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Interactive comment on "Numerical tools to estimate the flux of a gas across the air-water interface and assess the heterogeny of its forcing functions" by V. M. N. de C. da S. Vieira

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Dear reviewer1.

I acknowledge the patience and dedication to perform such thorough revision yielding a significant improvement in the article quality and readability. I performed most of the recommendations (51 of 55). I reply below justifying my point of view. I present a few extra corrections of my own. I ask for the reviewers and topic editor feedback on all this, so that I may act accordingly.

I send my replies already so that reviewer 1 as enough time to verify I effectively implemented the changes and judge about whether these are satisfactory. To enable it I C398

also provide the new pdf.

General comments:

I trust we all agree the article is too long and therefore, I took some effort to shorten it up. In the end several text pages, 2 equations and 4 figures were removed.

Introducing more text about the dataset and a new section describing the observations with detail is only secondary to the objective of the work. I propose the dataset be supplied in a supplementary table available online, so as not to burden further the bulk article. The article already has a section (3.2) dedicated to the field methods, which was improved. Reference to the supplementary table could be inserted here.

Furthermore, I recall a clear description of the software structure is available in the software tutorial available with the software package. While the scientific groundings for the choices the reader can make are already in the article, how to implement these in the software is also thoroughly explained in its tutorial. It is not necessary to burden the article further with software details and instructions. This is standard procedure in articles proposing software as is an example Vieira (2012b, in Computational Ecology and Software).

Specific comments

Page 911, line 2: important reference missing regarding transfer velocity from lake observations: Cole and Caraco 1998: "Atmospheric Exchange of Carbon Dioxide in a Low-Wind Oligotrophic Lake Measured by the Addition of SF6" Reply: Done I would also like to take this chance to include a reference to Salhée et al 2011 as I am very keen about it.

Page 912, lines 11-24. I think this text (describing the examples) could be removed from the introduction, in order to shorten the manuscript. It does not add any new information. Reply: Done

Row 25: "During the course of work" etc. Here the author is describing how the work

has progressed, which isn't important for the reader, please reformulate. Reply: Done

Page 913, equation 1, The convention is to write the equation first and then describe the terms in the equation on the following rows. The author has shifted this order and describes the terms first and then presents the equation, I think this need to be reformulated (it goes for all equations in the manuscript). Reply: Done. But equations 1 and 3 were embedded in the text.

Page 913-914, lines 11- 4(914): I think these two paragraphs are a little bit to detailed, in order to shorten the manuscript please consider revising this text. For instance, it isn't necessary to keep the sentence on what letter Zhao et al use for the Bunsen's solubility coefficient or why he is making this choice. Reply: Done.

Page 914, line 17: U10 doesn't have to be the measured wind at 10m, it can also be the estimated wind at 10m by using a measured wind at some other height. It is sufficient to say: "10m wind speed" or similar. The many references listed after this statement (8 of them) are not motivated in my opinion. Reply: Done

Page 915, line 4: The first paragraph should start with equation 2 (see previous comment) Reply: Done

Row 13-24: This is a lot of detail (too much) on the Schmidt number. This could be shortened considerably. Reply: Done

Page 917, line 18: Please specify how air temperature and pressure affects the air transfer velocity "in a mild manner". Reply: Done

Page 918: lines 9! Here you describe how the flux across the air water interface can be estimated. This has in principle already been described in the previous section. If the intention is to describe the actual software please make this clearer. The text here can also be shortened, for instance it is not necessary to in detail describe the concept of concentration difference across an interface and how it affect the direction and strength of the flux (as is done in the list on this page). In addition, I think the

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language here needs to be checked e.g. on row 10 "the gas concentration in the water and in the air gave the direction..". What is meant here by "gave"? Is this what the user needs to give the software (input)? If so, please make this clearer. Reply: Done These paragraphs were redundant and are better off removed. It implied some adaptations in the remaining text.

My understanding is that the author intends to describe the details of the model in Section 3 and how a user should use it. However, the author consequently uses the past tense here (preterit) which make it hard to clearly understand the intention/meaning of this text in this section (what has been made or what the user should be doing) Reply: Done See reply to the previous comment.

Page 919: line 3 (as an example) Again, it is not clear the users has the possibility to choose between several different chemical enhancement parameterizations or if the author is describing how the software was developed. If the latter is true, then this entire paragraph could be removed. Reply: Done See reply to the previous comment.

Lines 14! Please remove the text which describes how the author developed the algorithm. Reply: Done

Row 23: Surface roughness is primarily dependent on the waves, please reformulate. Reply: Done

Page 920. It is clear that the author has limited knowledge in micrometeorology. Atmospheric stability is not related to advection of warmer air, please see any meteorological text book. This is also basic knowledge and doesn't need to be described in detail in a research paper. Reply: Done The removed reference was to Atmospheric Stability 'sensu lacto' and not 'sensu strictu' to atmospherically stable conditions as opposed to atmospherically unstable ones.

Eq(6): The Psi function should be specified in direct connection to the equation. Reply: Done

The Psi-function should also have an index "m" to specify which function it is. Reply: Done I called the index 'u' following the implemented by Fairall, Grachev and others that I cite, as it is the vertical wind gradient being discussed and throughout the article I refer to wind as 'u'. I realize many other authors (Businger, Mahrs, Zhang, Smedman, etc) use 'm'. I am available to change it to 'm' if the reviewer wishes so.

It should also be stated that the Psi function is the integrated non-dimensional gradient (fi-function). Reply: Done

The author presents a psi-function which only applies for stable conditions (see e.g. Stull 1988, page 385). This is a serious flaw, a function dealing with unstable stratification must also be included. Reply: Pendant Yes, I was aware of that. This issue has been one of my major concerns. For long I have been intending to add alternative functions but struggling with lack of time. The works by Businger et al (1971) and Dyer (1974) were on the top of the list. It seems now is the time to do it. The work by Lee (1997) in Journal of Applied Meteorology has a few more formulations. Does the Reviewer agree with the addition of these? I will also take a look at Stull (1988). I hope to have them added to the software within the provided timeframe of one month.

also the reference for the Psi-function is unusual. Reply: Done This set of equations (now eqs. 4 to 6) is widely used and accepted, and therefore does any longer require references.

The unit of H is usually written as W m-2 (not J m-2 s-1) Reply: Being these equal, I prefer to keep as it is as it facilitates checking the model units for conformity between the left and right hand sides of the equation.

Page 921, lines 1-21. This is text book knowledge and shouldn't be included in a research paper. Reply: Done

Rows 24: what are you missing to determine L? Reply: Done. Explained in the text.

Page 924, lines 2-8: This part describes results and should be removed from the "Meth-

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ods" section. Reply: Done

Page 924: I think it should be made clearer that the difference is calculated for only the actual parameters implemented in the model. What if the difference is due to some unknown process, not included? How does the algorithm deal with measurement errors and measurement uncertainties? Reply: Done Just below equation 11 (former equation 13)

Eq 12: Why not use the index ref and env to avoid confusion? Reply: Because index 'a' and 'b' is the standard in all advanced calculus textbooks I have red. I have not yet seen a single one doing differently. Therefore, I would prefer to stick to that. Also, I have used 'obs' and 'est' in the alteration implemented due to the comment above, which is also standard. Along the remaining text 'a' and 'b' contrast more with these than 'ref' and 'env'.

Page 926-928. It shows that this is the author's expertise. However, I think this text described too many details and should be shortened to make it easier to read. Also, again, remove the text which describes how the work progressed (e.g. in paragraphs 2-3 on page 926 and paragraph 1 on page 928). It also not necessary to know all the details in the implementation (e.g. the comment on Matlab indexing on line 9 page 925). Reply: Done

Page 928. A Measurement section should be included prior to the Result section. Reply: I am trying to shorten the article as it is too long. Section 3.2 already refers to measurements and has been improved. Nevertheless, I would like to indulge the reviewer by adding to it a supplementary Table with the dataset used.

Extra changes by the author: Figure 3 was removed. Un-interesting text was removed from section 4.1 Un-interesting text was removed from the first paragraph of section 4.2

Page 930, lines 17-20, lines 27-28: You cannot say anything about under/ overestima-

tion since you don't compare with measurements Reply: Done Furthermore, I removed un-interesting text from this paragraph.

Row 28: "The Raymond and Cole (2001) was an exponential function" was? I guess it still is an exponential function, please revise the text. The problem with writing in the past tense is appearing at several occasions in the text (as stated earlier in this review). Reply: Done

Extra changes by the author: Figure 9 was removed. First 5 lines with un-interesting text were removed from section 4.3 Figure 11 was removed. Last 4 lines with uninteresting text were removed from section 4.3

Page 932: Which wind speed is used in Fig 10? Reply: 0.1m/s. It is specified on the figure legend.

Page 938, lines 8-9: How can you say that the linear functions underestimate the transfer velocities at high wind speeds due to lack of such data? If you don't have any data to compare with you cannot evaluate the parameterization. Reply: Done The text was clarified

Page 940, lines 2-4: Stability is physical concept, not something "developed for air over land", please rewrite this or remove. Reply: Done It was removed. Nevertheless, I meant to say the physical concept was first experimentally tested for air over land.

Line 8, A drag coefficient of 3.91 is at least 1000 times to large, it is normally of the order 0.001. If you have used this value in the algorithm then something is wrong. Please comment. Reply: Done It is a typo of my responsibility. It was supposed to be 3.1*10^-3. I used equations 18 and 19 from Sethuraman and Raynor (1975).

Line 12: If you cannot use L, use the bulk Richardson's number to evaluate stability. Reply: I am not shore about what the reviewer is referring to as there is no reference to L in this page. I 'll take a guess that the reviewer is referring to using the bulk Richardson number instead of playing with the drag coefficient and the work by Sethuraman

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and Rainor (1975). I do not have data at two different heights, meaning no du/dz, no $d\theta/dz$, nor dq/dz. I am unaware of how can I estimate the bulk, flux or gradient Richardson numbers given these constrains. Neither do I have the covariance of vertical wind speed fluctuation with whatever else. I would love to use L or the dimensionless stability parameter, but I am unaware of how can I do it given the current constrains.

Page 942, line 26: It is not as simple as "solely" evaluate u* from z0, wind sped must be included somewhere. Reply: Done Yes, and precisely this was already stated in the following line 27. The word 'solely' was misplaced and has been removed.

Figures Figure 1. It should be made clear that no algorithm has been compared with measurements at high wind speeds (e.g. up to 30~m/s). Reply: Done In section 5.1, paragraph 3.

Rephrase the figure text, (a) shows k for wind speeds in the range 0-30, (b) is a close up showing k in the wind speed range 0-8 (not 5 as is stated in the figure caption). Reply: Done

Fig 4, Formatting of y-axis label: superscript on cm2 Reply: Done

Technical corrections Firstly, all subfigures should clearly be marked with (a), (b) etc. not with (up) (down) (left) etc. Reply: Done

Some figures use a figure heading, some don't, please be consistent. Reply: Done

Also be consistent with the formatting of the figure legend (use box or not). Reply: Done

Express ratios using exponents e.g. meters per second as m s-1 not m/s (in the current versions both formats are used). Reply: Done

Page 909 Title: "Heterogeny" change to heterogeneity (?) Reply: Done

Page 934: DDF is a new abbreviation and should be written out. Reply: Done In section 3.3

Page 944, lines 9-10: "take forever" please rephrase. Second paragraph, this repeats what is described earlier, could be shortened. Reply: Done

- Fig2-3 Please be consistent with the formatting of the figure Legend (sometimes it has a box around it, sometimes not). Reply: Done
- Fig 5. Please use the Greek letter and not "alfa". Reply: Done
- Fig 7: Figure caption, what is the capital letter referring to and why use a semi-colon?
- Fig 9, 14: y-axis label, please correct the dot between mmol and m-2. Reply: Done

Fig 10b and 11b Demand is introduced on the y-axis label, this should be reformulated as ïAËZDËĞ CO2 Reply: Done

Fig 10a: y-axis label, use capital letter on the F in "flux". Reply: Done

Fig 12.13 Different formats are used for the dates, be consistent. Reply: Done

Fig 13: Please be more specific in the figure caption. In what sense does the figure display "the transfer limiting phase"? Reply: Done But in the results text and not in the caption

Fig 18. Caption: "Difference" don't use capital letter. Write out the meaning of the abbreviations used on the x-axis. Y-axis label, correct the "dot" between m-2 and d-1. Reply: Done

Kind Regards, Vasco Vieira

Please also note the supplement to this comment: http://www.ocean-sci-discuss.net/9/C398/2012/osd-9-C398-2012-supplement.pdf

Interactive comment on Ocean Sci. Discuss., 9, 909, 2012.

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