

# Supplementary information to "Determining the core temperature at the end of accretion: effect of chemical disequilibrium during metal-silicate partitioning"

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## ABSTRACT

This is the supplementary material for the paper entitled 'Determining the core temperature at the end of accretion: effect of chemical disequilibrium during metal-silicate partitioning'. Most of the figures are the final concentrations of each element in the mantle and the core (Fig. S4 to S19). Five sections has been added to tests the limits of the model: effect of liquidus temperature (S.1), effect of Moon-forming impact (S.2), sensitivity of the number of solution to the definition of a solution (S.3), sensitivity of the number of solutions to the number of scenarios tested (S.4), estimation of the error on the final temperature (S.5)

Keywords: Accretion model, Core temperature, metal silicate partitioning

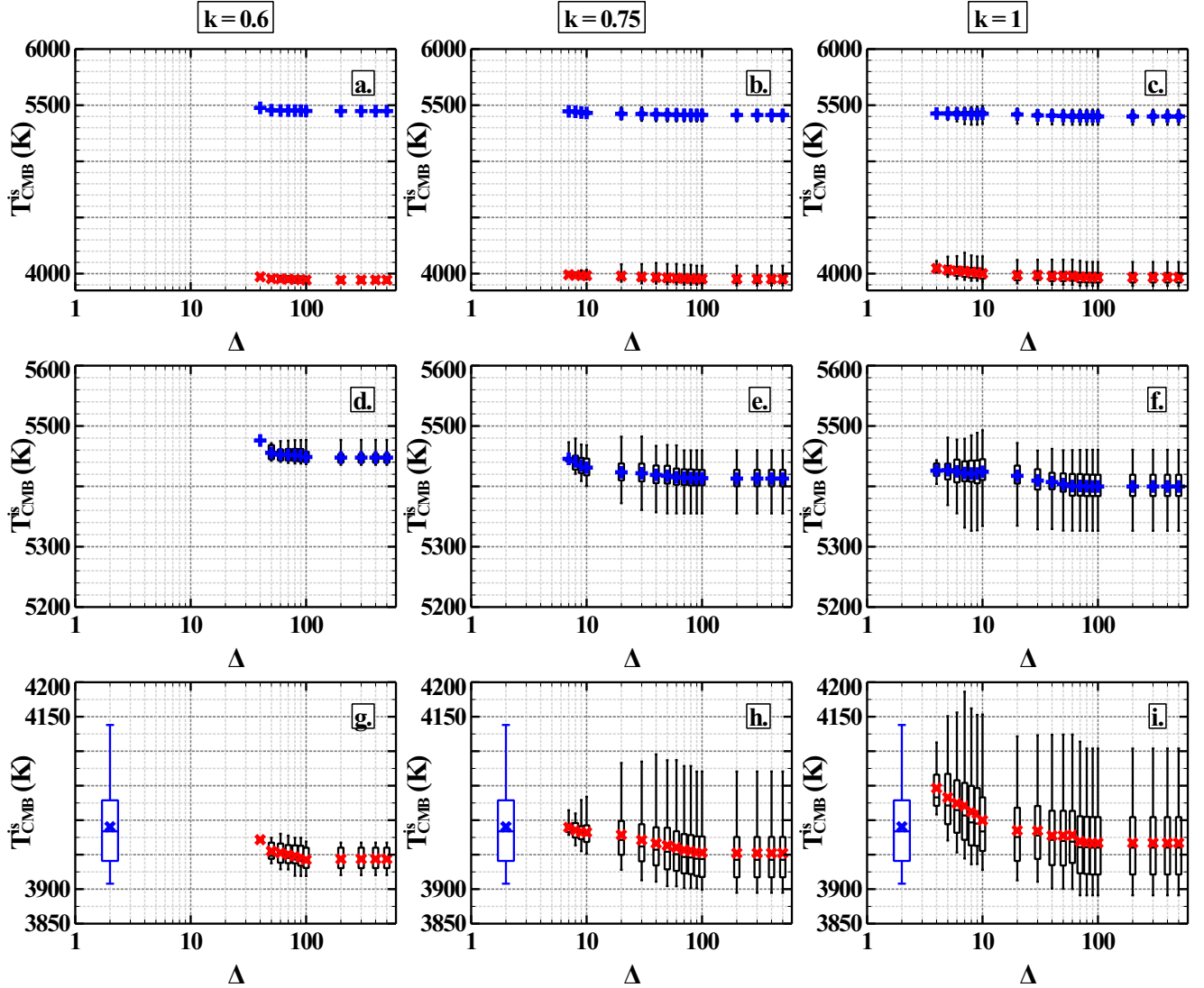
## S.1 CHOICE OF LIQUIDUS TEMPERATURE

The liquidus temperature is that of [Andrault et al. \(2011\)](#), as it was used in the original study of [Fischer et al. \(2015\)](#) whose parameterization has been used in our chemical model. This liquidus is calibrated for chondritic composition, which we used in the model. Therefore, this liquidus seems to be appropriate for our models, especially that it allows for comparison with our previous study ([Clesi & Deguen, 2023](#)), and other studies that use the same liquidus (e.g., [Boujibar et al., 2014](#); [Fischer et al., 2015](#)). However, as the liquidus temperature is the first temperature anchoring the subsequent evolution, choosing another liquidus or a temperature between solidus and liquidus will change the absolute values. A proper study of this effect is necessary, and this section is a first attempt to give hint on how this study should look like. Indeed, we did try to use the [Fiquet et al. \(2010\)](#) liquidus instead, so as to estimate the effect from the other side of the spectrum. This new temperature is given by equation:

$$T_{eq} = 2803 \pm 432 \left( \frac{P_{eq}}{35 \pm 44} + 1 \right)^{\frac{1}{2.41 \pm 0.99}} \quad (S.1)$$

which is the same as Equation (1) in the main text, with slightly different parameters. Unfortunately, running test with this temperature of equilibrium did not yield any results for  $k = 1, 0.6, 0.5$  and  $0.1$  (all  $\Delta$  tested). This indicates that choosing the liquidus for the magma ocean cannot be made without taking into account the parameterization of partitioning. Indeed, the parameterization used for this study has been calibrated for compositions and temperatures that are close to the [Andrault et al. \(2011\)](#) liquidus and therefore makes it possible to obtain solutions. As soon as a hot liquidus has been chosen,

the parameterization became invalid (no solutions could be found). Therefore, studying the effect of equilibrium temperature needs to be coupled with studying the effect of the parameterization to be impactful. Nonetheless, since we did not obtain chemically coherent solutions with the liquidus presented in Eq. (S.1), and still wanted to analyze the effect of changing the initial temperature on the final results, and especially how the relationship between  $T_{CMB}^{is}$  and  $k, \Delta$  variations are affected, we calculated the compositions using [Andrault et al. \(2011\)](#) (Equation (1) in the main text) and the temperature using as initial temperature of the metal given by Equation (S.1). This lead to a decoupling of the chemical and thermal part of the model, but do allow for an estimation of the effect of the initial temperature on the final heat content. We tested this for  $k = 0.6, 0.75$  and  $1$  and the full range of  $\Delta$ . The results compared to the main text are presented in Figure S.1.



**Figure S.1.** Temperature output ( $T_{CMB}^{is}$ ) using [Fiquet et al. \(2010\)](#) liquidus (blue cross) and using [Andrault et al. \(2011\)](#) liquidus (red crosses) for different values of  $k$ . Panels a to c: comparison of the results on the same plot. Panels d to f: Results only with [Fiquet et al. \(2010\)](#) liquidus. Panels g to i: Initial results presented in the main text.

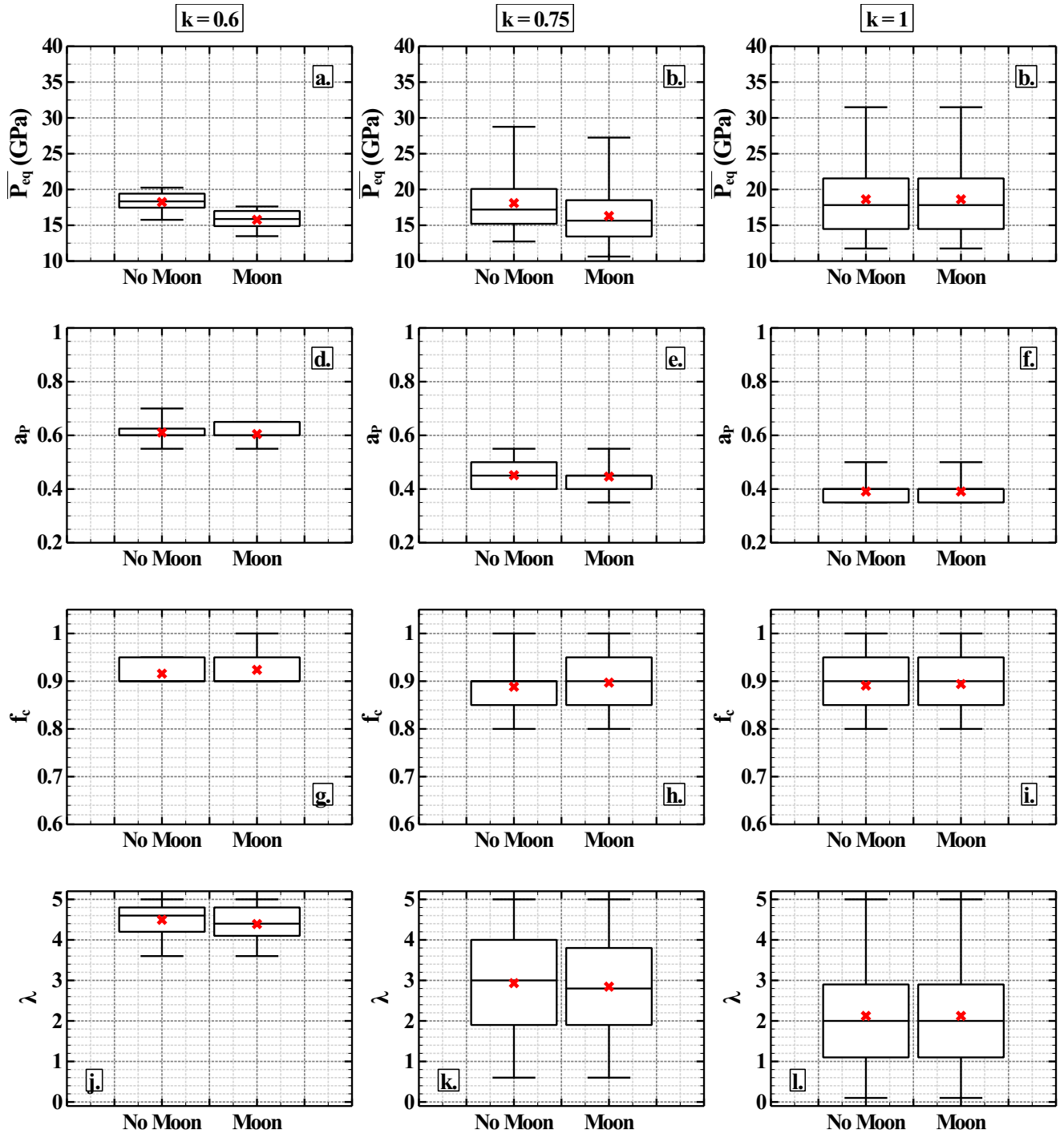
These figures shows that increasing the initial temperature of the metal tends to transpose the results to

higher temperature, but with a similar effect of at least  $\Delta$ , and most probably  $k$  (only 3 values were tested, but the trend is similar to that of Figure 7 and 8 in the main text). The range of output is within 400 K for both liquidus models, and the variability is lower for [Fiquet et al. \(2010\)](#) liquidus. However, this is for a decoupled chemical and thermal model, meaning the initial temperature is very high and the subsequent compression is not realistic and small since it is calibrated for a lower liquidus, thus inducing less changes in the temperature of the metal, and therefore explaining the flatter trend observed here. There is still a trend, the high values of  $\Delta$  tend to yield lower mean values than lower values of  $\Delta$ : this is particularly visible in panel f of Figure S.1.

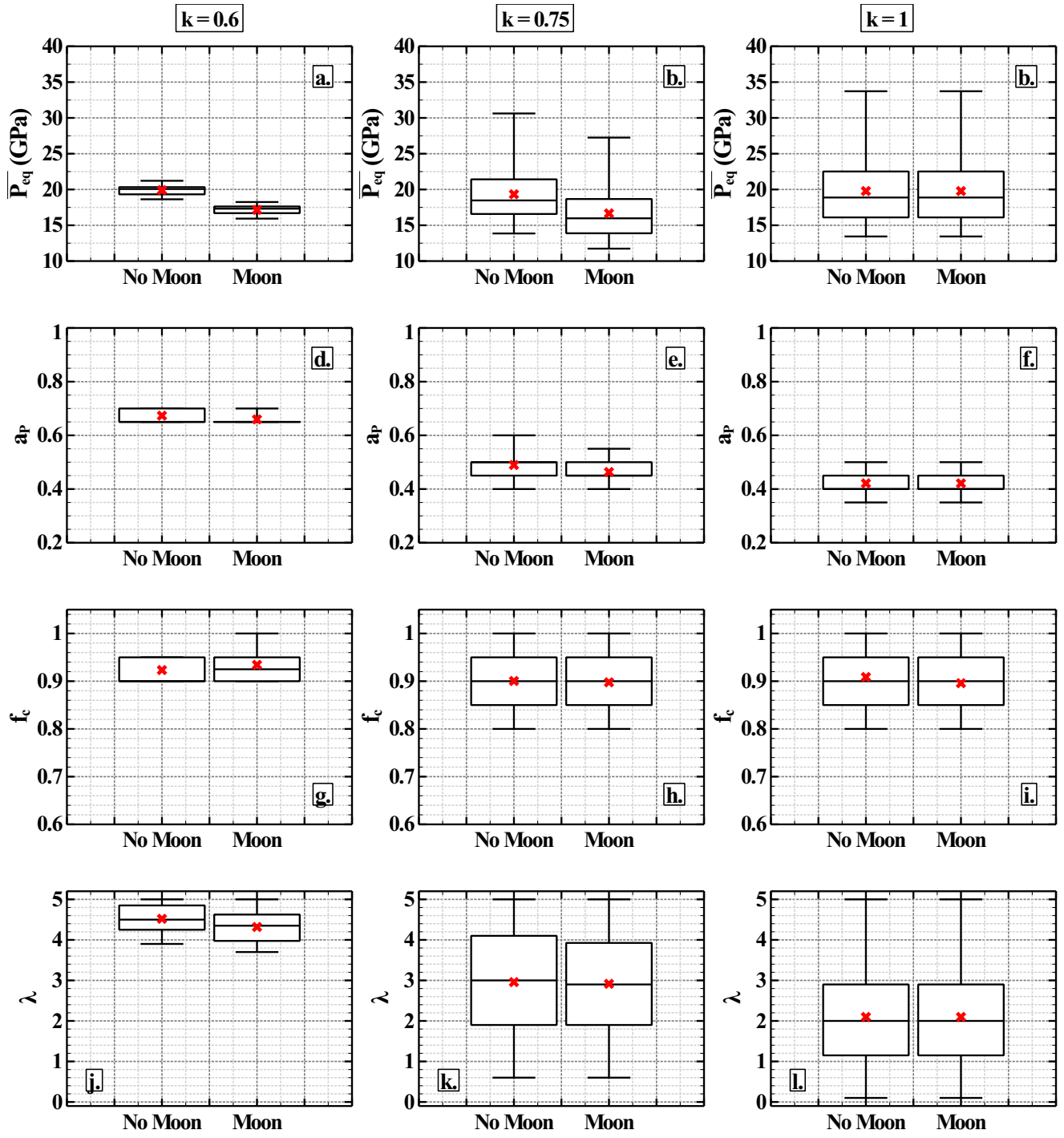
To conclude on this matter: the initial temperature does not change the trend of variability with  $k$  or  $\Delta$ , but changes the absolute values of  $T_{CMB}^{is}$ , all things kept equal. Unfortunately, keeping the link between temperature and composition will necessitate not to keep things equal, and therefore change the initial composition of impactor, the parameterization of partitioning and the overall outputs. A proper study of this effect will have to take be performed to properly estimate the effect of  $T_{eq}$  on the final  $T_{CMB}^{is}$ .

## S.2 MOON-FORMING IMPACT MODELING

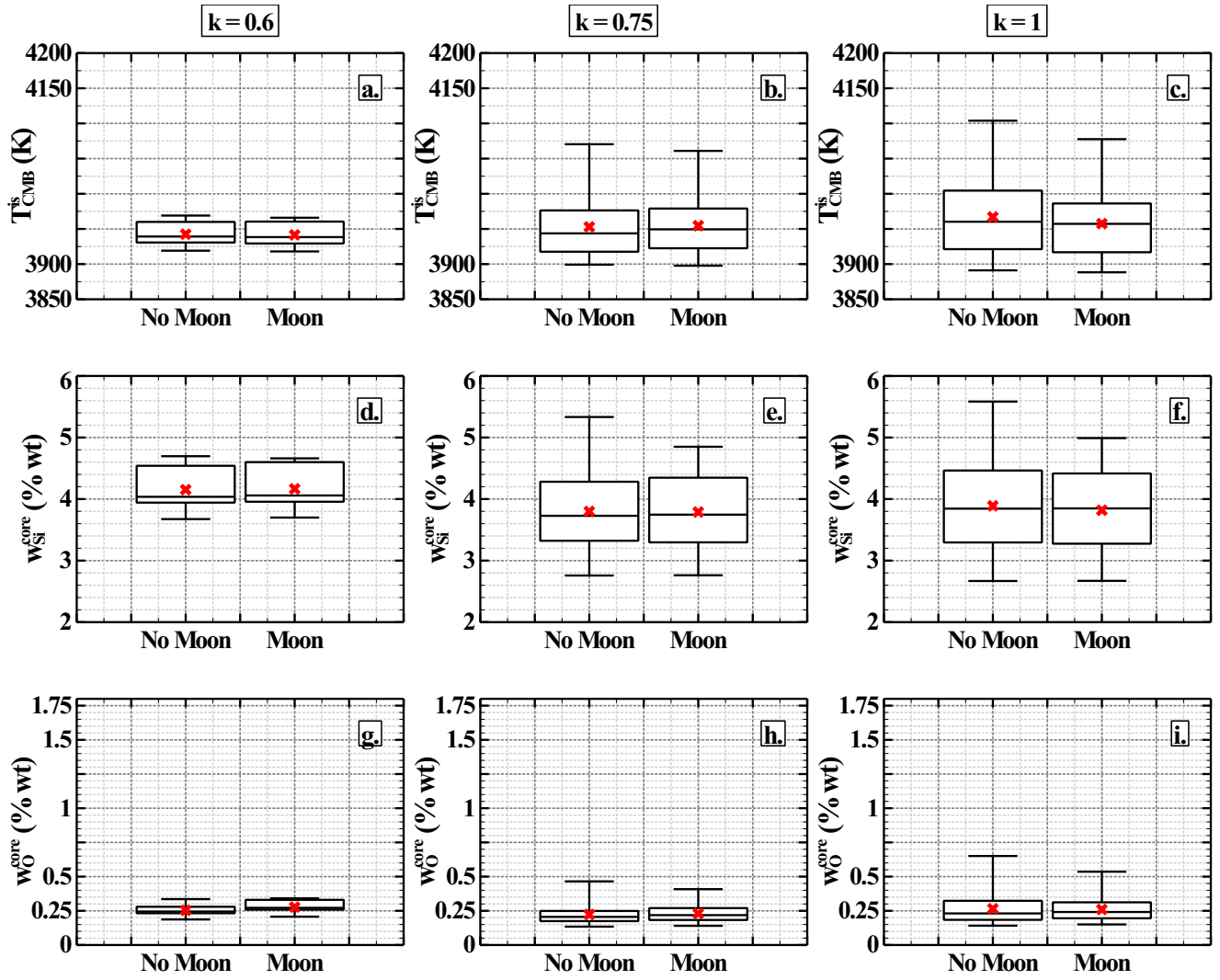
To model the Moon-forming impact, we modified the discretization of our model to match the model C20+T described in [Clesi & Deguen \(2024a\)](#). With this modification, the last 10% of accretion happen in one step, thus modeling the mass accreted by a Moon-forming impact ([Canup, 2004](#)). We did not include a specific parameterization of the value of  $k$  and  $\Delta$ , using existing parameterization for giant-impacts ([Deguen et al., 2014](#); [Landeau et al., 2016](#); [Nakajima et al., 2021](#); [Landeau et al., 2021](#)). We also did not add a specific model of thermo-chemical accretion for Theia, which would have changed both composition and thermal state of Theia's core. In the case of the core-merging scenarios ([Landeau et al., 2016](#); [Zhou et al., 2022](#)), both variables should change the final temperature and composition of the core. With these caveats in mind, we ran the models using the C20+T discretization to compare in a first approximation what would be the effect of a final giant impact for  $k = 0.6, 0.75$  and 1 and all values of  $\Delta$ . The number of solutions is roughly the same (a little bit below those presented in the main text). The average values of inputs Parameters ( $a_P, f_c, \lambda$ ) and the average value of the resulting  $\overline{P_{eq}}$  are presented for  $\Delta = 100$  in Figure S.2 and for  $\Delta = 50$  in Figure S.3, in comparison with the initial model presented in the main text. The output temperatures  $T_{CMB}^{is}$ , Si and O concentrations of the core are presented in Figure S.4 and Figure S.5 for  $\Delta = 100$  and  $\Delta = 50$ , respectively. Finally, the effect of  $\Delta$  on the temperature for Theia-like discretization for  $k=0.6, 0.75$  and 1 is presented in Figure S.6.



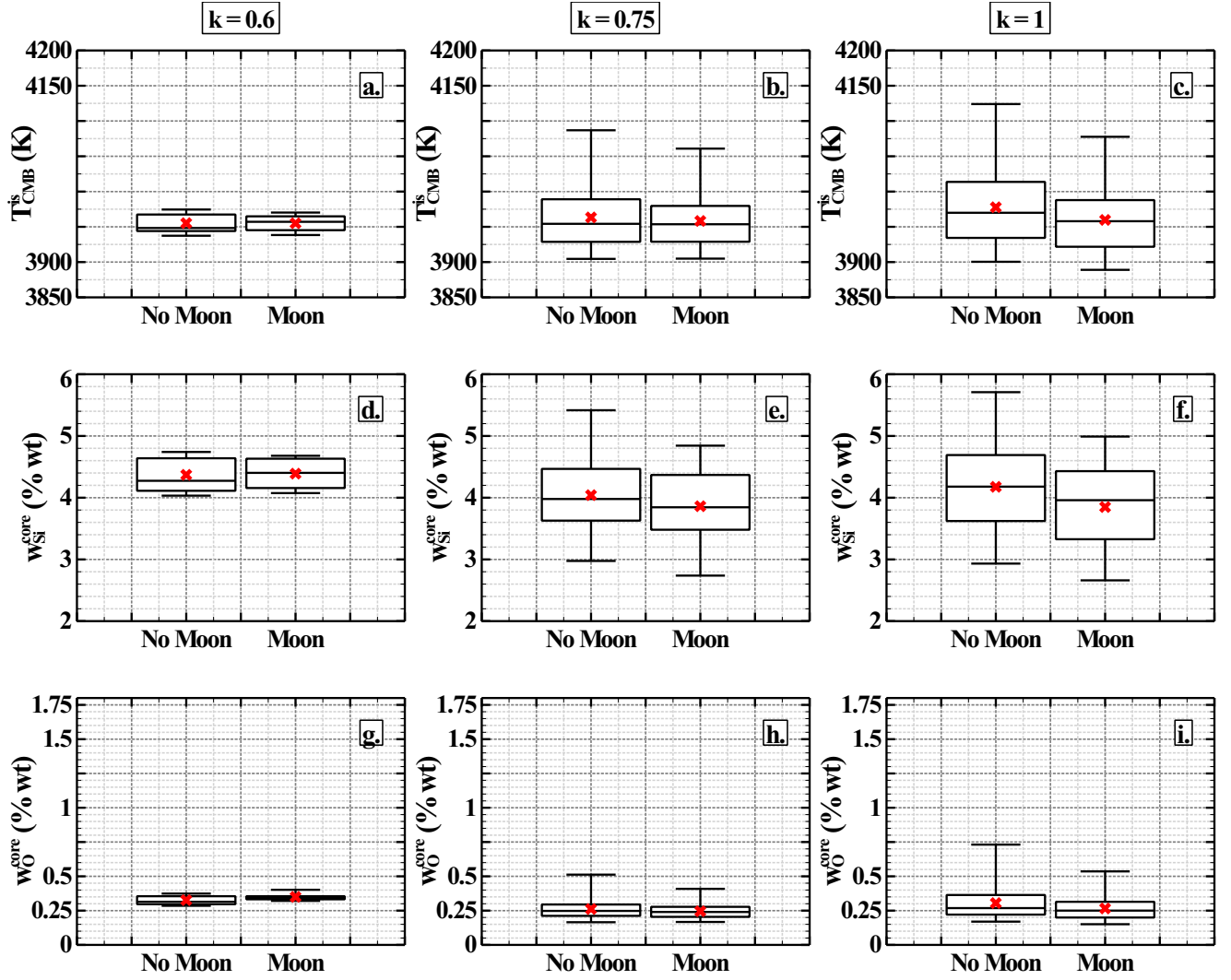
**Figure S.2.** Comparison of input parameters between the main text model, and the model including a Moon-forming impact (No Moon and Moon) for  $\Delta = 100$  and  $k = 0.6$  (panels a., d., g. and j.),  $0.75$  (panels b., e., h. and k.) and  $1$  (panels c., f., i. and l.)



**Figure S.3.** Comparison of input parameters between the main text model, and the model including a Moon-forming impact (No Moon and Moon) for  $\Delta = 50$  and  $k = 0.6$  (panels a., d., g. and j.),  $0.75$  (panels b., e., h. and k.) and  $1$  (panels c., f., i. and l.)



**Figure S.4.** Comparison of output parameters between the main text model, and the model including a Moon-forming impact (No Moon and Moon) for  $\Delta = 100$  and  $k = 0.6$  (panels a., d. and g.),  $0.75$  (panels b., e. and h.) and  $1$  (panels c., f., i.).



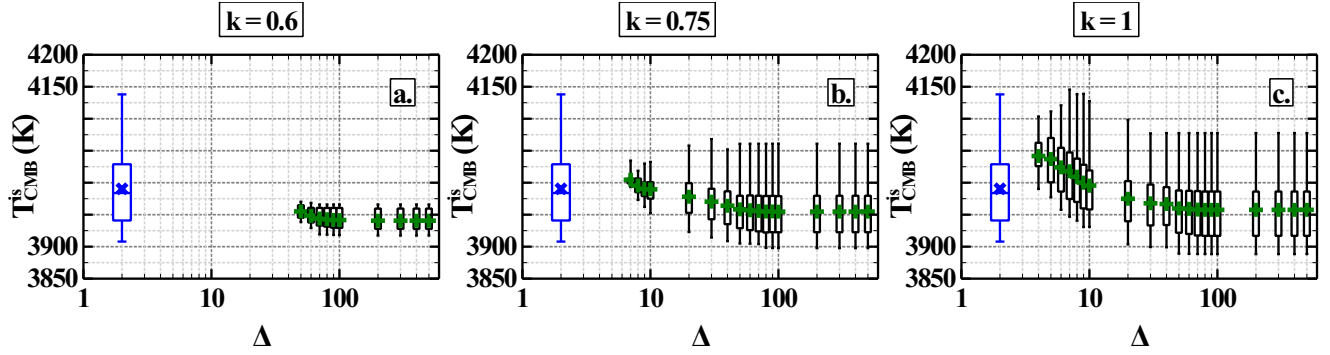
**Figure S.5.** Comparison of output parameters between the main text model, and the model including a Moon-forming impact (No Moon and Moon) for  $\Delta = 50$  and  $k = 0.6$  (panels a., d. and g.), 0.75 (panels b., e. and h.) and 1 (panels c., f., i.).

As can be seen on Figures S.2 to S.6, the effect of varying the discretization and nothing else does not change the output of the models significantly: the maximum  $T_{CMB}^{is}$  is 50 K below the initial model, but average and minimum are unchanged. The trend of increasing temperature with decreasing equilibrium rate is unchanged (Figure S.6).

This confirms the result of Clesi & Deguen (2024a) that discretization by itself does not change the results of accretion model if at least 10 steps are considered.

A proper way of improving the model would be:

- Link the discretization to scaling law for melting (Nakajima et al., 2021)
- Calculate the value of  $k$  and  $\Delta$  for each impact (Deguen et al., 2014; Landeau et al., 2021)
- In parallel, model the thermo-chemical evolution of Theia, and define its effect, for instance core-merging (Landeau et al., 2017; Canup et al., 2023; Zhou et al., 2022)



**Figure S.6.** Effect of  $\Delta$  on output temperature  $T_{CMB}^{is}$  for  $k = 0.6, 0.75$  and  $1$  (panels a, b and c, respectively). The blue box at  $x=2$  is the reference model as defined in the main text. The green cross shows the mean values.

- Link the discretization to a variation in the composition of the impactor: for instance small impactor masses with less metal and more reduced composition, and bigger impactor masses being both more oxidized and oxidizing (Henningsen et al., 2025)
- Apply all the previous step to a successful N-body simulation (Jacobson et al., 2017; Rubie et al., 2015)

In the end, our model does correctly predict the BSE composition and can be used as first estimation of the thermo-chemical evolution of the Earth, but does not accurately model the strong impact that the Moon formation is believed to have on core formation (Nimmo et al., 2010; Rudge et al., 2010).

Therefore, the values of  $k$  and  $\Delta$  proposed in our study should serve as a general approximation of the average degree of equilibrium throughout the accretion necessary to obtain the BSE, but do not apply to a specific part of the accretion process.

### S.3 EFFECT OF FILTER SIZE ON THE MODEL'S OUTPUTS

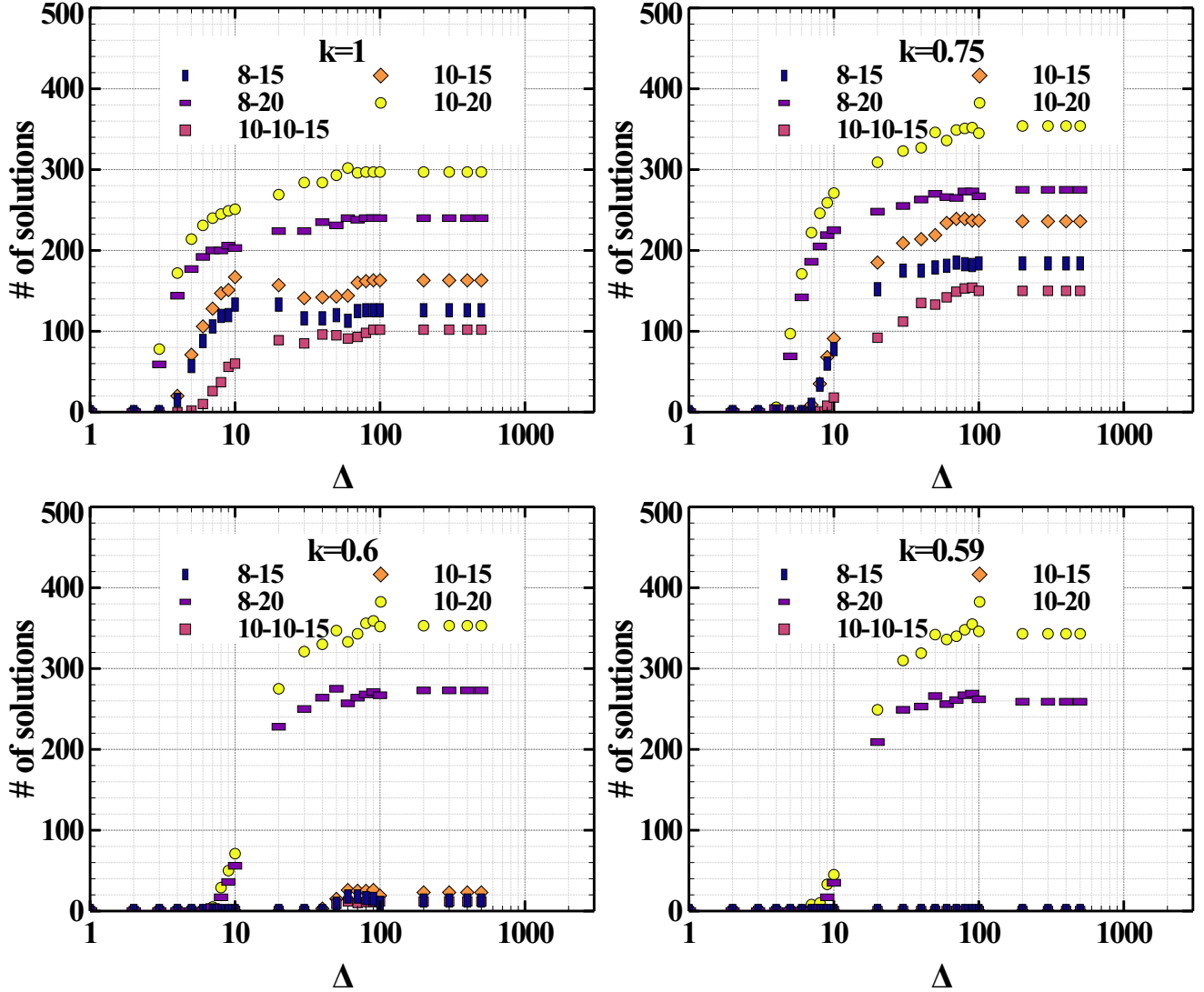
In Figure 4 of the main text, we show that no solution exists for  $k < 0.6$ , thus increasing the accepted minimum equilibrium degree of the metal derived from Hf-W study of  $k \sim 0.3$  (Rudge et al., 2010; Gu et al., 2023). This should be sensitive to how we define a solution: indeed, if we change (precisely, widen) the concentration range for the different elements present in the model, the number of solutions should increase (see supplementary material of, Clesi & Deguen, 2024a, especially for the low degree of discretization). However, the tolerance for the concentrations is not chosen randomly: in McDonough & Sun (1995), the major element error is 10%, Ni and Co are at 10% and V and Cr at 15%. With our threshold at 15 % for Ni, Co, V and Cr, we actually overestimate the number of solutions.

A full out sensitivity study being beyond the scope of the present study, but we tested a few scenarios with different limits and compared the input parameters which yield a solution. In those tests, we defined the concentration range around the BSE concentrations (see main text for the values) within a predefined range for each element. These limits are explicitly described in Table S.1.

In Figure S.7 and S.8, the number of solutions obtained in these sensitivity studies are presented as a function of  $\Delta$  (absolute number and relative success rate, respectively). For  $k = 0.59$ , we get solutions only if the ranges tested are higher than 20% for the trace elements. The numbers stay below 400 for 20 000 scenarios (success rate below  $\sim 2\%$ , Figure S.8). In Figure S.9, are presented the range of input parameters ( $\overline{P_{eq}}$ ,  $a_P$ ,  $f_c$ ,  $\lambda$ ) yielding solutions for different thresholds on major and trace elements,  $k$  of

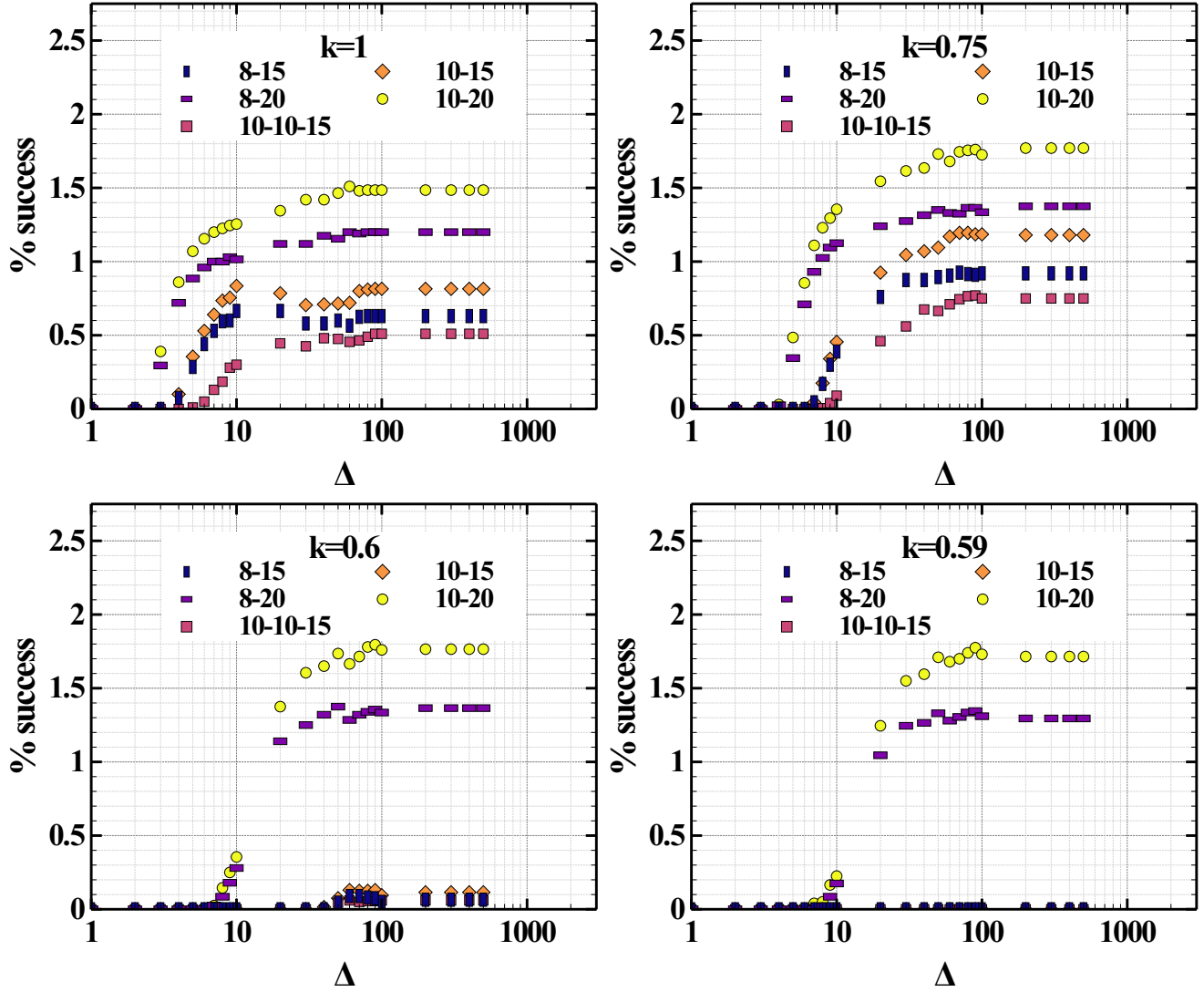
| Name     | Major elements range (%) | Ni and Co range (%) | V and Cr range (%) | Comment                                                    |
|----------|--------------------------|---------------------|--------------------|------------------------------------------------------------|
| 8-15     | 8                        | 15                  | 15                 | Major element range narrower than main text                |
| 8-20     | 8                        | 20                  | 20                 | Major element narrower and trace wider than main text      |
| 10-15    | 10                       | 15                  | 15                 | Same as main text                                          |
| 10-10-15 | 10                       | 10                  | 15                 | Ranges given in <a href="#">McDonough &amp; Sun (1995)</a> |
| 10-20    | 10                       | 20                  | 20                 | Trace element range wider than main text                   |

**Table S.1.** Name of the models tested for  $k = 0.59, 0.6, 0.75$  and  $1$ . The temperature was not calculated, as we focused on the number of solutions. These names are used in Figure S.7 and S.8.



**Figure S.7.** Number of solutions yielded by the different models defined in Table S.1 as a function of  $\Delta$ , for  $k = 1$  (top left),  $0.75$  (top right),  $0.6$  (bottom left) and  $0.59$  (bottom right)

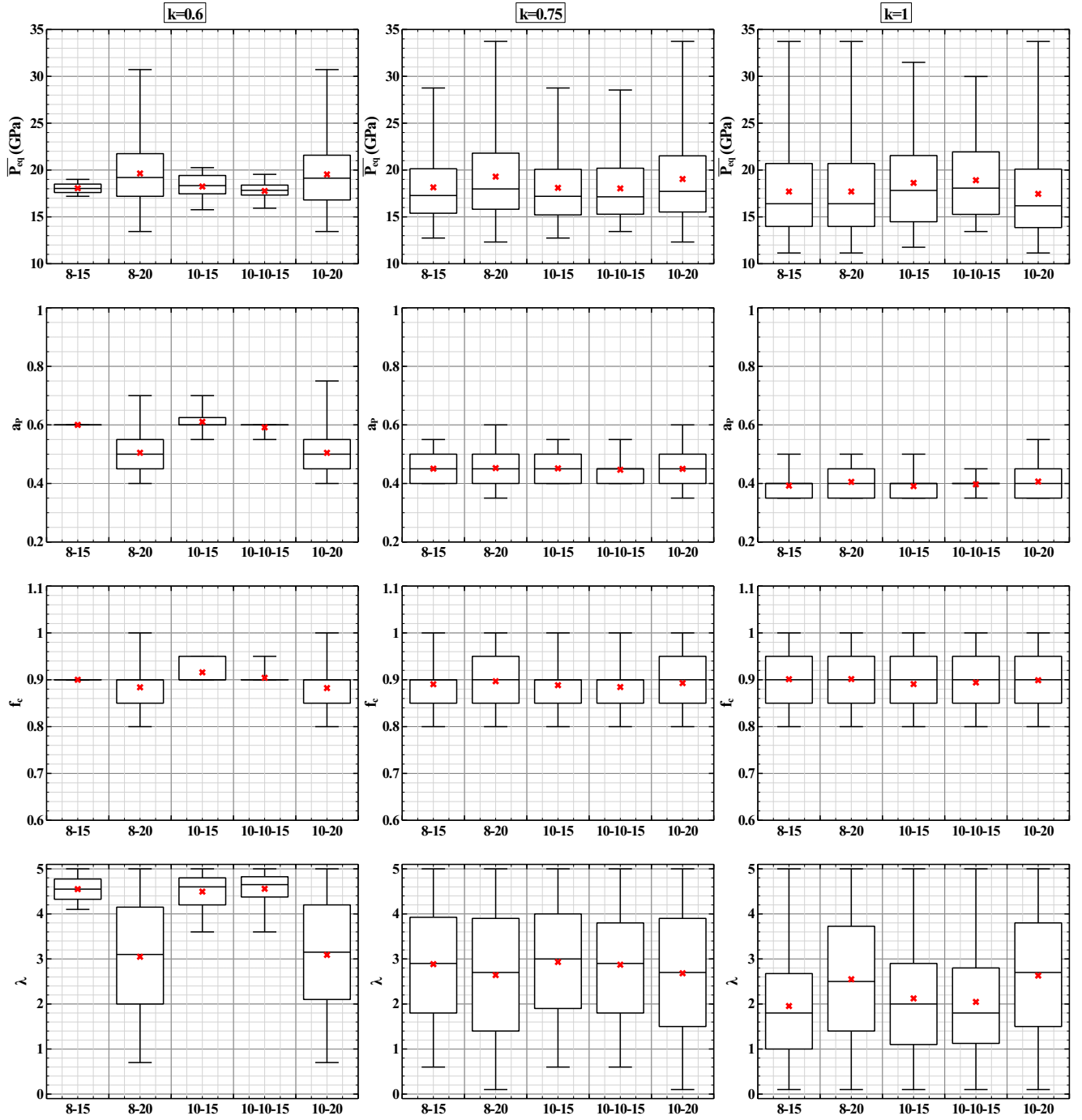
$0.6, 0.75$  and  $1$ , and  $\Delta = 100$ . This figure shows the input parameter ranges are a bit wider when the trace elements range for concentration are wider, but the values are comparable to what we observe in the main study (model 10-15). Therefore, the temperature range should be relatively comparable to the one presented in the main text of this article. In any case the range of concentrations in core and mantle are comparable, as evidenced by Figure S.10 focusing on NiO and CoO in the mantle. As expected, the



**Figure S.8.** Success rate (number of solution/20 000 scenarios), expressed in percentage, yielded by the different models defined in Table S.1 as a function of  $\Delta$ , for  $k = 1$  (top left), 0.75 (top right), 0.6 (bottom left) and 0.59 (bottom right)

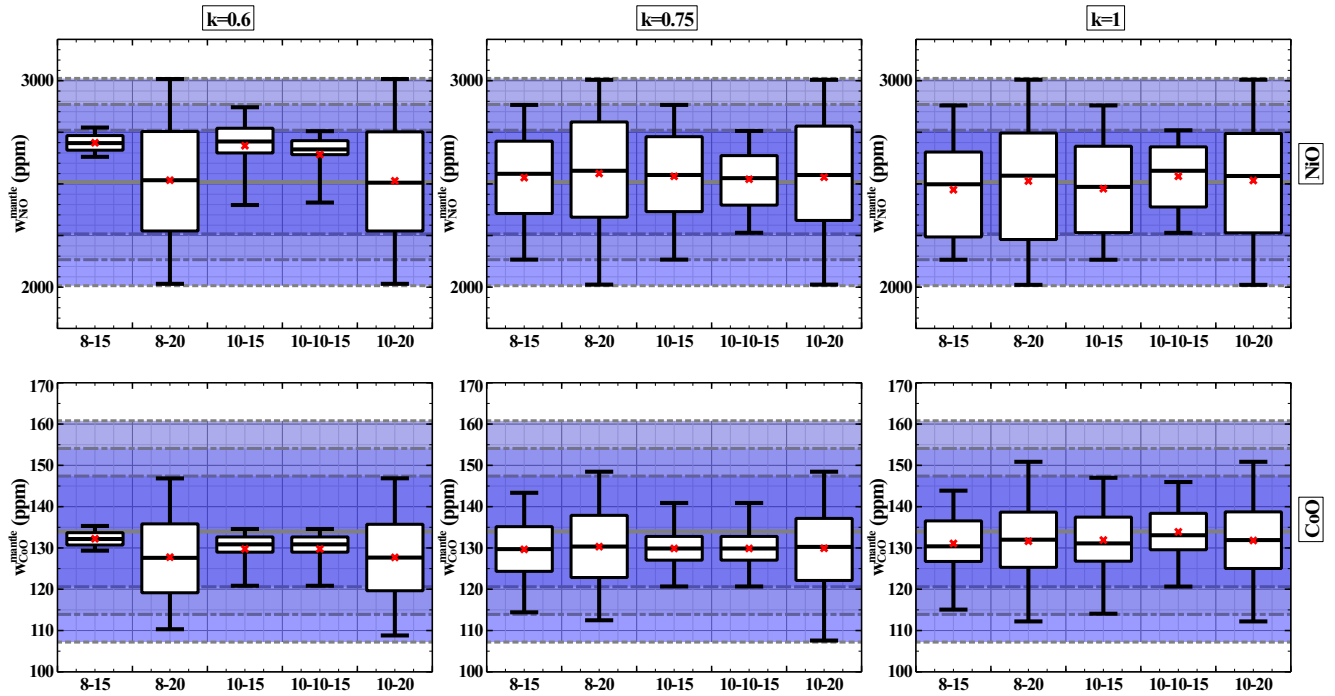
mean values are the same, increasing the range of solution only add composition further from the BSE composition. Figures S.7 to S.10 show that widening the threshold for a solution will tend to lower the minimum values of  $k$  and  $\Delta$ , but as argued in the following text, this comes with the cost of accepting models that are less representative of the Bulk Silicate Earth.

As the trace elements are the limiting factor for the number of solutions (see main text and supplementary materials of Clesi & Deguen, 2023, 2024a), we used the case of  $k = 0.55$  and  $k = 0.3$ , with  $\Delta = 100$  in both cases, to find what is the minimum range that will yield solution for at least one case where  $k < 0.6$ . For  $\Delta = 100$ , this range has to be 18% minimum for  $k = 0.55$  and 23% for  $k = 0.3$ , which is a significant increases compare to what is accepted as the standard error on the BSE as given in McDonough & Sun (1995) (between 80% and 130 % increase for Ni and Co, between 20% and 55% for V and Cr). If anything, the standard error of the BSE is lower than the one given in McDonough & Sun (1995) (as hinted in McDonough, 2003). The BSE compositions obtained by wider range of concentrations tend to



**Figure S.9.** Solutions ranges for  $\Delta = 100$  and the different thresholds for solutions defined in Table S.1. First row:  $\overline{P}_{eq}$  (GPa) for  $k=0.6$  (left),  $0.75$  (middle) and  $1$  (right). Second row:  $a_p$  solutions range for the same values of  $k$ . Third row:  $f_c$  solution range. Bottom row:  $\lambda$  solution range.

scatter the output compositions away from what is expected in the BSE. In Figure S.11, an example of this phenomenon is plotted for  $k = 0.6$ ,  $\Delta = 100$ , and the 4 trace elements (NiO, CoO,  $V_2O_3$  and  $Cr_2O_3$ ) for the models 8-15 and 8-20. For this value of  $k$  and  $\Delta$ , the number of solution is low enough that it is possible to see the complexity induced by increasing the threshold in the definition of a solution. Indeed,

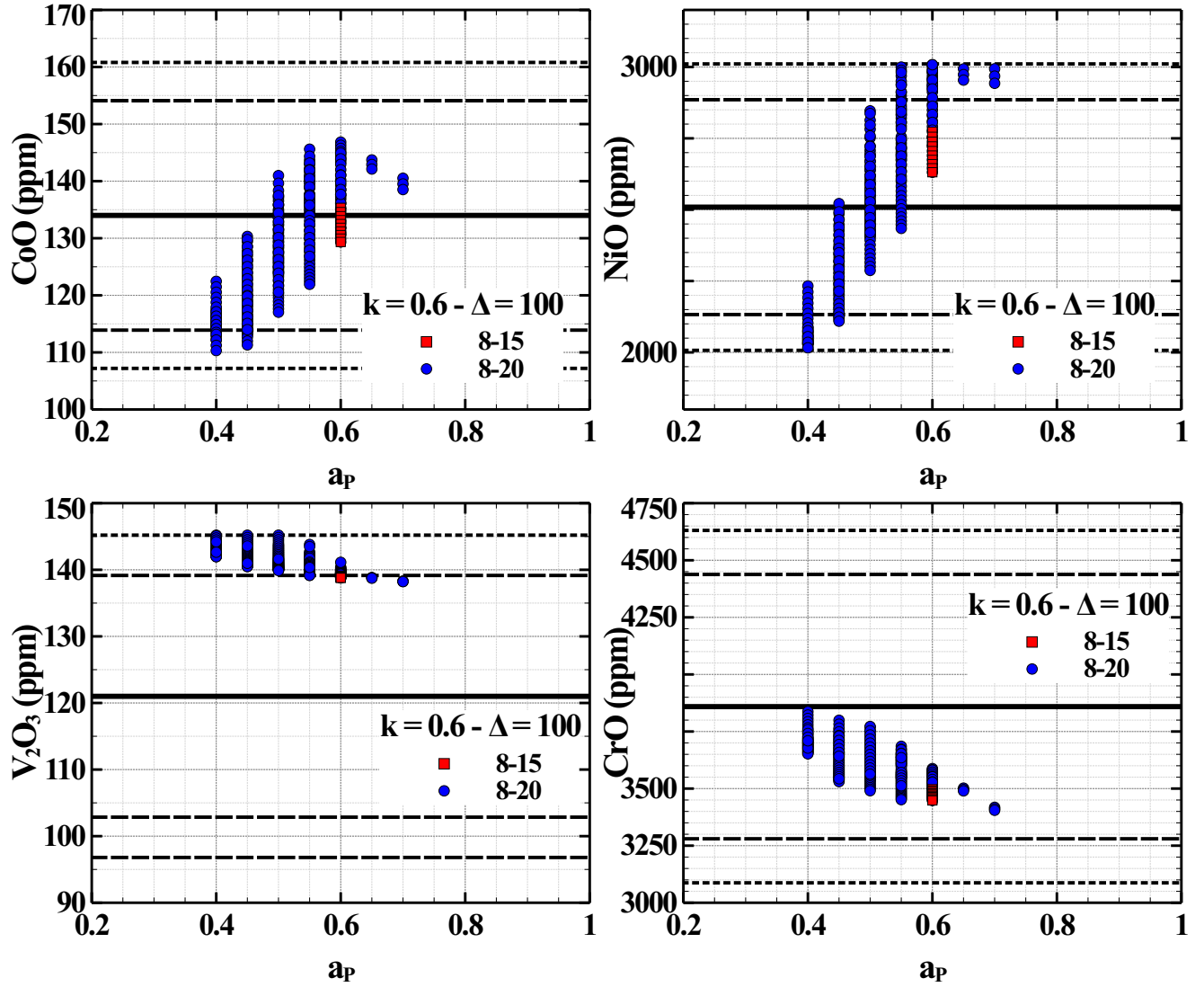


**Figure S.10.** Output concentrations range of NiO (top row) and CoO (bottom row) for the different models defined in Table S.1,  $\Delta = 100$  and  $k = 0.6$  (left column), 0.75 (middle column) and 1 (right column). The BSE concentration from McDonough & Sun (1995) is figured by the gray full line. The blue area and the dashed and dotted gray lines of different shading represent the different ranges (10, 15 and 20%) around the BSE value used in the study to define a solution.

for a threshold at 15% of the BSE value, the number of solutions is quite low, but all are close to the BSE, in particular Ni and Co. Increasing the thresholds tends to produce more solutions which are closer to the BSE for V and Cr, but these solutions tends to move the values of Ni and Co away from their expected BSE value. The same effect exists in reverse: scenarios with Ni and Co concentrations closer to the BSE value tends to yield V and Cr concentrations which are further away from their expected BSE values.

This result is dependent on the BSE model, so the value of  $k = 0.6$  is valid only if we consider the BSE chondritic model as given in McDonough & Sun (1995) (which is the standard in most studies) to be realistic. Using other BSE models as reference (Allegre et al., 1995; Javoy et al., 2010; Korenaga, 2009) might lead to other results, but it is highly unlikely as their proposed composition all fall within a range of 10% of each other for the elements used in this study: Allegre et al. (1995) and McDonough & Sun (1995) are for instance very close. As for Javoy et al. (2010), they lower the amount of FeO in the mantle compared to the previously cited models ( $6.5\% \pm 1\%$  which overlaps with the  $8\% \pm 0.8\%$  we used in our study), but the concentrations of the other elements proposed in their study are very close and overlapping with the BSE model we used.

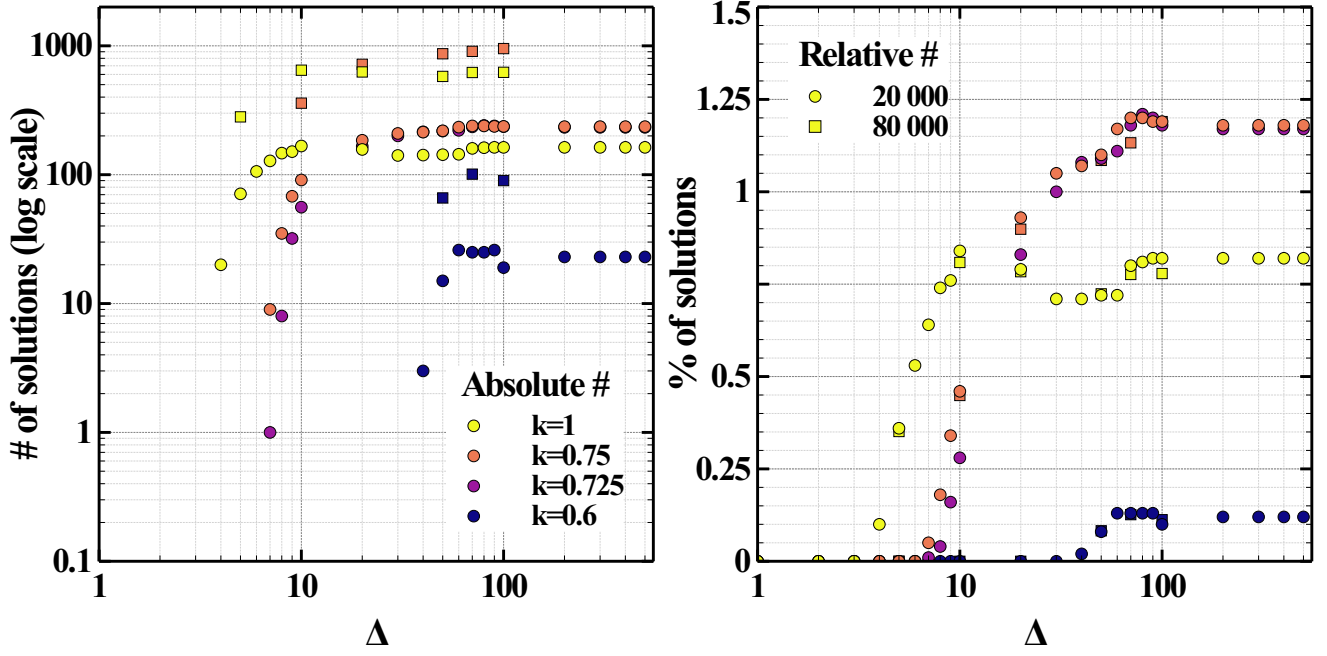
All of this tends to support the conclusions of the main text that at least 60 % of the metal needs to be equilibrated on average, all things kept equal, and in the optics of fitting a relatively chemically coherent Earth with the BSE standard composition. Changing the initial composition (number of elements, parametrization of partitioning, temperature of equilibrium) and/or BSE compositional model might change this number, but a proper study would have to be conducted separately.



**Figure S.11.** Comparison of two models (8-15, red squares, and 8-20, blue circles) compositional outputs for trace elements (CoO, top left, NiO top right,  $V_2O_3$  bottom left, and  $Cr_2O_3$  bottom right) as a function of the corresponding values of  $a_p$ , for  $\Delta = 100$  and  $k = 0.6$ . The black full line is the expected BSE concentration as defined in [McDonough & Sun \(1995\)](#), the dashed line are the 15 and 20% maximum variation threshold.

## S.4 EFFECT OF SAMPLING DENSITY ON THE MODEL'S OUTPUTS

One parameter that could alter the results is the initial number of scenarios tested. In the main text we tested 20 values of  $a_p$ , 20 values of  $f_c$  and 50 values of  $\lambda$  with all values combined leading to 20 000 scenarios being tested, while several more could be added, which would change the overall ratio between number of solutions presented in Figure 4 of the main text and the outputs of the model. In this section, we performed some tests with a higher number of parameter: 40 values of  $a_p$  (between 0.025 and 1, by steps of 0.025), 40 values of  $f_c$  (between 0.025 and 1, by steps of 0.025) and 50 values of  $\lambda$  (same as in the main text, as this parameter already span a very large range). The number of scenarios tested is 4 times the one presented in the main text (80 000), which tends to increase the time of calculation by 2.6. We calculated the number of solutions for  $k = 0.6, 0.75$  and 1, and  $\Delta = 5, 10, 20, 50, 70$  and 100; and did



**Figure S.12.** Absolute number of solutions (left) and relative success rate (right) as a function of  $\Delta$  for different values of  $k$ . The color scale in both panel represents the value of  $k$  (key in left panel). The square in both panel represent the bigger sampling range (80 000 scenarios tested) and the circles the sampling range used in the main text (20 000)

a specific calculation for the maximum number of solutions from Figure 4:  $k = 0.725$  and  $\Delta = 80$ . The number of solutions normalized by the number of the calculations for variable  $\Delta$  and  $k$  are presented in Figure S.12, along with the same ratio from Figure 4 in the main text. The difference the two sampling methods have on the selections of input parameters is compared in Figure S.13.

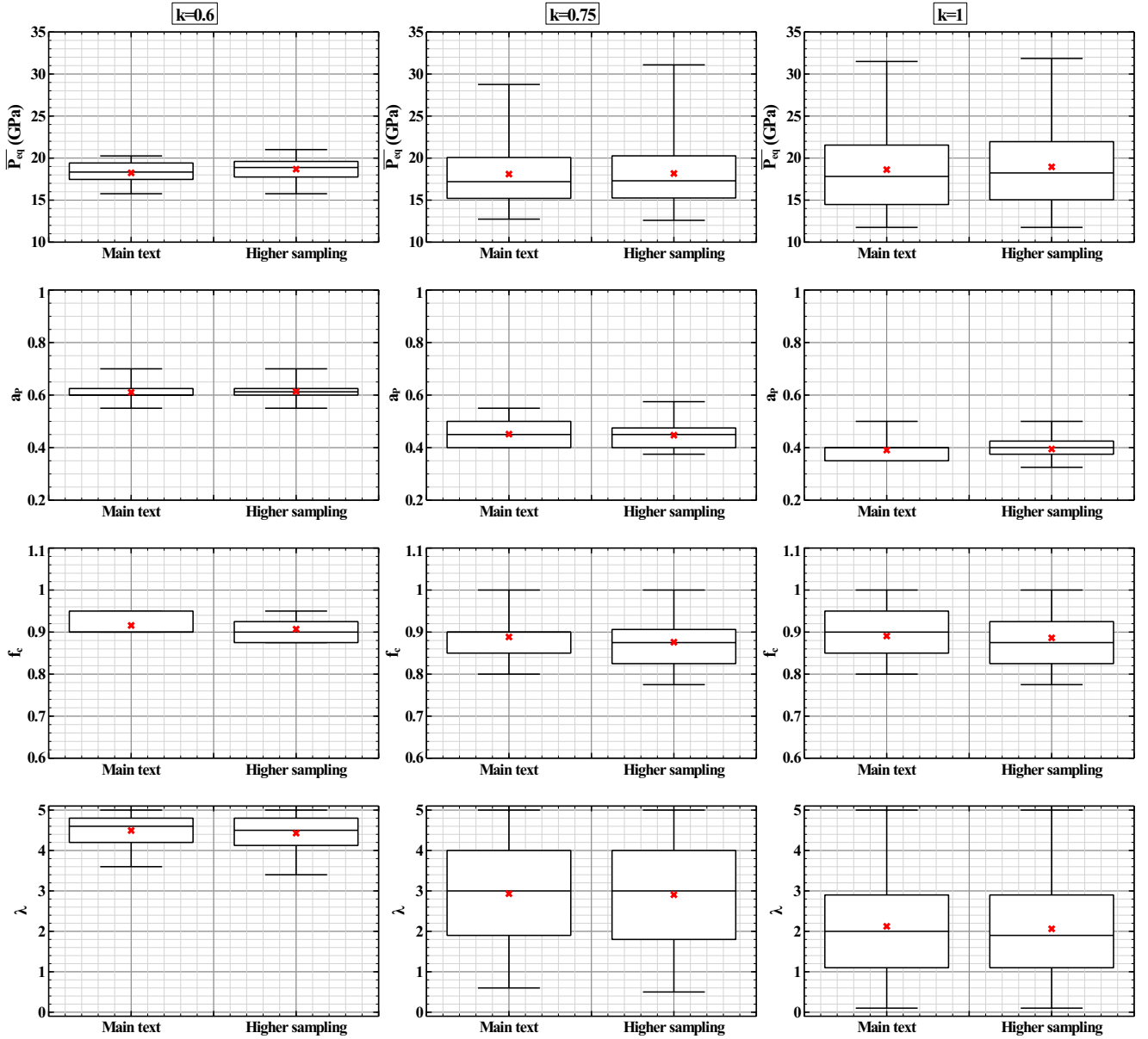
If we focus only on the maximum highlighted in Figure 4, we found 913 solutions with the new sampling of  $a_p$  and  $f_c$ . The solution rate is therefore  $913/80000 \sim 1.14\%$ , compared to the  $241/20000 \sim 1.21$  in the initial figure, which is roughly the same.

As shown in Figures S.12 the absolute number of solution increases when increasing the number of scenarios, but the ratios are comparable (barely visible squares in the right panel of the Figure S.12). The mean values and ranges of the input parameters ( $a_p$ ,  $f_c$ ,  $\lambda$  and  $\overline{P_{eq}}$ , Figure S.13) are comparable to the one in the main text, thus yielding similar compositions and temperatures in similar conditions.

All said and done, the model is not very sensitive to the number of scenarios tested, as long as the range  $a_p$  and  $f_c$  tested correctly spans the total values possible:  $a_p$  must be positive (a magma ocean must exist) and below 1 (the magma ocean maximum extent must not be higher than the CMB);  $f_c$  must be comprised between 0 and 1 as matter cannot accrete before the planet starts to grow, or after the planet has grown.

## S.5 ERROR ESTIMATION ON THE TEMPERATURE MODEL

The model is dependent on several parameters, measured or calculated more or less precisely. The error induced by the number of steps used in the numerical integration is negligible, increasing the number of steps changes the temperature only for the second decimal, i.e. the order of magnitude of the relative error is  $10^{-3}\%$  ( $\sim 0.00003$  K in absolute value variation). However, there are three main sources of relative



**Figure S.13.** Comparison of the results for a larger sampling distribution with the main text results for  $\Delta = 100$ . First row:  $\overline{P}_{eq}$  (GPa) for  $k=0.6$  (left),  $0.75$  (middle) and  $1$  (right). Second row:  $a_p$  solutions range for the same values of  $k$ . Third row:  $f_c$  solution range. Bottom row:  $\lambda$  solution range.

error for the final temperature. The first one is the error on the liquidus temperature as given by equation (1) of the main text. The second source of error is the error on  $K_s$  in Equation (2) of the main text and the third one is the error on  $\gamma$  in that same equation. The initial liquidus temperature carries a maximal error of 150 K for the maximum temperature of 4750 K (Andraut et al., 2011). This translates to a relative error  $\varepsilon_{T_{eq}}$  of 3.17 % that will be carried to the end. The main variation of temperature is due to compression, which depends on the  $K_s$  and  $\gamma$ . For the  $K_s$  as defined by this study, the values of  $K_0$  and  $K'$  were obtained by fitting a Murnaghan equation of state to a PREM based model (Clesi & Deguen, 2023). Therefore, the error on this parameters is the same error as the overall error on the PREM model (Dziewonski & Anderson, 1981), which is given between 2 and 4%. To be conservative, we use a relative error for  $K_s$  of

4% (hereafter  $\varepsilon_{K_s} = 0.04$ ), which yields the absolute errors on  $K_0$  and  $K'$  as given in the main text. For  $\gamma$ , we used the results of a previously published sensitivity study (Clesi & Deguen, 2024b) for the Al'Tshuler et al. (1987) formalism. Using the  $\chi^2$  given in Clesi & Deguen (2024b), we calculated the relative error induced by the Grüneisen parameter to be 6%, in the following calculations  $\varepsilon_\gamma = 0.06$ . Then combining these three relative errors ( $\varepsilon_{T_{eq}}$ ,  $\varepsilon_{K_s}$  and  $\varepsilon_\gamma$ ), the final relative error on temperature  $\varepsilon_{total}$  is therefore:

$$\varepsilon_{total} = \sqrt{(\varepsilon_{T_{eq}})^2 + (\varepsilon_{K_s})^2 + (\varepsilon_\gamma)^2} = 7.22\% \quad (\text{S.2})$$

This 7.22 % relative error is applied uniformly throughout the main text. The error for  $T_{CMB}^{is} = 4200K$  is  $\pm 300K$  (maximum value and maximum error) and the error for  $T_{CMB}^{is} = 3800K$  is  $\pm 274K$  (minimum value and minimum error). Finally, the error on the trend given for Figure 9 arises from the fit of temperature. From Table 2 in the main text and the same propagation of relative error in Equation S.2 applied to the formula of Equation (23) in the main text we get:

- $\varepsilon_{\Delta T} = 1.3 \times 10^{18}\%$  for the model of variation with  $T_{CMB}^{is}$  min values. This high error is due to the lack of  $\Delta$  dependency yielding a poor fit.
- $\varepsilon_{\Delta T} = 3.85\%$  for the model of variation of the  $\overline{T_{CMB}^{is}}$  values. The absolute error on the effect of disequilibrium is therefore comprised between 2 and 4 K.
- $\varepsilon_{\Delta T} = 15\%$  for the model of variation of  $T_{CMB}^{is}$  max values. The absolute error on the maximum variation is therefore 38 K for  $\Delta T(k, \Delta) = 250K$

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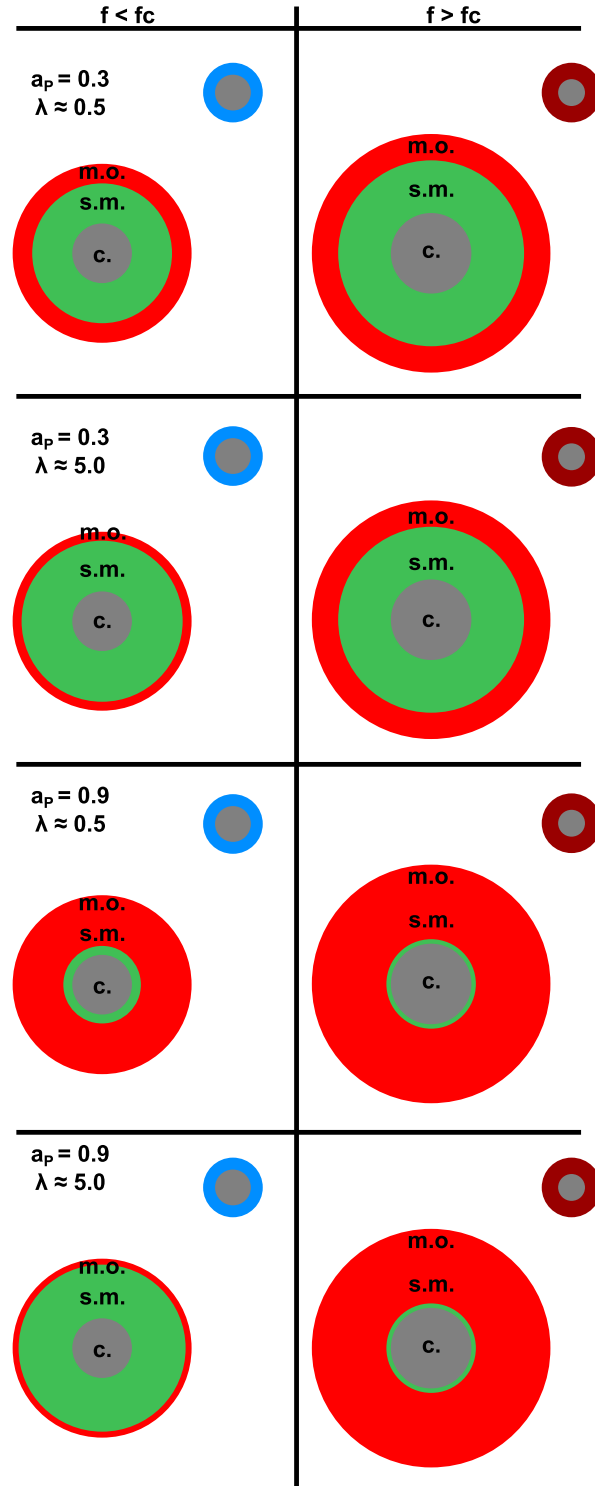
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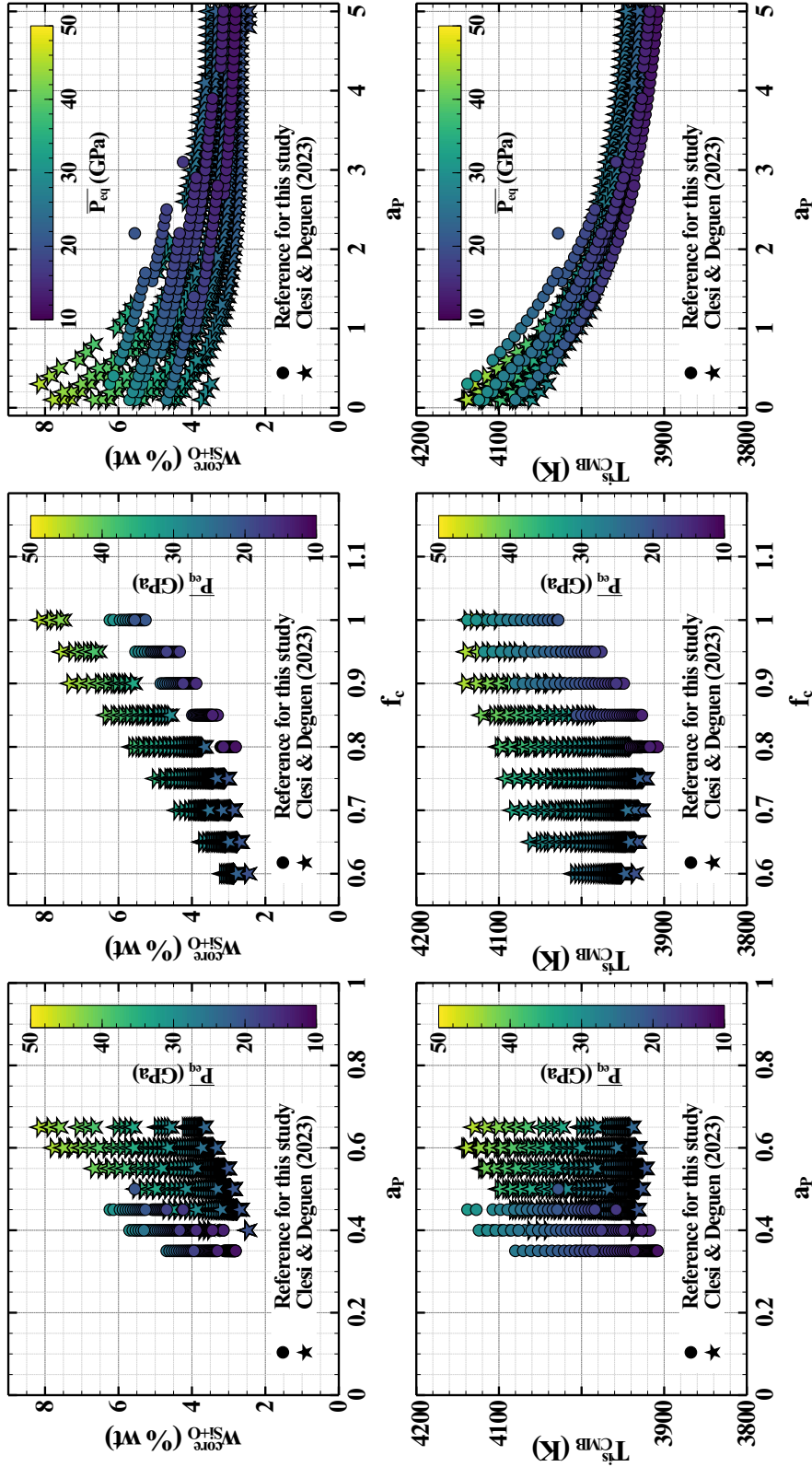
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## **ADDITIONAL FIGURES CITED IN THE MAIN TEXT**

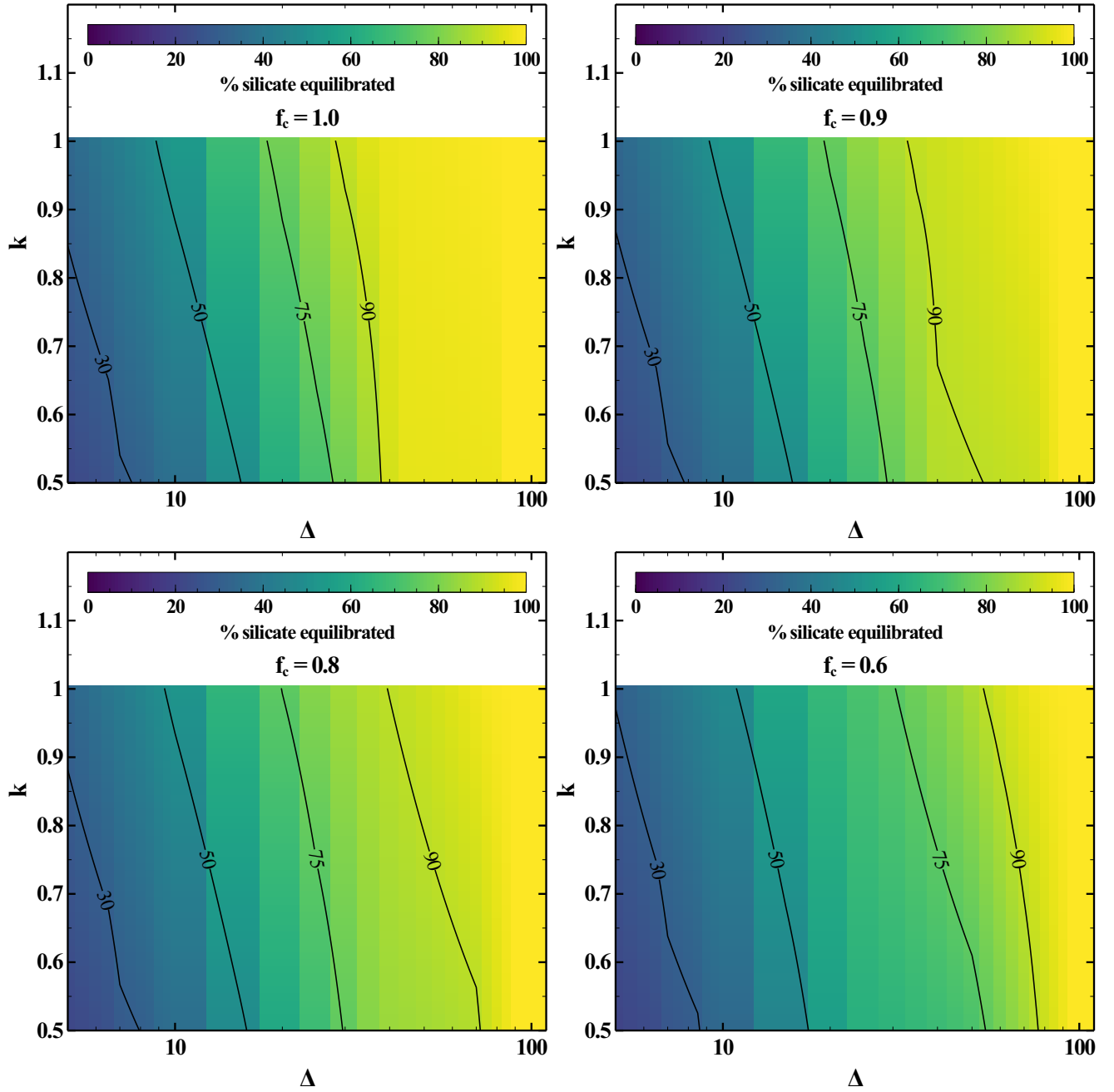
In this section are presented the Figures cited in the main text which are not related to the additional sections in the present document.



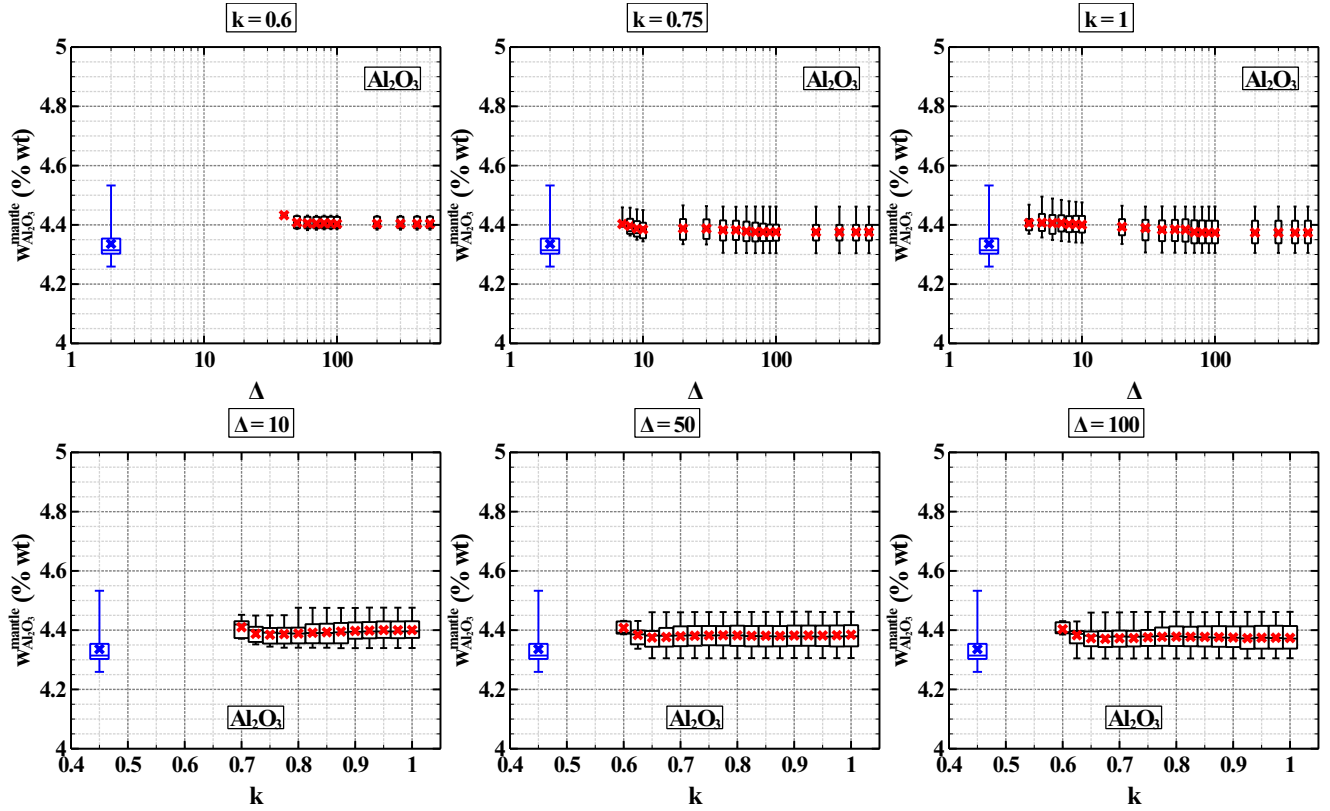
**Figure S.14.** Schematics of the physical meaning of the parameters  $a_p$ ,  $f_c$  and  $\lambda$  used to parameterize the models of accretion. This Figure has been published in [Clesi & Deguen \(2024a\)](#) and is reproduced here with the authorization of authors. The left column shows the early part of accretion ( $f < f_c$ , more reduced impactor in blue). The right column how the later stage of accretion ( $f > f_c$ , more oxidized impactor in dark red). The two first lines show the effect of  $\lambda$  for a low values of  $a_p$  on the depth of the magma ocean throughout accretion. The two bottom lines show the effect of  $\lambda$  for high values of  $a_p$  on the evolution of the depth of the magma ocean during accretion. m.o. = magma ocean (red), s.m. = solid mantle (green) and c. = core (grey).



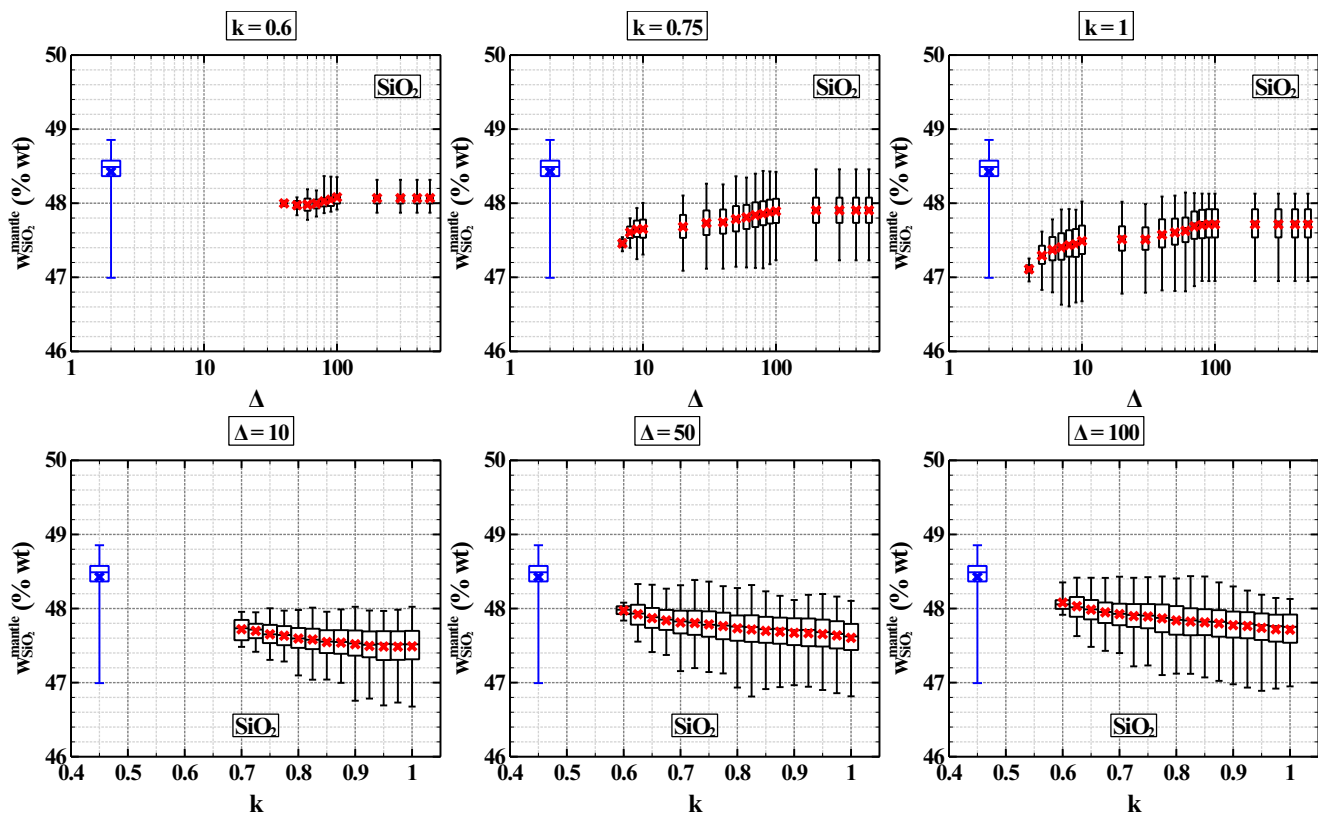
**Figure S.15.** Comparison of the reference solutions that are used in this study (round symbols) with the solutions obtained in [Clési & Deguen \(2023\)](#) with another filter (stars). The format of this figure is the derived from Figure 8 of [Clési & Deguen \(2023\)](#) to better highlight the differences between the solutions. The overall correlations are the same, with the weighted mean filter selecting for higher pressures models. The first row shows the correlation between light elements in the core with the three input parameters on each column:  $w_{Si+O}^{core}$  vs  $a_p$  on the left panel,  $w_{Si+O}^{core}$  vs  $f_c$  on the middle panel,  $w_{Si+O}^{core}$  vs  $\lambda$  on the right panel. The second row shows the correlation between the isentropic temperature at the CMB ( $T_{CMB}^{is}$  with the three input parameters presented in the same order. The color scale in all panel is the composite input parameter  $\overline{P_{eq}}$  in GPa.



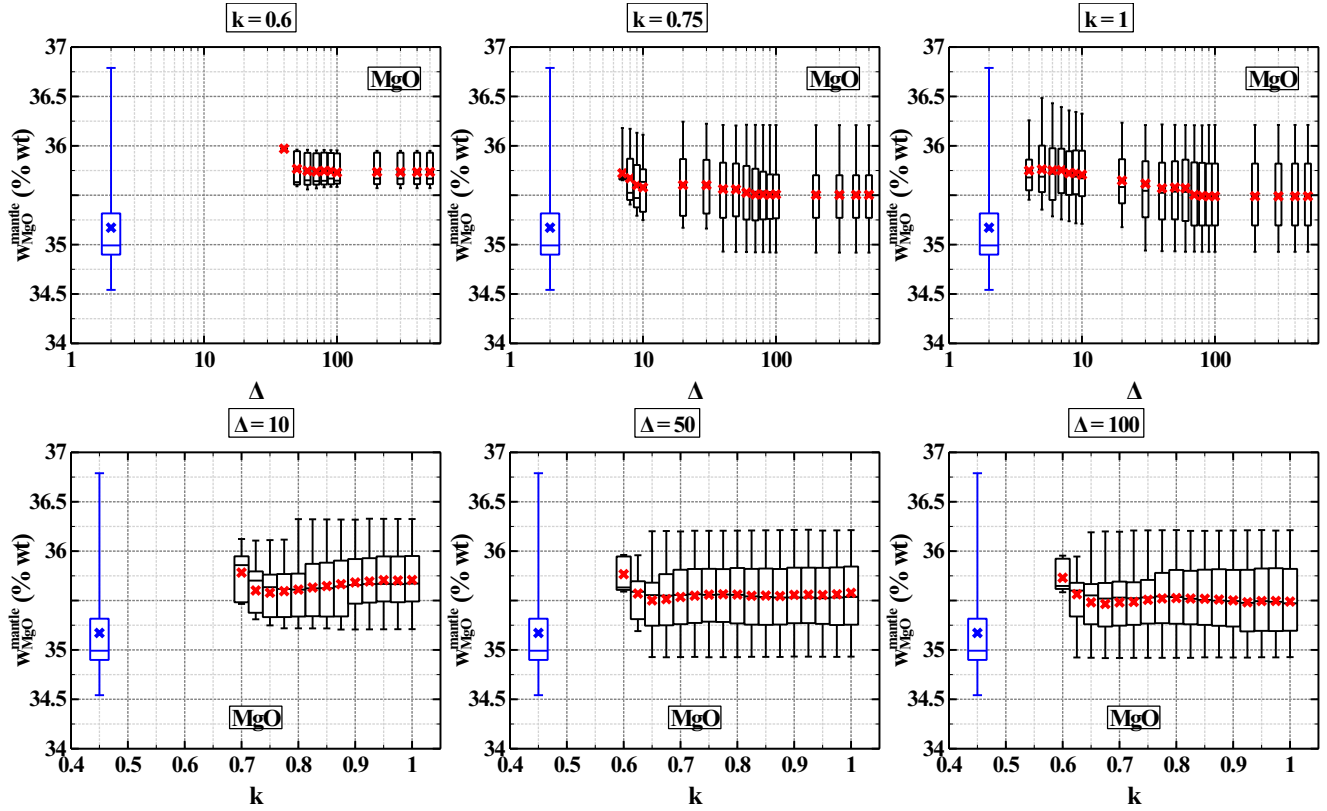
**Figure S.16.** Percentage of equilibrated mantle (color map) as a function of  $k$  (y-axis) and  $\Delta$  (x-axis) for  $f_c = 1$  (top left),  $f_c = 0.9$  (top right),  $f_c = 0.8$  (bottom left),  $f_c = 0.8$  (bottom right). Full equilibrium is reached for  $\Delta > 100$  in all relevant cases.



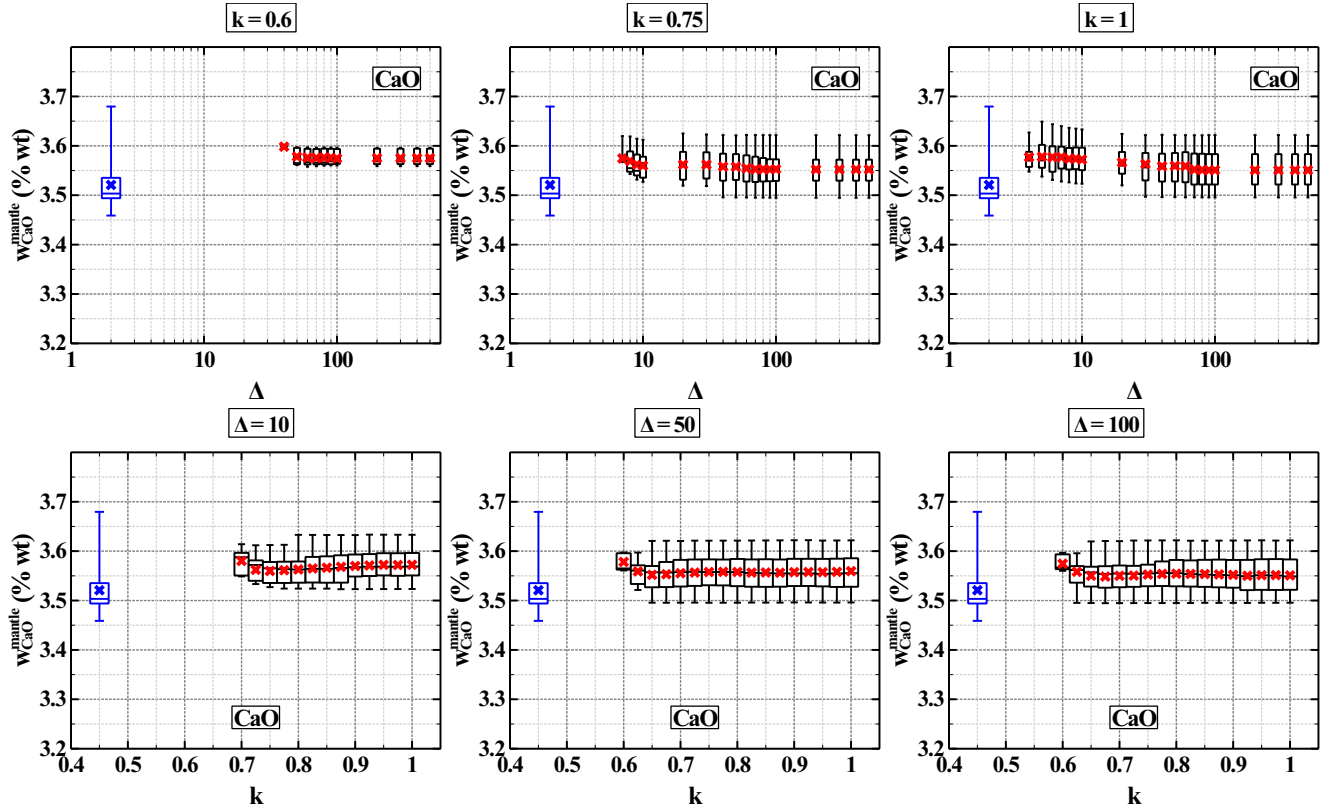
**Figure S.17.** Evolution of  $\text{Al}_2\text{O}_3$  concentrations (% wt) in the mantle as a function of  $\Delta$  for fixed values of  $k$  (top row), and as a function of  $k$  for fixed values of  $\Delta$  (bottom row). In each panel the entire solutions range are presented as boxplots, with the red cross being the mean value of the parameter, the white box delimiting the 1st and 3rd quartile, the horizontal line the median value and the vertical lines the minimum and maximum values. The reference model dataset is presented in blue with the same type of plot for comparison.



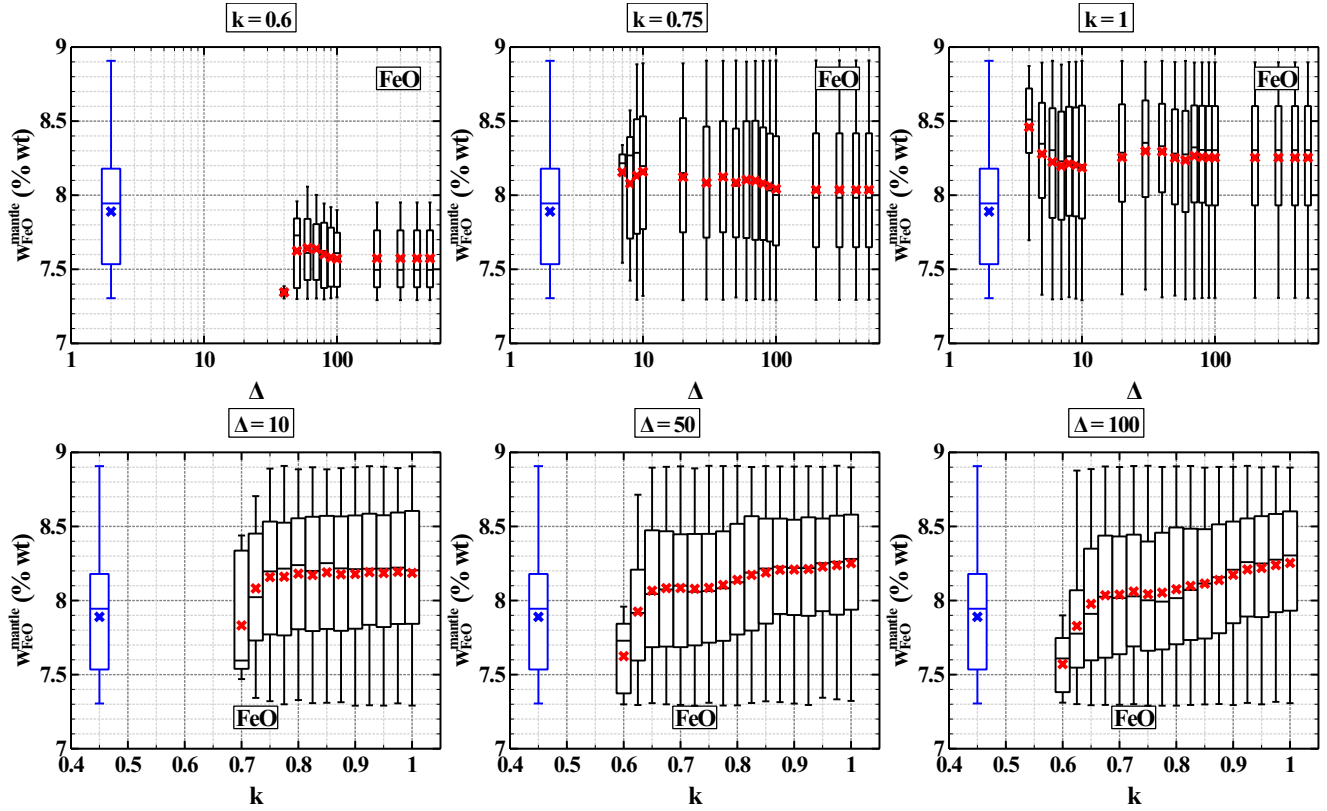
**Figure S.18.** Evolution of  $\text{SiO}_2$  concentrations (% wt) in the mantle as a function of  $\Delta$  for fixed values of  $k$  (top row), and as a function of  $k$  for fixed values of  $\Delta$  (bottom row). In each panel the entire solutions range are presented as boxplots, with the red cross being the mean value of the parameter, the white box delimiting the 1st and 3rd quartile, the horizontal line the median value and the vertical lines the minimum and maximum values. The reference model dataset is presented in blue with the same type of plot for comparison.



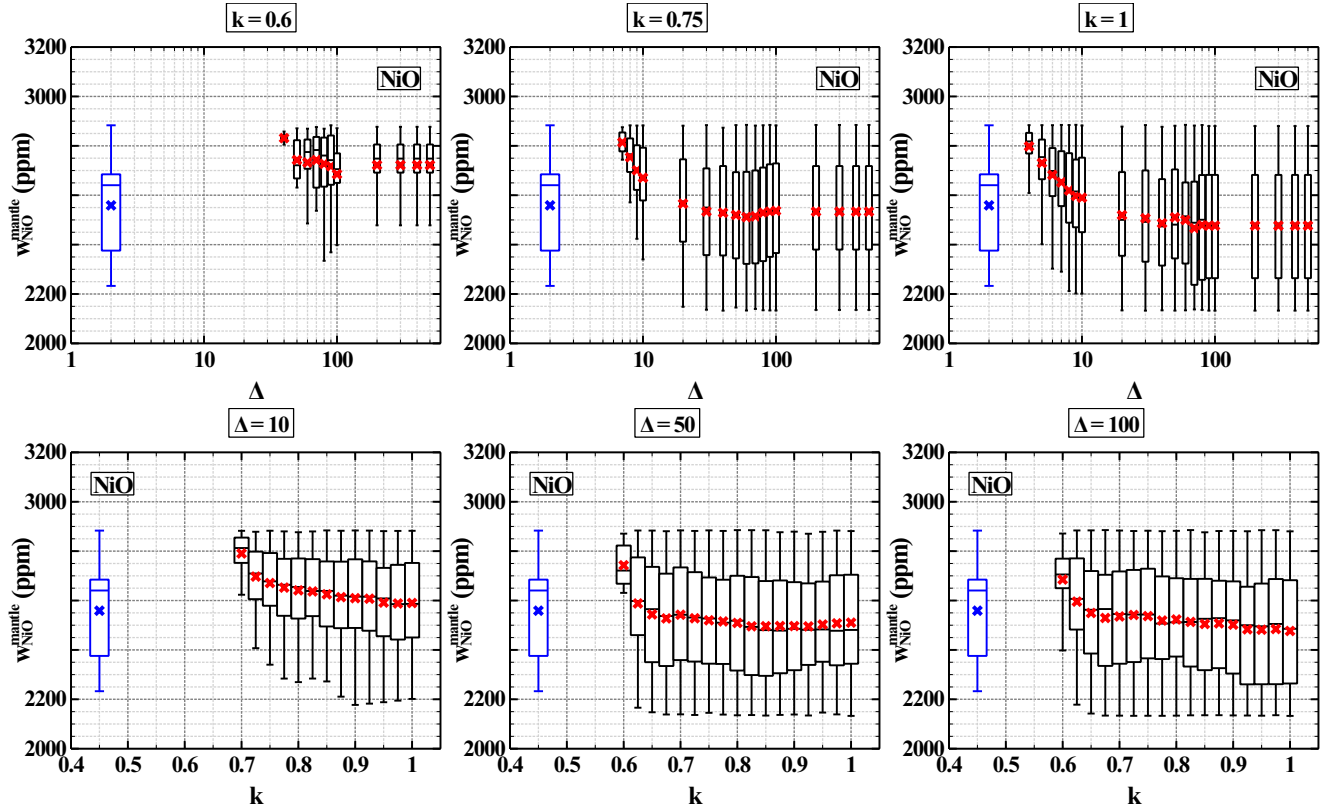
**Figure S.19.** Evolution of MgO concentrations (% wt) in the mantle as a function of  $\Delta$  for fixed values of  $k$  (top row), and as a function of  $k$  for fixed values of  $\Delta$  (bottom row). In each panel the entire solutions range are presented as boxplots, with the red cross being the mean value of the parameter, the white box delimiting the 1st and 3rd quartile, the horizontal line the median value and the vertical lines the minimum and maximum values. The reference model dataset is presented in blue with the same type of plot for comparison.



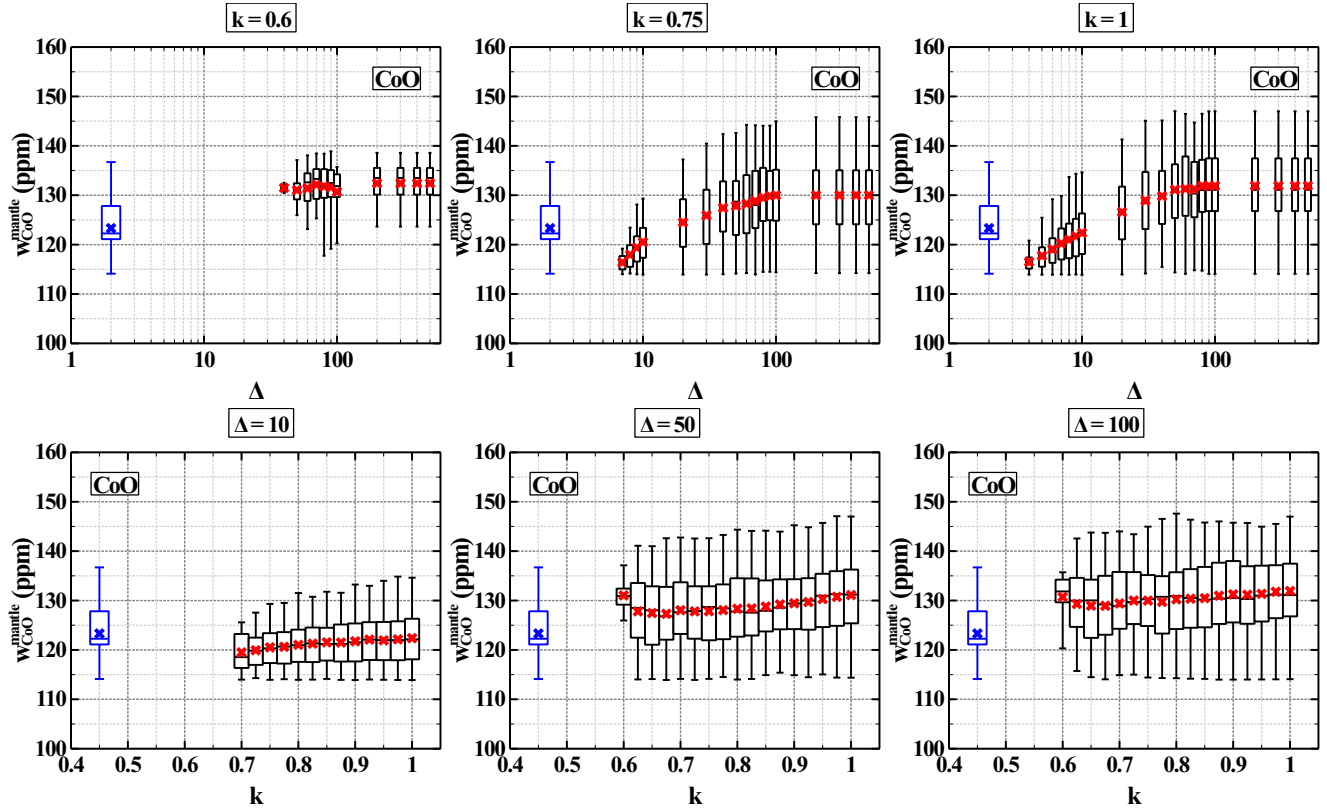
**Figure S.20.** Evolution of CaO concentrations (% wt) in the mantle as a function of  $\Delta$  for fixed values of  $k$  (top row), and as a function of  $k$  for fixed values of  $\Delta$  (bottom row). In each panel the entire solutions range are presented as boxplots, with the red cross being the mean value of the parameter, the white box delimiting the 1st and 3rd quartile, the horizontal line the median value and the vertical lines the minimum and maximum values. The reference model dataset is presented in blue with the same type of plot for comparison.



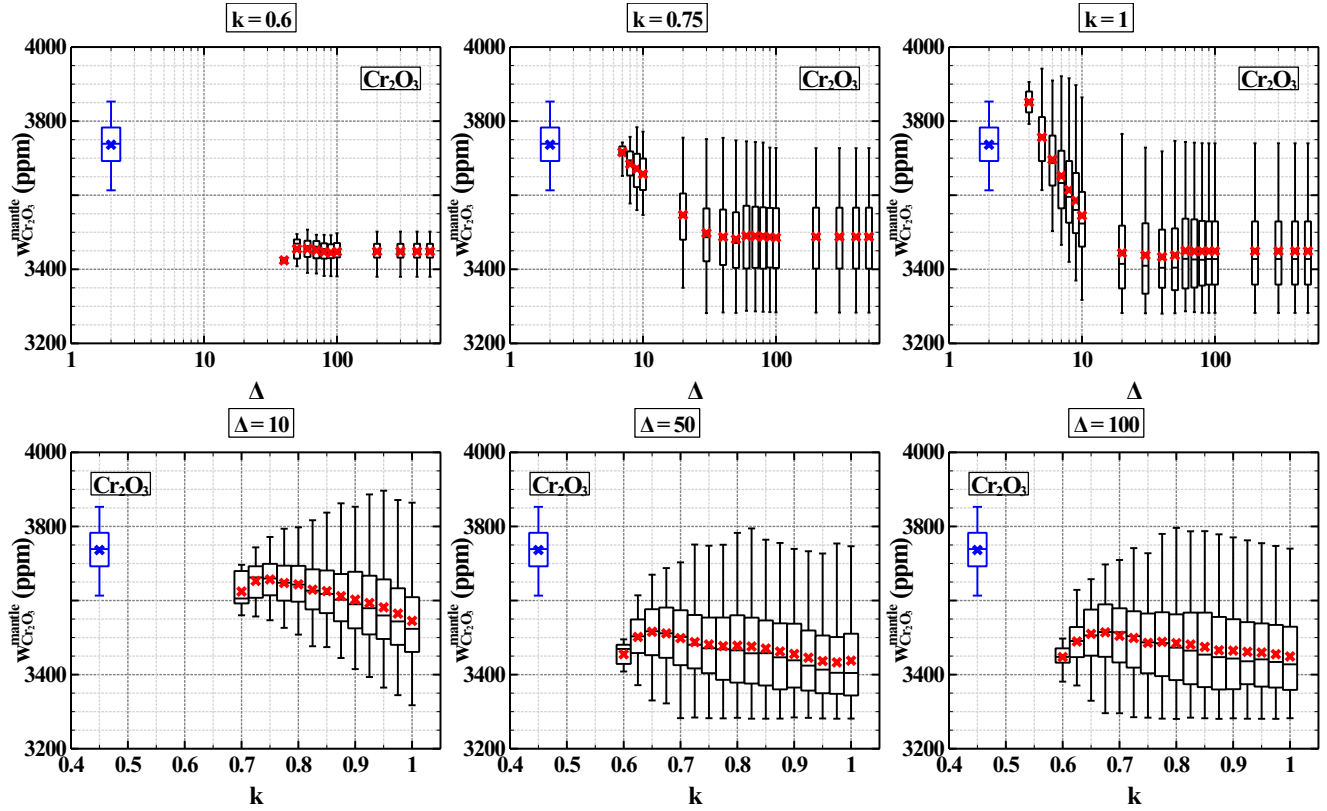
**Figure S.21.** Evolution of FeO concentrations (%wt) in the mantle as a function of  $\Delta$  for fixed values of  $k$  (top row), and as a function of  $k$  for fixed values of  $\Delta$  (bottom row). In each panel the entire solutions range are presented as boxplots, with the red cross being the mean value of the parameter, the white box delimiting the 1st and 3rd quartile, the horizontal line the median value and the vertical lines the minimum and maximum values. The reference model dataset is presented in blue with the same type of plot for comparison.



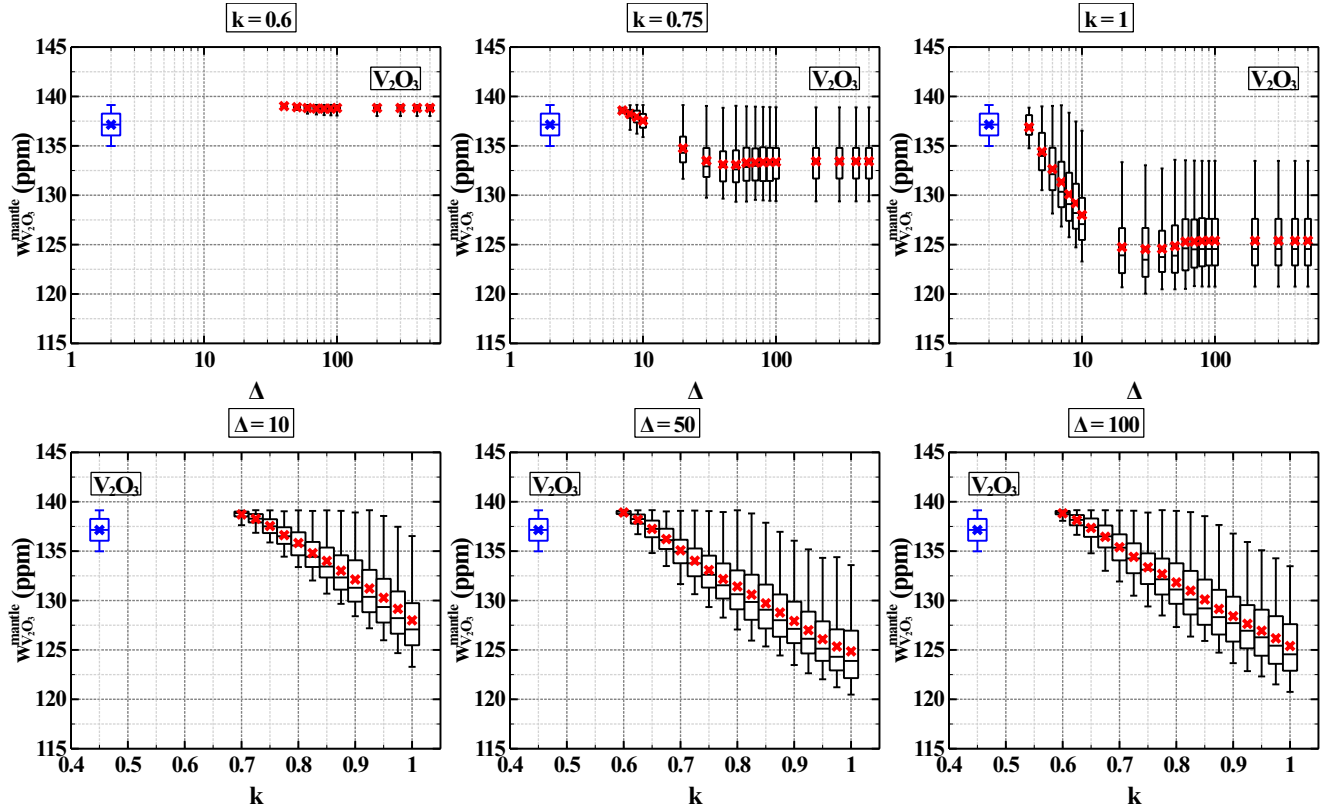
**Figure S.22.** Evolution of NiO concentrations (ppm or  $\mu\text{g/g}$ ) in the mantle as a function of  $\Delta$  for fixed values of  $k$  (top row), and as a function of  $k$  for fixed values of  $\Delta$  (bottom row). In each panel the entire solutions range are presented as boxplots, with the red cross being the mean value of the parameter, the white box delimiting the 1st and 3rd quartile, the horizontal line the median value and the vertical lines the minimum and maximum values. The reference model dataset is presented in blue with the same type of plot for comparison.



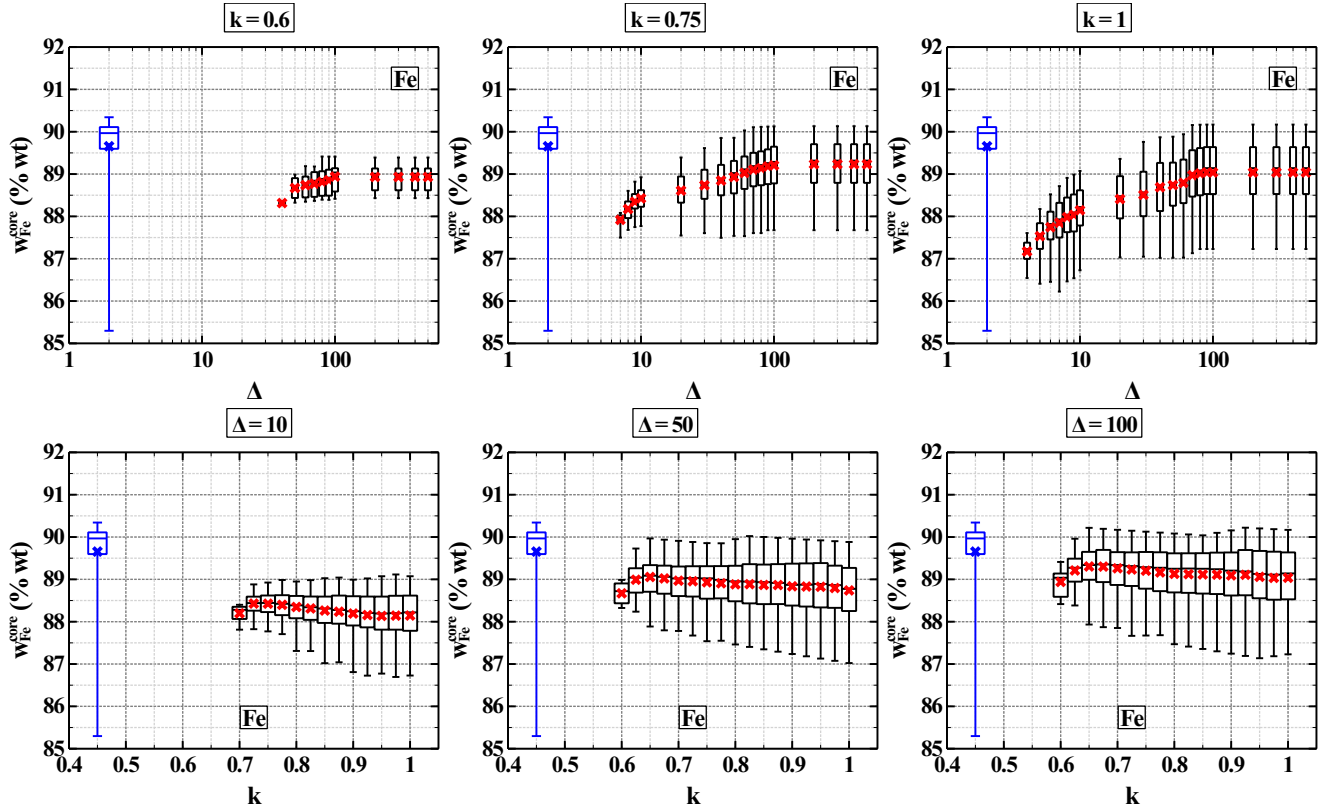
**Figure S.23.** Evolution of CoO concentrations (ppm or  $\mu\text{g/g}$ ) in the mantle as a function of  $\Delta$  for fixed values of  $k$  (top row), and as a function of  $k$  for fixed values of  $\Delta$  (bottom row). In each panel the entire solutions range are presented as boxplots, with the red cross being the mean value of the parameter, the white box delimiting the 1st and 3rd quartile, the horizontal line the median value and the vertical lines the minimum and maximum values. The reference model dataset is presented in blue with the same type of plot for comparison.



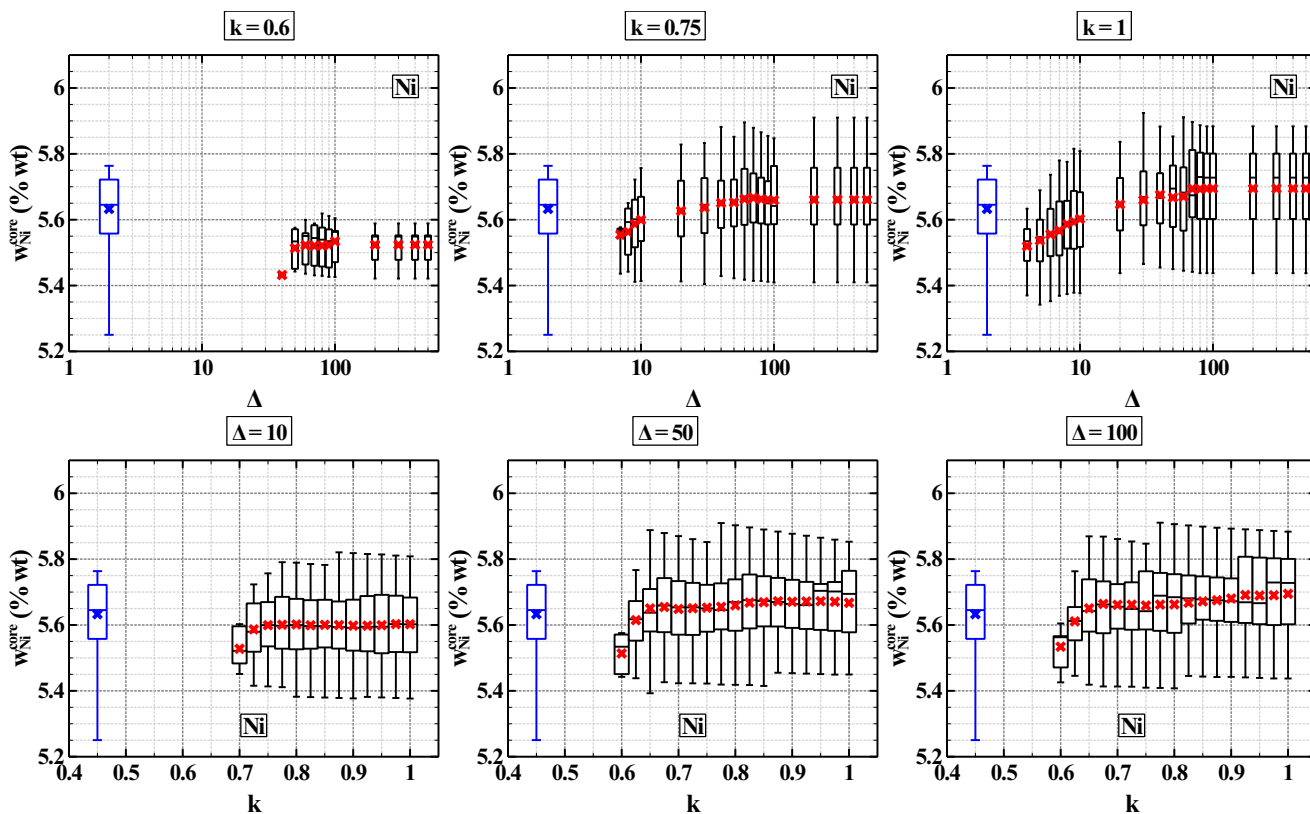
**Figure S.24.** Evolution of  $\text{Cr}_2\text{O}_3$  concentrations (ppm or  $\mu\text{g/g}$ ) in the mantle as a function of  $\Delta$  for fixed values of  $k$  (top row), and as a function of  $k$  for fixed values of  $\Delta$  (bottom row). In each panel the entire solutions range are presented as boxplots, with the red cross being the mean value of the parameter, the white box delimiting the 1st and 3rd quartile, the horizontal line the median value and the vertical lines the minimum and maximum values. The reference model dataset is presented in blue with the same type of plot for comparison.



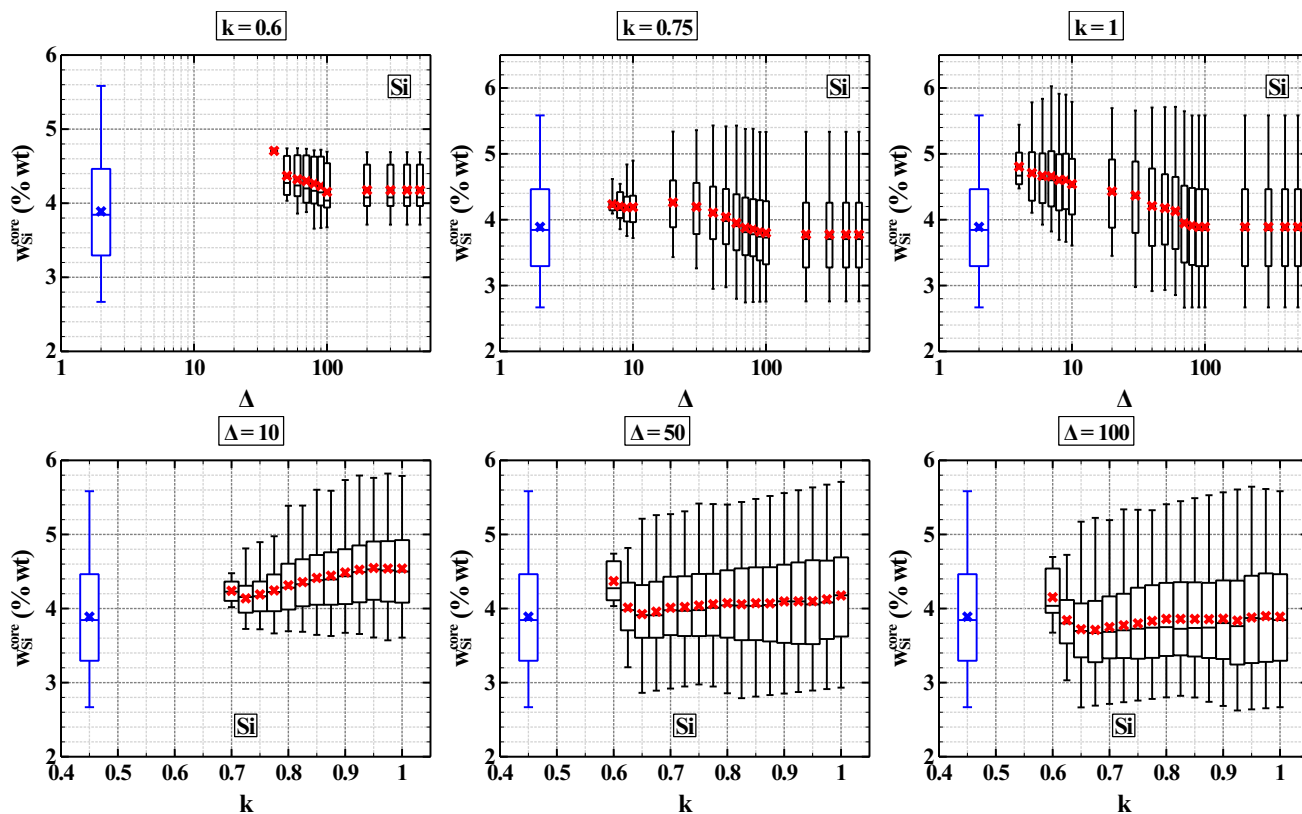
**Figure S.25.** Evolution of  $V_2O_3$  concentrations (ppm or  $\mu g/g$ ) in the mantle as a function of  $\Delta$  for fixed values of  $k$  (top row), and as a function of  $k$  for fixed values of  $\Delta$  (bottom row). In each panel the entire solutions range are presented as boxplots, with the red cross being the mean value of the parameter, the white box delimiting the 1st and 3rd quartile, the horizontal line the median value and the vertical lines the minimum and maximum values. The reference model dataset is presented in blue with the same type of plot for comparison.



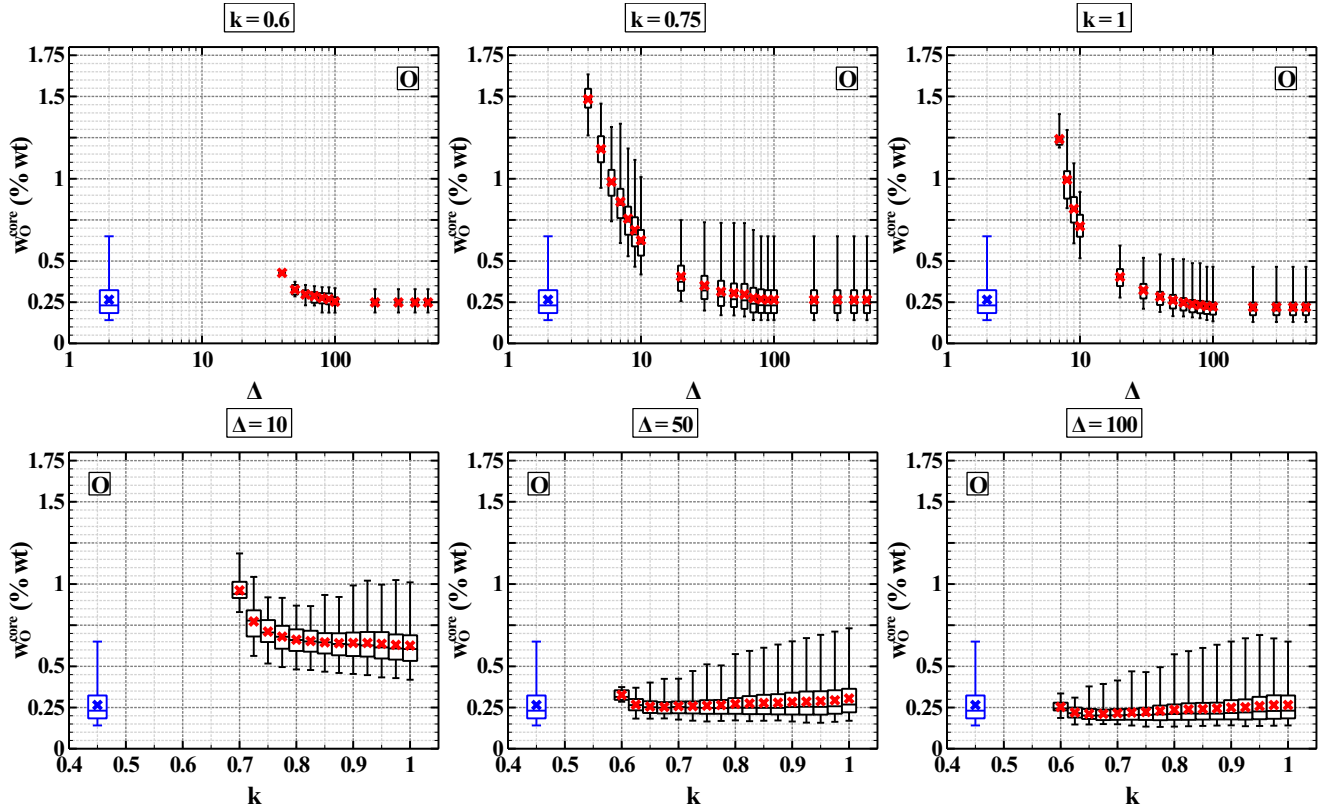
**Figure S.26.** Evolution of Fe concentrations (% wt) in the core as a function of  $\Delta$  for fixed values of  $k$  (top row), and as a function of  $k$  for fixed values of  $\Delta$  (bottom row). In each panel the entire solutions range are presented as boxplots, with the red cross being the mean value of the parameter, the white box delimiting the 1st and 3rd quartile, the horizontal line the median value and the vertical lines the minimum and maximum values. The reference model dataset is presented in blue with the same type of plot for comparison.



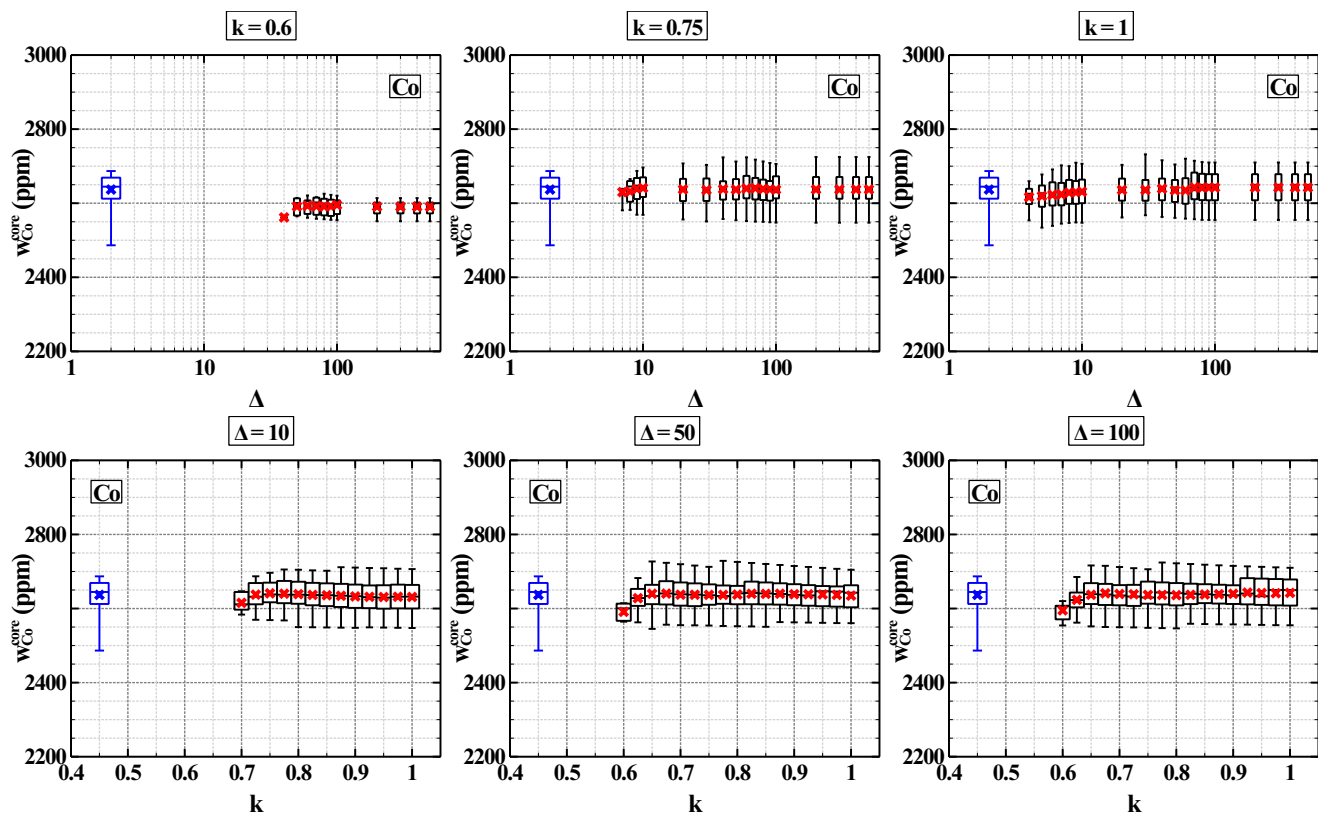
**Figure S.27.** Evolution of Ni concentrations (% wt) in the core as a function of  $\Delta$  for fixed values of  $k$  (top row), and as a function of  $k$  for fixed values of  $\Delta$  (bottom row). In each panel the entire solutions range are presented as boxplots, with the red cross being the mean value of the parameter, the white box delimiting the 1st and 3rd quartile, the horizontal line the median value and the vertical lines the minimum and maximum values. The reference model dataset is presented in blue with the same type of plot for comparison.



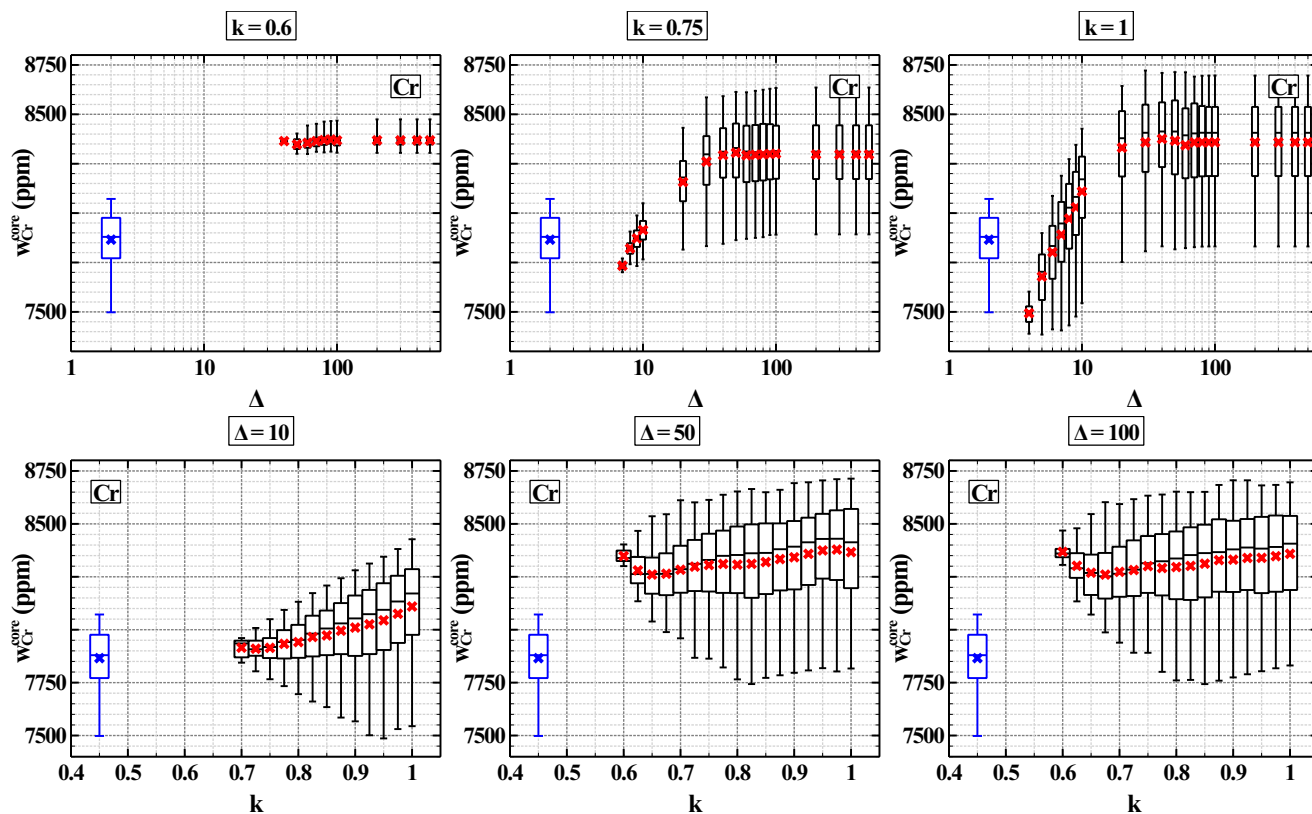
**Figure S.28.** Evolution of Si concentrations (% wt) in the core as a function of  $\Delta$  for fixed values of  $k$  (top row), and as a function of  $k$  for fixed values of  $\Delta$  (bottom row). In each panel the entire solutions range are presented as boxplots, with the red cross being the mean value of the parameter, the white box delimiting the 1st and 3rd quartile, the horizontal line the median value and the vertical lines the minimum and maximum values. The reference model dataset is presented in blue with the same type of plot for comparison.



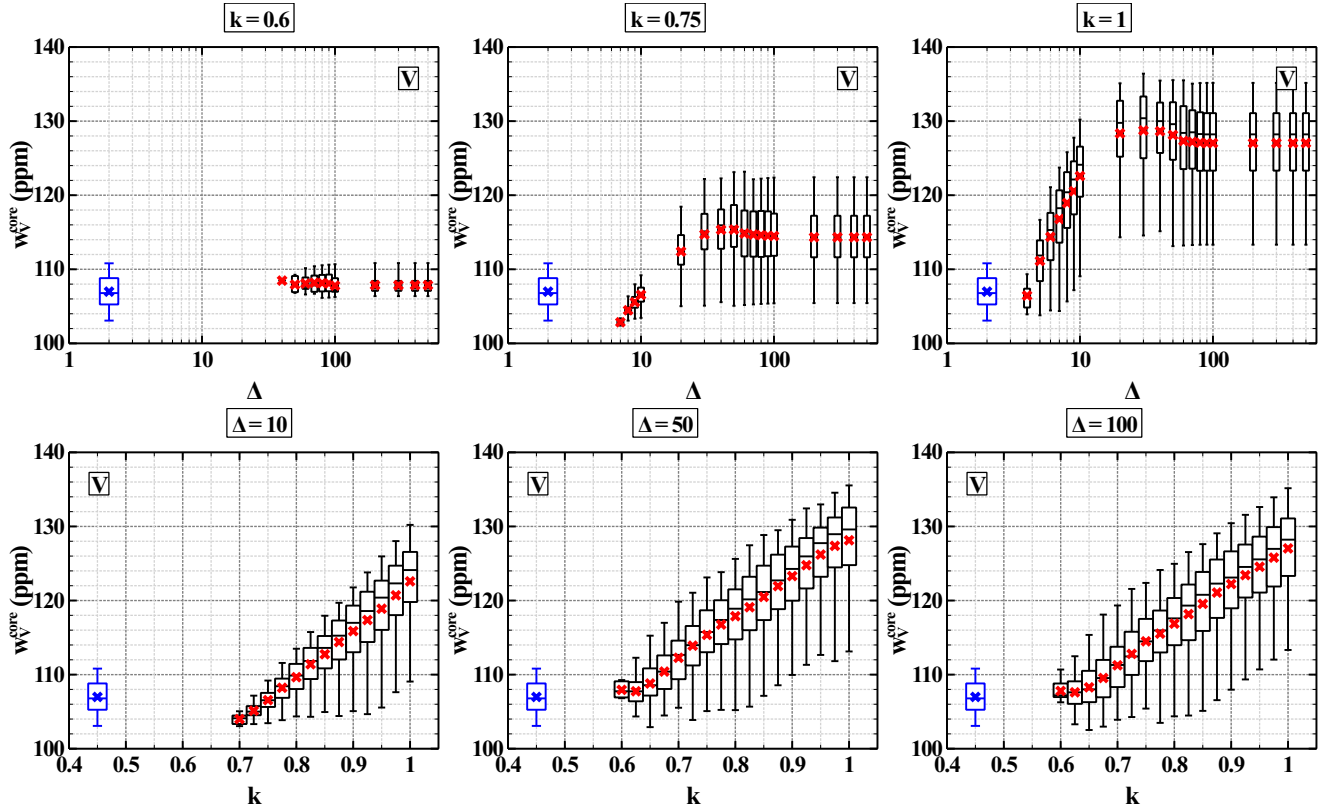
**Figure S.29.** Evolution of O concentrations (% wt) in the core as a function of  $\Delta$  for fixed values of  $k$  (top row), and as a function of  $k$  for fixed values of  $\Delta$  (bottom row). In each panel the entire solutions range are presented as boxplots, with the red cross being the mean value of the parameter, the white box delimiting the 1st and 3rd quartile, the horizontal line the median value and the vertical lines the minimum and maximum values. The reference model dataset is presented in blue with the same type of plot for comparison.



**Figure S.30.** Evolution of Co concentrations (ppm or  $\mu g/g$ ) in the core as a function of  $\Delta$  for fixed values of  $k$  (top row), and as a function of  $k$  for fixed values of  $\Delta$  (bottom row). In each panel the entire solutions range are presented as boxplots, with the red cross being the mean value of the parameter, the white box delimiting the 1st and 3rd quartile, the horizontal line the median value and the vertical lines the minimum and maximum values. The reference model dataset is presented in blue with the same type of plot for comparison.



**Figure S.31.** Evolution of Cr concentrations (ppm or  $\mu g/g$ ) in the core as a function of  $\Delta$  for fixed values of  $k$  (top row), and as a function of  $k$  for fixed values of  $\Delta$  (bottom row). In each panel the entire solutions range are presented as boxplots, with the red cross being the mean value of the parameter, the white box delimiting the 1st and 3rd quartile, the horizontal line the median value and the vertical lines the minimum and maximum values. The reference model dataset is presented in blue with the same type of plot for comparison.



**Figure S.32.** Evolution of V concentrations (ppm or  $\mu g/g$ ) in the core as a function of  $\Delta$  for fixed values of  $k$  (top row), and as a function of  $k$  for fixed values of  $\Delta$  (bottom row). In each panel the entire solutions range are presented as boxplots, with the red cross being the mean value of the parameter, the white box delimiting the 1st and 3rd quartile, the horizontal line the median value and the vertical lines the minimum and maximum values. The reference model dataset is presented in blue with the same type of plot for comparison.