Geosci. Model Dev. Discuss., 8, C616–C619, 2015
www.geosci-model-dev-discuss.net/8/C616/2015/

Geoscientific Model Development Discussions
Open Access

Interactive comment on "PyXRD v0.6.2: a FOSS program to quantify disordered, layered minerals using multi-specimen X-ray diffraction profile fitting" *by* M. Dumon and E. Van Ranst

Anonymous Referee #1

Received and published: 5 May 2015

The Ms "PyXRD v0.6.2: a FOSS program to quantify disordered, layered minerals using multi-specimen X-ray fiffraction profile fitting" submitted by M. Dumon and E. Van Ranst for publication in Geoscientific Model Development: Discussions describes a program designed to allow determining quantitatively structural parameters and relative proportions of disordered clays (mixed layers) from their X-ray diffraction (XRD) patterns. The described program allows this determination to be based on the simultaneous refinement of different XRD patterns collected on the same sample (multi-specimen method). This program clearly represents a step forward in the right direction for the quantitative structural determination of complex clay minerals assemblages. As such I think it would be a good thing to get this article published in Geoscientific Model

Full Screen / Esc
Printer-friendly Version
Interactive Discussion
Discussion Paper

Development: Discussions and the program available to the clay community. I think however that the present version requires significant improvements before it could be formally accepted for publication. These modifications are threefold: - The first requirement of a new routine allowing the calculation of XRD patterns from complex mixtures of disordered/interstratified phyllosilicates is consistency with available routines. Although these routines may not all be easily accessible, some of them are and I think an essential step would be to use to developed program to fit XRD patterns calculated with a different calculation algorithm (for a complex mixed layer) to make sure that ALL structural parameters (for both phases and components) are introduced and considered in the right way in the new algorithm. In addition I think that refinement of at least one experimental dataset (for example a known mixture of pure clays, or published datasets with determined structural parameters) would be a convincing evidence for the performance of the reported program. - A second important feature of the multi-specimen approach is its ability to deal with swelling layers which may behave differently depending on experimental data collection conditions: A mono- or bi-hydrated layer in the AD state may for example incorporate 1 or 2 planes of ethylene glycol upon solvation. From the Tables, it seems that all swelling layers are considered as a unique layer type in PyXRD, but precisions are clearly needed with respect to this major and specific aspect. This is especially important for ordered mixed layers (Reichweite parameter >= 1, which are not dealt with in the reported examples) because of the implications on junction probabilities. - Third, I think that the conclusions as to the ability of the proposed refinement algorithm to determine relevant structural (and quantitative) parameters from a single XRD pattern is misleading and should be modified. The main objective of the multi-specimen approach, as described in the abundant devoted literature is NOT to determine better or more accurate parameters but rather to release possible identification ambiguities from different structure models leading, for one of the data collection conditions, to similar XRD patterns. If this was not the case, the multi-specimen approach (and thus the present program) would be essentially useless, the more common and faster refinement of a single pattern being sufficient...

GMDD

8, C616–C619, 2015

Starting from computed XRD patterns, the ambiguity is easily overcome but this may not be the case when dealing with natural samples. Accordingly, all sections (including conclusion and the abstract) dealing with this aspect should be re-written. I agree with the authors however that refinement of a single pattern may be sufficient once possible identification ambiguities are released (by using the multi-specimen approach).

Finally, reference list is far from being complete. XRD profile modeling has developed significantly over the last two decades because of the increased availability of computing resources and calculation routines. Most of the latter had however been developed and used in the 1970's, and it would be reasonable to cite these pioneering works. It is for example striking that Newmod is cited as one of the available calculation routines with no reference to its original author (R.C. Reynolds, Jr.).

Minor remarks: p. 2497: Avoid acronyms in the title p. 2499, l. 1-4: References needed p. 2499, l. 8-11 / p. 2499, l. 21-25: Additional (older) references could be added. In particular reference to the original modeling works of Reynolds (for Newmod), and of the Russian group (Drits and Sakharov) from early 1970's could be included. p. 2500, l. 16-17: References to Meunier and Lanson are not relevant (at least not as presently written) here as they essentially review existing literature. p. 2500, l. 27-28: This statement contradicts the conclusions of the article (as the authors show that it is possible to obtain equally good structural/quantitative determination from a single XRD pattern). From the previous lines, one interest would be to obtain a faster refinement and an improved consistency of the structure models derived from different XRD patterns. p. 2502, l. 17-18: Probably not necessary to consider ionic species the effect being strongly correlated with thermal motion. p. 2503, l. 10-12: This is wrong as Newmod also includes uniform (or custom) distribution, MLM2C/3C Ergun's distribution, . . . p. 2503, l. 18: Projection is along c* not c p. 2504, l. 12-14: This possible constrains appear similar to those that were considered inadequate for other programs (see for example p. 2500, l. 8-11) p. 2505, l. 9-20: I am not sure all acronyms are necessary especially as they are (very) seldom used in the rest of the article. Remove

GMDD
8, C616–C619, 2015

acronyms. p. 2507, l. 5: Why not just consider statistical counting noise [sqrt(I0)] p. 2507, l. 8: Such a noise level corresponds to ∼40000 counts which is seldom achieved experimentally on mixed layers. p. 2508, l. 10-11: Systematic discrepancies should be described and an explanation sought. p. 2509, l. 1-2: Meaning unclear. p. 2510, l. 26-27: Again, XRD profile modeling was used before 2010!

Interactive comment on Geosci. Model Dev. Discuss., 8, 2497, 2015.

GMDD

8, C616–C619, 2015