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Interactive comment on "The implementation of a MiXed Layer model (MXL, v1.0) for the dynamics of the atmospheric boundary layer in the Modular Earth Submodel System (MESSy)" *by* R. H. H. Janssen and A. Pozzer

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Reply to anonymous referee 3

General comment The manuscript clearly describes the MXL model implemented in MESSy. The manuscript is well written and the objectives are clearly included in the subjects treated by GMD. In spite the title of the manuscript, the paper is mainly devoted to explain not the implementation of MXL in MESSy but the structure of the mixed–layer model, which is not a new model at all. Most of the manuscript is devoted to explain

the mixed–layer model. This model, as it is mentioned in the manuscript, has been developed, and its description already published by previous authors (e.g. van Heerwaarden, 2011, or some of the works by J. Vilà among others). On the contrary, the novelty of the work, which is the implementation of MXL in MESSy, is only described in one and a half pages (7219–7220). Finally, the authors use only two pages to show the results of the new MXL/MESSy and how these results compare with observations recorded during the DOMINO campaign and MXLCH numerical simulations obtained by van Stratum et al. (2012). In this comparison, I cannot see what is the improvement of the inclusion of the MXL submodel in MESSy. For these reasons, specially considering that most of the manuscript is devoted to describe the MXL, a model not developed by the authors, the manuscript cannot be published in GMD in its present form, and intensive major changes are needed.

We thank the reviewer for acknowledging the qualities of the MS and for pointing out what he/she sees as its weak points. In the following, we hope to clarify some of the choices that we have made in writing the MS. The comments are printed in italics and our replies in normal font.

Major comments 1. Keeping in mind that authors did not develop the MXL model, I have serious concerns about the publication of the manuscript in its present form. More than 75% of the manuscript (section 2, the largest one) is devoted to explain the MXL model, something that has been already published by several authors. The authors are perfectly ware about this fact, and, for this reason, they include many references where the model is described and used for different boundary–layer studies. To my opinion the manuscript should avoid most of the explanations about the MXL model, focus on its implementation in MESSy and check the improvements of this implementation by comparing the results against additional observations, and MESSy/without MXL and MXLCH numerical simulations.

As pointed out by the referee, we are aware that the MXL model is not new and that is has been published before in several publications, but not in this its complete form as it is here: in the work of Van Heerwaarden et al. (2009, 2010, 2011), there is no description of the equations for the chemical species (since their work does not deal with atmospheric chemistry) and in the work of Vilà et al. (2009, 2011) the land surface and soil model are not described (because their work does not deal with BL-land surface interactions). Moreover, we think that the complete description of the MXL model here is useful because the model as described in the current MS will form a reference for MXL to the MESSy community and a starting point for further developments of a 1D model within the MESSy framework (as mentioned in Sect. 5). People working with MXL/MESSy may find it helpful to get an overview of all equations used in this model in one paper. Besides, special care has been taken to explain the boundary layer model also to atmospheric chemists, as they are foreseen to be the main users of MXL/MESSy, e.g. in interdisciplinary studies that aim at crossing the border between atmospheric chemistry and dynamics.

2. If I'm not wrong, the authors never mention how MESSy worked before the inclusion of the MXL submodel. For instance, how the boundary layer depth was estimated? To my opinion, it would be necessary to clearly show the improvement of the model a comparison for the same data set of MESSy with and without the MXL submodel.

Perhaps we should further clarify that MESSy is an interface, and not a model by itself. It combines a basemodel (which can be a box, 1D or 3D model) with submodels that calculate the individual processes relevant to atmospheric chemistry and dynamics (see also Fig. 3). Before the implementation of the generic1D model VERTICO, MESSy was available as box model (CAABA/MECCA, Sander et al. 2011), regional model (COSMO/MESSy, Kerkweg et al., 2012) and a global model (ECHAM5/MESSy (also EMAC), Jöckel et al. 2010). We have included VERTICO as a column model to be able to perform types of studies that are not possible with a box or 3D model, and MXL is implemented as the first dynamics submodel in VERTICO, focusing on interactions between BL dynamics and atmospheric chemistry (see the Introduction on p. 7198 lines 12-26 and p. 7199 lines 1-3). A comparison of boundary layer depths

between MXL/MESSy and MESSy without MXL is not an option, since MXL is a type of submodel that was not available to MESSy before (i.e. one that explicitly accounts for BL dynamics in a single column). For a complete information: ECHAM5/MESSy boundary layer depth is diagnosed using the bulk Richardson number. We will rewrite parts of the Introduction and Sect. 3 to clarify this point.

We will change the introduction (p. 7198 line 16): 'Here we describe the implementation of a MiXed Layer model for the dynamics of the atmospheric boundary layer (ABL) and a generic 1D basemodel called VERTICO (VERTIcal COlumn) in the Modular Earth Submodel System (MESSy, Jöckel et al. 2010). The implementation of the latter is necessary because of the structure of the MESSy framework: in this framework, a basemodel determines the basic configuration of the coupled model, which can be a box, 1D or 3D model, and the individual processes are represented by basemodel independent process submodels that are coupled to the basemodel through an interface layer (Jöckel et al., 2010).'

And we will rewrite Sect. 3 (p. 7219, line 1-8): 'For the implementation of MXL, a generic 1D basemodel is created in MESSy, called VERTICO. VERTICO contains calls to modules for time and tracer management, the time loop which integrates the model equations and in VERTICO tracer concentrations are updated each timestep, combining the tracer tendencies from each active submodel. It is de facto a 3D basemodel in which the horizontal resolution has been reduced to a single grid box, to facilitate the submodel coupling within the MESSy framework. This also facilitates the possible development of a column model that includes more vertical levels in both boundary layer and free troposphere.'

3. Regarding the results obtained for the DOMINO campaign (section 4), I cannot see a clear improvement when MESSy results are compared against MXLCH (see Fig. 6 of the manuscript). I cannot see any comment about this point. Moreover, to my opinion, it would be necessary to compare more than one day or dataset to check the validity of the model.

Indeed, MXL/MESSy and MXLCH perform equally well for the DOMINO case study. Since the dynamics are equal, we conclude that the two chemical schemes that are used in MXL/MESSy (MIM2, Taraborrelli 2009) and MXLCH (the reduced scheme as in Van Stratum et al 2012) both perform satisfactorily under the conditions of the DOMINO case study, i.e. in a low-NOx, low-isoprene regime. We should underline that the main goal of this test was to prove that the two model implementations do not present any clear differences, i.e. the implementation of the MXL physics does still reproduce the expected results for well established cases.

We will comment on this in the revised MS (p. 7221, line 24): 'For this case study under conditions of low NOx and isoprene concentrations, MXL/MESSy with MIM2 chemistry and MXLCH with its reduced chemical scheme perform equally well, given the degrees of freedom available to tune the boundary conditions for the chemical species for each of these chemical schemes.'

The dynamics of MXL have been validated in various studies in comparison to LES results and field observations (e.g. Pino et al. 2006, Van Heerwaarden et al. 2010, Ouwersloot et al 2012), and since these are unchanged we do not see the point of further evaluation of the dynamics here. It is, however, important to note that the ability of the MXL model to reproduce the diurnal dynamics of the BL depends on the careful selection of a case study for which the assumption of a well-mixed boundary layer is valid (i.e. a clear and sunny day during which turbulence generated by buoyancy is strong enough to uniformly mix scalars and chemical species over the whole depth of the BL). Besides, it is important to select a day which has a dataset which is as complete as possible in term of observations of both dynamics as chemistry. Therefore, a comparison of the model to data from other days in the DOMINO campaign is not straightforward.

We will add the following comment on p. 7220, line 17: 'Van Stratum et al. (2012) selected one day from this campaign, the 23th of November 2008, as a case study for disentangling BL dynamics and chemistry. On this particular day the influence of

synoptic scale flows on the BL dynamics was relatively small, there were no clouds, and wind speeds and background pollution levels were low. This assures that local processes (BL dynamics, chemistry, emission and deposition) were the main drivers of the observed chemistry. Moreover, this day was during an intensive observation period, assuring that both BL dynamics and chemistry are well-characterized by observations.'

What is new in comparison to previous implementations of MXL, is that our implementation in MESSy and the coupling to process submodels available there, opens up a range of options not available before in combination of the MXL model. For instance, the coupling to more comprehensive chemistry schemes (e.g. Taraborrelli et al 2009), emission modules (e.g. MEGAN, Guenther et al., 2006) or a more elaborate organic aerosol module as before (Tsimpidi et al., 2014) is now possible. However, the performance of the coupled model will depend very much on the submodels that are used in combination with MXL and an evaluation of different combinations of MXL with other MESSy submodels would be beyond the scope of this paper.

Finally, the aim of the manuscript is to document the algorithms and the implementation of the code in its actual status (therefore the submission to GMDD). Further analysis of additional datasets would not add any significant information to the manuscript and would be well beyond the scope of the manuscript and (possibly) the scope of the journal itself.

Minor comments 1. The title is not a description of the content of the manuscript because most of the pages are devoted to explain the MXL model and not to explain its implementation in MESSy.

We will change the title into: 'Description and implementation of a mixed-layer model...'

2. Page 7202, lines 15–20, eq. 3. I don't understand why you need to introduce ? in your notation. If ! = Div(U), please use only Div(U). Note that you use also U for the velocity module, which includes also the convective velocity (see eqs. 21, 41, and 60).

In fact, it is ω that we prescribe as a boundary condition to the model, so we think it is useful to introduce it here. Instead, we will leave out the definition of ω as Div(U), since it is not further used. In this way, we also avoid the ambiguity caused by using U in two different contexts. The sentence on p. 7202, line 17-18 becomes:

'where ω represents the large scale velocity that is a function of the horizontal wind divergence in s^{-1}.'

3. Page 7204, line 1: please include any reference for the choice of the value of the entrainment flux ratio.

We will include a reference to Pino et al. (2003) here.

4. Page 7207, eq. 21. You are using the same symbol (U) for two different definitions of the velocity (compare with eq. 3 and the lines below).

We will remove U from the text below Eq. 3 (also see point 2 above), so it will be used for one definition of wind velocity only.

5. Page 7212, line 9. Please introduce in the text zsl = 0:1h to define the surface layer as you did in page 7213.

will do

6. Page 7218, line 12. I'm quite sure Vilà–Guerau de Arellano et al. (2015) were not the first, or the only ones to suggest the parameterization of the momentum surface fluxes. Please include previous references, for instance Stull (2000).

That is off course true, we will include a reference to Stull (1988) here.

7. Page 7219, line 9. Figure 4 is referred before Fig. 3. Please change the order of these figures.

Will do

8. Page 7220, line 26: include "(see Table 1)" after ": : : despite the positive latent flux

: : :".

will do

9. Page 7221, line 11: "MESSY/MXL" to "MXL/MESSy".

Will do

10. Page 7221, line 23. "a.m" to "LT".

Will do

11. Page 7222, line 7. This is not a new result at all. Previous works (de Arellano et al., 2004; Casso–Torralba et al., 2008 among others) have already pointed out the importance of morning entrainment on the mixed–layer concentration of compounds. Please comment.

We do not claim to show a new scientific result here and we think that that is also not the point of a model description paper. Indeed has the effect of entrainment been shown for CO2 before in the papers mentioned by the reviewer and here we show qualitatively the same result for O3 as already shown by Van Stratum et al (2012) in their Figure 6a. We just show (Fig 7.) and describe (p. 7222, lines 1-11) a budget calculation for O3 as an example of the ability of MXL/MESSy to derive the contribution of the different processes to the budget of a species.

12. Caption Fig. 2. "Typical midday mixed–layer profiles : : :". Please clarify that the arrows don't mark the actual direction of the fluxes.

The last line of the caption already reads: 'the arrows indicate the direction in which the flux is defined positively.'

13. Figure 7. Superscripts are needed for the units of the y–axis.

Will do

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