Dear Editor:

Thank you for your efforts so far in managing the revision process thus far and ensuring the high quality of this publication. At this stage of the review, we are very encouraged by the positive feedback from Reviewers 1 and 2. The minor issues requested by Reviewer 2 has been fully addressed. Concerning Reviewer 3, there are a number of issues with the critiques of Reviewer 3 that we would like to bring to your attention. It is in our hope that, with your input, we could come up with a reasonable course of action.

In particular, the Authors believe that the critical comments from Reviewer 3 are predicated on a misunderstanding of interpreting the hash map approach as a verbatim replacement of a 3D array. The Authors further emphasize that this approach enables emission source to be represented only at the source location only, which offers significant savings in runtime memory and storage. Additional clarification has been introduced in § 2.1. And, along with various minor comments, the Authors hope that the amendments will be satisfactory, and that the overall implementation has been sufficiently detailed not to hinder reader's understanding.

In light of the above arguments, the Authors will proceed to disseminate the comments from Reviewers 2 and 3, and to address all necessary and outstanding issues. The original reviewer comments will be presented in indented italics, and abridged only to clarify the Authors' understanding. The line and section references to the manuscript refers to the first revision.

As emphasized in the previous discussions already, in the current version of the MS, the width of Figure 10 has been shrunk from 17 cm to 12 cm so that it will completely fit on the page in manuscript move. Once accepted for publication, Figure 10 should revert to 17 cm for better visualization.

Sincerely yours,

The Authors.

## **Response to Reviewer 2**

**Comment 1:** Equation (10) assumes that 100% of the energy consumption is used for heating. In reality, a certain fraction of the energy is used for water heating (and cooking with gas) that does not depend on the temperature deficit.

**Response 1:** A note will be added in §3.1 to bring this to the readers' attention. This change will be considered for implementation in future releases of this module.

Comment 2: Page 12, line 346: typo: "boarder".

Response 2: This has been corrected.

**Comment 3:** Section 4: give a list of input data for the emission calculation that needs to be provided by a user to reproduce the exemplary model run on domestic heating emissions. Which checks of the input (in addition to minimum height and footprint) are performed to ensure that the calculated volume sources are physically sound?

**Response 3:** The Authors have introduced Appendix C, indicating user-defined and default values for all namelist parameters used in the domestic model, as well as all relevant building-specific input data in the PALM \_static file. Additional information on input and runtime checks have been introduced at the end of § 3.2. The implicit understanding here is that the model can only rectify faulty input and calculated values to the extent of preventing system crashes, usually by replacing it with default values during initialization, and imposing a zero lower limit in emission source values during runtime.

**Comment 4:** *Page 15, line 460-461: rephrase wording of the sentence "This indicates mixing of the PM10 still lingering …"*.

Response 4: "still lingering" has been replaced with "that remains".

## **Response to Reviewer 3**

**Comment 1:** [*T*]*he implementation makes the hash tables as large as the model's 3D grid ... Crucially, this offers no space savings over a simple 3D array.* 

**Response 1:** The Authors believe there is a misunderstanding. The hash map approach was chosen so that only cells identified as emission sources are stored in the data structure, thus offering significant savings in runtime memory and storage. The motivations are stated in §2.1, LL 83-84, that the emissions sources "are only defined at sparse, discrete regions", and thus, in LL 89-90, "it is strongly preferred to consider [emissions] only at discrete locations where the emission source is present." The present implementation functions under the principle that the number of volume sources is not equal to the number of grid points.

At the suggestion of the Editor, the Authors have introduced an additional clarification in § 2.1 to justify the adaptation of the hash map approach over the traditional 3D array.

**Comment 2:** Equations (3) to (6) essentially implement indexing in a multidimensional array. I cannot see any reason why the re-implementation is preferable to just using a multidimensional array, which is very efficient in Fortran. The memory cost is the same, and the native Fortran implementation is easier and also faster, as the divisions and modulo operations in (4) to (6) can be avoided.

**Response 2:** Please refer to Response 1 regarding the memory cost of the hash map, and Response 7 for the status of Equations (4-6).

**Comment 3:** What prevents me from recommending publication is the highlighting of the importance of using a hash function, followed by an implementation that offers no benefit but comes at the cost of both performance and clarity. Additionally, the implementation is still not explained clearly enough, see the minor points below where several unclear statements are noted. These flaws are especially severe for a journal such as GMD, focused on model implementation and a clear description of it. "ideally, the description should be sufficiently detailed to in principle allow for the re-implementation of the model by others, so all technical details which could substantially affect the numerical output should be described." (from point 3 of GMD's guidelines for Model Description Papers).

**Response 3:** Please refer to Responses 1 and 2. In the first author's practice in computational model development, particularly in the private sector, hash tables are commonly used as a memory efficient method to represent sparse, discrete data. As such, the Authors are pleasantly surprised such classic concepts still find novel uses. On the other hand, as a fundamental data structure, there already exists an abundance of comprehensive resources on the theory and machinery of hash tables. The Authors thus add no scientific value to this article by deviating its focus from its application in organizing emission sources to a rudimentary exposition of its implementation, a topic that has been thoroughly covered in textbooks on computer data structures and algorithms, with Corman et al (2009) is one of the most accessible to the readers.

Having said that, aside from the indicated minor comments, no further details are given on the reason or manner in which the implementation is not satisfactorily explained. The Authors assume that addressing these comments will remedy any concerns from the Reviewer.

**Comment 4:** As a side note, when storing the emission sources in a simple 3D array, there is a simple optimization: Store the emission sources from the surface up to  $k_{max}$ , the height level of the highest emission source. For cases where sources are

located between the ground and the highest smoke stacks, this can already save a substantial fraction of the memory.

**Response 4:** The Authors would also like to point out that, at lower grid resolutions (i.e., regional and global scale) models, increasing  $k_{max}$  by one can cover the vertical dimension by tens to hundreds of meters. In urban scale models such as PALM, the same vertical space must be covered by 10 to 20, or even more vertical layers due to the high spatial resolution. At this stage, the memory consumption, while substantially reduced in the Reviewer's opinion, can still severely restrict model scalability and runtime performance.

**Comment 5:** *Line 195: The sorting procedure alluded to here is very unclear. Why is it needed at all? Why is the reverse lookup not achieved through Eqs 4-6 this time? If it's a crucial part of the implementation it should be explained carefully, perhaps together with the global hash map H.* 

**Response 5:** Line 195, and by extension §2.3.2, do not refer to any reverse lookup (see Response 7). However, the Reviewer is correct, the sorting algorithm (§2.3.2, L194) "facilitate[s] the hash key lookup" such that the runtime scales only with the logarithm of the number of emission sources using bisection search. This will be added to the MS.

**Comment 6:** Line 115, Equation 7: It is still not well explained what is stored in h<sup>m</sup> (h with superscript m). I expect h<sup>m</sup> to give a source intensity for each grid cell with an emission source from sector m. But it's also said that f depends on the location, making that interpretation seem redundant. There is a notation problem: if h<sup>m</sup> is the mapping between (i,j,k) and kappa defined in Eq. (2), what does it mean to multiply h<sup>m</sup> with f in Eq (7)?

**Response 6:** The definition of  $h^m$  is given in Eq. (2), in which (§ 2.1 LL 98-100) "the spatial association between the ... emission source location and the corresponding ... cell index locations in the computational domain are maintained ... for which ... a hash key  $\kappa$  is assigned for each source location[.]" The function  $f_p^m$  (the source function) calculates the intensity of emission. The dot product operation ( $h^m \cdot f_p^m$ ) in Eq. (7) is not redundant as  $f_p^m$  is continuous (that is, it produces a value as long as there are input parameters), and the dot product implies that  $e_p^m$  is only defined where  $h^m$  is defined (i.e., at the respective volume sources). A short clarification will be added to L 116 to reinforce the idea that  $e_p^m$  is only defined at volume source locations.

**Comment 7:** *Line 110: "It should be noted that Equations (4 - 6) must be performed in the order presented." this seems to no longer apply to the revised version, where the three equations are independent.* 

**Response 7:** After reviewing the source code, Equations (4-6) are not used in the emission module aside from model diagnostics. They, and the descriptions associated with them, have been removed from the MS to improve overall clarity.

**Comment 8:** *Line 111: "or by using bitwise operations" it seems hard to guarantee the hash map is still collision free in this case, however that's a side point.* 

**Response 8:** As a (side) point of interest, the Reviewer is correct; bitwise operations do not unconditionally guarantee collision-free hash keys as Eq. (3) does. In practice, the use of bitwise operation for unstructured and moving meshes has not (yet) resulted any hash key collision, at least for the Authors, in this application in other research and commercial model codes. It should also be added that the method proposed by Teschner et al (2003) is particularly effective in minimizing such collisions.

**Comment 9:** *Line 244: "using Equation (7) in the function The function f, as a function of time" something wrong in the sentence, maybe just a missing "."* 

**Response 9:** The Reviewer is correct. L 244 should read "... hash key  $\kappa$  – using Equation (7)." And the remaining text should be removed. It will be corrected.

**Comment 10:** *Line 391: "4.1 Temnperature deficit" typo[.]* 

**Response 10:** The Reviewer is correct. It will be corrected.

Comment 11: Fig 4 and Table 2 caption: I'd suggest to omit empty unit brackets

**Response 11:** The empty unit brackets emphasize that the terms in question carry no units. Their inclusion is also to introduce stylistic consistency with other caption labels.

**Comment 12:** *[T]he "2.1E-4" etc notation for powers of 10 doesn't look good in text. Also, the numbers could probably be given with fewer digits.* 

**Response 12:** Prior to the initial submission, the Authors have experimented with different notations, and concluded that the "E" notation offered the least bad option in terms of space and clarity. The five significant digits used throughout the manuscript is to partially reconcile the vast difference in orders of magnitudes of the tabled values, particularly in Table 2.

## **References:**

Cormen et al (2009) "Introduction to Algorithms" MIT Press 253-280. Teschner et al (2003) Proc 8 Int Fall Workshop Vision Model & Vis.