Response to Reviewer 2 Comments

The manuscript focuses on harmonizing input data for Atmospheric Transport and Dispersion (AT&D) modelling as mentioned in the abstract. I think that it is a very meaningful study. However, I found it is organized confusedly so that it can’t be understood well. What are the factors behind these discrepancies? Is it related to harmonizing input data? What are the problems that the unharmonized input data leads to? The author should clarify how to harmonize the input data in this study? I strongly advise that the authors reorganize the manuscript according to why, how and what relating to harmonizing input data.

Response 0 :

The authors have restructured the manuscript by incorporating additional information about context and objectives in sections 1, 2 and 3. Additional information about the input harmonization topic as indicated in the title has been also incorporated in section 2.14 and a new section (2.15) has been created.

The meaning of “harmonization” has been cleared; it is written in the paper as follows:

Section 1.1: “In the paper, the term “harmonization” is employed to describe the process of constructing and employing AT&D models. This harmonization is essential to guarantee that, regardless of the specific model employed within its designated scope, the results remain highly comparable. Among these disparities, three primary categories can be distinguished: those attributed to the model itself, those linked to the input data utilized, and those arising from user choices.

The aim of the harmonization process is threefold:

• To offer direction during model development, ensuring consistent representation of physical phenomena, especially concerning the relationship between atmospheric turbulence and the diffusion coefficient for pollutants.

• To offer guidance on constructing input data for the model, including factors like the atmospheric wind and turbulence profile, the appropriate roughness value, and the specification of the source term within the AT&D model.

• To provide users with guidance that constrains potential individual choices, particularly concerning numerical parameters or mesh settings.

As atmospheric dispersion modelling continues to evolve as a research area over time, it becomes evident that certain decisions must be made. These decisions should be of a generic nature, guided by harmonization principles, rather than being tailored individually for each study.”

Section 1.3: ”The harmonization process ensures that the mathematical and theoretical representation of physical phenomena remains consistent, regardless of the level of simplification used by the model. Additionally, harmonization implies that the input data used for modelling are sufficiently well-defined to eliminate any need for interpretation during use.”

Specific comments:

**Point 1:**

(1)   1.1 Atmospheric dispersion accidents

The title should be revised. Air pollution accidents?

Chernobyl, 1986. Fukushima, 2011. should be referred.

**Response 1:**

The title has been revised:” 1.1 Toxic gas atmospheric dispersion accidents”

Chernobyl, 1986. Fukushima, 2011. have been referred.

**Point 2:**

(2)   Line 38-52, Please make the content related to the topic more closely.

**Response 2:**

Section 1.1 has been restructured and completed, and we hope it is clearer.

However, from the authors' point of view, it is necessary to introduce the French regulatory context and lines 38-52 have been kept.

**Point 3:**

(3)   Line 58-60, Please clarify some reasons behind these discrepancies. Is one of them related to harmonizing input data？

**Response 3:**

Harmonization input data is one of them; the definition of “Harmonization” has been documented in Section 1.1 (See “response 0”). It is written as follows:

“There are numerous reasons behind these disparities, stemming from various sources, and they underscore the clear necessity for harmonization. In the paper, the term “harmonization” is employed to describe the process of constructing and employing AT&D models…..” ;

**Point 4:**

(4)   I think context of AT&D model uses is not important for readers. Instead, the authors should describe the specific input data for AT&D models. I don’t know if Line 109-112 is the description of the input data, but I can ensure they are not enough.

**Response 4:**

From the authors' point of view, the context of AT&D model uses is important. Indeed, the need of harmonization of input data and modelling practices is more significant in the regulatory context. The authors have documented the reasons to making certain decisions in terms of harmonization in Section 1.1, as follows:

« As atmospheric dispersion modelling continues to evolve as a research area over time, it becomes evident that certain decisions must be made. These decisions should be of a generic nature, guided by harmonization principles, rather than being tailored individually for each study.”

The authors have documented when the context plays some roles.

See section 2.15

“Some simplifications describing ABL, particularly in the regulatory context, are sometimes necessary such as the stationary nature of ABL over the modelling period.”

**Point 5:**

(5)   Line 81-85, I agree that source term is typically unknown, but what is the difference of the wind? Please clarify it.

**Response 5:**

There are many ways to build an inlet wind profile starting from meteorological conditions such as described in regulation. Indeed, meteorological conditions may be described in a very simple way such as user choice is required.

See Section 2.2

There is, unfortunately, no bijection between Pasquill stability classes and the Monin Obukhov length and a user choice is required [29] for a given roughness, especially for classes A and F.

In the revised version, the authors have added documentation about the influence of the inlet profile formulations.

See section 3.7 The choice of inlet profile formulations for RANS CFD should be done consistently with the choice of sub-model turbulence for RANS approach [26, 31] to reach a satisfactory equilibrium state for ABL

**Point 6:**

(6)   What does Figure 1 mean?

**Response 6:**

An explanation about the meaning of figure 1 has been added.

See Sec 2.

“A diagram showing the main steps of AT&D modelling within the context of risk assessment is presented in Figure 1. This figure shows the most important topic to be considered in a harmonization process, with the three points of view mentioned in sec-tion 1.2, the model, left and right on the figure, input data, in green in the centre, and user, who will run the model and make the choices. In the subsequent section of this chapter and in the following chapter, each element depicted in the figure will be comprehensively explained, outlining its potential impact on dispersion outcomes.”

**Point 7:**

(7)   2.1 Background about theoretical approaches, It is recommended to summarize their input data.

**Response 7:**

The authors have added section 2.15 in order to summarize the fundamental parameters.

See 2.15 :

“At the end, a harmonization of meteorological data pre-process means focusing on fundamental values describing ABL, such as Monin-Obukhov Lenght (LMO), friction velocity u\*, wind speed (m/s) at an altitude reference, the roughness, and the turbulent sensible heat flux.”

**Point 8:**

(8)   2.2 From my stand, Gaussian model is used in a simplified scene or an early emission stage in which lacking sufficient meteorological data or for a rapid assessment since its assumptions are those, such as uniform continuous turbulent flow field…… When there are available sufficient meteorological data, more sophisticated models can provide better results though it will spend more calculation time. In this case, what are the reasons for harmonizing these models with different purposes.

**Response 8:**

The meaning of “harmonization” has been clarified, it is written in the paper as follows:

See section 1.1

“In the paper, the term “harmonization” is employed to describe the process of constructing and employing AT&D models. This harmonization is essential to guarantee that, regardless of the specific model employed within its designated scope, the results remain highly comparable. Among these disparities, three primary categories can be distinguished: those attributed to the model itself, those linked to the input data utilized, and those arising from user choices.”

**Point 9:**

(9)   Through the section 2, I don’t yet understand how the authors make the harmonization between the models.

**Response 9**

The authors have restructured the manuscript by incorporating additional information about context and objectives in sections 1, 2 and 3. Additional information about the input harmonization topic as indicated in the title has been also incorporated in section 2.14 and a new section (2.15) has been created.

**Point 10:**

(10) Table 4 lists the input data for SLAB model and CFD approach. However, how are they harmonized?

**Response 10**

The purpose of the table is to show the common parameters that would require in-depth study and the specific parameters that would require to take decisions guided by harmonization principles, rather than being tailored individually for each study.

**Point 11:**

(11) Line 537-539, descriptions for Figure 9, the study should be considered as an essential stage for validate the use of CFD model in the context of regulatory studies …… Therefore, the manuscript seems to be for a validation for CFD model application, and does it have to do with the harmonizing?

**Response 11**

The authors deem that the validation of a model by comparison with experimental data should be a generic rule for practice harmonization in the context of regulatory studies.

The authors have added explanation on the objectives of section 3.

See section 1:

“In Section 3, the focus shifts to the application of AT&D models to a massive release across various model types. The primary objective of this section is to emphasize the significance of harmonizing each aspect when utilizing AT&D models. This section is then not directly focussed on the application of harmonization practices, since those practices are most relevant for prediction cases within the regulation context. Instead, Section 3 illustrates how each parameter can significantly impact the results, under-scoring the importance of harmonizing these practices.”

**Point 12:**

(12) Figure 9, which is better of the results from FDS and Code\_saturne model? And why？What does this result mean? I can’t understand the idea of the author

**Response 12**

The goals were not to compare the CFD model's results with others. Instead, the authors aimed to provide straightforward comments regarding potential overestimations or underestimations from their perspective.