*General comment*

The authors have answered to the first comments and additional parts have been added in the revised version of the manuscript. The major suggestions of this review focus on the new parts added in the manuscript in the aim to strengthen these parts. Additional minor comments concern the other parts of the manuscript.

*Major comment*

**Results**
**3.1 Model validation using discrete phases**

The title of this paragraph should be changed because this paragraph deals with the comparison of calculated XRD patterns from PyXRD and Sybilla[©]. In addition, the comparison does not only consider discrete phases, comparison of calculated mixed layer minerals is also performed. The title could be: "Comparison between Sybilla[©] and PyXRD results: calculated *00l* reflections for single discrete clays and MLMs".

Among the clay minerals which were chosen for this comparison, the MLMs and their structural characteristics should be modified in order to be more relevant. Indeed, authors have used the default setting of the different illite-smectite MLMs that are proposed in Sybilla[©] and in some cases studied, the interest of these examples is still limited. For instance, XRD calculated pattern of R1 illite-smectite (Wi = 0.6; Pss = 0.5) is very closed to the R0 illite-smectite (Wi = 0.6; Pss = 0.4) and also does not largely differ from the R0 illite-smectite chosen (Wi = 0.5; Pss = 0.5). In addition, the choice of the default setting from Sybilla[©] is also limited for MLMs with higher Reichweite (R2 and R3) because of the too low mean CSDS of 4 that limits the influence of the stacking order (R3 or R0 MLMs illite-smectite have quasi-similar XRD calculated profiles with mean CSDS of 3). Thus the parameters of the MLMs chosen need to be modified and I suggest presenting R1, R2 and R3 MLMs illite-smectite with mean CSDS of 10 or more with MPDO (maximum possible degree of ordering) for R1. In addition, I would suggest exposing the calculated XRD patterns for these MLMs in a figure. The XRD patterns calculated with PyXRD (solid line) could be plotted over the XRD patterns calculated using Sybilla[©] (crosses) with the difference plot below. The figure 4 presented in the revised manuscript could be also improved (I do not obtain with Sybilla[©] the same calculated XRD pattern for the R2 illite-smectite MLM presented in figure 4 that motivate the presentation of calculated XRD patterns).

In the Table 1, the authors give the residual error (Rp) obtained between XRD patterns calculated with PyXRD and Sybilla[©]. Although quite low, they remain significant, particularly for the talc with a Rp equal to 6.4%. This value is higher than Rp obtained for the comparison of experimental and calculated XRD profiles on natural samples and consequently need more explanation in the text or a new calculation. The explanation in the manuscript l294-298 does not support this difference otherwise such difference should be present on each XRD calculation exposed. In addition, I suggest to the authors to also calculate the Rwp (weighted profile R-factors; Howard and Preston, 1989) that could be more relevant in the present case.

*Howard, S.A. and Preston, K.D. (1989) Profile fitting of powder diffraction patterns. In D.L. Bish and J.E. Post, Eds., Modern Powder Diffraction, 20, p. 217–275. Reviews in Mineralogy, Mineralogical Society of America, Chantilly, Virginia.*

## 3.2 Model validation using assemblages

As for the part 3.1, I would like to suggest a title. The title could be: "Comparison between Sybilla$^©$ and PyXRD results: calculated *00l* reflections for mixtures of discrete clays and MLMs".

The authors mention that Sybilla$^©$ "does not have an easy way to calculate a pattern for a certain mixture of phases (or in any case this feature is unknown to the authors), while PyXRD does" (l305-306). This is possible using Sybilla$^©$ however, I agree with the authors that an easy way does not exist. To create this type of file with Sybilla$^©$, you need to first have a .txt file with the angular range of your XRD pattern (for example a XRD pattern calculated with PyXRD as performed in the manuscript). After opening the XRD pattern and writing the diffractometer parameters in the dialog box (fitting>add gene phases>select phases) and selecting the phases (for example kaolinite and illite as for the first mixture), you just have to save the calculated pattern (fitting>save all). You have saved an .xml file with the structural parameters of the mixture. Open this file with notepad and then you will able to modify in this file all that you need (for example, phase content in the present case). After performing the modifications, save this file as an .xml with another name and open this file in Sybilla$^©$ with fitting>add from input file. The mixture modified should appear. Save the fit pattern in .csv file (fitting>save fit pattern). Open the .csv in a spreadsheet program and you have the file needed.
*N.B.: I have added a .xml file and a .csv file that give an example for the first mixture kaolinite, illite.*
Using this procedure, the authors should directly compare the output from Sybilla$^©$ with the output of PyXRD for mixture and improve the validation test for the weight fractions. In addition, I suggest to the authors to give in Table 2 the Rp and Rwp values between the XRD patterns of mixtures calculated with Sybilla$^©$ and PyXRD. Moreover, I suggest adding a figure that show the comparison between the calculated XRD patterns from the two software as mentioned above for the part 3.1.

Finally, the authors should also add the Rp and Rwp values for the four assemblages calculated. These R-factor values will help the reader to estimate the order of magnitude of the misfits that could remain in the theoretical cases exposed.

*Minor comment*

L31-32: "… might be sufficient", precise for the cases studied.
L34: remove "very" before useful
L101-102: add references, other authors have used this approach or precise "and reference therein"
L118: "… or at least more robust)…". This part of the sentence is not necessary. I suggest to remove it.
L130: replace "model" by software
L251: add a space between strategy and algorithm
L291: replace "diffrerent" by different
L384-385: "these results…excellent results". I suggest to remove this sentence that is not necessary.
L398: remove a space after "strategy"
L460-462: "If…more parameters". This sentence is unclear. Remove this sentence or precise the idea.