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Comment on acp-2021-614

Anonymous Referee #1

Referee comment on "Technical note: Interpretation of field observations of point-source methane plume using observation-driven large-eddy simulations" by Anja Ražnjević et al., Atmos. Chem. Phys. Discuss., https://doi.org/10.5194/acp-2021-614-RC1, 2021

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The technical note „Interppretation…" by Raznjevic at al. is very interesting lecture about the application of LES model to understand problem with application of inverted GPM for point sources.

Personally, I would like to congratulate the authors of good work done with this paper. I think that a time spent for reading it is definitely not lost.

However I'm surprised that this is submitted under the technical note format. The main topic of the article focus on the estimation of methane emission rate from O&G installation in Romania during the campaign in year 2019. I hoped that application of complex LES model will be deeply interpreted for some good and bad examples of plume behaviour. Here, I mean the well known structure of the plume (I suppose that smoke would be much better medium to do the study than methane). The authors had another idea of the story, which is not bad but a bit hard to follow.

So, at the beginning they present the description of measurement site and methodology, than touch a bit of LES set-up and some hints for further statistical analysis of gas plumes. All this., including introduction takes full 9 pages and not much details are presented anyhow. The LES model (authors refers to the github repository of microHH) applicability should be tested on the known source during well designed experiment with the well measured state of boundary layer, including wind profiles and convection scales. This requires some extra instruments like doppler sodar, windcube wind profilers and perhaps a lidar.

Authors were completely unprepared for the experiment and choose the one of the measurements done during the campaign instead of using the multitracer (instrument can measure almost all possible gases) release tests, which for sure they were able to organize. If the finding of emission rate from a single gas well was a target of the article – it's not enough to give the impression of the method validation. In general it is hard to understand why do the authors use the oil well as the emission source. If the applicability of LES is a target – they should prove the success on many other cases/sources so the reader will get some statistical information. Finally, if the interpretation of LES is a target than lets run it in different scenarios of landscapes (flat vs steep, meadow vs forest etc.).

The technical note should be as straight and technical as possible with only important definition and graphs. Most of the first 9 pages are a description without the big importance for the case study presented later in the "results" chapter. The whole article is 24 pages long and the next chapters present an incoherent and still not technical style of text. There isn't any uncertainty calculations regarding the emission estimates. All statistics is used only descriptive way – qualitatively. My advice for authors is to cut down the unnecessary sentences, some repetitions and input a bit more technical data but overall work over the coherent and consistent data, not shuffling with new model results for each section. Conclusions of the article have no support in real measurements nor in quantitative calculations.

I will try to express my point in a detailed review, but before I do that I would like to underline that I spent some time in reading and perhaps didn't follow the all authors suggestions and I put much time to help authors make the next, better approach to final text:

Line 74 – 81 : nice summary of the paper but it was just described in lines 59 – 73.

87 What is the particular name of plain and mountain ridge where the experiment took place, Carpathians are 1700 km long.

87 is "actual site" a single oil well? If this would be the very well measured oil well I would feel that its OK but later authors declare that it was just multiple transects on one road in some distance from the well (repeated cross-sections in same place). In this case we really use the cannon to shoot the sparrow.

89 and 90 and Fig1 – If length of the road is 150m and the bisection of the segment is not passing the source, it means that the mean distance between source and receptor is NOT the distance to the middle of the road segment.

Fig 1. What for the North direction is reported? Average wind direction would fit better. The wind direction during the measurement was 50 till 150 degrees (let's say on average

100), so the road was mostly not in the central plume. It would require wind direction of 120 till 200 degrees. Wasn't any better point for the presentation?

Fig 2. A) why the pressure situation is presented for a whole Europe – its just enough to present the region with large distances between isobars (here geopotential is not necessary as we discuss the low winds only). B) measurements of heat fluxes require basic meteorological instruments, there is no need to use the model when real data are easy to access. The experiment was obviously not planned during the campaign.

95 – 98 the synoptic situation is not referring to the Fig2a. as there is no high pressure over the Baltic sea visible. All the story can be shorten to sentence in lines 98 – 100. Fig2a is a bit useless.

104 – 105 The windcube information would be welcomed for such experiments so the wind vertical gradient can be verified experimentally. Again, no need for comparisons of models if only experiment is well planned.

111 "…LARGE scale advection was SMALL…" ð□□□

120 Concentration is not referring to ppb value but any unit per unit of volume. Use the molar fraction instead.

121 What does B20 means regarding the flask type?

122 NOAA (WMO) scale doesn't cover 5000ppb, ICOS scale as well. Please describe how does the linking procedure looks like or explain why it is not important.

122 The accuracy of measurement is the important parameter, please provide, including all internal uncertainties (calibration, averaging, etc).

158 Why domain was chosen so large(almost 5km) and horizontal resolution was chosen to be so low (5m), Can MicroHH model be run on resolution of single meters?

162 The oil well is usually less than 1m wide (area max =3m2)and in LES model it is the area of 10x10m = 100m2? If yes, than it is far from realistic situation. Maybe other oil or rather gas facilities would be a better choice.

176 initiated FOR -> initiated AT

175 and 177 Simulation was run for 7h or 7.5h? Nudging was started 0.5h after the model started?

183 what does “local” refers to? What are the explicit “local influences” and how they were represented in LES?

186 “all other specifics….identical” – Table 1 points differences in columns 4,5,6

192 “realistically” – what is this term referred to? Please explain why wind speed at 2m force the whole BL to be realistically simulated. Especially in case of “local influences” like the slope flow.

Fig3. What is the message from this profiles, especially for wins speed measured at 2m above ground and receptor located aprox. 100m from the source?

199 is uref=umeas? Why is it differently subscripted? Why authors didn’t use the simple Gaussian model for a comparison as it is frequently used tool in such situations? Why authors didn’t refer to

Fig 5. It is not explained in the text nor in the title of this figure why and how was the cross-section of plume chosen. Why at 3m? Receptor was at this height, right? So why wind measurements were done on 2m height? The source is located at 3600,3600, why not to show larger part of the plume and if it is settled up for the measurement scale – why not to show the transects (i.e. road segment). Why time between snapshots are not equal (nether the less it is not important).

233 Authors claim that “local effects…” not mentioned what exactly they introduced to keep the local condition “realistic” beside the (somehow) averaged wind speed.

248 How exactly release of N2O is measured? Give the uncertainties or accuracy estimation.

251 How one can tell the periodic behaviour of period 55min from 90min time scale figure?

Fig 6. A) what does 17 means on the time scale description. Why A) is in different timescale than C)? is B) plot on other timescale? If not you can bond the plots and use only one scale. Is legend at C) referring to B)?

252 It is a bit of speculation with no reference, some link to the observations of orography influence on period of wind speed should be added.

258 At what frequency wind was rotated, to average values or each 1min average of measured wind dir, if other please specify.

259 What measure does the "comparability" has? Be precise.

261 What was the time averaging period for mole fraction measurements, was it 20Hz or 1Hz or 1min as well? Not specified in "measurements" section

265 There is no information during how many transect no plume should be observed according to the wind direction. Was this percentage in agreement to LES? Assuming 1 transect every min – we have 10% success for first 30 min and a bit more, up to 30% for the next periods. Is this poor recovery in agreement with LES?

269 Fig2 shows the heat flux, not the surface flux of potential temperature – it is the same but please harmonise the variables

271 "…looks smoother…" is not technical nor quantitative description

272 – 273 Why not to take only this simulation which potentially is able to be recorded by the receptor

275 "…by 50" is not in agreement with line 264 where we find 40

276 – 284 – The averages of measured and simulated methane source efficiency don't

contain uncertainties – whole comparison is qualitative – what is not welcome in technical notes. One can't compare the values.

284, 285 "…contribute to the error", "…estimation error might…" – do authors refer to uncertainty, difference between the results or real computational error? In all cases it should not be left unspecified. Also quantitatively!

286 It is not clear what "…not Gaussian shape…" is referring to and how authors made this statement – none of the curve on all 3 parts of Fig 7 looks Gaussian but there are some statistical test to make such statement, even if human brain is a powerful tool for curve recognition.

- Is it possible that from this section on all material is not referring to the earlier conditions?

297 How does the averaging works for the plume this time? Is it 30 min average?

How do the integration works – is it same as averaging or rather adding up the plumes? Width and depth of plume are the dimensions not a cross-sections of plume.

Fig 7. The N2O and CH4 averaged plumes are very similar however there is no quantitative measure to c confirm that from the figure. If the mass fraction (why mass fraction is used instead of molar fraction?) would be scaled or normalized to emission rate than figure would be more informative.

315 Again authors do not present the measure of dispersion or uncertainty of values. How hBL is calculated so precisely (congratulations!), it refers to particular moment or whole period (11:30 – 14:30). Usually in this time it is rising slightly due to entrainment and heat fulxes, maybe not much but definitely larger than 1cm.

Fig 8. The scales on the plot affect the plume shape very much. Here X and Y scale are different while X and Z are the close. It gives very wrong impression that plumes are narrow. Also the integration of the plumes gives the wrong effect of plume density (what is especially important for instantaneous plumes). Taking into account the aim of the paper – cross-section would be more appropriate.

321 What "…starts" mean, how it was estimated and how it refers to value 1.9 (what are

uncertainties?).

324 Is top of BL 500m this time?

326 It is hard to judge but on Fig 9 there is much more plumes than 30

335 From fig 8d the reader gets impression that the maximum of methane mole fraction stays deep below the mean of the plume centrelines till 2000m – here the skewness suggest 1500m, could authors give the deeper explanation of the difference. It is very doubtful however that someone would measure the oil well methane plume 1.5km from the well.

Fig 9. Scales on the figure are also different for each of the space dimension. It makes the plots equally wide but one can scarify it for sake of reality. Also Y distribution and horizontal shape of plume would be more visible. The first 50 - 100 m there is a negative skewness of y distribution, it is important from the point of view of measurement done in this region. Authors should comment on it. Why fig 8 has X distance up to 4320m and this one only 3000?

338 First approx.70 m has a skewness (negative), so not all distances are Gaussian shape. From the data presented in the paper it is not clear than all transects of the plume are Gaussian shape – it should be tested and results presented on the plot.

340 Even small eddies will make the plume wider with distance. What is the background of sentence "….with bigger and bigger eddies."

335 – 345 Quantitative description should replace the qualitative one. The oscillation of single centreline is induced by the eddies but its not obvious that it will result with oscillation of sigma y as well. Shouldn't the turn of the plume make it narrower not wider?

Fig10. The distribution of Z plume dimension 1500m from the source is not in accordance with fig 8 but is in accordance with fig 9 (are this figures from same simulation groups?).

355 It is not clear which dimension of plume authors mean (X,Y,Z)?

358 Again the conclusion of "bigger and bigger" is not confirmed

Fig 11. "…(left row).." refers to left column and next to the right comlumn

366 What means "virtually"?

369 The dimension of plum might be also in X dimension. Replace "row" with column.

371 "…is much larger…" can it be expressed quantitatively?

374 – please explain the variables , sigma v and t was not introduced earlier

379 – 380 Can it be confirmed? The size of distribution and size of eddies not necessarily might be corelated. Smaller eddies may make the overall plume spread by bigger distance with time (Csanady equation) its not obvious that vertical scale boundary induces other eddy-plume relation.

387 – Y variable is not important as we are describing the vertical distribution only (equation 9 is only referring to Z)

388- 390 Usually sources of methane related to O&G are not higher than few meters. It will not change the picture. Authors do not present any simulation for higher emitters nor the thermally elevated plumes.

Paragraph 4.3 has no quantitative results from modelling. I would expect it from technical note.

Fig 12. In title please exchange "rows" with columns. Dimensions (Y and Z) of the plumes are not consistent (even not consistent ratio) – as the shape, moments and distribution of methane the topic of the article it makes completely illusive picture for a reader.

415 the definition of ic implies the shape of it. Authors don't propose any deeper conclusion with application of relative coordinate system. It looks it is unnecessary here. All can be explained in absolute dimensions as well.

418 – 421 It is the statement that one should do the measurements close to the downwind direction and on longer street segments when going further from the source. Did it really required LES?

423 There are some numbers from the LES indicating the distance 300m as the less "fluctuative" area of plume – how does it refer to fig 5 where authors present substantial changes in plume direction and real measurement where only 10% of plume were captured?

How the conclusion about weak meandering in a distance farther than 1500 came out. As it is very important for the topic of the article authors should give more numbers and physics here.

426 "..far from the source….highest chance of measuring" It looks good when one can fly with drone but is it referring to ground base measurements as well?

438 It has inverted U-shape

448 beta was not introduced earlier, p as well but it is explained in line 449

Fig.13 The X distances are 100,600 and 3000m? Is the ic Marro in distance of 100m indeed 600m wide? I doubt eq 10 gives this shape, even unoptimized. Scales are again making the mess from plume shapes. How does the asymmetry of (icr,LES) in Y dimension come at large distance?

Fig.14 Linear scale is not working well for lognormal distributions. If gamma function is proposed as a PDF shape some statistical quantitative verification is required. Please use the test.

Conclusions are mostly descriptive and completely not in the agreement with measurement results (discussed earlier).

490 "…which can help…" please use the specific arguments and show the areas where LES gives additional valuable information which cannot be acquired directly at the field.

497 "…correctly." There is no quantitative prove that it gives better results than simple

Gaussian model.

507 – 510 Give the uncertainty and perform the discussion

520 L also has some uncertainty.

Final comment: The simulations presented by author assumed that the methane is a conservative tracer which behaves in a same way as the air but usually industrial release is not following this assumption. Methane as a part of natural gas coming from the oil reservoirs deep in the crust may be much wormer than the air, it can be also colder as expanded from the point leak. So, the information about the temperature of the source gas is very important when analysing large releases with close distanaces, but not present in the paper.