Dear Editor:

Please find attached the Authors' response to the comments from the three reviewers on the following pages. In the mean time we would like to thank you for your efforts in organizing the discussion of this manuscript.

Please note that, 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 1

The Authors would like to thank Reviewer 1 for the encouraging comments. Please find our response on the corresponding comments below, with reference to the Reviewer's original comments in indented italics.

> **Comment 1:** *Page 3: Equation 1: PM10 particles contain large particles with diameter > 5 micrometers. Such large particles can experience gravitational settling, which requires another term in the transport equation (1). I would say the transport equation applies to smaller particles within PM2.5 that do not experience gravitational settling. Is it fair to say that the modeling approach is more suitable for PM2.5 than PM10? If you agree, then the model should be advertised as a transport model for PM2.5. If larger particles are to be accounted for correctly, then a gravitational settling term should be added to the transport equation.*

Response 1: The PM emission factors for domestic heating from Struschka and Li (2019) is only applicable to PM_{10} and is accordingly indicated throughout the MS.

However, the Reviewer is correct, that gravitational effects (i.e., settling) may alter the dispersion characteristics, and can be activated through PALM dry deposition module (Khan et al, 2021). This has not been considered in the MS for two reasons. First, this MS is primarily a model description of an extended, generalized approach for emissions source treatment in the prognostic equations, and as such the application to domestic heating serves as a demonstration of said approach. Second, the bulk and turbulent flows are frequently the dominant modes of particulate transport. A note has been introduced at the end of § 3.1 to indicate that gravitational effects have not been considered.

> **Comment 2:** *Section 3: Particles emissions from domestic heating are only present when fossil fuels (e.g. natural gas or diesel) are used which result from combustion processes in HVAC furnaces and water heaters. However, many buildings rely on heat pumps for heating, which only consume electricity. In such a case there will not be particle emissions from heating. Does PALM allow for such heating technologies? If so, particle emissions from heat pumps should be set to zero.*

Response 2: Yes, under LOD2, the user has a much greater degree of control over the location, mode, and the amount of pollutants emitted into the solution domain. This has been indicated in §§ 2.3.1, 2.3.3, and 3.2 of the MS. Further, if the building in question employs heat pump, it is expected the emissions would originate from the power plant(s) where the electricity is generated, assuming coal-fired or gas, instead of the building stack directly. This results in a displacement of both the geographical location of the emission source, as well as the assignment of emission GNFR sector C to GNFR sector A. Quantifying the corresponding change in emission inventory is conceivable but is beyond the scope of this MS.

> **Comment 3:** *Equation 12: This equation is used to consider heating requirement for buildings as a function of $T_{outdoor}$-$T_{setpoint}$, however, I think it is more appropriate to use heating degree days instead. Even in the absence of a building energy system, T_{indoor} can be higher than $T_{outdoor}$ due to internal heat gains (people, equipment), conductive-convective-radiative heat transfer, and thermal inertial of buildings. An energy balance in the absence of building energy systems results in degree days. Would it be more appropriate to estimate the building heating needs using the degree-day approach, rather than $T_{outdoor}$ – $T_{setpoint}$ one can use $T_{outdoor}$-T_{indoor} in the absence of building energy systems? In summary, fundamentally, degree-days ($T_{outdoor}$-T_{indoor}) estimates are different from temperature deficits ($T_{outdoor}$-$T_{setpoint}$). Weather and climate models calculate degree-days considering an*

energy balance model between buildings and the outside environment in the absence of a building energy (heating/cooling) system.

Response 3: The parameterized domestic heating module uses a generalized form of heating degree day (HDD) to characterize emissions at a much higher temporal resolution than once-on-a-daily basis. Since the definition of HDD can be effectively regarded as a deficit between the ambient and target temperature, this generalized approach is thus termed "temperature deficit", described in § 3.1 of the MS.

However, the Reviewer is correct. The indoor temperature should be calculated at each building. At the time of implementing the domestic heating emission parameterization, and subsequently the preparation of this MS, such module, while it exists for PALM (Fröhlich and Matzarakis, 2020), does not have a functional interface with the PALM chemistry module (Khan et al, 2021). Thus a set point temperature was introduced as a placeholder input, with a default value of 15 °C has been adopted according to guidelines provided by VDI (2013). The latter reference has been added to the MS.

References:

Fröhlich and Matzarakis (2020) GMD 13-3055-2020.
Khan et al (2021) GMD 14-1171-1193.
Struschka and Li (2019) "Temperaturabhängige zeitliche Disaggregation von Emissionen aus Feuerungsanlagen der Haushalte und Industrie für Berlin im Rahmen des MOSAIK-Projektes."
VDI (2013) VDI-Richtlinie 4710 Blatt 1.

Response to Reviewer 2

The Authors would like to thank Reviewer 2 for the meticulous comments. Please find our response on the corresponding comments below, with reference to the Reviewer's original comments in indented italics.

> **Comment 1:** *[I]t is strongly recommended to perform tests treating domestic emissions as either buoyant or nonbuoyant volume sources. The heating exhaust should be a warm plume, which rises by buoyancy, especially in winter when air temperatures are low. The buoyancy effects might be less effective than the turbulent mixing, however, this needs to be investigated for the conditions of this study. It is referred to a study by Langner and Klemm (2011), who demonstrated that dispersion models work acceptably for nonbuoyant volume sources, but don't cope with buoyant volume sources. Another aspect of PM10 emissions from domestic heating is that they are partly volatile. Residential emissions of organic carbon are largely semi-volatile and intermediate volatility compounds (S/IVOCs). The authors should explain how the modular emission concept can be extended in the future to handle the volatile fraction of emissions and incorporate the emissions of S/IVOCs. They should also discuss the representativeness of the meteorological conditions in the 48-hour simulations for the winter period.*

Response 1: Volatility of emitted particles has not been considered in this work due to performance constraints, as these calculations are computationally expensive. However, PALM integration with existing other aerosol models, that is SALSA 2.0 (Kurppa et al, 2019) and ISORROPIA (Nenes et al, 1998; Fountoukis and Nenes, 2007) are available, where the PALM chemistry module, and by extension the present emission module, can operate seamless with these models, should this be of scientific interest.

Buoyancy effects, otherwise referred to as plume rise, is currently not implemented in the PALM Model System. However, in the context of domestic stacks featured in § 3.2, they are often small and will disperse quickly into the surrounding atmosphere, which means explicit treatment of buoyancy effects are of secondary importance, though out of prudence they should not be overlooked, as pointed out by the Reviewer.

These aspects have been added to § 3.1 of the MS for emphasis.

> **Comment 2:** *Introduction (P3, line 58-61): The two examples (trees and exhaust emissions from aviation) given here do not have much in common. Which vertical resolution is meant in relation to trees and aircraft? Approaching and starting airplanes emit in a height up to 900 meters within several kilometers around airports, potentially affecting ground concentrations. Further, the phrase "sufficiently low horizontal resolutions" sounds strange, as models generally try to achieve high resolution.*

Response 2: The Reviewer has pointed out a very important point that led to the implementation of the emission module. On one hand, emission production mechanisms are vastly different, from biogenic, to road traffic, to aviation. On the other hand, treatment of the emission source terms at the prognostic equations is the same irrespective of production sources. Thus, one of the main design considerations for this emission module is to provide an efficient and uniform framework for the assignment of emission sources into the prognostic equations, while allowing the flexibility of taking into account the variability in emission mechanisms defined, for instance, in each emission sectors. How this aspect of the emission module has been implemented PALM is discussed in §§ 2.2 and 2.3.

On grid resolution, PALM is currently considered a high-resolution model. As such some techniques used in regional or global models no longer apply (i.e., definition of vertical emission profiles) as emissions can (and must) be explicitly assigned to individual cells. However, there is always a trade-off between detail and performance, and as such model runs might need to be conducted at lower grid resolutions, say, 10 m or 50 m. This is still very high in comparison with regional or global models, but can be “sufficiently low” that a cell could include multiple emission sources from different sectors

> **Comment 3:** *Introduction (P3, line 64-65): Volume sources are a quite common way to treat diffusive sources in dispersion models. Mention how other models for the urban scale, e.g. AEROMOD and AUSTAL deal with (nonbuoyant) volume sources.*

Response 3: While the Authors agree with the Reviewer on the treatment of volume sources, PALM is a non-steady Eulerian model, while AEROMOD is a steady-state Gaussian dispersion model and AUSTAL is a Lagrangian dispersion model. As such, the treatment of volume source terms is thus quite different in each model, and, after some contemplation, the Authors have decided to refrain from referencing these two models, at the risk of misrepresenting familiarity in their usage and implementation, as well as implying any functional equivalence in source term treatment with PALM.

> **Comment 4:** *Model description (P5, line 123-125): While the hash map is described as a clear connection between the emission database and the cell coordinates (i,j,k) where the emission of a source is added to the prognostic equations, it is not clear what happens for different cell sizes and volumes of the defined grid. How is it assured that the emission source is allocated to the correct cell when the grid cell size and volume is changed in the model configuration?*

Response 4: In PALM, the prognostic equation (Eq 1) undergoes volume integration after the emissions have been assigned. Emission inputs will be adjusted to the required grid cell size without user intervention. Volume integration is standard in models based on the finite difference / volume approach and therefore is not explicitly mentioned in the MS.

> **Comment 5:** *What is the footprint of a building and how is it calculated (P8, line 213)?*

Response 5: The footprint is the projected area of the building on the ground. This information is provided as input, as indicated in § 3.2. This information is typically available from the city’s planning department as part of the GIS data. This has been clarified in § 3.1 when this term first appears.

> **Comment 6:** *Module implementation: It is not clear how the height level of the building stack is considered. The module implementation section only mentions the (i,j) cell location of each building stack. The volume source is probably defined at the height of the stack exit and not the entire building is the volume source. Are there any plausibility checks of the user-provided emissions? There should be some internal control in the emission modules that check the plausibility of finally calculated emission rates and gives warnings when emission rates are unrealistic or not defined.*

Response 6: For domestic parameterization (LOD 0), the stack volume sources will be introduced unconditionally in the cell above the roof of the corresponding building at horizontal stack location (i, j). While there is no plausibility check during calculation of the volume sources, which would otherwise be quite time consuming, rigorous checks are implemented on the parameterized input to ensure the calculated volume sources are physically sound given the user input. On the other hand, under LOD 2, described in §§ 2.3.1, 2.3.3, and 3.2 of the MS, emissions sources are provided as external data, the onus is on the user to ensure correct specification.

> **Comment 7:** *It would be interesting to see a more generalized approximation of the vertical profiles shown in Figure 9 for sampling sites A-F as time average, for example in steps of 10 m above ground. The average vertical profiles should be compared to more generic vertical profiles of heating emissions in urban areas found in the literature.*

Response 7: As a model description paper, the case runs and corresponding results discussed in §§ 3.2 and 4, are conceived and presented to serve the sole purpose of demonstrating consistency of input and output data in the context of the model. Interpretation of the model output beyond verification of the functionality of said model, as well as any of their comparison with published data, is *ultra vires*.

> **Comment 8:** *Define the reference height (P16, line 476). What causes the vertical mixing of heating emissions, does buoyancy of the heating plume play a role here or not? The occurrence of down-wash and accumulation should be explained in terms of meteorological conditions, not only in terms of trapping in building enclosures.*

Response 8: The reference height (36.87 m above sea level) is calculated internally by PALM for computational reasons, as the topology of the solution domain is not flat, and cells lying underground, and those inside urban structures, will remain unused. The description of the reference height in § 4 has been expanded for clarification.

Vertical transport in open areas is mainly caused by the prevailing wind. In urban enclosures, the turbulent shear layer at the roof region restricts momentum, heat and mass exchange above and below the buildings (Bright et al, 2013; Chan and Butler, 2021; Driver and Seegmiller, 1985; Oke, 1988) which also attenuates the effects of ambient meteorology significantly.

However, the instance of "vertical mixing" indicated by the Reviewer has been corrected to "vertical transport" to indicate a more general transported mechanism than a purely meteorological concern, which is used throughout the MS.

> **Comment 9:** *Figure 10: in top row (A) the vertical cross-section shows a hotspot at 20:00 at around 30 m, despite there seem to be no emission stacks of buildings close-by.*

Response 9: The emission sources lie outside of the cutting plane in the figure in question. That the urban structures around sampling location (A) are not aligned with the cutting plane makes the visualization more difficult. A note has been provided in the last paragraph of § 4.3 to remind the readers of this.

> **Comment 10:** *The Concluding remarks should address the limitations of the domestic emission parametrization. The uncertainties of the emission factors are large and cannot be ignored. Also the diurnal variation in domestic heat usage can be locally different from the one defined in CAMS for other stationary combustion.*

Response 10: The CAMS profile used in this MS is the default configuration, but the user can introduce other profiles that are deemed more suitable for the particular model run. This is indicated in §3.2 of the MS. A more geographically refined emissions specification is also possible, either through LOD 2 or the generic emissions mode (§ 2.3.3). Clarification has been introduced in § 5 on the additional limitations of the parameterized domestic emissions module.

References:

Bright et al (2013) Atmos Environ 68 127-142.
Chan & Butler (2021) GMD 14 4555-4572.
Driver & Seegmiller (1985) AIAA J 23 163-171.
Fountoukis et al (2007) ACP 7 4639-4659.
Kurppa et al (2019) GMD 12 1403-1422.
Langner & Klemm (2011) J Air Waste Manage Assoc 61(6) 640–646.
Nenes et al (1998) Aquat Geochem
Oke (1988) Energ Buildings 11 103-113.

Response to Reviewer 3

The Authors would like to acknowledge the efforts of Reviewer 3. Please find our response on the corresponding comments below, with reference to the Reviewer's original comments in indented italics. In terms of language-related issues, they have all been addressed unless otherwise stated.

> **Comment 1:** *In general, what is meant by "hash map"? The relation in Eq (3) and (4)-(6), or an array (or other data structure) of emission sources indexed by kappa?*

Response 1: A "hash map", otherwise known as "hash table", is a fundamental data structure that provides a computationally efficient access to data, through the use of aptly called "hash keys". In the context of this MS, the hash map (h^m or H) is a linear array which is associated with discrete emission sources in the computational domain using unique hash key values (κ) derived from their corresponding grid locations (i, j, k). Each emission module described in §§ 2.3.1 and 2.3.2 maintains its own hash map (h^m), as defined in line 100 of the MS, and subsequently Eq (2). The bidirectional relationship between the grid indices and hash key is defined in Eqs (3-6). A reference (Cormen et al, 2009) has been included in § 2.1 to provide additional background information for the interested reader.

> **Comment 2:** *What I miss is a description of the data structure of emission sources. How is it organized? For a given cell (i,j,k), how are the emission sources in this cell found? (i,j,k) maps to a single kappa value. How are the emission sources found then?*

Response 2: Please refer to Authors' response to Comment 1.

> **Comment 3:** *If the array of emission sources is shorter than the number of grid cells, there should be a search operation to find the sources corresponding to a given grid cell. If the array of sources has the same length as the number of grid cells (which makes look-up easy), it seems one could just use a full 3D field of source strengths instead, with the same memory cost but less complicated code.*

Response 3: As indicated in lines 92-93, and subsequently demonstrated in §§ 3.3 and 4, emissions sources are non-contiguous and, except for artificial test cases, only found in a small number of grid cells. This makes the use of the hash map approach critical, as it affords significant savings in terms of input storage and application memory. The search of the cell index is also accomplished by looking up the sorted hash keys in the hash map (see lines 188 and 199 of the MS).

> **Comment 4:** *A comment of how the implementation handles domain decomposition would be helpful. The list of emission sources is presumably prepared for each MPI process?*

Response 4: The Reviewer is correct. An additional sentence has been introduced at the end of the second paragraph of §2.3.1 to emphasize this point.

> **Comment 5:** "3. The interface between the prognostic equation solver and the emission module should be implemented to allow only localized data access to prevent propagation of data corruption into other emission sectors." *I don't understand this statement. Data corruption would be an error in the implementation. Isn't it an obvious design objective that the implementation should be error-free?*

Response 5: The Authors agree with the Reviewer in principle. Further, based on the Authors' practice in various development projects including the one outlined in this MS, having a software architecture that localizes code and data access will help isolation of source(s) of implementation error and subsequent deployment of corrective measures. Thus, while achieving an error-free implementation is the obvious goal, a sound data and code encapsulation strategy will help achieve this goal much more effectively.

Comment 6: *Eq (2): the notation feels unnecessarily convoluted, with the W sets with multiple indices. Additionally, in "W* ∈ 0, 1, 2, · · · up to the corresponding upper bound *N" presumably the set does not include N, but this is not clear from the formulation.*

Response 6: Eq (2) is the mathematical definition of the hash table as indicated in the Authors' response to Comment 1. An equivalent, graphical representation can be found in Figure 1. Given the complexity of the overall module design, it is in the Authors' opinion, that Eq (2) cannot be further simplified. Further, the range of *W* has been made to explicitly indicate "up to but not including" in the MS.

Comment 7: *The mapping in eq. (3) is quite trivial, just enumerating all the grid cells. Usually a hash function implies something more, e.g. that the output space is smaller than the input space (although this is no strict of formal requirement).*

Response 7: The Reviewer is correct that the output space (hash table size) can be smaller than the input space (the emission sources). This will result in hash key collision, however, which requires additional resolution strategies. Eq (3) is seemingly trivial due to the use of a Cartesian grid system in the PALM model framework. Another common approach is the so-called bitwise operation, as described in Teschner et al (2003) or, more classically, in Jenkins (1996), which are used in other model systems involving moving and/or unstructured grids. For the purpose of the MS, Eqs (3-6) provide a sufficient function without adding complexity. This point, as well as the additional reference, has been incorporated in § 2.1 of the MS.

Comment 8: *Eq. (4) is wrong, it should have a division not mod. Additionally, there is an implied rounding down after the divisions, which could be indicated with a floor function or with round-down vertical-bars-with-hooks symbols. I don't understand Eq. (8) or the explanation above it. Additionally something is missing in the sentence "...p is the union all emission sectors".*

Response 8: The Reviewer is correct, Eq (4) should be a `div( )` operation, instead of the `mod( )` operation that is currently being shown, and this has been corrected in the MS. Further, the functions `div( )` and `mod( )` are understood to provide integer outputs. As the inputs to these functions, as defined in Eqs (2-5), are subset of integers (i.e., whole numbers), there should be no further ambiguity in the form they are currently presented in Eqs (4-6) on the MS.

Comment 9: *Eq. (9) What's meant by the union of hash maps?*

Response 9: The union operation adds all values of the same hash keys across all hash maps. Referring this to "addition" imply each hash map contains identical sets of hash keys and thus are directly commutable, which is not true in this case. This has been clarified in § 2.1 of the MS.

Comment 10: *line 268: "specifies the annual cumulative temperature (in degrees) to be heated above the ambient temperature to the target temperature, with a default value of 2100 K." It's not obvious what annual cumulative temperature is. If it is something like degree days, the unit is wrong.*

Response 10: The Reviewer is correct. The unit of both heating degree day (i.e., temperature deficit) and annual cumulative temperature should be in degrees. All instances indicating otherwise have been corrected throughout the MS.

References:

Cormen et al (2009) "Introduction to Algorithms" MIT Press 253-280.
Jenkins (1997) Dr Dobbs J 22(9):107.
Teschner et al (2003) Proc 8 Int Fall Workshop Vision Model & Vis.