Comment on amt-2022-6
Anonymous Referee #1

Referee comment on "Air pollution monitoring: development of ammonia (NH₃) dynamic reference gas mixtures at nanomoles per mole levels to improve the lack of traceability of measurements" by Tatiana Macé et al., Atmos. Meas. Tech. Discuss., https://doi.org/10.5194/amt-2022-6-RC1, 2022

This paper is clearly written and well organized. The introduction presents the article and context well. Figures and tables are comprehensive and helpful.

However, a few minor points deserve consideration.

Pg 1 line 17: why choosing an amount fraction range between 1-400 nmol/mol? It could be interesting to argue this choice in order to know the limits of this method development.

Pg 2 line 33 (+abstract): Need reference for effect on human health? Which guidelines? In fact NH₃ at ambient levels have mostly effect on ecosystems. Direct effect on human health occurs at higher concentration (for instance in livestock buildings).

Pg 2 line 37: « In 2016, estimations suggested 4.2 million premature deaths worldwide caused by suspended particles (WMO, 2018). » not exactly à 4.2 million premature deaths worldwide caused by ambient air pollution and 2.5 million for PM2.5 exposure.

Pg 2 line 42: 60 %? à precise on which spatial scale?

Pg 2 line 46: « continuously increased » à precise since when?
Passive sampling isn’t the only « indirect method » à add active sampling via denuder or on-line gas-liquid interaction systems (like MARGA, AIRMONIA, etc.) + ref to « Bobrutzki, Kristina & Braban, Christine & Famulari, Daniela & Jones, Stephanie & Blackall, T. & Smith, Thomas & Blom, M. & Coe, H. & Gallagher, Martin & Ghalaieiny, M. & McGillen, M. & Percival, C. & Whitehead, James & Ellis, R. & Murphy, J. & Mohacsi, A. & Junninen, H. & Pogany, A. & Rantanen, Sami & Nemitz, Eiko. (2009). Field inter-comparison of eleven atmospheric ammonia measurement techniques. Atmospheric Measurement Techniques Discussions. 2. 1783-1835. 10.5194/amtd-2-1783-2009. » / For passive sampling, add reference to EN 17346 :2021 « Ambient air - Standard method for the determination of the concentration of ammonia using diffusive samplers » and to « Braban, Christine F.; de Bree, Frans; Crunaire, Sabine; Fröhlich, Marina; Fromage-Mariette, Anne; Goelen, Eddy; Hafkenscheid, Theo; Hangartner, Markus; van Hoek, Caroline; Martin, Nicholas A.; Michen, Benjamin; Noordijk, Erik; Stoll, Jean-Marc; Twigg, Marsailidh M.; Tang, Y. Sim; Cowan, Nicholas; Poskitt, Janet. 2018 Literature review on the performance of diffusive samplers for the measurement of ammonia in ambient air and emissions to air. Edinburgh, Centre for Ecology & Hydrology, 85pp. ».

Verify « spectrometry » à mass spectrometry? + add « conductimetry »?

These methods are often poorly characterized and they do not allow reliable measurements taking into account effective quality assurance and quality control procedures (QC/QA) (calibration, traceability, maximum allowed expanded uncertainty, etc.) à not right for passive sampling because a standard exist!

The results obtained by METAS during the study showed a very good stability in the generation of NH3 with short response times, even at very low amount fractions. à what is « good stability » ? « what is short response times » à add values / precise these terms.

In order to know the robustness of the system it could be important to specify the precision and the resolution of the balance and the temperature sensor.

The diagram seems simplistic and merits better specification of the constraints linked to this generation such as temperature and air flow control.

« 2M PROCESS » à precise country?

We know that oven temperature control is crucial for permeation. This paragraph does not indicate how this parameter is controlled. It would be interesting to add validation tests to measure the temperature in the oven, in order to control the absence of a gradient and cinetic between the heating element and the probe which allows control of the heating of the oven. The diagram could illustrate this.
significant addition to this development

Pg 7 line 181 : The normal molar volume : \( l_n / \text{mol} \)

Pg 8 para. 4.2.4 : Takes up the remark made earlier. It seems important to be more detailed by test results the fact that you consider the correction accounting for the stability of the temperature in the oven as equal to zero

Pg 9 table 1 : This table seems useless since we find in figure 4 the graph. Can be just indicate the mean and the standard deviation on the evolution of the permeation rate over time.

Pg 13 line 300-304 : It could be interesting to indicate the references of the filter and its filtration efficiency in order to guarantee the residual amount fraction

Pg 14 table 4 : Standardize the results of the weight column

Pg 14 para. 6.1 : Regarding the calibration what are the concentration levels and what were your results. The contribution of tables and graphs would make it possible to validate this calibration

Pg 15 para. 6.2 : You indicate that this is a repeatability test.

In the paragraph there is no indication how many times you have to repeat the different levels just that the standard deviations calculated over the last 30 minutes of génération for each of the 9 points. On reading it is more of a linearity test than repeatability

Pg 17 table 7 : Standardize the results of the Intercept column

Pg 17 line 382 \( u^2(F) \) <> \( u^2(xref) \)

P19 line 430-433 : It could be interesting to apply a table identical to table 9 for your own results in order to be able to compare the same things and this even if the concentrations are different from that of METAS
Pg 20 table 10 : indicate the units

Pg 20 para. 8 : You specify measurement levels between 1 and 400 nmol/mol. Except your graph presented in figure 6 only shows the results between 1 and 300 nmol/mol. What is the reason?

In addition, which analyzer did you use to perform this test presented in fig 6 and how do you explain the greater measurement dispersion when the concentration increases?

Pg 22 figure 7 : What is the point of having so many figures concerning the regression line and $R^2$