Interactive comment on “High resolution modelling of aerosol dispersion regimes during the CAPITOUL field experiment: from regional to local scale interactions” by B. Aouizerats et al.

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To Reviewer#1,

The authors appreciate the constructive and helpful comments provided by Reviewer#1. Its comments helped to improve our manuscript. The paper has thus been modified to take into account the recommendations given. Below, we have copied the referee comments in italics and inserted our responses in standard font where
appropriate.
We also would like to mention that a bug has been found in the management of scalar tracers (as aerosols) by the shallow convection scheme. The aerosol concentrations are thus a little bit modified, especially for the ground concentrations of secondary species during the night, which is now lower. In that context, and in order to present a rigorous work, we redone the simulation with the bug corrected. therefore, the figures show different values, but the objectives and conclusions of this study remain the same. Moreover, we added a new figure showing the comparison of dynamical parameters between observations and model results. Finally, the fourth subfigures (previously 8d and 9d) were replaced by the horizontal cross section of the turbulent kinetic energy showing the roll structures along the whole third domain, and not only beginning where the aerosols are emitted.

Regards,

Benjamin Aouizerats

1 Specific comments

1. The abstract states that Observations show that local dynamics is driven either by convective cells coexisting with rolls or only by rolls depending on the day-regime. This statement is not directly backed up in the text of the paper. A discussion is given about the ratio between the boundary layer height and the Monin-Obukhov length. However, no direct observations of the convective plumes or roll structures are presented. This is important because the regional
topography could impact the type of mesoscales structures that form. For example, the wind conditions identified by one of the soundings may not be representative of the larger region when the flow is channeled through mountains, e.g., the Autan wind from the southeast.

It is true that the observations do not prove the presence of rolls or convective cells. However, the ratio between the boundary layer height and the Monin-Obukhov length indicates that the turbulent situation differs between the two days of the IOP, and may show different structures at local scale. The text was modified in that way.

The location of the mountains remains relatively far from the city of Toulouse in comparison with the size of the mesoscales structures. A figure was added showing the comparison of dynamical parameters, including 10-m wind direction and velocity observed at several station located over the large region of Toulouse and the results of the simulation. The wind structures observed and modelled over this large area show that the different wind regimes occurring over Toulouse show the same pattern as over a greater area. The text has been adapted to take this new comparison into consideration.

2. The major regional emission sources are due to cities on the corners of the second domain, as shown in Figure 1. Are the domains configured with two-way interactions so that the plumes from the middle grid can advect out onto the outer grid? By having the cities on the very edge of the domain there could be issues with recirculation patterns in and out of the domain edge causing the emissions from the cities to not be advected into the correct areas of the inner domain. Because the middle domain boundary appears to go through areas of complex topography this could become an issue.
Indeed, the grid-nesting configuration includes a two-way interaction between each domains. This precision has been added in the text. Moreover, it should be noted that the intensity of the emissions from the regional cities located on the corners of the middle domain are relatively low compared to the emissions from Toulouse. We didn’t see major issues or discrepancies at domains edges.

3. **Is the model properly spun up by 3 July?** The aerosol concentrations shown in Figure 2a appear like they are still evolving to establish the proper regional background characteristics. If the model were started a day earlier, would the aerosol field on 3 July 10 UTC be very close to what has been used for this study?

The 2-day spin up performed before the 2-day IOP appears to be enough to correctly initialise the model. Moreover, the three domains were introduced gradually: 1st spin up day with the largest domain, 2nd spin up day with the two largest domain, and finally the 2-day IOP with the three domains. We think that the relatively low concentrations of background aerosols at the beginning of the situation (ie Figure 2a) are mainly due to the meteorological situation. Indeed, before the IOP, the meteorological situation was windier, with lower temperature, and therefore less favourable to high photochemistry. Moreover, as mentioned p.29574 l.12-14, the model runs since the the 1st of July 0 UTC with the largest domain. We think that a two-day spin-up is enough to establish the background concentrations.

4. **The model is used from a resolution of 10 km down to 500 m. How is the turbulence and clouds handled differently between these scales?** 500 m is essentially LES and requires appropriate sub-grid handling of turbulence that is different from a PBL parameterization used with 10-km grid spacing. Does
Meso-NH produce a proper energy cascade for use as an LES model?

At 10km and 2.5km resolutions, boundary layer physics are supposed mainly unidimensional (along the vertical). The turbulence is 1D (Cuxart et al, 2000) and mixes all quantities on the vertical (wind, potential temperature, water quantities, chemistry and aerosols). This turbulence scheme mixes each layer with the layers above and below. In addition, a scheme parameterizes the boundary layer thermals and shallow cumulus clouds (Pergaud et al 2009). It simulated the vertical non-local mixing by organized structures in the boundary layer. All quantities mentioned above are also mixed by this scheme.

At 500m however, one enter the limit of the LES: for a boundary layer height of approximately 2km (in our case), one reproduces explicit eddies in the model. We use then a 3D turbulence scheme (also described Cuxart et al, 2000), that takes into account the effects of all horizontal gradients. As the organized eddies are explicitly resolved by the model, the thermal and shallow cumulus cloud parameterization is no longer used. MesoNH has been extensively used as an LES model, either for convective, neutral or stable boundary layers, with or without clouds (cumulus, stratocumulus), and the energy cascade has been tested; see e.g.:

Pergaud et al., 2009; Sandu et al., 2008; Couvreux et al., 2007; Drobinski et al., 2007; Tomas et al., 2006; Couvreux et al., 2005; Cuxart et al., 2007; Cuxart et al., 2000.

5. Accurately handling secondary organic aerosols is difficult in models. How accurate are the secondary organic aerosols in this simulation? Results are shown comparing secondary vs. primary aerosols. These need to be defined.
What species are included in each of them? Do the secondary species only include the SOA species? Or, do the authors also include the other secondary species such as sulfate?

The aerosol module has been evaluated, and a special effort has been made to estimate the production of SOA species. The reaction scheme used is based on CACM scheme (Griffin et al., 2002) which is able to produce the SOA precursors. The equilibrium scheme between gases and SOA is MPMPO (Griffin et al., 2006) which is also known to reproduce the main SOA formation branches by VOC oxidation. However, the SOA formation by droplets are not considered. Concerning the primary and secondary species, as mentioned P29574 l.1-4, the primary species include black carbon and primary organic carbon, and the secondary species include the inorganic ions $NO_3^-$, $SO_4^{2-}$, $NH_4^+$, as well as ten classes of SOA and water.

6. p. 29571 l. 5 Coarseness of a model grid does not imply the model results are averaged over several hours as stated in the text. Does the author mean that coarse model grids are best compared to observations averaged over several hours, assuming that variability in space and time can be considered similar under certain conditions? This should be stated more clearly.

As Reviewer#1 mentioned, this part was not clear in the previous version of the text. We meant that the dynamical variables at each time steps are usually interpolated between the dynamical fields from the coupled meteorological analyses. It may be the source of errors, especially when there are high spatial or temporal gradient between the two coupled dynamical fields used for interpolation. It has now been modified in the new version of the paper.
7. The statement is made that the background aerosols are set up using CO concentration. More detail is needed since the two are not directly comparable, even though they have similar emission sources. This is of particular concern because the background concentration of BC appears high in the model. In Figure 5a the modeled values are higher than the observations during the low-concentration periods.

For particles, the background aerosols were set up by deriving the CO concentration with a ratio obtained from Cachier et al., 2005 and which is similar to observations during the CAPITOUL campaign. The CO concentration in the atmosphere is initialised by the MOCAGE analyse fields corresponding to that period. The main assumption is indeed that the initialisation of aerosol particle concentrations can be derived from the CO concentration obtained from the MOCAGE analyses. However, this assumption is only used for the initialisation of the modeled atmosphere, before the two-day spin-up, in order not to start the spin-up with a aerosol free atmosphere. The background aerosol concentration at the beginning of the IOP mainly comes from the emissions during the spin-up. Concerning the BC values modeled, the constant overestimation seem to come from the previous bug on shallow convection which is now corrected. The new modeled values do not show the same behaviour.

8. The regional and sub-regional sections of the paper add little to the analysis beyond a basic description of the meteorological conditions. They could be significantly strengthened if they included observational comparisons for both meteorology and aerosols. This would help readers know how well the model reproduced reality on the larger scale feeding into the boundaries of the high-resolution domain. Also, the two sections could probably be combined.
As Reviewer#1 suggested it, we added a Figure presenting the comparison of meteorological variables (2-m temperature, relative humidity and 10-m wind) observed by stations located over the large second domain. Unfortunately, there were no more aerosol observation available than those already presented in Figure 5. We also agree in the fact that these sections present a well known classic pollution plume at regional scale. On the other hand, we find it interesting to keep this section in the present form in order to be compared with the simulation results at local scale, but if Reviewer#1 really thinks that this subsection should be removed, we will do so.

9. Figure 5 shows the range of model observations within the Toulouse region along with averaged observations. How much range is there in the observations? And, how many observation stations are included in the comparison? Because the study compares the model at 500-m resolution this detail is important. Is the high-resolution domain able to properly capture the small-scale variability? Some statistics showing the difference between the different model resolutions would help with this comparison.

This section was not clear in the previous version of the text. Figure 5 shows the range of model values and compare them with the observation. There is only one observation point. The measured values are compared with the model values located at the 21 grid points corresponding to the location of the 21 dynamical station, which basically cover an area of 4 by 4 km centered over the aerosol observation site. In that way, this figure shows that the 500-m resolution model simulates high variability. However, due to the lack of other aerosol observations, we cannot compare the simulated aerosol variability with the reality. On the other hand, the new figure shows the comparison of the 2-m temperature observed by the 21 stations and modeled at the correspondind grid points.
10. The conclusion talks about the importance of high resolution. Models do reproduce more detail at high resolution, but is the detail realistic? No observations have been given to demonstrate that the detail is realistic.

Indeed, there were no observations allowing to confirm the presence of rolls during the IOP. Reviewer#1 is right to mention that there are no observations allowing to back up the simulation of rolls. However, roll observations have been carried (Grossman, 1982; Weckwerth et al., 1995; Moeng et al., 1994; Hartmann et al., 1997) in the past, and show the same characteristics than those modeled in this study. In that context, the modeled situation seems realistic. One of the point of this study is to highlight that in order to reproduce mesoscale structures such as rolls, which may drive the pollutant dispersion at local scale, a high resolution model is needed. We think that considering plume dispersion at local scale and pollution variability is a new thing and may lead to next field campaigns to adapt the experimental network in order to measure those meso-scale structures.

11. Also, when smoothed back out to the coarser scale that can be resolved in the outer grids, is the added detail adding any value by improving the mean value of the concentration on the coarser grid?

The two-way nedging method applied in our case allow the values computed over the 500-m resolution domain (where the physics is more precisely resolved) to be injected as a recall value. Thus, mean values on the third domain compared with the corresponding coarser grid point show very little differences. The largest differences between domains is on the spatial structures and variability.
12. It is stated that the model correctly reproduced the dynamical and aerosol fields. This was never clearly shown in the paper. One figure was given that shows the BC and total aerosol concentrations for the Toulouse region as a time series. However, this is insufficient to know how well the mesoscale features were reproduced.

Indeed, Reviewer#1 is right, and the few aerosol observations does not allow to state about the mesoscale aerosol pattern. We have now modified the text. Concerning the dynamical situation, the new figure shows the evolution of dynamical parameters observed by stations located all over Toulouse and at the main regional cities (pointed as A, SG, C and CC). We have added a section to consider this comparison.

13. Of particular concern to this reviewer is the issue of spinning up the small-scale features within the model domain. A relatively few number of grid points are in the highresolution domain, which uses LES type resolution. Unlike typical LES simulations, this paper uses a model with realistic topography and inflow outflow boundaries. Because of this, a much larger domain is required than in a traditional LES model because the small-scale structures must develop from the coarse inflow conditions. Both on 3 July and 4 July it appears that the structures shown in Figures 8 and 9, respectively, develop about half way into the domain and then blow out the outflow boundary. Should these structures have developed closer to the inflow boundary? Is the structure just becoming evident because emissions from Toulouse are injected from around the middle of the domain? It is very hard to tell from the figures whether the features are just plumes from point sources or if they are due to mesoscale flow patterns.

We do understand the limitation of the few grid points at high resolution to
the formation and development of mesoscale structure. A sentence has been added. Unfortunately, the high numerical cost of such simulations which include high resolution, chemical and aerosol solving does not allow us to extend the number of grid points. Concerning the location of those mesoscale structures, the new subfigure drawing the horizontal cross section of the turbulent kinetic energy shows that the roll structures develop from the boundaries of the domain (around 5 grid points). The reason why the rolls concentrating the aerosols are only visible from the middle of the domain is because the main apportionment of primary particles comes from the city of Toulouse which is located on the middle of the domain.

14. Minor comments

We thank Reviewer# for the minor comments, which all have been taken into account into the new version of the study.