Review of 'Quantifying horizontal and vertical tracer mass fluxes of a daytime valley boundary layer' by Leukauf et al.

The authors investigate the transport and mixing of pollution in an idealized valley during daytime using large-eddy simulations with WRF. The purpose of the manuscript is to quantify the horizontal and vertical tracer mass fluxes in dependence of surface sensible heat flux and initial stratification. Several sensitivity tests were performed systematically varying the surface sensible heat flux amplitude and the Brunt-Väisälä frequency. The valley volume is distributed in 3 different volumes and tracer mass fluxes between these volumes and the total exported tracer mass out of the valley volume are calculated. The total exported tracer mass significantly drops when increasing atmospheric stability and decreasing the surface sensible heat flux. The authors propose a single parameter to describe the combined effect of initial stratification and surface forcing on the total export of tracer mass.

The transport of pollution in valleys is an important research topic which has been studied extensively in the past, but still needs further investigations. The authors specifically address the role of horizontal fluxes from the slope wind layer into the stable core of the valley. Although the assumed atmospheric conditions and valley geometries are highly idealized and not necessarily realistic, I believe that the manuscript provides interesting results. However, I have several minor and some major comments regarding the definitions of valley volumes and the clarity of the result section. The presentation quality is mostly good too excellent, but there are multiple English spelling and grammar flaws and I recommend having the manuscript checked by a native speaker. In my opinion the manuscript is suitable for publication in ACP provided that the authors conduct a substantial review considering my comments given below.

Major comments

1. Definition of volumes: While I can follow the definition of volume V1, I have concerns about the definitions of the other volumes. The authors define everything above the level of the valley ridge as free atmosphere (V4). However, slope winds and a CBL, which forms on the plateau at ridge height, occur above this level. They are surely not part of the free atmosphere but rather part of a boundary layer affected by the terrain. Thus, the conclusion that the total export of tracer mass into the free atmosphere is described by fluxes at the tops of V3 and V2 is not correct in my opinion. A possible solution could be to simply define V4 as the volume outside the valley atmosphere, whereat the valley atmosphere goes up to the valley ridge.

In Fig. 1 it seems like a neutrally stratified layer forms above the stable core (V3) topped by an inversion. Maybe a definition of the top of V3 taking into account the level of this neutrally stratified layer might be more appropriate than simply using a constant upper level for this volume.

2. Readability and clarity of the result section: I understand that the evolution of the tracer mass fluxes in the different simulations is very complex and requires a detailed analysis. The authors divide the analysis in 5 subsections and describe the different aspects in great detail in the respective sections. However, the amount of details significantly affects the readability and clarity of this section and makes it rather hard to follow for the reader. Especially section 3.2, 3.3 and 3.4 are difficult to read. Thus, I strongly encourage the authors to revise these sections and to focus on the most important features instead of describing everything in detail. This would improve the manuscript a lot.

Minor comments

Title: "Quantifying horizontal and vertical tracer mass fluxes in (?) a daytime valley boundary layer" Abstract: The abstract is rather long (especially the part after l. 12) and the authors should consider shortening it by reducing the number of detailed information (specific surface heat flux or stability, percentages). Instead they should focus on the most important results.

1. 19-20: How can the authors quantify a transport to the stable core when a complete neutralization of the valley atmosphere is reached?

1. 22: "The total export of tracer mass out of the valley atmosphere ..."

1. 29: How is the valley atmosphere exactly defined? Up to ridge height?

1.31: stably-stratified instead of stable as stable can also refer to stable in time

1. 32: The authors use buoyancy frequency as well as Brunt-Väisälä frequency for the same parameter.

1. 38: "but" does not make sense here.

1. 39-40: The aims of the study do not belong here. They rather belong to the end of the introduction where they are already mentioned in 1. 91-93.

1. 51-52: How is turbulence generated when the HI penetrates the stable core? Due to shear? Please clarify.

1. 66 and 1. 70: The abbreviation for convective boundary layer has to be given at its first occurrence and should be used consistently thereafter. The same applies to other abbreviations (e.g. HI).

1. 70: Per definition mixed layer and CBL are not the same, as the CBL consists of a surface layer, mixed layer and entrainment layer. If the authors choose to use both terms CBL and mixed layer (ML)

I recommend to distinguish clearly between both terms. However, I do not see the point of using both terms as the authors mostly refer to CBL in their manuscript.

1. 73-76: Other important mechanisms for pollution transport are the upward transport of polluted air over the mountain ridges due to slope winds (mountain venting, e.g. Fast and Zhong 1998) and the horizontal downstream advection of polluted air from over the ridges with the large-scale flow (advective venting, e.g. Kossmann et al. 1999). These mechanisms substantially affect the evolution of the boundary layer over mountainous regions and in particular over valleys and should be mentioned.

1. 77-84: This detailed paragraph on plain-to-mountain winds is not relevant for the study.

1. 89-90: The order of the references is not uniform.

1. 93: It would be interesting to get some information on the chosen setup already in the introduction. For example, what are the valley dimensions and what was the motivation for that? Are they similar to a typical alpine valley? What is the range of surface forcing? Are the conditions typical for summer, winter, fall conditions?

1. 93: The authors also investigate the total export of pollutants out of the valley atmosphere which would be interesting to mention here.

1. 93-95: This sentence does not fit here. It rather belongs to the motivation at the beginning of the introduction.

1. 97: a detailed list of the presented results would be helpful for the reader.

1. 109: Motivation for valley dimension? See previous comment

1. 117-118: Motivation for amplitude of surface sensible heat flux?

1. 123ff: How realistic is the chosen setup? The authors chose a uniformly stratified atmosphere at rest for initialization. I do not see how this resembles any realistic conditions. What about a valley floor inversion? I suppose this would significantly influence the results. The authors should at least discuss this.

1. 130: A table summarizing the different runs would help for clarity.

1. 142: What is the reason for 41 minutes averages?

1. 147:Please specify the difference between volumes and bulk fluxes.

1. 148: As long as the valley atmosphere is ...

1. 154: What does more useful mean?

1. 157: What time is sunrise? At initialization time? Please clarify.

1. 159-160: How is the breakup detected? I believe that once the stable core is eroded the heat flux criterion detects the inversion around ridge height as h_cbl.

l. 166: Why is that useful?

1. 174-175: Are the budgets for the different volumes closed? What about sub-grid scale fluxes? Did the authors quantify these?

1. 196: Do the authors have an explanation for the large difference?

1. 216: What are the similar characteristics?

1. 232: It is not so much a failure but rather results from the criterion itself.

1. 234: The heat-flux criterion is not used for the upper boundaries of V2 and V3. The authors should be more precise here.

1. 235: How is the boundary between V1 and V2 determined?

1. 243: What does in the morning mean? I guess heating starts once the simulations are started? CBL instead of mixed layer

1. 244: the description of the SWL is not necessary as it is already introduced. Why is the SWL and CBL not indicated in Figs. 2a, b?

1. 247: here and thereafter: once the abbreviation HI is defined it should also be used.

1.252: description of HI not necessary anymore.

1. 254: CBL instead of mixed layer.

1. 260-263: Did the authors investigate the variability of HI for the different output times? This might be interesting to know.

1. 264-265: How did the authors detect the turbulent mixing?

1. 271-274: This rather belongs to the description of the other simulations in the next section.

1. 267-268: Where does this second and stronger circulation come from? Is this symmetric, i.e. does it occur on the other ridge as well? This circulation is right at the boundary of the model domain. Is this a numerical boundary effect? Why did the authors choose the boundaries of the model domain so close to the valley? Did the authors perform sensitivity runs with other domain boundaries? According to the definition of the authors this circulation occurs in the free atmosphere, which is somewhat contradictory as it obviously is a boundary layer process (see major comment 1).

1. 278: into the CBL

1. 284: If regime 2 is never reached in S1N10 it can't be reached earlier or later in other runs.

1. 290: bulk or volume fluxes? See previous comment.

1. 293: the authors use SWL and V2 synchronous (here and at several locations in the text). It would improve readability if the authors used only one term.

1. 312: How can the normalized flux exceed 100%? The definition of the top of volume V1 during regime 2 is not clear to me. How deep was the neutrally stratified layer? The authors stated that is exceed the ridge height (1.272). See also major comment 1.

1. 338-339: This sentence is irrelevant.

1. 341: How is the total tracer mass calculated? Between 6 and 12 LT or between 6 and 18 LT as it is stated in Fig. 5?

1. 364: Why does the surface sensible heat flux decrease sharply at 18 LT? I thought it follows a sine curve?

1. 374: Dependence on forcing amplitude and initial stability?

1. 378-379: english: For simulations with different than ???

1. 381: As far as I understand F_12 is defined at height h_cbl and the horizontal extent of the area reaches from the bottom of the slope (x = 2 km) to the slope. With different surface heating I expect the height h_cbl and thus the horizontal area to vary strongly. How does this affect the fluxes and what does this mean for the comparability of the different runs? Do the authors consider this in the analysis?

1.390: What is "usual meaning"? I do not understand lower end of the SWL? Please clarify.

1. 393: SWL into the free atmosphere. See major comment 1.

1. 423: Change the title of this subsection so that it reflects its content better. E.g. Definition of a dimensionless parameter

1. 439: English: not further conclusions...

1. 441: ... important for what?

1. 446-447: .. with strong stability and/or weak forcing ... implies weak stability and/or strong forcing ...

1. 448: As B is defined as the ratio between required and provided energy it does not depend directly depend on the breakup time. It is rather a measure of total mixing. Only its sign gives some information if the breakup is reached (B<1) or not. Thus, I do not understand why the authors call it breakup parameter. In my opinion, this is misleading. Something like "mixing parameter" or "export parameter" would be more appropriate.

1. 459ff: The discussion section should be improved. At the moment it is rather long and repeats a lot of previous studies (e.g. 1. 495-503 or 1. 523-526) but often misses a critical discussion of the findings of this manuscript to other studies (e.g. 1. 489-494).

1. 464: What is inhomogeneous? The terrain or the atmosphere?

1. 463-488: The sensitivity of the tracer fluxes to the different definitions of the volumes is very interesting. The discussion would benefit from an additional figure visualizing the sensitivity.

1. 495-503: this is pretty much a summary of previous studies. It would be more interesting to discuss the aspects related to terrain geometry (depth, width, slope angles, ...) which have not been considered in this study and maybe speculate about their impact.

1. 553: referring to V2 and V3 in the summary is not ideal, as a reader only reading the summary would not understand it.

1. 555-558: Some more details on the how?

1. 570-571: Testing the dependence on realistic atmospheric stratifications (i.e. several elevated inversions) would be interesting too.

Fig. 2: How long are the time averages? Are the wind vectors time averaged as well?

Fig. 4: Are the shown fluxes averaged in time or instantaneous? It would be helpful to include the total export into V4 (f_24+f_34).

Fig. 8: ".... Of the forcing amplitude, A_shf, ..."

References:

Fast JD, Zhong S (1998) Meteorological factors associated with inhomogeneous ozone concentrations within the Mexico City basin. J Geophys Res 103(D15):18927–18946

Kossmann M, Corsmeier U, De Wekker SFJ, Fiedler F, Vögtlin R, Kalthoff N, Güsten H, Neininger B (1999): Observations of handover processes between the atmospheric boundary layer and the free troposphere over mountainous terrain. Contr Atmos Phys 72:329–350