature-dependent viscosity combining basal heating and 446 internal heating (see Figure 3), the scaled and non-scaled cylindrical geometries show 447 large disagreements in all studied metrics. Nevertheless, even in the spherical annulus, 448 the mean velocity and the CMB heat flux present the largest errors among the investi-449 gated quantities. 450

In Figure 7, we show the results of the thermal evolution for a Mercury-like setup. 451 Here we used two sets of simulations in order to illustrate the case of a initially weakly 452 convecting mantle with a reference viscosity set as  $\eta_{ref} = 10^{21}$  Pas resulting in a Rayleigh 453 number of  $Ra = 3.49 \times 10^4$ ; and the case of a mantle presenting a stronger initial con-454 vection with a reference viscosity lowered by two orders of magnitude, thus increasing 455 the Rayleigh number to  $Ra = 3.49 \times 10^6$ . Here again the global trend previously seen 456 for Mars and the Moon emerges. As shown in figure 4, the spherical annulus geometry 457 again reproduces best the 3D results with an approximate error of less than 1%, with 458 a notable exception for the velocities, which are highly overestimated (more than 90%459 of relative error). The very high relative error of the  $v_{rms}$  is explained by the present-460 day state of the Mercurian mantle. In our simulations, a Mercury-like planet falls into 461 a quasi-conductive state after a couple of Gyr of evolution irrespective of the geometry 462 (Figure 7), which in turn gives very low absolute  $v_{rms}$  values. Yet the absolute differ-463 ence of velocity between the geometry is very small (less than  $1 \times 10^3$  cm/year). De-464 spite these high relative error values in the velocities, the stagnant lid thickness is, how-465 ever, quite well reproduced by the 2D geometries, giving a maximum relative error of 466 19 km (or an underestimation of 6.5%). 467

# 468 4 Discussion

Our results show that the spherical annulus can reproduce the 3D spherical shell
geometry better than the cylindrical geometry, consistent with previous studies by Hernlund
and Tackley (2008). Our systematic study, using simulations of increasing complexity,
shows for the first time in great detail the difference in using a 2D geometry instead of
a more realistic 3D spherical shell domain when modeling thermal convection in planetary mantles.

When using the cylindrical geometry, whether scaled or not, the results show substantial differences to the 3D geometry results in steady-state and thermal evolution simulations. The necessity of choosing between a scaled and a non-scaled cylinder in modeling geodynamic processes inevitably results in a trade-off between an accurate repre-



Figure 6: Timeseries of a Moon-like case with an initial crust of 50 km and with 4 different geometries (2D non-scaled cylindrical, 2D scaled cylindrical, 2D non-scaled cylindrical, 2D spherical annulus and 3D spherical shell). For a description off the values investigated, see Figure 5.



Figure 7: Timeseries of a Mercury-like case with an initial crust of 50 km, with 4 different geometries and 2 different reference viscosities. For a description off the values investigated, see Figure 5. The dotted lines represent simulations with a reference viscosity of  $\eta_{ref}=10^{19}$  Pa s while the solid lines represent the cases with a reference viscosity of  $\eta_{ref}=10^{21}$  Pa s. The maximum and minimum of the output quantities are not displayed here, since these variations are negligible.

sentation of the deep interior structures in the case of the non-scaled cylinder, especially
important when studying thermochemical structures (Stegman et al., 2003; Nakagawa
& Tackley, 2004; Yu et al., 2019; Kameyama, 2022), and a correct representation of the
heat fluxes as well as root mean square velocity in the domain (Deschamps et al., 2010;
Mulyukova et al., 2015) for the scaled one. To circumvent these inaccuracies, the systematic use of the spherical annulus in reproducing thermochemical convection in 3D is
thus strongly recommended.

In the case of steady-state simulations, we showed that the spherical annulus has the largest error in the high radius ratio scenarios (i.e, f = 0.6 and 0.8). The efficiency of the spherical annulus in reducing the error to the 3D (compared to the results of the scaled cylinder) is most visible in the case of a low radius ratio configuration (i.e., f =0.2), while nonetheless displaying large discrepancies in the mean temperature in the case of bottom heated and temperature-dependent setups, as also seen by Guerrero et al. (2018).

Concerning the heating modes, as reported by Hernlund and Tackley (2008), the 492 purely internally heated cases show the largest difference between the 2D and 3D geome-493 tries, while the mixed heating cases (bottom and internal heating) tends to be the heat-494 ing mode for which the spherical annulus exhibits the smallest errors in comparison to 495 the spherical shell, as the difference in the temperature distribution between the spher-496 ical annulus and the spherical shell tends to disappear (see Figure S6 of the SI). This 497 particularity becomes quite useful when trying to model more realistic processes such as thermal evolution models of terrestrial planets, as the silicate mantles of planets will 499 invariably show heating induced by both the presence of radiogenic elements in the man-500 tle and by the core. The smaller error between the 2D spherical annulus and 3D spher-501 ical shell observed in mixed heated cases makes the spherical annulus an acceptable al-502 ternative to model more complex scenario (Figure 4), for which a 3D geometry is too ex-503 pensive. The trend of the relative error in the steady-state stagnant lid simulations with 504 mixed heating is also observed in the case of thermal evolution models: the errors in the 505 surface heat flux and stagnant lid thickness increase with increasing radius ratio (cf. the 506 errors obtained for the Moon and Mars in Figure 4). However in the case of Mercury, 507 while the steady-state simulations would predict the largest errors, the low Rayleigh num-508 ber in thermal evolution models and the transition to a conductive state during the ther-509 mal evolution strongly reduce the discrepancy between 2D and 3D geometries. 510

The results presented here show that the spherical annulus is to be preferred to the 511 cylindrical geometry, whether for steady-state simulations or thermal evolution simula-512 tions. However, in the case of the thermal evolution simulations one should question whether 513 this geometry is sufficient to approximate the 3D spherical shell. Some observables such 514 as the heat flux, the mechanical thickness of the lithosphere and the crust produced by 515 partial melting of the mantle are used to evaluate the thermochemical evolution of a planet. 516 But an important question is whether the 2D spherical annulus is accurate enough to 517 reproduce the results of a 3D spherical shell for the above mentioned quantities, and which 518 of these observables can be affected the most. 519

Additional post-processing has thus been conducted in order to better character-520 ize the differences of more complex processes in the spherical annulus compared to the 521 spherical shell. We exclude from this comparison the cylindrical geometry given its lack 522 of accuracy in reproducing 3D. Moreover, the areas and volumes in the 2D cylindrical 523 geometry are truly 2D and thus difficult to compare to the 3D spherical shell. Melting 524 in the mantle, the thickness of the mechanical lithosphere, and heat fluxes are shown in 525 Figure 8 as a function of time. For the calculation of the mechanical lithosphere thick-526 ness, we follow the approach of Grott and Breuer (2008). The calculations involving par-527 tial melting of the mantle are highly simplified and do not include the effects of latent 528 heat or mantle depletion. While the quantities presented in Figure 8 are based on sim-529 ple post-processing of the thermal evolution results, they are meant to provide first or-530 der implications for the thermal evolution modeling with 2D and 3D geometries (for ad-531 ditional information concerning the post processing, see S11, S12). 532

When reproducing 3D simulations, the spherical annulus is well suited to replicate melting, mechanical thickness and heat fluxes. In particular the heat fluxes, and especially the CMB heat flux (Figure 8g, h, i) are especially well reproduced in terms of values and trend of evolution. The largest errors were observed for a Mars-like structure with an overestimation of less than 1.5 mW m<sup>-2</sup> compared to the 3D for the surface heat flux and an almost identical CMB heat flux (less than 1 mW m<sup>-2</sup> lower values compared to the 3D case).

The mechanical thickness for a Moon-like interior structure will be underestimated 540 on average by 5% for the spherical annulus, while the amount of melting will be over-541 estimated by 10% as in the case of Mercury. Since the computation of the amount of par-542 tial melting in the mantle through time relies on the temperature profile of the simula-543 tion, it is not surprising to see on one hand the underestimation of the mechanical thick-544 ness and on the other hand a systematic overestimation of partial melting by the spher-545 ical annulus compared to the 3D. The main reason explaining these differences is that 546 the spherical annulus will consistently overestimate the overall mantle temperature, lead-547 ing to a hotter temperature profile, thus directly affecting the degree of melting and the 548 thickness of the mechanical lithosphere. 549

In the case of a Mars-like structure (Figure 8b, e) the differences between 2D and 550 3D are larger, in particular in the case of partial melting, which the annulus will over-551 estimate by a maximum of 30% at around 1.5 Gyr. The mechanical thickness will be un-552 derestimated on average by 10 %. In particular the differences in partial melting could 553 lead to an overestimation of the crustal thickness in the 2D spherical annulus geometry. 554 This in turn could lead to more crustal production due to a mechanism called "crustal 555 blanketing" (e.g., Schumacher & Breuer, 2006), in which the reduced thermal conduc-556 tivity of the crust will prevent efficient cooling of the mantle. A higher crustal produc-557 tion rate could then lead to a stronger depletion of the mantle in crustal components and 558 volatile elements. Hence, care should be taken when the spherical annulus geometry is 559 employed to study partial melting and subsequent crust production or degassing in par-560 ticular for planets with an intermediate radius ratio, like Mars or Venus. These processes 561 and the differences between 2D and 3D geometries for such scenarios need to be quan-562 tified in future studies. 563



Figure 8: Timeseries of the three scenario investigated (from left to right; the Moon, Mars and Mercury). First row shows the fraction of molten mantle (in %) at a given time in the evolution for each planet, second row shows the mechanical thickness of the lithosphere (in km) during the evolution, and the third row shows the CMB and surface heat fluxes (in mW m<sup>-2</sup>). Since the cylindrical geometry shows the largest difference to the 3D, it was not included in this comparison. All the equations used in order to compute these quantities are described in the SI.

# 564 5 Conclusions

The main goal of this study is to provide a systematic comparison between different geometries in order to determine how accurate can 2D geometries reproduce 3D results. To this end, we investigated (scaled and non-scaled) 2D cylinder, 2D spherical annulus, and 3D spherical shell geometries in a series of scenarios. We started with isoviscous steady-state models, included the effects of a temperature dependent viscosity, and finally tested the different geometries for thermal evolution setups. Our main findings are the following:

5721. While it is obvious that a 3D geometry should be preferred over a 2D one, due to573the high computational cost, this may not always be feasible. Applying models574with different complexities, we demonstrated that the 2D spherical annulus ge-575ometry is able to reproduce the 3D models much better than the 2D cylinder, in576particular for the low radius ratio setups. The latter is also clearly seen when mod-577eling the thermal evolution of the Moon.

578	2.	For steady-state scenarios, our models show that the 2D geometries will mostly
579		overestimate the mean temperature compared to 3D, a result largely explained
580		by the geometry of mantle plumes (i.e., sheet-like in 2D vs. columnar-like in 3D).
581		This discrepancy decreases with an increasing Rayleigh number but is more ac-
582		centuated for low-radius ratio cases, a result already observed by Guerrero et al.
583		(2018). The differences in temperature between the 2D and 3D geometries decreases
584		for mixed heated cases (i.e., heated both from below and from within). This is es-
585		pecially true in the case of the spherical annulus, since the spherical annulus is a
586		geometry which uses the same cell volumes as a 3D spherical shell.
587	3.	We find that for intermediate ratios of the inner to outer radius (e.g., Mars-like
588		thermal evolution case), the differences in the results for the 2D and 3D geome-
589		tries are larger than for extreme radius ratios. In contrast to the temperature-dependent
590		steady-state cases, where the difference in surface heat flux and stagnant lid thick-
591		ness between 2D geometries and 3D geometries is largest for high radius ratios,
592		the difference obtained for Mercury-like evolution parameters is minimal. This is

due to the low Rayleigh number of Mercury that leads to the transition to a conductive state during its thermal history.

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4. Care needs to be taken when studying melting processes with the spherical annulus in thermal evolution setups with intermediate radius ratios (e.g., Mars and Venus), as this geometry might overestimate crustal production by up to 30% compared to a 3D simulation leading to a different thermal history of the interior.

Future studies need to test the accuracy of the 2D spherical annulus in reproducing the 3D spherical shell geometry in more complex scenarios considering variable thermal conductivity and expansivity (Tosi, Yuen, et al., 2013), chemical buoyancy (Nakagawa et al., 2010), as well as partial melting of the mantle and its influence on thermal evolution.

# <sup>604</sup> Data Availability Statement

<sup>605</sup> Supplementary datasets containing all values shown in tables and figures are available <sup>606</sup> upon request on Zenodo : https://doi.org/10.5281/zenodo.8047757

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# **@AGU**PUBLICATIONS

# Geochemistry, Geophysics, Geosystems

Supporting Information for

# Supporting Information for "Approximating 3D Models of Planetary Evolution in 2D: A Comparison of Different Geometries"

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- 2. Datasets concerning temperature dependent simulations; Figure S6
- 3. Datasets concerning thermal evolution simulations; Figure S7

# Introduction

In Section S1 we present the scaling factors used in this study, as listed in Table S1. Section S2 displays in Table S2 all the parameters used to create the grids employed in this study for the thermal convection model GAIA. Section S3 details the differences between the cylindrical and the spherical annulus geometries used in our thermal convection code GAIA. Section S4 provides a short comparison between the study from Hernlund and Tackley (2008) and this study for isoviscous stead-state cases. Section S5 presents how the relative error is calculated. In Section S6 we give briefly the equations used for internal heating and the decay of heat producing elements in our model. In Sections S7 and S8 we list the tables displaying all the present-day values of the investigated output quantities for the thermal evolution scenario in an homogeneous setup (S7) and in a setup with a 50 km crust (S8); these data are available as CSV files provided at . Section S9 presents the temperature profiles at present day and at 1 Gyr into the evolution for each thermal evolution scenario with a 50 km crust. Section S10 shows the calculation of the stagnant lid thickness for the thermal evolution models. Section S11 displays the calculation of the partial melting in the mantle, as a post processing step for the thermal evolution models. Section S12 gives the formulation to calculate the thickness of the mechanical lithosphere as a post processing step. In the Section S13, three different comparisons of stagnant lid simulations (see Section 4), are displayed as slices for both the 3D spherical shell and the 2D spherical annulus geometry, with the 3D on the left and the 2D geometry on the right.

# S1 Scaling table

The conservation equations used to model mantle convection are expressed in non-dimensional form. The non-dimensionalisation is obtained by multiplying the parameters by a well-suited scaling factor. Parameters with a star represent the non-dimensional ones and are calculated as follows:

Quantity	Non dimensional
Temperature	$T^* = \frac{T - T_0}{\Delta T}$
Length	$x^* = \overline{\frac{x}{D}}$
Time	$t^* = \frac{\kappa_0}{D^2}t$
Velocity	$u^* = \frac{uD}{\kappa_0}$
Pressure	$P^* = \frac{PD^2}{\eta_0 \kappa_0}$
Stress	$\sigma^* = \sigma \frac{D^2}{\eta_0 \kappa_0}$
Density	$\rho^* = \frac{\rho}{\rho_0}$
Thermal expansivity	$\alpha^* = \frac{\alpha}{\alpha_0}$
Heat production rate	$H^* = \frac{H\dot{D}^2}{\kappa_0 cp\Delta T}$
Viscosity	$\eta^* = \frac{\eta}{\eta_0}$
Activation energy	$E^* = \frac{E}{\Delta TR}$
Activation volume	$V^* = \frac{V\rho_0 Dg}{\Delta TR}$

Table S1: Table of the non dimensional values used in the study

In the remainder of this study, all the non-dimensional parameters are used without the star for better readability.

Setup	Geometry	Aspect ratio	Radial resolution	Lateral resolution	Total points	Rayleigh number
	2 - D	0.2	48 shells	227 p.per.shell	11350	$10^4 - 10^5 - 10^6$
	2 - D	0.4	48 shells	352 p.per.shell	17600	$10^4 - 10^5 - 10^6$
	2 - D	0.6	48 shells	604 p.per.shell	30200	$10^4 - 10^5 - 10^6$
	2 - D	0.8	48 shells	1358 p.per.shell	67900	$10^4 - 10^5 - 10^6$
	2 - D	0.2	120 shells	556 p.per.shell	69052	$10^7 - 10^8$
	2 - D	0.4	120 shells	880 p.per.shell	107360	$10^7 - 10^8$
	2 - D	0.6	120 shells	1508 p.per.shell	183976	$10^7 - 10^8$
Isoviscous	2 - D	0.8	120 shells	3393 p.per.shell	413946	$10^7 - 10^8$
	3 - D	0.2	48 shells	40962 p.per.shell	2048100	$10^4 - 10^5 - 10^6$
	3 - D	0.4	48 shells	40962 p.per.shell	2048100	$10^4 - 10^5 - 10^6$
	3 - D	0.6	48 shells	40962 p.per.shell	2048100	$10^4 - 10^5 - 10^6$
	3 - D	0.8	48 shells	40962 p.per.shell	2048100	$10^4 - 10^5 - 10^6$
	3 - D	0.2	70 shells	40962 p.per.shell	2949264	$10^7 - 10^8$
	3 - D	0.4	70 shells	40962 p.per.shell	2949264	$10^7 - 10^8$
	3 - D	0.6	70 shells	40962 p.per.shell	2949264	$10^7 - 10^8$
	3 - D	0.8	70 shells	40962 p.per.shell	2949264	$10^7 - 10^8$
	2 - D	0.2	100 shells	472 p.per.shell	48144	$Ra = 5 \times 10^6; Ra_Q = 5 \times 10^7$
	2 - D	0.5	100 shells	943 p.per.shell	96186	-
T-dependent	2 - D	0.8	100 shells	2828 p.per.shell	288456	-
	3 - D	0.2	70 shells	40962 p.per.shell	2949264	-
	3 - D	0.5	70 shells	40962 p.per.shell	2949264	-
	3 - D	0.8	70 shells	40962 p.per.shell	2949264	-
	2 - D	Mars $\rightarrow 0.544117$	155 shells	1 650 p.per.shell	259050	$Ra = 2.14 \times 10^6; Ra_Q = 5.91 \times 10^7$
	3 - D	-	70 shells	40962 p.per.shell	2949264	_
Thermal	2 - D	$\mathrm{Moon} \rightarrow 0.224137$	135 shells	670 p.per.shell	91790	$Ra = 5.35 \times 10^5; Ra_Q = 8.70 \times 10^6$
evolution	3 - D	-	64 shells	40962 p.per.shell	2703492	_
	2 - D	Mercury $\rightarrow 0.827868$	84 shells	2803 p.per.shell	241058	$Ra = 3.49 \times 10^4; Ra_Q = 8.00 \times 10^4$
	3 - D	-	46 shells	40962 p.per.shell	1884252	

**Table S2:** Grid parameters for each simulation in this study. For each grid, the number of shells displayed is the number of layers in the "active" part of the grid, meaning that it does not account for the two ghost layers at the base and at the top of the grid, which are used to set the boundary conditions.

# S2 Grid parameters

This table provides all the grid parameters used in this study for the steady state simulations as well as the thermal evolution models.



**Figure S1:** Representation of the elementary volumes of the cylinder in blue and of the spherical annulus in red. In a regular two dimensional representation of the spherical annulus grid, we only see the area of the elementary volume bisected by the equatorial plane (red filled areas).

# S3 Spherical annulus geometry

The principal difference between the 2D spherical annulus and the 2D cylindrical geometry lies in the formulation of the areas and volumes for each grid. The cylindrical geometry will have a purely 2D formulation of its areas and volume whereas the spherical annulus use the same formulation as a 3D spherical shell. The effective degree of curvature for each cell goes then from 1 in the case of the cylinder to 2 in the case of the spherical annulus. For the mathematical formulation of the grid geometry, we refer to *Hernlund and Tackley*, 2008

# S4 Comparison to results of Hernlund and Tackley 2008

This table presents the comparison between the study from *Hernlund and Tackley*, 2008 and this study for isoviscous steady state cases considering basal heating and internal heating, respectively, with Rayleigh numbers between  $Ra = 10^4$  to  $Ra = 10^5$ . For the radius an Earth-like value is used (f= 0.55) for the 3D spherical shell and the annulus, while the scaled cylinder uses f= 0.3025. The values are averaged over the last 20% of the simulations.

		Bottom heated		
$Ra = 10^4$	Geometry	3D	Spherical annulus	Scaled cylindrical
	v <sub>rms</sub>	42.3	37.7	35.6
Hernlund	$v_{\rm rms}$ peak-peak	0	0	0
&	<nu></nu>	3.85	4.18	3.99
Tackley 2008	<Nu> peak-peak	steady	steady	steady
	V <sub>rms</sub>	42.1	43.1	37.3
This	$v_{\rm rms}$ peak-peak	0	0	0
study	<nu></nu>	3.84	4.12	4.08
	<Nu> peak-peak	steady	steady	steady
$Ra = 10^5$				
	V <sub>rms</sub>	160	160	165
Hernlund	$v_{\rm rms}$ peak-peak	11	14	90
&	<nu></nu>	7.27	7.39	6.2
Tackley 2008	<Nu> peak-peak	0.5	0.3	2.1
	V <sub>rms</sub>	163.9	160.0	158.1
This	$v_{\rm rms}$ peak-peak	1	10	0
study	<nu></nu>	6.62	7.16	7.75
	<Nu> peak-peak	0.03	0.4	0.2
		Internal heated		
$Ra = 10^4$	$Ra_Q = 3.4 \times 10^4$			
Hernlund	V <sub>rms</sub>	23.3	23.5	22.8
&	v <sub>rms</sub> peak-peak	0	0	0
Tackley 2008	<t></t>	0.311	0.308	0.319
	v <sub>rms</sub>	22.6	23.3	21.4
This	v <sub>rms</sub> peak-peak	0	0	0
study	<t></t>	0.311	0.312	0.334
$Ra = 10^5$	$Ra_Q = 6.6 \times 10^5$			
Hernlund	V <sub>rms</sub>	60.5	78.5	77.0
&	v <sub>rms</sub> peak-peak	7	36	75
Tackley 2008	<t></t>	0.322	0.349	0.384
	v <sub>rms</sub>	76.7	84.6	79.7
This	$v_{\rm rms}$ peak-peak	2.2	9	10.5
study	<t></t>	0.337	0.3443	0.387

**Table S3:** Comparison of the spherical annulus used in this study and the study of *Hernlund and Tackley*, 2008. The top part of the table are the results from *Hernlund and Tackley*, 2008 and the bottom part of the table present the results from this study. The values displayed are the root mean square velocity ( $v_{\rm rms}$ ), mean temperature (<T>), and Nusselt numbers (*Nu*), which are computed once a statistical steady state is attained.

# S5 Error computation

The error presented in the main manuscript to illustrate the difference between 2D and 3D geometries was computed as follows:

$$Error = -\frac{(3D_{value} - 2D_{value})}{max(3D_{value}; 2D_{value})} \times 100$$
(S1)

The absolute error for the thermal evolution simulations on the other hand is calculated as:

$$Error = 2D_{dimensional value} - 3D_{dimensional value}$$
(S2)

in order to determine whether a 2D geometry over or under-estimates the 3D geometry results.

# S6 Internal heating and heat producing elements decay

In our thermal evolution scenarii, we also take into account the decay of the heat producing elements, here being the  $Ur^{238}$ ,  $Ur^{235}$ ,  $Th^{232}$  and the  $K^{40}$ , thus giving us the heat production rate which is determined from present day amounts of heat sources and is given by equation 28 from *Breuer* (2009).

# S7 Table of results for the thermal evolution simulations without crust

This table gives all the present-day values in a dimensional form for the thermal evolution simulations without crust.

Planet	Parameter (Unit)	3D sph. shell	2D sph. annulus	2D scaled cylinder	2D cylinder
Mars	$T_{\rm mean}$ (K)	1697.1	1713.9	1752.8	1846.3
	$T_{\rm CMB}$ (K)	2146.8	2150.2	2189.3	2171.1
	$v_{\rm rms}~({\rm cm/yr})$	0.767	1.04	1.05	1.32
	$q_{\rm top}~({\rm mW/m^2})$	21.68	22.95	24.10	27.12
	$q_{\rm bot} \ ({\rm mW/m^2})$	2.10	2.12	1.91	1.07
	$D_{ m lid}~( m km)$	302.5	297.1	281.52	247.7
Moon	$T_{\rm mean}$ (K)	1367.6	1372.7	1552.6	1661.8
	$T_{\rm CMB}$ (K)	2379.7	2403.6	2473.2	2287.9
	$v_{\rm rms}~({\rm cm/yr})$	0.216	0.374	0.527	0.472
	$q_{\rm top}~({\rm mW/m^2})$	14.533	14.47	17.05	18.15
	$q_{\rm bot}~({\rm mW/m^2})$	0.959	0.910	0.723	-3.35
	$D_{ m lid}~( m km)$	415.1	427.5	377.2	358.5
Mercury	$T_{\rm mean}$ (K)	1049.3	1048.0	1069.8	1155.6
	$T_{\rm CMB}$ (K)	1689.0	1685.1	1715.9	1829.2
	$v_{\rm rms}~({\rm cm/yr})$	5.7 E-4	3.1E-07	5.9E-07	7.7E-05
	$q_{\rm top}~({\rm mW/m^2})$	12.85	12.83	13.56	15.29
	$q_{\rm bot}~({\rm mW/m^2})$	10.20	10.15	10.10	10.74
	$D_{ m lid}~( m km)$	294.9	252.9	248.2	244.0

**Table S4:** Output quantities at present day for various geometries and planets in anhomogeneous set.

S8 Table of results for the thermal evolution simulations with a 50 km crust

TT1-:	± - 1-1 -		1 +1			f + 1	<b>1</b> 1 1	1+ <sup>1</sup>		: + 1-	
$1 \mathrm{ms}$	table	gives a	n the	present-da	y values	for the	unermai	evolution	simulations	WIUII	crust.

Planet	Parameter (Unit)	3-D sph. shell	2-D sph. annulus	2-D scaled cylinder	2-D cylinder
	$T_{\rm mean}$ (K)	1700.4	1741.8	1774.4	1846.1
Mars	$T_{\rm CMB}$ (K)	2123.4	2147.5	2169.2	2109.2
	$v_{\rm rms}~({\rm cm/yr})$	0.73	1.00	1.03	0.92
	$q_{\rm top}~({\rm mW/m^2})$	21.78	23.22	24.15	26.53
	$q_{\rm bot}~({\rm mW/m^2})$	1.65	1.29	1.19	-1.68
	$D_{ m lid}~( m km)$	277.00	259.80	254.61	233.17
	$T_{\rm mean}$ (K)	1456.9	1481.6	1658.1	1756.8
	$T_{\rm CMB}$ (K)	2404.7	2435.1	2504.9	2296.6
Moon	$v_{\rm rms}~({\rm cm/yr})$	0.24	0.35	0.68	0.50
	$q_{ m top}~({ m mW/m^2})$	14.63	14.53	16.95	17.93
	$q_{ m bot}~({ m mW/m^2})$	0.38	0.30	0.22	-1.86
	$D_{ m lid}~( m km)$	368.2	370.9	327.3	305.7
Mercury	$T_{\rm mean}$ (K)	1049.3	1048.7	1070.5	1155.5
	$T_{\rm CMB}$ (K)	1689.0	1686.9	1716.7	1830.1
	$v_{\rm rms}~({\rm cm/yr})$	5.7E-04	5.1E-05	6.2 E- 07	1.6E-3
	$q_{ m top}~({ m mW/m^2})$	12.8	12.8	13.6	15.2
	$q_{ m bot}~({ m mW/m^2})$	10.2	10.1	10.8	10.1
	$D_{\rm lid}~({\rm km})$	294.8	292.7	275.7	296.5

**Table S5:** Output quantities at present day for each planet in various geometries for the thermal evolution simulation with a 50km crust.

All the present day output quantities are available in the online CSV files of this study.



Figure S2: Profiles of temperature throughout the entire mantle for the Moon, Mars and Mercury. The profiles are shown at 1 billion years into the evolution and at present day. Every geometry studied is represented here; in the case of Mercury, only the simulations with a reference viscosity  $\eta_{ref} = 10^{21}$  Pas are shown.

# S9 Temperature profiles for thermal evolution simulations



**Figure S3:** Calculation of the stagnant lid thickness adapted from the work of *Hüttig and* Breuer (2011). The thickness is determined by finding the depth where the derivative of the averaged velocity profile  $\frac{dV}{dR}$  is the highest and intercepting it with the y axis. The red line is the averaged velocity profile in the domain, the blue line is the derivative of the velocity profile, the green dashed line is the depth of the stagnant lid, and the black line is the depth of the absolute value of the velocity derivative is the highest. All units are non dimensional.

# S10 Stagnant lid calculation

In the calculation of the stagnant lid we use two different methods to determine its thickness. The first is from the work of *Hüttig and Breuer* (2011) and is illustrated by the Figure S3 The calculation of the stagnant lid becomes difficult with the velocity gradient method (*Hüttig and Breuer*, 2011) when the veolocity are too low. Therefore a second method, relying on the Peclet criterion is used in the case of Mercury when it falls into a quasi conductive state. The determination of the stagnant lid with a Peclet criterion, is determined with a threshold, that we set here as 5% of the averaged  $v_{rms}$  at the studied time step. The thickness is then the depth at which the  $v_{rms}$  profile becomes smaller than our threshold (or Peclet criterion).



**Figure S4:** Melting curves from *Takahashi* (1990) and the minimum, mean and maximum temperature profile for a present-day Mars-like case.

# S11 Partial melting calculation

We compute the averaged fraction of molten mantle at every time-step during the thermal evolution of the planet as a post processing step. It is used here as a simple comparison between the geometries. We use the melting curves from *Takahashi* (1990), as seen on Figure S2. However a cutoff is imposed at a depth of 7 GPa in the case of Mars. To calculate the volumetrically averaged degree of melting, we use eq 20. from *Morschhauser et al.* (2011) which is as following :

$$m_a = \frac{1}{V_a} \int_{V_a} \frac{T(r) - T_{sol}(r)}{T_{liq}(r) - T_{sol}(r)} \, dV,\tag{S3}$$

with  $V_a$  being the volume of the meltzone,  $T_{sol}$  the temperature of the solidus,  $T_{liq}$  the temperature of the liquidus, and T(r) the calculated mantle temperature profile. We then compute the total volume of melted mantle and compare it with the total mantle volume.

Parameter	Crust	Mantle
$\dot{\epsilon} (s^{-1})$	$10^{-17}$	$10^{-17}$
$Q \; (kJ  mol^{-1})$	488	540
$B (\operatorname{Pa}^{-n} \operatorname{s}^{-1})$	$1.1\times10^{-26}$	$2.4 \times 10^{-16}$
n (-)	4.7	3.5
$\sigma_y$ (MPa)	15	15

**Table S6:** Rheological parameters used in the equation S6, as appropriate for dry diabase crust and dry olivine mantle, for more information see *Plesa et al.* (2016), *Grott and Breuer* (2008).

# S12 Mechanical thickness calculation

In this study we calculate the mechanical thickness, by using the strength envelope formalism McNutt (1984) for a structure comprised of a mantle layer and a crust layer. This mechanical thickness of the lithosphere represents the depth at which the plate looses its mechanical strength due to ductile flow *Grott et al.* (2007). This depth, or temperature equivalent is then calculated as following :

$$T_e = \frac{E}{R} \left[ log \left( \frac{\sigma_B^n A}{\dot{\epsilon}} \right) \right]^{-1}, \tag{S4}$$

in which E, A and n are rheological parameter listed in Table S6, R is the gas constant,  $\sigma_B$  the bounding stress, and  $\dot{\epsilon}$  being the strain rate. The total elastic thickness of this system depends then on whether the two layers act as a single elastic layer or are separated by an incompetent layer of crust. If the layers are separated, the elastic thickness  $D_e$  is then calculated as:

$$D_e = (D_{e,m}^3 + D_{e,c}^3)^{\frac{1}{3}},\tag{S5}$$

where  $D_{e,m}$  and  $D_{e,c}$  are the thicknesses of the elastic parts of crust and mantle, respectively Burov and Diament (1995). However, if  $D_{e,c}$  is greater or equals the local crustal thickness, then no layer of incompetent crust exists between the crust and the mantle and the effective elastic thickness is given by the sum of the two elastic layers:

$$D_e = D_{e,m} + D_{e,c} \tag{S6}$$

The decoupling of the system will strongly reduce the total elastic thickness as seen in eq. S5 and will mostly happen in regions with a thick crust. In the case of our simulations with a laterally homogeneous crust thickness we don't have any zone with a local thicker crust. To compute the local elastic thickness, a strain rate  $\dot{\epsilon}$  profiles of  $10^{-17} \ s^{-1}$  is used. The parameters used for this calculation are available in the Table S5.



**Figure S5:** Temperature slices in a temperature-dependent viscosity case with purely basal heating, left is 3D spherical shell and right is 2D spherical annulus. Two plumes are present in both geometries, however the distribution of the temperature is much more diffuse in the case of the annulus, as seen in *Guerrero et al.* (2018).

# S13 Slices comparison 3D-2D in stagnant lid simulations

The plots presented here show special cases of comparison between 3D and 2D spherical annulus for different heating mode in temperature-dependent viscosity setups.



Figure S6: Temperature slices in a temperature-dependent viscosity case with basal and internal heating. We note the disappearance of the error of the temperature distribution seen in Figure S1 by the addition of internal heating.



Figure S7: Temperature slices in a temperature-dependent viscosity case with purely internal heating. The amount of downwellings in a slice for the 3D case is far larger than what can be seen for the 2D spherical annulus (2D).

# Supplementary datasets

The following datasets are available upon request on Zenodo : https://doi.org/10.5281/zenodo.8047757

# Datasets concerning isoviscous simulations

Tables containing the time averaged (on the last 10% of the run) values for all the outputs and geometry studied. There is one table per Ra number with a given heating mode. In total there are 15 tables for each scenarios (i.e., three different heating modes and five different Ra numbers).

# Datasets concerning temperature dependent simulations

Tables containing the time averaged (on the last 10% of the run) values for all the outputs and geometry studied for temperature dependent viscosity simulations. Only one Ra is investigated. In total three tables, for three heating modes.

# Datasets concerning thermal evolution simulations with and without crust

Tables containing dimensional present day values of all the investigated outputs for different geometries and planet scenarios for cases with and without crust. In total six tables, for three planets.

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