

## ***Interactive comment on “Soot and SO<sub>2</sub> contribution to the supersites in the MILAGRO campaign from elevated flares in the Tula Refinery” by V. H. Almanza et al.***

**Anonymous Referee #2**

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General Comments:

This paper describes an investigation of the contribution of flare emissions to local and regional air quality in Mexico. The relevance of this study extends beyond this specific application since flare emissions are poorly understood and contribute significant uncertainty to air quality modeling in areas with intensive petrochemical operations. The introduction does a good job describing the relevance of this work, reviewing previous studies on flame emissions, and giving background on the Tula area and its emission activities. While Sections 1 and 2 read well and are clearly presented the later results sections are rather disjointed, rambling, and difficult to follow. Also, grammatical

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and word choice errors are more prevalent in these latter sections. There are many parts of the paper that should be clarified and there are many technical corrections that are needed. I think that if these questions are addressed and the text is clarified in the indicated sections along with thorough editing, the paper may be acceptable for publication.

Specific Comments:

The study uses a CFD combustion model to compute emissions from the Tula flares. By necessity, the set up of this model is largely prescribed with a single constant wind profile and gas stream. The composition fractions of the gas stream are specified (page 15184) but the mass flux is not given or described as to how it was derived. I would think that given the difficulties in calculating emissions that agree with other estimates, particularly for soot, that some sensitivity model runs should be made where winds and gas components and fluxes are varied. Perhaps this is part of the other paper that is repeated mentioned; if so, this should be mentioned along with a clear description of what the other paper is about and how in compliments this paper.

The description of the emission calculations for the slices in Section 3.1.1 is quite confusing. For example, I don't understand why there is inflow and outflow along the slice. Isn't the flow through the slice? Also, what are the quadrants? Perhaps another diagram would help me visualize the process. I am also confused about how the emissions from the single modeled flare are scaled to the three flares. In Section 3.1.2 (pg15189) the IMPei estimates for the 3 flares is used to extrapolate the model calculations of one flare to all 3. It is not described how this is done, but from the values given it seem that the model is taken to represent F1. However, on pg15191 a similar extrapolation for soot seems to be inconsistent. If the model is assumed to represent F1 as for SO<sub>2</sub> then the total for the 3 flares would be about 0.88 g/s which is about an order of magnitude greater. It seems that in this case the modeled flare is assumed to represent F3. Please explain and justify these calculations.

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The description of the WRF-Chem setup in Section 2.2.1 (pg15186) raises some questions about data assimilation (FDDA). They state that FDDA is used for the 2 coarse grids only for the first 24 hours. However, in Section 3.3.1 (pg15196) they credit FDDA for the good agreement of the model with observations on March 23 which is after the initial 24 hours. Also, in the conclusions (pg15204) there is a statement about the importance of analysis nudging for the whole period. First, why is FDDA used only for the first 24 hours? Which 24 hours, during the 2 day spin-up or on March 22? Is analysis nudging using the 1 degree FNL only? Clearly the meteorology simulation could be improved by using obsgrid to reanalyze with observations or using observation nudging and apply FDDA for the entire simulation period. In fact, Fast et al. (2009) is cited and noted that they used observation nudging and reported reasonable predictions. Why not follow this previous work?

Another point of clarification: the lowest layer is said to be 50 m. Is this the height of the mass level (layer mid-point) or the full layer? If the lowest mass level is 50 m, this is much higher than is typical. Also, when reporting the meteorology model performance it would be good to also show the model mean biases for all of the evaluated parameters.

Important results of this work are the average contributions of MHR emissions to the concentrations at the supersites which are reported on pg 15198 and in the abstract. However, it is not clear how these are calculated. Please explain.

Technical Corrections:

Abstract: "IMP" is used before it is defined

Pg15182ln2: Capitalize Environmental in EPA.

Pg15182ln24: What is meant by "soot radiation"?

Pg15183ln24: What is "Favre-averaged"?

Pg15185ln2: Should the gamma be in "the nucleation ( $\alpha\tilde{\gamma}$ )" ?

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Pb15186ln3: Why: "in sub-grid scales"? "...different aerosol and photolysis schemes"; different from what?

In several places the word "specie" is used (which means coined money) when "species" is intended

Pg15188: "The initial and boundary conditions are the default values computed by the model." What are these default values and how were they "computed by the model". Also, since no emissions are used other than from the MHR, it is not clear how the ICs and BCs should be set.

Pg15189ln19: Should be "about a g/s"

Pg15190lns11-19: This paragraph is not very clear. For example, it is not clear how resolution effects the eddies and how the eddies affect the SO<sub>2</sub> concentrations. Is higher resolution expected to increase or decrease SO<sub>2</sub> concentrations downwind? Also, the term "crosswind" is confusing since this is a 2-d simulation and crosswind usually means at right angle to the mean flow. "This imply to lower hydrogen sulfide concentration." should be "This implies that hydrogen sulfide concentration should be lower. "

Pg15192ln8: Should "1.07" be "3.37"?

Pg15192ln9: It would be better to say "is too high" rather than "can be lower".

There are many places where new paragraphs are started where they shouldn't be, such as pg15192ln16, pg15197ln21, pg15200 and pg15204ln4. I suggest merging these paragraphs with the previous paragraphs.

Pg15194ln10: Insert "did" between "simulation" and "not".

Pg15195ln24: "For NO<sub>x</sub> the same estimate of NO<sub>2</sub> and NO..." Same as what?

Pg15196ln22: Should "timing" be "magnitude"?

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Pg15197ln19: "form" should be "from"

Pg15197ln23: What is meant by "increment of emissions"?

Pg15201ln3: "form" should be "from"

The Figures should be improved. Many, particularly figs 1, 6, and 7 are too small and blurry to read. The line plots in figs 3, 4, and 5 could also be expanded with times of the day added to the x-axis. On Fig 7 it would be good to label T0, T1, and T2 and add the location of the TIC.

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Interactive comment on Atmos. Chem. Phys. Discuss., 12, 15177, 2012.

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