

Evaluating the Impact of HCL Atmospheric Dispersion caused by an Aborted Rocket Launch in different Stability Conditions

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Abstract— An aborted rocket launch may occur because of explosions during pre-launch operations or launch performance, which generates a huge cloud near ground level comprising hot buoyant exhaust products. This action occurs within a few minutes, and populated areas near the launch centre may be exposed to high levels of hazardous pollutant concentrations within a short time scale — from minutes to a couple of hours. Although aborted rocket launch events do not occur frequently, the occurrence rate has increased in the past few years, making it mandatory to perform short and long-range assessments to evaluate the impact of such operations on the air quality of a region. In this work, we use a modern approach based on the Model for Simulating the Rocket Exhaust Dispersion (MSRED) and its modelling system to report the simulated impact of a hydrogen chloride (HCl) exhaust cloud, formed during a hypothetical aborted rocket launch, on the atmosphere near the earth's surface at the Alcantara Launch Center, Brazil's space-port. The results show that when a launch occurs under stable atmospheric conditions, the HCl concentrations near the ground can reach levels that are extremely hazardous to human health.

Keywords— aborted rocket launch, CMAQ, HCl dispersion, MSRED, rocket exhaust cloud.

I. INTRODUCTION

Rocket launches generate gas emissions produced from burning fuels that are re-released into the atmosphere and transported and dispersed by the wind. Thus, before the launch, it is crucial to analyse the potential trajectory of these gases. Several models are presented in the literature, as in Denison et al. [1], Brady et al. [2], Bennett et al. [3], Bernhardt et al. [4], Koch et al. [5], Voigt et al. [6], and Bauer et al. [7], which deal with the impact that rocket exhaust pollutants cause in the stratosphere without focusing on the impact they cause in the region of the atmospheric boundary layer (ABL), notably at the time of the rocket launch and thereafter. This is due to the strong interest in evaluating the impact that these pollutants cause in the ozone layer where a large amount of hydrogen chloride (HCl) and alumina (Al_2O_3) is emitted during the burning of the propellant. Particles of Al_2O_3 can provide a heterogeneous HCl conversion surface to other chlorinated compounds, which in turn play an important role in depleting the ozone layer [8].

Likewise, it is important to study the impact caused in the lower troposphere, mainly owing to the problem of air quality. To solve this problem, some approaches use

computational fluid dynamics (CFD) techniques for modelling the formation of the exhaust plume; however, the computational cost of this methodology is very high, which pre-vents its use in the operating environment [5,7]. Other researchers use an approach based on Lagrangian models [9,10,11,12] to model toxic gases, whereas others use Gaussian approaches. Some of these models include the Rocket Exhaust Effluent Diffusion Model (REEDM) [13], which was operationally employed by the National Aeronautics and Space Administration (NASA) to evaluate the impact of rocket exhaust clouds. It was recognized that the REEDM model does not adequately represent cases with greater atmospheric turbulence, because it uses a unique turbulence scheme to simulate the dispersion in the launch centre region and its environment [14]. In addition, Anderson and McCaleb [15] present a study which concluded that the REEDM model is deficient for cases of aborted launches caused by explosions, when the results are compared with the CALPUFF model which obtained better solutions in these types of situations. Further-more, it is important to stress that this model is not available to the scientific community for use and

evaluation of its performance and accuracy. The Open Burn/Open Detonation Dispersion Model (OBODM) [16] does not focus on modelling the impact of the rocket exhaust cloud. Instead, it was designed to assess the impact of open-air explosions using the mechanism in the REEDM as a basis.

The Stratified Atmosphere Rocket Release Impact Model (SARRIM) [17] is employed by the France's space agency to evaluate the environmental impact of rocket effluent emissions at the Kourou spaceport in French Guiana; however, like REEDM, this model is not available for use by the scientific community.

The Plume Tracker [18] software package seeks to simulate the elevation, transport, stabilisation, and subsequent deposition and precipitation of particles from the ground cloud generated by rocket launches. Its focus is basically modelling the plume motion process starting at 6,000 ft above sea level, from cloud ascent and stabilisation to pre-collecting particulate matter, without concerns about cloud formation from an actual rocket launch, and the concentration of gaseous pollutants and the involved chemical reactions; therefore, it is not fully suitable for modelling the dispersion of toxic rocket gases, which is the focus of this work.

Developed by Moreira et al. [19] for use by the Institute of Aeronautics and Space ('Instituto de Aeronáutica e Espaço', in Portuguese) at the Alcântara Launch Center (ALC), the Modelo Simulador da Dispersão de Efluentes de Foguetes (MSDEF, in Portuguese) was designed to calculate peak concentrations with dry and wet depositions. Advances in the field were made by the work of Nascimento et al. [20] that presented the first effort to represent exhaust clouds from rocket launches using the Community Multi-Scale Air Quality (CMAQ) modelling system for the ALC region. Recently, Nascimento et al. [21] presented a new model called the Model for Simulating the Rocket Exhaust Dispersion (MSRED), emphasising its ability to simulate the formation, rise, stabilisation, expansion, and dispersion of rocket exhaust clouds for short-range assessment. This model is based on a semi-analytical three-dimensional solution of the advection-diffusion equation utilising a modern parameterisation of the atmospheric turbulence, which uses meteorological input from the Weather Research and Forecasting (WRF) model [22]. For long-range and chemical transport assessment, this model couples with the CMAQ model [23] by generating a ready-to-use initial conditions file to be input to CMAQ. Thus, the MSRED system represents state-of-the-art in the atmospheric modelling field for this unique type of air quality problem. Furthermore,

Nascimento et al. [21] presented the study and simulation of the meteorology, dispersion, and chemical transport of rocket exhaust pollutants in the region of the ALC, Maranhão state, Brazil, by employing this hybrid system to assess the impact of normal launches on the atmosphere. Recently, Nascimento et al. [24] conducted an evaluation of the MSRED model application for the blast event of the SpaceX Falcon 9 rocket launch test on September 1, 2016 at the Cape Canaveral Air Force Station.

In this study, we considered an aborted case at the ALC to analyse the impact of the HCl compound, selected because of its hazardousness when released in ambient air. HCl can be perceived at low concentrations of approximately 0.8 ppm [25] and is corrosive to the skin and mucous membranes (such as the eyes). Acute exposure in a short period of time can cause coughing, hoarseness, inflammation and ulceration of the respiratory tract, chest pain, and pulmonary damage [26,27]. Previous studies about HCl dispersion in the atmosphere have focused on the chemical composition of the ground cloud and, more importantly, the arrangement of tons of HCl produced in approximately the first 10 s after the launch [28]. It was concluded that the ground cloud rises owing to thermal thrust, stabilises according to atmospheric conditions, is carried by the wind, and finally undergoes decay caused by entrainment of dry air and natural diffusion. This is a simplification of a complex process that inspires study and is a field quite open to research.

Accordingly, this work aims to provide a background for the simulation of aborted rocket launches considering HCl atmospheric dispersion. Hence, this work is divided into the following sections: Section II presents the methodology and Section III discusses the results. The conclusions are presented in Section IV.

II. METHODOLOGY

The modelling domain was defined in the WRF model using five domains wherein each domain's horizontal resolution was 8.1 km, 2.7 km, 900 m, 300 m, and 100 m, respectively, and 70 vertical levels in an episode ranging from March 18, 2013 to March 22, 2013. The case was simulated considering a hypothetical aborted launch of the satellite launch vehicle (VLS, 'Veículo Lançador de Satélites', in Portuguese) for different atmospheric conditions — unstable, stable, and neutral. The emission rate and effective heat of the propellant for an aborted launch are 1.36×10^5 g/s and 103 cal/g, respectively [21].

The constituents of the exhaust cloud are fractions of the total weight of the products released in the firing of

the propellant. They are used to determine the emission rate of each contaminant in each cloud partition, multiplied by the release rate defined by the operator. The MSRED model is capable of simultaneously processing the contaminants that come from the burning propellant. The constituent compounds that impact air quality are carbon dioxide (CO_2), carbon monoxide (CO), HCl, and Al_2O_3 . The first three are the main gases, and the last is a particulate material.

For an aborted launch case, MSRED considers that the exhaust cloud, after its formation, rise, growth, and stabilisation, has a cylindrical shape. The cloud is then divided into n partitions, where n is the number of vertical levels that the cloud intercepts, which are the same vertical levels configured in the WRF modelling. Each partition is treated as an independent source, and the MSRED computes the concentration at a receptor by calculating the contribution of each source in that receptor. More information about the details of the mathematical and computational modelling developed in MSRED can be found in Nascimento et al. [21]. As no contaminant concentration data are available to perform quantitative analysis of the results, a qualitative analysis was performed to evaluate how the modelling system simulates each event.

2.1. Short description of the model

The solution to the three-dimensional advection-diffusion equation obtained for a vertically inhomogeneous ABL is described in Nascimento et al. [21]. The solution is semi-analytical, as no approximation is given throughout the derivation process, with the exception of the stepwise approximation of the eddy diffusivities and longitudinal wind speed, and the numerical Laplace inversion of the transformed concentration. Some details regarding the computational strategy developed in the model that were not presented in previous articles are now described in Section 2.2.

2.2. Computational strategy for parallel processing

The MSRED is designed to enable the use of high-performance computing during its execution in addition to the traditional serial approach. The chosen strategy for balancing the computational effort was to divide the dataset according to the number of available processors. The model verifies the number of processors available for its execution and divides the domain in the longitudinal direction — x -axis of the computational grid — in q equal parts, generating subdomains with dimensions $(x/q, y, z)$. This strategy ensures consistency between the diverse variables that are calculated throughout the execution and

the scalability of the model, because it guarantees that the amount of processing time is inversely proportional to the number of processors available for its execution, thereby avoiding race conditions and bottlenecks in the communication between processes and in the execution of the various calculations.

To develop this strategy, the distributed memory parallelism approach was chosen using the Message Passing Interface (MPI) paradigm which is widely used in high-performance computing, including the WRF and CMAQ models.

2.3. Representation of the rocket exhaust cloud

The representation of the source term is one of the main challenges in modelling the environmental impact caused by rocket exhaust effluents in the atmosphere, notably in the region of the ABL. According to Simmons [29], rocket exhaust plumes exhibit a characteristic structure. For the formation of the cloud (stabilisation time, format, stabilisation height, cloud division, etc.), the approach presented in the MSDEF model was followed; however, it included the addition of important improvements aiming at a better representation of the source term which will be described in the Section 2.3.1. The parameterisation of the turbulence was the same as in Nascimento et al. [21,24].

2.3.1. Rise of the exhaust cloud

Determining the exhaust cloud stabilisation height for normal releases and the plume generated for launch failures are important factors in calculating the concentration of pollutants because, in general, the maximum concentration calculated on the earth's surface is inversely proportional to the cube of the stabilisation height [13]. For the aborted or explosive launch case the best option is the continuous plume rise model.

The exhaust cloud, once stabilised, may exceed the height of the atmospheric boundary layer. In this case, two distinct regions are considered to calculate the concentration: first, delimited in the lower part by the terrestrial surface and in the upper part by the ABL; and second, extending from the ABL height to a maximum of 3,000 m. The pollutants are assumed not to penetrate the region above the second region (above 3,000 m) and below the first region (below the earth's surface). It is assumed that the gases coming from the second region do not penetrate at its base (or at the top of the ABL); however, for particles, it is assumed that penetration always occurs.

2.3.1.1. Continuous cloud rise

In the case of an aborted launch or a blast, the time for a continuous plume to reach the height z_k is given by Eq. (1) [13]:

$$t_k = s^{-0.5} \arccos \left[1 - \left(\frac{su\gamma_x\gamma_y z_k^3}{3F_c} \right) \right], \quad (1)$$

where s is the stability parameter given by Eq. (2):

$$s = \frac{g}{\theta} \frac{\Delta\theta}{\Delta z} \quad (2)$$

where:

u : wind speed velocity

$\frac{\Delta\theta}{\Delta z}$

Δz : vertical gradient of potential virtual temperature (K/m)

$\theta = 0.0098$ K/m: dry adiabatic lapse rate

$\gamma_x, \gamma_y, \gamma_z$: coefficients of longitudinal, transverse, and vertical entanglement, respectively

In this work, the vertical gradient of potential virtual temperature will be obtained by a more accurate calculation that uses the meteorological variables provided by the meteorological model WRF [30]. The term F_c (m^4/s^2), which is the thermal thrust term of the continuous boom, is given by Eq. (3):

$$F_c = \frac{gHQ}{\pi\rho_c T} \quad (3)$$

where:

$g = 9.8$ m/s²: acceleration of gravity

H : effective heat contained in the fuel (J/g)

Q : emission rate (g/s)

T : ambient air temperature (K)

ρ : air density (g/m^3)

c_p : 1.004832 J/gK: specific heat of the air at constant pressure

Thus, the stabilisation height of the continuous boom z_c is given by Eq. (4):

$$z_c = \left(\frac{6F_c}{u\gamma_x\gamma_y s^{1/2}} \right)^{1/3} \quad (4)$$

The constants γ_x and γ_y assume the value of 0.5, respectively [13].

2.3.2. Dimensions of the cloud (source term)

The longitudinal r_x , transversal r_y , and vertical r_z radiuses of the cloud at the stabilisation time t^* are given by the Eq. (5):

$$\begin{cases} r_x = \gamma_x z_c \\ r_y = \gamma_y z_c \\ r_z = \gamma_z z_c \end{cases} \quad (5)$$

For the aborted launch case, it is assumed that the cloud is cylindrical in shape [13]. Thus, the radius of each cloud partition is simply the radius of the cylindrical cloud, given by Eq. (6):

$$r_c = \gamma_x z_c, \quad (6)$$

where $\gamma_x = 0.5$ [13].

III. RESULTS AND DISCUSSIONS

This section presents the results from modelling the dispersion and chemical transport of exhaust clouds from aborted rocket launches for different atmospheric stability conditions, using the MSRED model for short range evaluation and the CMAQ model for long range evaluation.

The meteorological information used for each scenario and its respective atmospheric stability condition is presented in Table 1 and refers to the location of ALC. The time reference is Greenwich Mean Time (GMT), and u_* , L , w_* , h , u_v , and u_d represent the friction velocity (m/s), Monin-Obukhov length (m), convective velocity (m/s), height of the ABL (m), wind speed (m/s), and wind direction ($^\circ$) at the surface layer (~ 10 m), respectively.

Table 1. Meteorological information of each modelling scenario.

Atmospheric Condition	Date and time (GMT)	Local date and time (GMT-3)	u_*	L	w_*	h	u_v	u_d
Stable	03/18/201 3 09:00 h	03/18/201 6 06:00 h	0.4	100.0	0.0	874.8	3.5	74.0
	03/18/201 3 16:00 h	03/18/201 6 13:00 h	0.6	-30.3	2.5	773.5	2.9	62.8
Unstable	03/18/201 3 22:00 h	03/18/201 6 19:00 h	0.6	180.0	0.0	733.0	4.0	63.6
	03/18/201 3 22:00 h	03/18/201 6 19:00 h	0.6	180.0	0.0	733.0	4.0	63.6

The ABL was discretised using the meteorological vertical layers defined in the WRF model. Fig. 1 presents the volume of each partition in relation to the total

volume of the exhaust cloud for each scenario. As shown, the behaviour of the vertical distribution of the partitions is consistent with the mathematical modelling of exhaust cloud formation for aborted launch cases, and the cloud has a cylindrical shape.

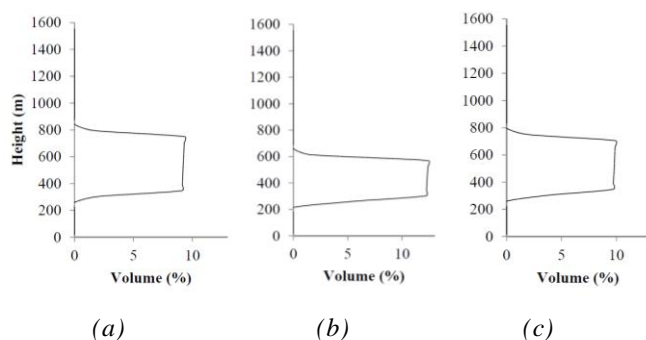


Fig. 1: Percentage volume of each partition in relation to the total volume of the exhaust cloud for the aborted launch case and the (a) stable, (b) unstable, and (c) neutral atmospheric conditions.

The propellant used by VLS is primarily formed by CO, CO₂, HCl, and Al₂O₃ [21]. The following figures show scenarios of the modelling with MSRED and CMAQ for the HCl pollutant (March 18, 2013). The MSRED model simulated all the processes regarding the formation, rise, expansion, stabilisation, and dispersion of the exhaust cloud for the first hour, evaluating its short-range impact. Thereafter, it generated the mean concentration scenario of the first hour after the launch, which was then used as the initial conditions input for the CMAQ model for the long range modelling of the exhaust cloud's impact.

The time for the hypothetical aborted launch case with an unstable condition was at 16:00 GMT (13:00 local time). A scenario for the mean concentration of HCl at the surface level was generated with a 20-minute interval and is presented in Fig. 2.

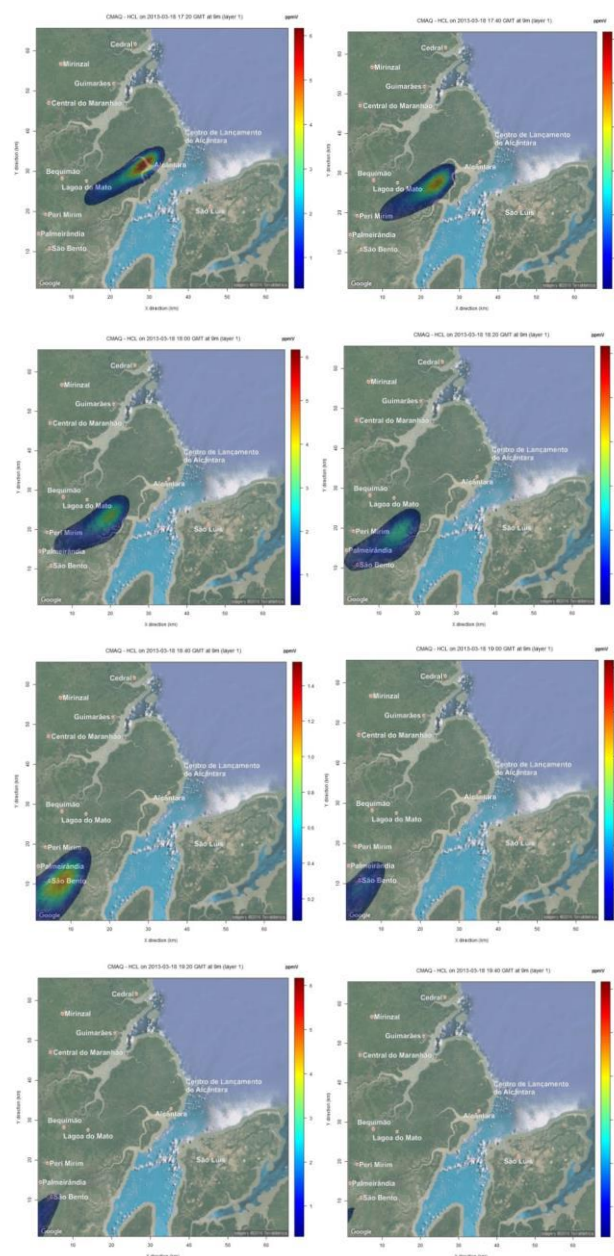


Fig.2. Scenario of the 20min average concentration for the HCl pollutant simulated by CMAQ using the initial conditions generated by MSRED, for a hypothetical aborted rocket launch case considering convective atmospheric condition.

At 17:20 GMT (first frame of Fig. 2), one can observe that the exhaust cloud travelled approximately 15 km from the launch pad, which is consistent with the surface wind speed (refer to Table 1). Each frame features the cities and villages near the CLA. As the time goes on, the HCl concentrations decrease below the concentrations at the beginning of the scenario. This occurs because of the physical and chemical processes that take place, leading to a decrease in the concentrations with the passing of time and as the plume travels along the domain.

The next scenario refers to the stable atmospheric condition for the aborted launch case, which is shown in Fig. 3.

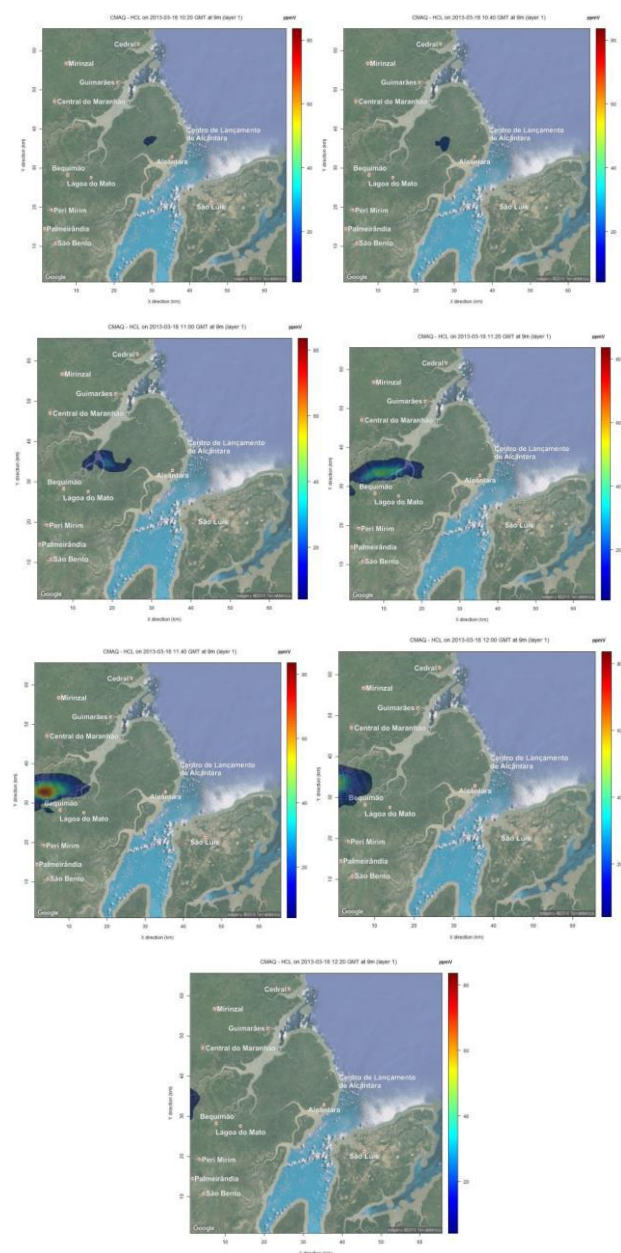


Fig.3. Mean 20 min concentration scenario for the pollutant HCL, modelled by the CMAQ for the aborted launch case with stable conditions, using the initial conditions generated by the MSRED model, from 10:20 until 12:20 GMT.

The concentrations in this scenario were the highest reported by the model for the aborted release case, and the presented concentration values had the potential to cause damage to human health or life. In this case, the cities most impacted by the exhaust cloud would be west of the CLA. It is important to note that higher

concentrations occur at greater distances from the launch centre.

Finally, the modelling scenario with the CMAQ, using the initial conditions generated by the MSRED, will be presented for the long range evaluation of the impact of the rocket exhaust cloud on ambient air in the case of a hypothetical aborted launch in a neutral atmospheric condition. Fig. 4 below presents this scenario.

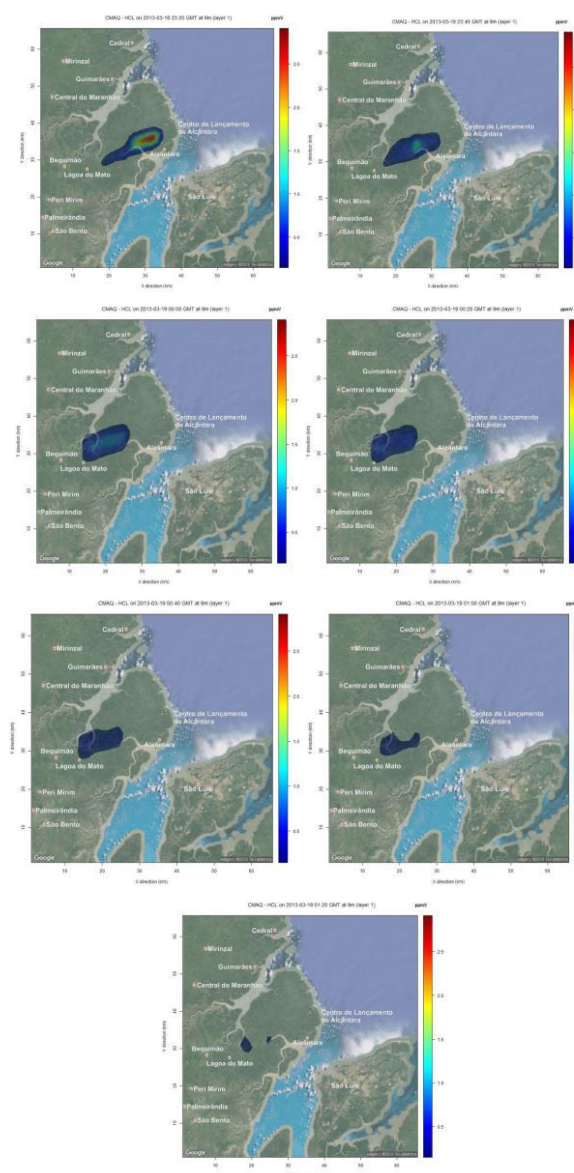


Fig.4. Mean 20 min concentration scenario for the pollutant HCL, modelled by the CMAQ for the aborted launch case with neutral conditions, using the initial conditions generated by the MSRED model, from 23:20 until 01:20 GMT.

It can be observed that the concentrations remained at lower levels than those presented in the stable condition scenario, although slightly higher than in the unstable

case. In addition, for both the unstable and neutral cases, the highest concentrations occurred at distances closer to the launch centre. It should be noted that all simulations conducted under the different atmospheric conditions were for a hypothetical case that utilised a rocket carrying a much lower amount of fuel than a conventional rocket launched in other parts of the world; hence, the concentrations could be much larger than those found in this work.

3.1. Parallelism performance

The following figures present a graphical analysis of the performance of the computational parallelism mechanism that was designed and developed in MSRED. For this analysis, the processing time (in seconds) of the concentration calculation for each grid receiving point was measured based on the emission of an exhaust cloud partition using a varying number of processors. Fig. 5 presents a graphical analysis of the performance of the computational parallelism mechanism showing a reduction in processing time as the number of processors is increased. Fig. 6, however, presents the graphical analysis of the MSRED speedup. Speedup is a measure of performance which measures the ratio of sequential to parallel runtime:

$$S_p(n_p) = \frac{T_e(1)}{T_e(n_p)}, \quad (8)$$

where n_p is the number of processors, $S_p(n_p)$ is the speedup, and $T_e(n_p)$ is the model execution time for n_p processors. Performance tends to be ideal when speedup approaches n_p .

Another important measure is the efficiency E_p , which deals with the relationship between speedup and the number of processors:

$$E_p(n_p) = \frac{S_p(n_p)}{n_p} \quad (9)$$

In the case where speedup = n_p , the efficiency would have value of 1 (100%), meaning a greater efficiency value is optimal. Its chart is shown in Fig. 7.

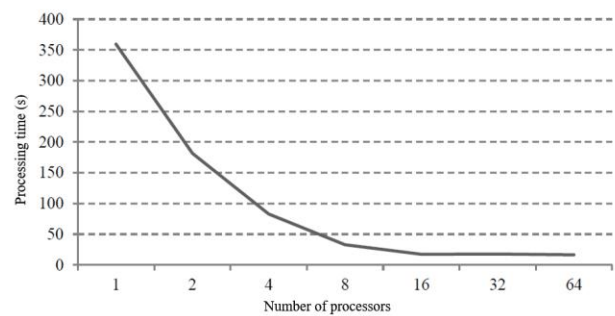


Fig.5. Percentage Reduction Graph of Processing Time.

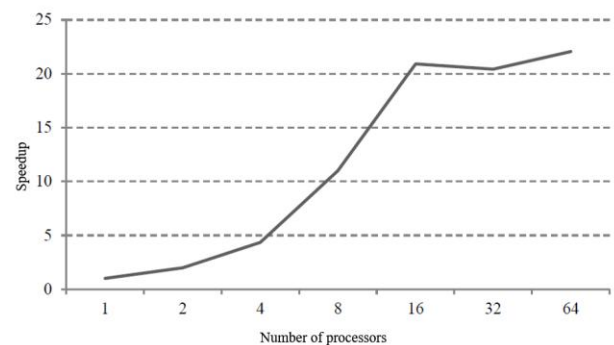


Fig.6. Speedup Chart.

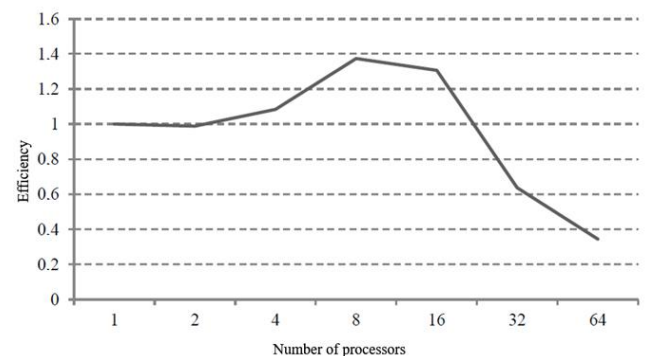


Fig.7. Efficiency Chart.

Table 2, in turn, presents the values of the processing time for each set of processors along with the percentage reduction, speedup, and efficiency. The tests were performed using 64-bit Intel Xeon 8-core computers, each with 2.133 GHz and 8 GB of RAM.

Table 2. Concentration processing time due to the issuance of an exhaust cloud partition for each processor set.

Number of processors	1	2	4	8	16	32	64
Processing time (s)	359.4	181.8	82.9	32.7	17.2	17.6	16.3
Reduction (%)	-	49.4	54.4	60.6	47.4	-2.3	7.4
Speedup	1	2.0	4.3	11.0	20.9	20.4	22.0
Efficiency	1	1.0	1.1	1.4	1.3	0.6	0.3

In analysing the presented performance indicators, it can be observed that as the number of processors doubles, the processing time reduces by approximately one half, and in some cases by even more than a half, such that the processing time of the model is inversely proportional to the number of processors allocated for its execution. This shows the MSRED model's ability to be scalable, that is, to increase performance as more capacity is added. However, it is also observed that as the number of processors greatly increases, the reduction in processing time is negligible; hence, the processing time is stabilised at an approximately constant value. This occurs when there are more processors available for executing the model than grid subdivisions, in cases where the number of processors is greater or equal to the number of receptor points in the x direction, which is the basis of the division strategy for the computational parallelism of the MSRED model.

IV. SUMMARY AND CONCLUSIONS

This work presented a qualitative analysis of a hypothetical aborted/explosion of a VLS rocket launch in the CLA, Brazil, considering HCl compounds and the impact on the air environment for different atmospheric conditions. The concentrations in the stable scenario were the largest reported by the model for the aborted release case and presented concentration values with the potential to cause damage to health or human life.

This study highlighted the importance of simulating this type of event owing to the large amounts of hazardous pollutants that are emitted in a short time scale. Though an aborted launch is not a frequent event, it can severely impact the surrounding populated areas, potentially causing serious damage to public health. Aiming to fill a gap in the scientific community, Nascimento et al. [21] designed a hybrid, integrated, and modern modelling system to address this issue. At its core is the MSRED model which was developed to accurately represent the exhaust cloud and the physical processes that are involved in the fast release, formation, rise, expansion, stabilisation, and dispersion of rocket exhaust gases for short-range evaluation, using meteorological input data from the WRF model, and to generate a concentration scenario based on the short-range scenario that is input to the CMAQ model to simulate the chemical transport for long-range assessment.

The results show the importance of utilising a modern, hybrid, and integrated model-ling system to assess the impact of rocket exhaust clouds on the environment by simulating the effects of aborted launch/explosion cases. This system is suitable for use in pre-launch planning

activities, post-launch environmental analyses, emergency plans, test missions, and in decision making studies regarding the spatial allocation of monitoring networks.

Likewise, it is important to mention that this modelling system can be applied to any launch centre in the world because of its degree of generalisation and parameterisation, and it can also be used to evaluate explosions which have characteristics similar to aborted rocket launches.

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