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# *Interactive comment on* "Aerosol-CFD modelling of ultrafine and black carbon particle emission, dilution, and growth near roadways" *by* L. Huang et al.

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We thank referee for their helpful comments. We will first address the General comments of the referee, followed by the Specific issues that they raised below.

Response to General comments

1) The paper entitled "Aerosol-CFD modelling of ultrafine and black carbon particle emission, dilution, and growth near roadways" by Huang et al. deals with CFD simulations using the ANSY FLUENT of ultrafine and black carbon emissions. The topic of the paper is very interesting and overall the attempt of including the chemistry in this

type of CFD simulations is of great relevance. Nevertheless I found that the manuscript itself is not properly constructed because I found little matching between what is written and what is shown. The manuscript also suffers from a poor use of Tables and Figures, too limited in my view which make the reading rather heavy. I suggest the authors to reduce to minimum the number of in-test numbers and to summarize them whenever possible in tables. The authors may have considered to use Appendices to provide all required details without distracting the reading from the main message. Given the complexity of the various elements composing the paper each requiring specific attention and depth, they are instead all mixed together failing in conveying robust conclusions. As a reader of a scientific publication I would search for details on novel ideas or models or maybe I could be interested simply in the treatment of boundary conditions and then how field data are fed into the CFD simulation. All I was hoping to find is missing.

We thank referee for their constructive criticism. We agree that a better use of Tables and Figures can be done to improve the delivery of our work. We modified Figures and added Tables wherever possible to minimize the number of in-test numbers. In response to the comment regarding the structure of the manuscript, we removed some technical details in our manuscript and put them into the Supplement. Please refer to our following response for details.

2) Despite in length the introduction focused on the justification of k-epsilon in versus LES, little is new in the CFD modelling. The treatment of ABL in CFD is rather known as well as the role of turbulence in the mixing process. Instead I was also surprise no mentioning of the diffusion process and no discussion on the Schmidt number. This may have a significant role especially considering the different phases of the aerosols dynamics. Why the authors believe that ABL parameterisation is more important than the diffusion part? There is evidence for ignoring this aspect? Nevertheless information on the Schmidt number needs to be provided and choice properly justified.

By synthesizing previous studies and conducting their own time-scale analysis on the two-stage dilution process (briefly described in the manuscript), Zhang and coauthors

(Zhang and Wexler, 2004;Zhang et al., 2004) qualitatively demonstrated that turbulent mixing and aerosol dynamical processes are the dominant factors governing dispersion and transformation of particles in the near-road environment. Thus, the goal of this study is to properly model the turbulence and the aerosol dynamics by implementing the latest development in CFD, rather than to develop new CFD theory or techniques. To our best knowledge, only one such attempt by Wang et al. (2013) can be found in literature. However, the major difference in our work is two-fold. First, we implement a novel ABLT treatment (Parente et al., 2011a, b), recently developed for the RANS approach to better model TKE and epsilon profiles in ABL with the presence of obstacles (vehicles). This approach allows a gradual transition in the dissipation rate source (Sepsilon) and a k-epsilon model constant (C$\mu$) from the fully developed ABL (dominated by ABLT) to the wake region (dominated by VIT) in one unified domain. A brief description of this aspect is added to the manuscript, and more detailed information on this is included in the Supplement. Second, due to the unique geometry of the highway under investigation, a periodic boundary condition is used to significantly reduce computational domain in the direction along the road. This, in turn, allows the very fine grid applied to the vehicle surfaces required to better model VIT. By validating modelled “inert” species (CO2 and BC) dispersion against measured data, we first demonstrated the computational accuracy and affordability of this approach and documented this in the original manuscript.

In this work, the diffusive mass flux in FLUENT is modeled as the sum of two components: molecular and turbulent diffusion (e.g. Eq 4 in (Di Sabatino et al., 2007)). Turbulent diffusion due to VIT and ABLT are the main dilution mechanisms for pollutants in the near-road environment (Zhang and Wexler, 2004;Zhang et al., 2004). The minimum of the FLUENT calculated turbulent diffusivity is about 10 times higher than the default molecular diffusivity for air (2.88x10-5 m2/s). Therefore, if “diffusion” in the above comments refers to molecular diffusion, the combination of ABLT and VIT dominates the diffusive mass flux in our case. If “diffusion” in comments refers to the total diffusive mass flux due to both molecular and turbulent diffusion, the two dominating

sources of turbulence (ABLT and VIT) have been included in our study. The impact of turbulent diffusion on dispersion of pollutant in our CFD modelling is through the turbulent Schmidt number (Sct), described below.

The key parameter governing modeled turbulent diffusion of pollutants using the RANS approach is the turbulent Schmidt number (Sct), defined as the ratio of the turbulent momentum diffusivity and the turbulent mass diffusivity. Derived as an empirical constant (0.7-0.9 commonly used) based upon experiments, Sct is required as an input to FLUENT to estimate the turbulent mass diffusion coefficient based upon its (assumed) correlation with turbulent momentum diffusivity. Analyzing a widely distributed range of 0.2-1.3 for Sct in literature, Tominaga and Stathopoulos (2007) confirmed that the value of Sct has a large influence on the prediction accuracy of mass transfer. More importantly, they pointed out that without correctly predicting the flow field (i.e. mean and fluctuating components), the discussion of the optimum values for Sct may be misleading. In their review, they found that for plume dispersion in open country for example, a smaller value of Sct might be used to compensate the underestimated turbulent momentum diffusion. They further suggested that the “standard” value should be adopted when this type of underestimation did not occur. Given the good agreement between modelled and measured data of both on-road and near-road TKE, the standard value (0.7) is used in our study. This value is also close to 0.6, which was determined based on field observation for near-neutral conditions (Flesch et al., 2002).

We accept reviewer’s suggestion and have included discussions on diffusion and the Schmidt number in Section 2.1 of the revised manuscript.

3) In general, the validation of the CFD is poor. No discussion has been included in the verification of the boundary dimensions and grid size. There is no statistics reported on the number of runs made and whether the assumption of stationary conditions hold Some comments should be added here. In general the paper requires some major restructuring before it can be considered suitable for publication. In my view is poor on both the experimental description and in the CFD.

The computation domain for the base case simulation, for example, is shown in Figure 1(a). The top of the domain is set to 50 m above ground so that the turbulent flow near the surface is not affected by the top boundary (the x-y plane in purple mesh). The horizontal dimension of 375 m perpendicular to the highway (x-axis) is determined by considering the availability of measurements and the extent of pollutant dispersion (Gordon et al., 2012a). Both dimensions of the domain are in compliance with the recommendations for CFD simulation of flows in the urban environment (Franke, 2007).

For the verification of the grid size used in our study, we carry out CFD simulations using a series of three grid cell sizes: coarse, current, and fine grids. Normalized by the values from the current grid configuration, the results show that for both turbulence quantities and pollutant concentrations, the improvement of the grid size refinement with the current grid configuration is negligible (less than 3%). However, grid coarsening would result in significantly overestimated turbulence, therefore, underestimated pollutant concentrations at Site B.

We believe the assumption of stationary boundary conditions is valid for the cases presented in this manuscript based on the following reasons. Firstly, the meteorological conditions remained relatively unchanged for the periods of investigation (i.e. 05:00-08:00 a.m. of 14 and 15 September 2010). The most relevant meteorological conditions to the near road dispersion of pollutants include the wind speed and direction and the atmospheric stability condition. The FEVER field study was designed to monitor pollutant gradients perpendicular to Hwy-400 under predominant wind from the west. Following the previous analysis (Gordon et al., 2012a), the measured turbulence and pollutant concentrations are filtered for winds within 45° of the highway normal, which results in removing less than 5% of the data. Previous results on the variations in the measured wind speed and atmospheric stability condition show persistent diurnal patterns (Fig. 2 in (Gordon et al., 2012a)). The case study period of 05:00-08:00 a.m. of 14 and 15 September 2010 is specifically chosen due to this ideal perpendicular wind condition (within 5° on average). Secondly, both the traffic volume and the travelling

speed show persistent diurnal patterns and stability within the period chosen (Fig. 2 in (Gordon et al., 2012a)). Finally, the residence time (of about 400 s) estimated based on 3-m wind speed measured on site is much less than the averaging period of 1 hour for the half traffic case (05:00-06:00 a.m.) and 2 hours for the base case (06:00-08:00 a.m.). Therefore, the assumption of stationary conditions is considered valid in our case study.

In response to reviewer's suggestions, we have included the above discussion in the Supplement.

Response to Specific issues

1) I found specifically that the description of the atmospheric conditions is limited or hardly documented e.g. the authors claim that the simulations refer to neutral conditions but the period of measurements is between 5-6am or 6-8am. . . now the time of the year is missing and generally at the sites' latitude 6-7 can be dark and cold and therefore typically stable conditions occur. . . unless we are in the summer, in this case it is more likely that a convective boundary layer is growing. Surely neutral conditions would require rather high wind speed – again wind speed information is missing! Another missing information is concerned the wind direction. Simulations are run for conditions perpendicular to the road. . . how many cases have been used?

We accept this suggestion and add Section 3.1 FEVER field study to the manuscript to better describe the atmospheric conditions using the measured wind speed, direction, and Monin-Obukhov length. The FEVER field study took place between 16 August and 17 September 2010. However, only data measured between 05:00-08:00 a.m. of 14 and 15 September 2010 are used in this study for model validation. This is because during this period, the predominant wind direction was almost perpendicular to the highway (within 5° of the highway normal) and the median Monin-Obukhov length (of 36.9 m) indicates near neutral stability conditions. A table (Table 1 in the revised manuscript) is added to summarize the atmospheric conditions during this period. Although relatively low wind speed of 1.4 m/s was measured during this period, it is comparable to the wind speed value of 1.5 m/s in one of the neutral conditions measured and modelled by Wang et al. (2013).

Our simulations for wind perpendicular to the road include 7 cases. There are two simulations for traffic flow conditions of 05:00-06:00 a.m. (54.9 vehicles/min) and 06:00-08:00 a.m. (104.3 vehicles/min). There are additional four simulations carried out for sensitivity tests on individual aerosol dynamical processes, which are listed in Table 6 of the manuscript. And one additional sensitivity run is carried out without maintaining ABL profiles.

The added section to the manuscript reads as follow:

3.1. FEVER field study

The Fast Evolution of Vehicle Emissions from Roadway (FEVER) study was conducted to monitor pollutant gradients perpendicular to a major highway north of Toronto, Canada (Hwy-400; 43.994 N, 79.583 W). The model developed and tested in this paper was designed to simulate the FEVER observations. A complete description of the monitoring strategies of the FEVER project were documented in (Gordon et al., 2012a;Gordon et al., 2012b), the BC emission rate for gasoline vehicles was estimated by Liggio et al. (2012), and the rapid organic aerosol production under intense solar radiation was investigated by Stroud et al. (2014).

The site under investigation was a 6-lane (25 m across from the lane edges) highway, mainly surrounded by flat agricultural fields and some trees lining the side roads, with negligible local pollution sources other than vehicular emissions. To validate modeled VIT, the on-road TKE data measured by the Canadian Regional and Urban Investigation System for Environmental Research (CRUISER) mobile laboratory was used for model comparison. The on-road TKE data was measured by two 3D sonic anemometers during passenger vehicle chasing experiments on six days between 20 August and 15 September 2010. To validate modeled near road dispersion, a case study period

of 14 and 15 September 2010 between 05:00-08:00 am was chosen for comparison. The near-road TKE data was measured by a 3D sonic anemometer at a 3-m tower located 22 m east of the road center. Wind speed and direction data was measured by an AirPointer system (Recordum GmbH), averaged every minute, 34 m east of the road center. As shown in Table 1, the predominant wind direction was approximately perpendicular to the highway and the median Monin-Obukhov length indicates near neutral stability conditions. The CRUISER mobile lab housed instrumentation to measure BC, CO2, and UFP while driving transects perpendicular to the highway. Following a previous study (Gordon et al., 2012a), data were filtered for winds within 45° of the highway normal, which results in removing less than 5% of the data. In addition, particle size distributions between 14.6 and 661.2 nm were measured at two fixed sites with an SMPS every 3 minutes and averaged for 05:00-06:00 and 06:00-08:00 am of 14 and 15 September 2010 for model validation.

2) Figures need substantial improvement. Fig.1 needs to include more details about dimensions and type of boundary. Perhaps a Figure showing the measurement site and physical distances would be helpful with an indication and a summary of the meteorological conditions including stability (perhaps through a Richardson number or the Obukhov length scales).

In response to the above suggestion, we modified Fig. 1 to include details of dimensions and type of boundary in the caption.

A figure showing the measurement site is already published in our previous study (i.e. Fig. 2 in (Gordon et al., 2012b)). To avoid repeating the same information, it is not included in the manuscript. However, it is duplicated here and in the Supplement (S1) for the convenience of readers.

A summary of the meteorological conditions is added to Section 3.1 and Table 1, including the measured wind speed and direction, the friction velocity, and the Monin-Obukhov length.

3) I suggest the authors clearly describe the different cases in the CFD simulation.

Our simulations for wind perpendicular to the road include 7 cases. The only difference between CFD simulations for 05:00-06:00 and 06:00-08:00 a.m. is the traffic flow conditions. While atmospheric conditions remained unchanged, the traffic flow increased significantly from 54.9 to 104.3 vehicles per minute. Assuming all 3 lanes are evenly occupied, the y-axis dimensions are determined to be 91 and 48 m for the above periods, respectively. Small values in the y-axis reflect higher traffic flow volume. This information is summarized in Table 2 of the revised manuscript.

For the model sensitivity analysis discussed in Section 4.2 of the manuscript, a total of five sensitivity runs were performed based upon the base case (06:00-08:00 a.m.). Four sensitivity runs are carried out by turning off a single aerosol dynamical process for each case, and the results are compared with the base case in Table 6. Finally, an additional sensitivity run is conducted without maintaining ABL profiles.

In response to the reviewer's suggestion, a description of the different cases and all sensitivity runs is summarized at the beginning of Section 4, before our results are presented.

4) I suggest to summarize somewhere the CFD validation (type of runs, how many etc) and indicate whether in simulating various types of cars you also changed the dimensions of the cars. If yes obviously this would require a further assessment of the grid influence on the solution.

There is a large variability in shapes and dimensions of the real on-road vehicles. It is beyond our computing power to include vehicles in such detail into our model. However, the size of vehicles during the period of our model simulations can be divided into passenger vehicles (>92%), medium-sized trucks, and heavy-duty trucks. As we are focusing on BC and UFP dispersion within approximately 30 to 300 m away from the road centre, we believe that the very small fraction of trucks can be ignored to simplify model simulations. The limitation of this simplification is already

discussed in the text (see Section 4.1.2 in the original manuscript). The 3D models of passenger vehicles used in this study are the generic models created by SketchUp® (https://3dwarehouse.sketchup.com), named "Mid-size brown SUV" and "Sedan". Both vehicle models are used in the on-road TKE simulations, but only SUV model is used in the near-road dispersion simulations. Based on the on-road TKE simulations, the modelled TKE for Sedan is biased slightly low compared to simulations for SUV.

The grid sensitivity test is summarized in the Supplement (S2).

5) An indication of the effect of the Schmidt number is mandatory.

We agree and accept this suggestion. Please refer to our response to the General Comment (2) for details. In response to this suggestion, a discussion on the effect of the Schmidt number has been added to Section 2.1 of the revised manuscript.

Response to Minor issues

1) Please revise the English whenever possible, I found not too technical in several occasions. Often the authors refer to pollution gradients which is incorrect.

We accept the suggestion. In some places, we use "horizontal gradient perpendicular to the highway" to be clear. In other places, we use "pollutant concentration" instead of "pollutant gradients" to be correct and precise in the delivery of our study.

2) Also they refer to "decay of turbulence mixing decay"? This is not clear.

We agree with the reviewer regarding "decay of the turbulent mixing strength" used on L21, 12250. The revised sentence should read: As a measure of the turbulent dilution under perpendicular wind conditions, near-road TKE is also modelled and compared to the measurements at a tower located 22 m east of the road centre.

Finally, we thank the reviewer for their helpful feedback and suggestions. This is very much appreciated.

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Please also note the supplement to this comment:
http://www.atmos-chem-phys-discuss.net/14/C6858/2014/acpd-14-C6858-2014-supplement.pdf

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Interactive comment on Atmos. Chem. Phys. Discuss., 14, 12235, 2014.

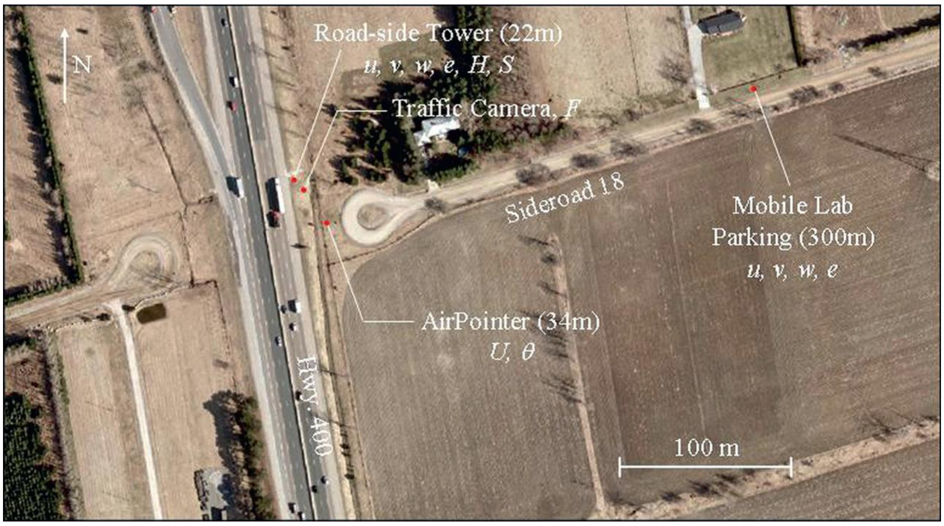

**Fig. 1.** FEVER study site map (originally from Fig. 2 in (Gordon et al., 2012b)).

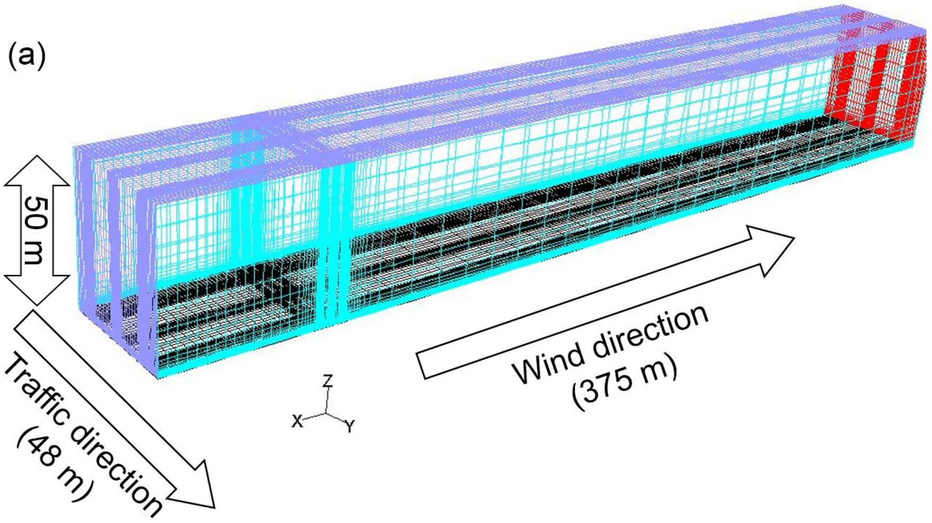

**Fig. 2.** Computational domain (a) and running vehicles and ground mesh (b). Purple mesh indicates velocity-inlet boundaries (left and top); Red mesh indicates pressure-outlet boundary (right); Black me