Integrating Short and Long Range Approaches for Modeling the Dispersion and the Chemical Transport of Rocket **Exhaust Clouds**

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ABSTRACT

Rocket exhaust clouds are composed by hazardous pollutants, e.g. alumina, carbon monoxide and dioxide, and hydrogen chloride, which are generated during the burning of rocket engines. In the case of vehicle launching, huge and hot clouds are generated near the ground level and are composed by the buoyant exhaust products, which will rise, expand, stabilize, entrain the ambient air, and they will start to be dispersed according to the atmospheric conditions. This process takes a couple of minutes to occur, and generally human receptors located in populated areas nearby the launching center may be exposed to high levels of concentrations within a few to tens of minutes, up to less than one hour. Also, these pollutants may be carried farther due atmospheric dispersion, and chemically interact with other atmospheric compounds, forming new pollutants, reaching and impacting other populated areas located in farther distances. The launch centers around the globe, like spaceports, need to operationally assess the impact of rocket launching events in the environment, requiring to evaluate both short and long range impacts prior to launchings through meteorological and air quality modeling. In general, however, air quality models do not account for calculating peak and average concentration for a short time scale, i.e. ranging from minutes to one hour. In addition, there is the fact that modeling rocket exhaust clouds formed due rocket/vehicle launching is quite a unique air quality problem. For this purpose, we chose to use a modern air quality model which targets this problem, named MSDEF. For long range assessment, we chose the CMAQ modeling system, since it represents the state-of-the-art in regional and chemical transport in air quality modeling, and due to its capability to deal with chlorine gases – which is a considerable part of rocket exhaust clouds. In order to couple both models, the MSDEF code is being rewritten using the I/O API library, making it possible for MSDEF to generate the initial conditions as input to CMAQ model. Thus, it forms the basis for a hybrid, modern and multidisciplinary system which, in conjunction with the WRF model, can be operationally used in different missions at the Alcântara Launching Center (ALC), the Brazilian gate to the space, as planning activities and environmental assessments, pre-and post-launching forecasts of the environmental effects of rocket operations.

INTRODUCTION

Although the assumption regarding the formation of the ground and contrail cloud (see Figure 1) is a major concern in rocket exhaust cloud modeling, it is also important to predict weather and air quality conditions in short and long range terms in order to operationally assess the impact in the environment of normal and aborted launching operations. Recently, the REEDM model [1] has been used in a hybrid system, in conjunction with other modeling tools to simulate the weather and the dispersion of toxic gases in launch operations. The French Space Agency (CNES) conducts simulations of the impact of rocket exhaust pollutants using a model called SARRIM (Stratified Atmosphere Rocket Release Impact Model), during normal or aborted launching operations in the European Spaceport in Kourou, French Guyana [3]. However, more recent works present the idea of using a more complete, multidisciplinary and hybrid approach in order to achieve the goal of assessing the impact of effluents released from launching operations for the European Space Agency (ESA). And the work presented in [4] presents a first-step effort for the Indian Space Agency to evaluate a hybrid approach in the assessment of the impact of rocket exhaust pollutants during launching operations.

Unfortunately, there is no model fully operational to meet these demands in ALC, the Brazilian Spaceport. Currently, a more complete, multidisciplinary, modern and hybrid approach is under development, which will be not only adapted to the Brazilian site characteristics, but will be also suitable to any spaceport site in the world wide. This work presents a qualitative analysis of the very first results of the application of this system to a hypothetical rocket launch event in the ALC region (see Figure 2).





Fig. 1 -The formation of the ground and contrail clouds, during a rocket launch [7]

THE SHORT RANGE DISPERSION MODEL - MSDEF

A modern approach has been developed by [2] called "Modelo Simulador da Dispersão de Efluentes de Foguetes", in Portuguese, which stands for "Simulation Model of Rocket Effluent Dispersion". It applies a stepwise approximation of the eddy diffusivity and wind speed, the Laplace transform to the diffusion-advection equation, a semi-analytical solution of the linear ordinary equation set resulting in the Laplace transform application, the construction of the pollutant concentration by the Laplace transform inversion through the application of the Gaussian quadrature scheme, the computation of first-order chemical reactions, and the discretization and the parameterization of the atmospheric boundary layer (ABL). Such as in the REEDM model, the MSDEF model assumes that the cloud released by the rocket can be initially defined as a single cloud that grows and moves, but remains as a single cloud during the formation of its ascending phase (see Figure 3). Thus, the discretization of the ABL is applied through the partitioning of the stabilized cloud in "disks", representing the different meteorologica vertical levels at different altitudes, each one having a single wind speed and direction that moves the disk into the same cloud. The hypothesis of transport in a straight line ignores the possibility of wind fields that can arise in complex terrain or may evolve during the passage of a sea breeze front or greater scale.



THE LONG RANGE CHEMICAL TRANSPORT MODEL – CMAQ

Once the short range model has been applied, for a time scale ranging from minutes to a couple of hours, it is important to assess how the rocket exhaust pollutants will impact in the region of the surrounding area of the launch site for the next hours after the launch event. Commonly, the launching centers are close to big and populated region/cities that may be affected by the gases released during the launchings. In the case of ALC, the capital city of Maranhão State, São Luís, with more than 1 million inhabitants, is located southwards far 30 km. Recently, [8] presented a work where the Community Multi-scale Air Quality (CMAQ) modeling system [10] were applied for regional scale modeling of the chemical transport of rocket exhaust pollutants in the region of ALC, which showed interesting and promising results. Therefore, since CMAQ represents the state of the art in regional and chemical transport air quality modeling, and due to its capability to deal with chlorine gases, it has been chosen to be applied in this hybrid system for long range assessment of rocket exhaust clouds.

METHODOLOGY

MSDEF needs a single layered profile of meteorological information such as wind speed and direction. It can be achieved by using sounding data collected in the launch site, or by using output from the Weather Research and Forecasting Model (WRF) [9]. Recently [5] validated WRF for the ALC region using radiosonde data collected during dry (2008) and wet season (2010) as a comparison. The reference [6] showed that the application of WRF-LES is quite interesting, since it provides very high resolution information about the atmospheric turbulence and terrain elevation for the air quality modeling, which is an important issue regarding the short range dispersion modeling. The domains were configured and modeled using WRF 3.6 model. The horizontal resolutions of the nested grids were 8.1 km, 2.7 km, 900 m, 300 m and 100 m, with sizes of 40 x 40, 64 x 64, 76 x 76, 76 x 76 and 112 x 112 grid cells for domain 1 to 5, respectively. It was necessary to process 3" terrain resolution from USGS to input into WRF in order to provide higher resolution to the model. The episode ranges from Mar 18th, 2013 to Mar 22th, 2013.

WRF 3.6 was ran with the large eddy simulation (LES) option enabled for real cases (WRF-LES), and its output was used as input to MSDEF (domain 5). Two hypothetical normal launch cases were set up: one for convective atmospheric conditions, and the other for slightly neutral conditions, with the launches occurring at Mar 18th, 2013 13:00 and 17:00 GMT-3, respectively. The emission rate for the launch was of 520 kg/s.

After MSDEF execution, its output was then post-processed in order to generate background concentrations as initial conditions for CMAQ. For this end, a ICON-like file has been produced for each case for the domain 3. It was the most important and hard task, since several data processing was needed to be performed, like grid rotation, matching of vertical layers, computation of concentration values from the finest domain (100 m) to the target coarser domain (900 m), I/O API programming, and so on.

Finally, CMAQ 5.0.2 was executed using the domain 3 configuration, with no emissions from any other source. The boundary conditions was also zeroed out, with only the initial concentrations computed by MSDEF being used as initial conditions to CMAQ.



In this sense, the model does forecast concentration ranging from 5 to 10 km from the launch pad. The model makes predictions of instantaneous and average concentration in time (typically 10 min and hourly average). A shorter average time is appropriate for exposure to the cloud of the rocket, because the source (cloud) typically goes on a receiver with a time scale of tens of minutes before the hour.

Figures 4 and 5 show a plot of HCI concentrations computed by MSDEF for one hour after the launching for each convective and neutral conditions, respectively, for the domain 5. Figures 6 and 7 present the scenario of HCI concentrations computed by CMAQ using the initial conditions from the MSDEF output, two hours after the launching.









The results show the importance of a hybrid and multidisciplinary approach in order to evaluate the impact of rocket exhaust clouds in the environment. While the MSDEF, acting as the short range dispersion model, provides a fast and robust way for computing the concentrations of the very first minutes after the rocket launching at different vertical altitudes for the entire domain, the CMAQ model deals with the simulation of the chemical transport processes at larger space and time scales. Although this is a qualitative work, it presents the basis of a framework, which is under development, that will represent the state of the art in the assessment of the regional impacts of rocket exhaust clouds in the environment.

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RESULTS



Fig. 6 - Scenario generated by CMAQ for HCI concentrations (ppmV) at ground level (10 m) for the convective case. Each frame represents the following two hours after the MSDEF first-hour scenario (15:00h and 16:00h GMT-3

represents the following two hours after the MSDEF first-hour scenario (19:00h and 20:00h GMT-3)

CONCLUSIONS AND FUTURE WORK

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