A NUMERICAL STUDY OF THE CONTAMINANTS DISPERSION IN ALCANTARA LAUNCH CENTER

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1. INTRODUCTION

The burning of rocket engines during the first few seconds prior to and immediately following vehicles launchings results in the formation of a large cloud of hot, buoyant exhaust products near the ground level, which subsequently rises and entrains ambient air until the temperature and density of the cloud reach an approximate equilibrium with ambient conditions. The NASA has computational codes, like the REEDM – "Rocket Exhaust Effluent Diffusion Model" (Bjorklund et al., 1982; Bjorklund, 1990; Bjorklund et al., 1998) that are designed to calculate peak concentration, dosage and deposition (resulting from both gravitational settling and precipitation scavenging) downwind from normal and aborted launchings to use in mission planning activities and environmental assessments, pre-launch forecasts of the environmental effects of launch operations and post-launch environmental analysis.

In this work, due the lack of experimental data from rocket exhaust clouds in the Alcântara Launch Center (ALC), located in the state of Maranhão, in the northern region of Brazil, our intention is to provide a framework that will allow the development of a more meaningful model that consider the Brazilian site characteristics. Therefore, the main purpose of this study is report a numerical study of the contaminant dispersion in ALC using the CMAQ modeling system. These simulations represent an effort in the construction of a computational tool for normal and/or accidental events during rocket launchings, making possible to predict or simulate the concentration in accordance with emergency plans and pre and post-launchings for environmental management.

2. METHODOLOGY

Fig. 1 and **Fig. 2** present the modeling domains and the ALC locations. These domains were modeled using WRF-ARW model (Skamarock and Klemp, 2008) to generate the meteorological fields, in a one-day simulation. Their horizontal resolution are 27km, 9km, 3km and 1km, and their horizontal dimensions in grid cells are 36x36, 54x54, 84x84 and 66x66, for domain 1 to 4, respectively. The innermost domain, highlighted in **Fig. 2**, was used to model a hypothetical normal rocket launch event in ALC using the CMAQ model, version 4.6 (Byun and Schere, 2006).

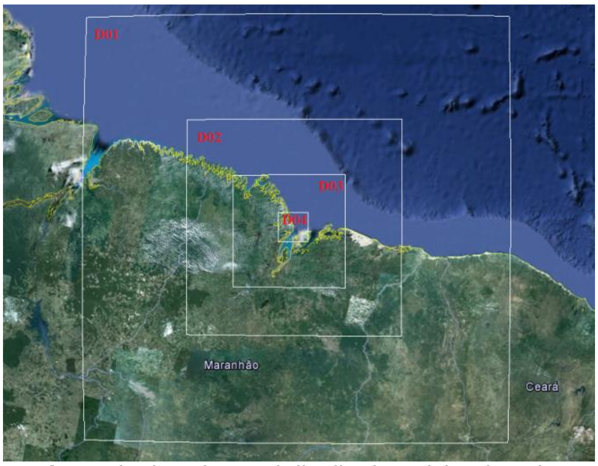

Fig. 1 The location and distribution of the domains modeled in WRF

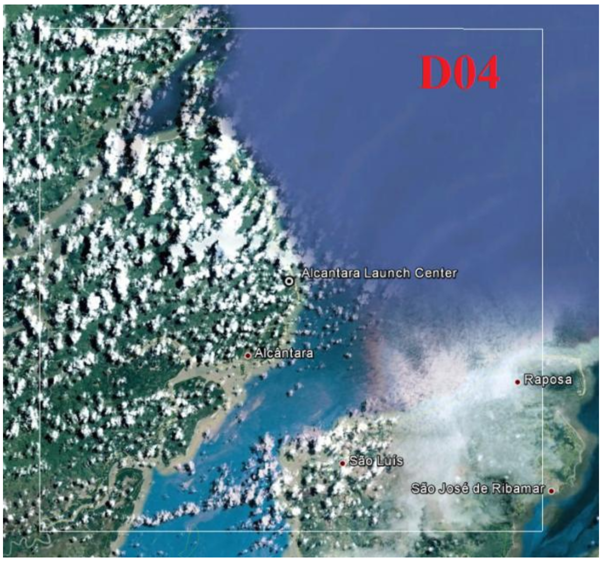

Fig. 2 The location of the domain used in CMAQ to model the rocket launch case

2.1. Building the Emissions File

Emissions from rocket launchings have some particularities that we had to address in order to run SMOKE to build the emissions file. **Fig. 3** shows the launching of Titan IV, in Cape Canaveral, USA, and the formation of the so called *ground-cloud* and *contrail-cloud*. It has been a practice in USA to consider only the emissions from ground to 3.000m in simulations, and the emission rate of a normal rocket launch is $5.2x10^5$ g/s (Bjorklund et al., 1982).

Since SMOKE was not designed to deal with such kind of use case, for each vertical level below 3.000m, we configured a virtual stack source emitting a certain amount of the total emissions, following the distribution presented in **Table 1**. Each virtual stack was positioned in the middle of its respective level. The virtual stacks located nearest to the ground have the main contribution in the emissions, simulating the ground-cloud effect. The remaining emissions were distributed along the highest levels.

Table 1 Distribution of the total emissions along the levels, represented by their corresponding virtual stack

Virtual Stack Id	Stack Height (m)	Distribution of Total Emissions (%)
0	11	20
1	53	30
2	81	10
3	120	7
4	180	6
5	233	5
6	285	5
7	524	4
8	704	4
9	1446	3
10	2195	3
11	2788	3

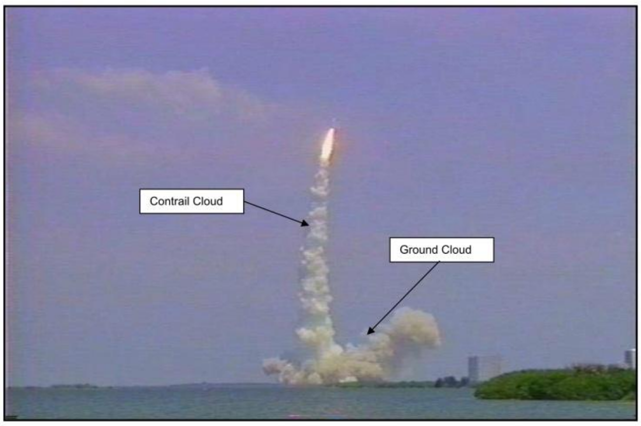

Fig. 3 Ilustration of the formation of the ground and contrail clouds, during a rocket launch (Nyman, 2009)

The inventory was composed of only one pollutant, representing the combustion gases of the propellant. **Table 2** shows the distribution of compounds that are emitted during the combustion, and their corresponding species in the chosen chemical mechanism (see section 2.2). For this simulation, we considered the three major emitted compounds: carbon monoxide (CO), hydrogen chloride (HCl) and alumina (solid Al_2O_3). Any other kind of anthropogenic or biogenic emissions were used in this work, only the emissions from the rocket launch. Regarding temporal allocation, we setup temporal profiles in SMOKE in order to have the entire emissions only at noon.

Table 2 Basic composition of the combustion gases of the propellant (Bjorklund et al., 1982)

Product	% m/m	Specie
Carbon Dioxide (CO_2)	4.4	-
Carbon Monoxide (CO)	27.6	CO
Hydrogen Chloride (HCl)	21.6	HCl
Alumina (Al_2O_3 sólido)	28.2	PMFINE
Water Vapor (H_2O)	7.0	-
Nitrogen (N_2)	8.4	-
Hydrogen (H_2)	2.8	-

2.2. Configuring the CMAQ Model

Once our emissions have HCl, we needed to build a special version of CMAQ and its accessories that is capable of deal with chlorine emissions. Though our work has no intention to evaluate the impact of the emissions in the region, but, as stated before, study how we can apply CMAQ to such case, we chose to model with chlorine emissions and evaluate how it would behave in this situation. **Table 3** shows the options used to build CMAQ. No initial or boundary conditions were applied, and the photolysis rates were calculated by JPROC according to the selected options used to build CMAQ.

Table 3 List of the options used in CMAQ for this work

CMAQ Build Property	Selected Option
Gas Chemistry	cb05cltx_ae4_aq
Aerosol Chemistry	aero4_tx
Advection	vyamo
Vertical Diffusion	acm2_tx
Solver	ebi_cb05cltx
Cloud Module	cloud_acm_tx

3. RESULTS AND DISCUSSIONS

Fig. 5 shows a sequential tile plot for alumina, which was modeled as PMFINE, and **Fig. 6** shows a sequential tile plot for carbon monoxide, both at the first level. In these figures, we can see how the ground cloud behavior after the rocket launch. Initially, it presents high concentrations at the location where the launching occurred, and after the first hour it presents a sensible decrease in the concentrations. Few hours later, the ground cloud was totally dispersed from the domain.

Fig. 7 and **Fig. 8** show a sequential 3D plot for alumina and carbon monoxide, respectively. As we can note, these figures shows the same behavior, where we can easily identify the ground cloud and contrail cloud formed after the launching. In the subsequent hours, the most of the concentrations remain near the ground.

Although the emissions of HCl were of a considerable amount (see **Fig. 4**), the concentrations in CMAQ output were of the order of 1.0×10^{-20}. We also evaluate other chlorine compounds, even ozone, but with no meaningful results. Despite of our efforts in modeling this case with HCl, it cannot be achieved at this time. We must take more time to evaluate modeling CMAQ with chlorine compounds.

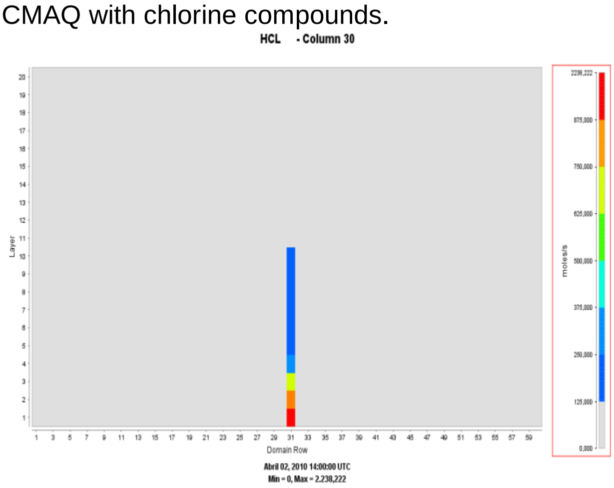

Fig. 4 Vertical cross section plot of the emissions of hydrogen chloride. The emissions near ground are in the order of 82 kg/s

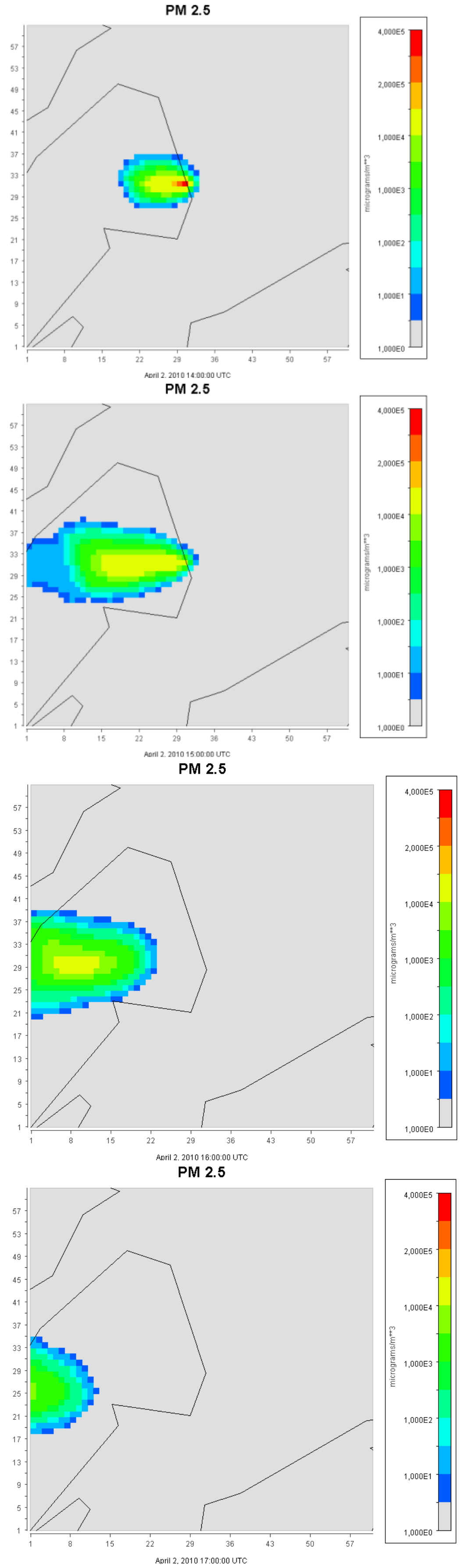

Fig. 5 Sequential tile plot for PM 2.5, representing the concentrations of alumina, for the first layer

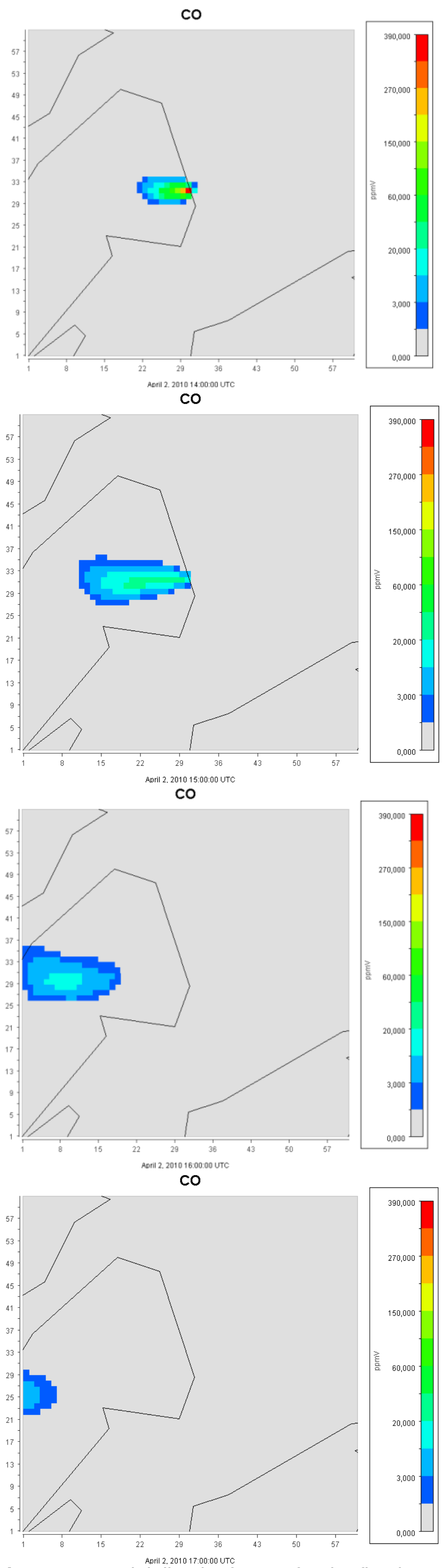

Fig. 6 Sequential tile plot for CO for the first layer

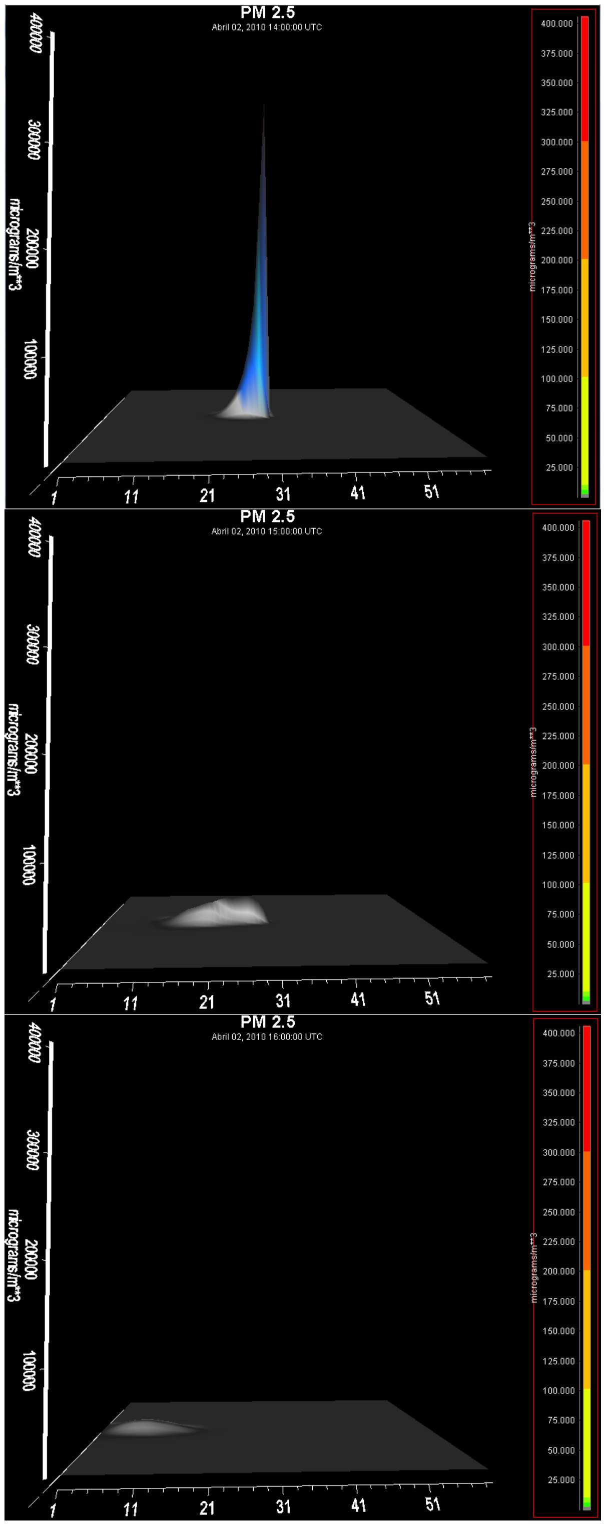

Fig. 7 Sequential 3D plot for PM 2.5

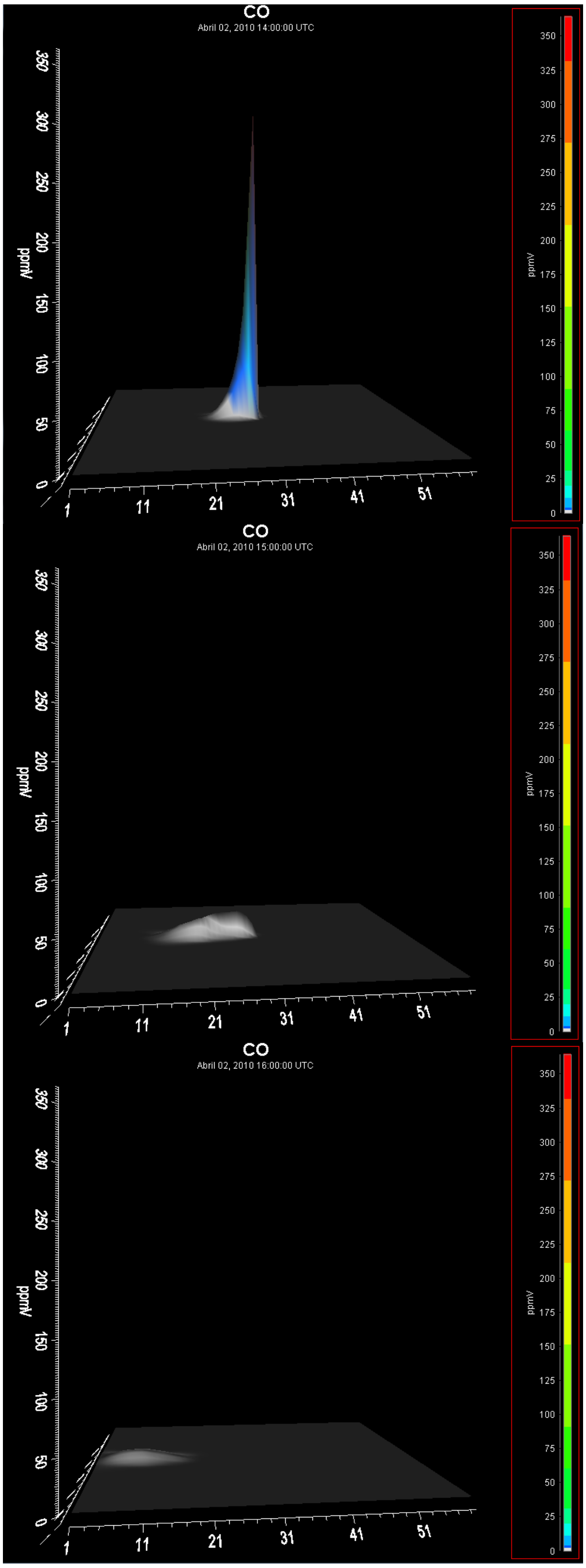

Fig. 8 Sequential 3D plot for CO

Based on the results, we consider that the use of CMAQ to model rocket launch cases is very interesting and promising. We faced some difficulties that we had to address in order to run the model. One of the biggest challenges was how to properly build the emissions file. Although we could manage to configure and run SMOKE to this case, we think that a specific tool should be created to achieve this purpose. The results of the concentrations of CO and PM 2.5 showed to be very interesting: the formation of the ground and contrail cloud and the dispersion of the ground cloud were very clear in the simulations. However, the chlorine issue must be better understood and properly applied to this case, since chlorine has a major impact in the emissions of the combustion gases of the propellant during rocket launch events.

4. SUMMARY

In this work, our main purpose was to apply CMAQ as a numerical model to simulate the dispersion of the contaminants emitted during a normal rocket launch event and evaluates the entire CMAQ suite – model and its accessories – for this case. Since it is a first step to provide a framework that will allow the development of a more meaningful model that consider the Brazilian site characteristics, in ALC, we found that the use of the model for this case is quite promising, despite of some difficulties we have encountered, as reported earlier.

5. ACKNOWLEDGEMENTS

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Figures 1 to 3 were produced using Google Earth, property of Google Inc. Figures 4 to 8 were produced using the VERDI application.

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