Responses to review comments of manuscript "Atmospheric Dispersion Modeling Applied to Assess the Contamination from a Mining Tailings Basin in the Semiarid Region of Bahia – Brazil" submitted to Anuário do Instituto de Geociências by Santos et al.

**Reviewer A:**

1. Does the title accurately describe the content of the article?: Yes

2. Does the abstract (summary) is in agreement with the article?: Yes

3. Is the manuscript appopriate for the journal?: 4

4. Is the problem significant, and concisely stated?: 5

5. Is the literature review done in a relevant manner?: 4

6. Are the methods described comprehensively?: 5

7. Are the results presented and discussed clearly and objectively?: 4

8. Are the interpretations and conclusions justified by the results?: 3

9. Is the scientific discussion made profoundly?: 4

10. Is the scientific language acceptable?: 3

11. Final score (sum up items 3 to 10):: 32

12. Comments and suggestions (please fill with the items which did not receive the maximum rate)::
General comments for "Atmospheric Dispersion Modeling Applied to Assess the Contamination from a Mining Tailings Basin in the Semiarid Region of Bahia – Brazil"

The paper's goal is to evaluate the dispersion of Lead emissions from a tailing in Bahia and its impact on streets and houses downwind the tailing. The authors developed an eulerian dispersion model which contemplates dispersion, advection, emissions, and deposition.

Page 3

Figure 1 is hard to read. Increase the label size. There are no units in the figure regarding the Lead concentration.

Also in figure 1. How did you perform the monthly average of wind direction?

It would be nice to see the wind rose of the data, additionally to the description of the data.

*We increased the label sizes in Figure 1 (as well as several other figures) and added the units of ppm in street sediments and ppm in house dust in the figure caption. It is now also mentioned in the captions that monthly wind directions are simple arithmetic averages of hourly measurements and that respective wind roses can be found in Santos et al. (2020).*

Page 8, equation 14 regarding the Lead deposition. The authors give a deposition value of 10-2/s. There is no reference corroborating this value.

Usually, the deposition of a particle is related to its size and density.

Can the authors explain the adopted value?

On the second step, the authors calibrated the deposition coefficient based on the modeled results/ observed concentration

*Due to reasons of mathematical tractability and limitations in data availability, variable particle sizes and densities are not considered in this study. This is now explicitly stated in sections 2.3 and 4. As now also stated in more detail before Equation 14, the initial estimate of λdep = 10-2 1/s is based on a particle deposition time scale of on the order of minutes, similar to the common observation of a dust cloud settling behind a driving car.*

The emissions and resuspension were adopted from Harris & Davidson (2005), which estimate these parameters based on wind speed and concentration of the pollutant. However, there are methodologies in AP-42 (USEPA) and EEA (Europe) that estimated these emissions. Have the authors considered using these methodologies and incorporated them into their models?

*Following this suggestion, we considered using these methodologies, but arrived at the conclusion that they are not immediately relevant to our problem. EEA-2019 provides factors for estimating emissions from vehicle abrasion, but not for resuspension of particulates that have previously been deposited. The guideline AP-42 (USEPA) and USEPS Moves (2020) present resuspension only in combination with emissions from vehicle abrasion.*

Review the English. Sometimes it looks like it was directly translated from Portuguese, such as "well below" on page 10.

*We changed this to “significantly below”. Following also Reviewer B’s suggestions and by our own thorough revisions, the Englisch style was improved throughout the whole manuscript.*

**Reviewer B:**

The Manuscript theme is quite relevant, but needs Major Revision. Only after Major Revision would this paper be suitable for publication.

The title is too long. I advise making the title shorter and more direct.

*The title was shortened to “**Modeling Urban Atmospheric Lead Dispersion from a Mining Tailings Basin in Bahia, Brazil”.*

*We included “urban” to emphasize the local (km) scale of the problem, as well as an indicator for the fact that concentrations in streets and houses are considered as inherent constituents of the model.*

**General comments**

1. This manuscript has no continuous line number, and it makes it difficult to add specific comments, this issue should be solved if it passes to the next revision.
2. The English grammar and style should be checked throughout the manuscript. It necessary a Moderate English changes.
3. The introduction does not provide sufficient background and does not include all relevant references. Must be improved.
4. The research design Must be improved.
5. The methods Must be improved.
6. The results are not clearly presented. Must be improved.
7. The conclusions Must be improved.

*We included continuous line numbers and addressed all other general comments with detailed responses below.*

**Abstract**

1. The Abstract needs major improvements. It does not provide some basic information. E.g:
What is the study period analyzed? Which year are you analyzing? How did you validate you results (in-situ observations? Remote sensing? Experimental campaigns?) Where’s the statistics of the model evaluation (put some results in the abstract - bias,rmse,pearson, etc.)?

*We improved the abstract in both language and content, including year of experimental campaign and RMSE of calibration.*

1. The English grammar need major revision. E.g:
“For this, a model was elaborated with three domains (houses, streets and air) in Matlab R2014a, having as input data the information related to the meteorological conditions of the region, specifically, direction and speed of winds, and using for calibration the chemical analyses of lead contamination obtained in street sediments and dust from houses distributed throughout the urban area.”
The phrase is too long and heavy; the authors should reformulate and split it.

*After reformulating and splitting the sentence, it now reads:*

*“For this purpose, a model was elaborated and implemented in Matlab R2014a considering houses, streets and air as three coexisting spatial domains. The model uses wind speed and direction as input data and results were calibrated (RMSE = 0.64 on decadal logarithmic scale) against existing measurements taken in 2014 of lead concentrations in street sediments and house dust within the urban area.”*

1. The phrase needs to be improved.
“In general, the model was able to reproduce the atmospheric dispersion process in the area and presented a satisfactory response in the estimation of lead concentrations in the analyzed domains, demonstrating to be appropriate to assist in the evaluation and management of contaminated areas through atmospheric dispersion.”
The phrase is too long, vague, and heavy; the authors should reformulate and split it.

*After reformulating and splitting this sentence, it now reads:*

*“Results suggested that particulate resuspension from streets and accumulation in houses may explain observed concentration patterns, and that the amount of suspended lead in the air is small compared to that in streets and houses. Additional simulations carried out for a hypothetical future remediation scenario showed that after 200 days the concentrations in the air and in the streets decreased considerably, while they stopped accumulating in houses. Hence, the model may be a potentially useful tool to assist in the evaluation and management of this and other urban areas affected by contamination through atmospheric dispersion.”*

**Introduction**

1. There are some long phrases in the Introduction section; I suggest the authors reformulate the entire Introduction with correction of the syntax

*The entire introduction was thoroughly reworked and expanded, while splitting long phrases.*

1. Paragraph 3 in page 2: *“The climatic adversities of the semi-arid region, characterized by low rainfall rates, irregularities in the distribution of rain events (Marengo 2008) and long cyclical droughts (Blamont et al. 2002), together with the low concentration of heavy metals found in groundwater, springs and cisterns of the municipality (Gomes et al. 2020), contributed to the formulation of the hypothesis that wind erosion would be the main process of dispersion of contaminants originating from the tailings basin.”*

The Paragraph is too long and heavy; the authors should reformulate and split this sentence.

*After reformulating and splitting, this passage now reads:*

*“The climatic adversities of the semi-arid region are characterized by low and irregular rainfall events (Marengo 2008) as well as long cyclical droughts (Blamont et al. 2002). Moreover, concentrations of heavy metals found in groundwater, springs and cisterns of the municipality are low (Gomes et al. 2020). These facts contributed to the formulation of the hypothesis that wind erosion and transport would be the main process causing the dispersion of lead (and other contaminants) originating from the tailings basin across the urban area of Boquira.”*

1. The Introduction section is short and needs to be improved. In this section, contamination by ore and lead should be discussed in a broader context such as the physical and chemical impact to the environment and human health. The authors should cite more important studies in a national and international approaches as well as the regulation and guidelines behind the ore and lead activities. Also, the social and economic impacts of the ore contamination. And the connection with atmospheric modelling dispersion (cite previous modelling studies applied to ore contamination, and different models and approaches used in others studies).

*The introduction was almost completely reworked following these suggestions. Note that mainly due to the suggested expansions of the introduction, methodology and discussion sections, the manuscript is now at the journal´s length limit. Please see the manuscript with changes marked for more details.*

1. In this section, you should first identify the “gap” in the literature, present a compelling argument why the “gap” needs to be filled, and convince the reader that their approach is appropriate and practical. In short, the study needs to convince the reader how exactly this study contributes to the field.

*After discussing various risks and damages caused by lead contamination in the first part of the introduction, the last paragraph is now dedicated to clearly defining the knowledge gap, why it should be filled, and how we attempt in this study to go about it.*

**Methodology**

1. The Methodology section is short and needs to be improved and better writing.

*The entire methodology section was thoroughly reworked, expanded and language edited. Please refer to the manuscript with changes marked and the following responses for more details.*

1. The Figure 1 needs to be reformulated in a higher resolution. See journal rules.

The figure 1 C and D is hard to see and understand. My suggestion is to increase the circles and fill it according with the color bar range. By the way, what does the color bar mensurating? Concentration of lead? In what unit (µg/m³, g/ m³)? It’s necessary to put a title in the color bar and the Unit.

*Figure 1 was generally improved in both resolution and increased font size. All figures are now in 300 dpi jpg-format according to journal rules and can also be uploaded as separate files, if necessary.*

*We filled the circles in C and D, but due to their small separation distance and resulting overlap in certain areas, we did not increase the circle size. The units of the color bars are ppm, which is now stated in the figure caption.*

1. There is information in the Methodology that would be better sit in the introduction. The CONAMA and WHO guidelines should be contextualized in the Introduction section.

*Both CONAMA and WHO guidelines are not discussed in the introduction.*

1. There should not be the subtopic **2.2 Conceptual model**. This is not Methodology, or at least not that way that was described. This should be adapted and moved to the Introduction section.

*We evaluated different options to address this comment, but concluded that the description of the conceptual model is an integral part of our model development and, hence, methodology. However, we improved the description of our particular conceptual model, while similar to suggestions for section 2.3 below, we extracted the more general statements*

*”Models of atmospheric pollutant dispersion are based on the mathematical description of transport processes including the mechanisms of suspension, advection, dispersion, deposition, resuspension and accumulation (Khan & Hassan 2021). Contaminants can be removed from the atmosphere by dry deposition processes through the action of gravity, and also by wet deposition consisting of the absorption of pollutants by raindrops and consequent removal by precipitation to the soil.”*

*and relocated them with slight modifications into the introduction.*

1. A better description of data quality and homogeneity is needed.

*More details on data acquisition, analysis and processing are now included in the last two paragraphs of section 2.1.*

1. The subtopic **2.3** should be reformulated.
There are paragraphs that should be adapted and moved to the Introduction. Would be better contextualized there. E.g:
“The mathematical modeling of atmospheric contaminant transport is based on the numerical solution of the mass conservation equation of a contaminant chemical species on a fixed space-time grid (Moreira & Tirabassi 2004). These models can be used to identify and study standard scenarios, generate diagnoses and simulate prognoses, supporting solutions to the problem of air pollution (Silva 2013).”

“The atmospheric dispersion of the particles is related to local turbulence and deposition, including precipitation and sedimentation, resulting in a downward movement of particles in the atmosphere (Khan & Hassan 2021). According to Seinfels & Pandis (2006), the deposition process is represented by three distinct steps. The first step represents the aerodynamic transport by the atmospheric layer to a very thin layer of stagnant air, adjacent to the surface, the second stage corresponds to the Brownian transport in this very thin layer, and the third step leading to the adherence at the surface.”

*These two paragraphs were adapted and moved to the introduction. We also expanded the introductory paragraph of section 2.3 including a more thorough discussion of assumptions taken.*

1. The subtopic **2.4** should be reformulated in an organized way.

*Old section 2.4 is now split into new sections 2.4 (Numerical implementation) and 2.5 (Calibration procedure). Each of these sections was also significantly expanded by including more comprehensive discussions of relevant details (please see manuscript with changes marked).*

**Results and Discussion**

1. My comments have been addressed in the Results section carefully.

*We are not sure how to address this comment, but it appears positive...*

1. Discussions on the main findings need further enrichment by comparing them with existing literature. There should be some indications on how the main findings are in line with previous studies. At the end of the Discussion section, the limitations of the study should be mentioned.

*We included references to previous studies at several locations throughout the discussion section for comparison to our own findings. Two new paragraphs at the end of the discussion section are now also dedicated explicitly to a summary of the limitations of our study. Please note again that our manuscript length is at or even slightly beyond the recommendation by the journal, such that we attempted to strongly summarize for brevity.*

1. It is missing statists. Where is Pearson, RMSE, bias, MAE to evaluate model results? The authors showed only Figures.

*All the suggested goodness-of-fit statistics are now reported in the caption of Figure 3.*

1. Is necessary to improve the Figures resolution (see journal rules).

*All figures were improved regarding resolution and font sizes. Note that the surface plots in Figure 5 are affected by the numerical resolution of the model, not the graphical resolution of the figure itself.*

**Conclusion**

1. In the Conclusion section, the authors should discuss the main implications of your findings and avoid using the inputs which are already mentioned in the previous sections.

*We renamed this section into “Summary and conclusion”, where the first two paragraphs provide an overview of our approach and outcomes, while the last two paragraphs discuss the arising implications and recommendations.*

1. Moreover, the theoretical and practical implications of this study should be stated in one paragraph.

*Please see response to previous comment.*

1. The language needs moderate revision to fix many style and syntax problems.

*We thoroughly revised English language throughout the whole manuscript.*

1. The Manuscript need Major Revision.

*Thank you for the thorough and constructive review!*