Use of CFD by IDQBRN for Radiological Defense Using CTBTO Radionuclide Measurements

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Abstract. The Institute of Chemical, Biological, Radiological and Nuclear Defense (IDQBRN) is part of the Brazilian Army's Chemical, Biological and Nuclear Defense System (SisDQBRNEx), based on the lines of research conducted in its laboratory complex. Through its Computational Fluid Dynamics Laboratory (LFC), has been inserting into its research activities the use of CTBTO data to simulate various scenarios containing the dispersion of radionuclides in the atmosphere, thus predicting response and specific emergency actions. In this work, data inversion was performed to determine the amount of $^{137}$Cs released during the Fukushima Daichi nuclear accident, followed by a CFD simulation to analyze the behavior of the radioactive cloud at obstacles near the emission source, the dose received and the concentration level of $^{137}$Cs in the atmosphere.

Keywords: CTBTO, Defense, Radionuclide, CFD, Dispersion.

1. Introduction

The Institute of Chemical, Biological, Radiological and Nuclear Defense (IDQBRN) is part of the Brazilian Army's Chemical, Biological and Nuclear Defense System (SisDQBRNEx), based on the lines of research conducted in his laboratory complex divided into three Defense sections illustrated in Figure 1.

In this context, IDQBRN Computational Fluid Dynamics Laboratory (CFL) performs computational fluid dynamics (CFD) simulations of chemical, biological, radiological and nuclear (CBRN) displacement in the environment, to advise prompt and command actions. response at defense events against CBRN agents.
The Computational Fluid Dynamic Laboratory (LFC) has multidisciplinary activity and focus on simulation of CBRN scenarios for scientific-technical advice on Research, Development, and Innovation (PD&I) of PRODE and emergency actions involving CBRN products. Applying Computational Fluid Dynamics (CFD) tools.

The volume of data generated by the four (4) measurement technologies, namely seismic, hydroacoustic, infrasound and radionuclide, provided by the Comprehensive Nuclear Test Ban Treaty Organization (CTBTO) Through its International Monitoring System, it is critical to validate various CFD simulations not only in the field of radionuclide dispersions but in several others in the Defense area.

For example, in the Fukushima Daiichi accident, more than 35 radionuclide stations that are part of the International Monitoring System (IMS) captured the propagation of radioactive particles and noble gases, as shown below in Figure 2, the $^{137}\text{Cs}$ activity concentration detected by Takasaki Station (RN38 and RN37).

The IDQBRN, as Brazilian Army technical-scientific advisor, has the specific objective of accompanying and advising on activities carried out by the Army with international entities related to the disarmament and non-proliferation of weapons of mass destruction and their vectors [16]. The use of CTBTO data related to radionuclide measurement technology from the global network of the
International Monitoring System, including 80 radionuclide stations around the globe, is included in its research activities [30, 10].

This allows simulating several scenarios containing the dispersion of radionuclides in the atmosphere thus predicting response and punctual emergency actions. In addition to obtaining radionuclide data that can also be used to study atmospheric processes [5] applied to defense research. Moreover, this technology is currently the only one capable of confirming whether an explosion detected and localized by others (seismic, infra-wave and hydroacoustic - employed by the CTBTO verification regime) is indicative of a nuclear test.

CTBTO’s International Monitoring System is designed to research undeclared nuclear activities such as nuclear weapon testing, but can also be used as a monitoring system for tracking released radionuclides from different sources [23].

For this detection, CTBTO uses the Atmospheric Transport Model where it can be used as a tool to estimate the time-dependent relationship between two locations in a global (or regional) grid. These two points are called source and receiver, and the relationship between them source-receiver sensitivity (SRS). If now a source emission or receptor concentration is known, the other parameter can be estimated via ATM [23].

The Atmospheric Transport Model (ATM) is a computational method for predicting the concentration and deposition on the earth's surface of point source air pollutants [18].

ATM is an application of the Gaussian feather model, which has been well described in previous publications, for example, Pasquill-Gifford [24]. With this model, for each point source, an image source was postulated at an equal distance below the earth's surface to make matter flow cross the zero surface. This practice has been described by [15] and is well accepted in air pollution studies [18].

Lagrangian particle dispersion models require meteorological fields as input and the uncertainty in driving meteorology is one of the main uncertainties in the results [2], the spread of uncertainty across the system is not simple, and has not been fully explored. Here, we take a type A uncertainty approach to estimate the uncertainty associated with calculating the inversion of the source term.

The atmospheric dispersion of radionuclides used today generally uses models using Gaussian plume models, which use the Pasquill-Gifford stability classes to determine dispersion coefficients [22, 26]. These models present results in agreement with experimental measurements on flat terrain and some adjustments can be made to take account of release height, boundary layer, deposition, and other factors.

There are even models such as AERMOD, which uses the Gaussian model only for horizontal and vertical treatment for stable conditions and a non-Gaussian probability density function for vertical treatment under unstable conditions [13].

However, they do not provide a more realistic approach to release conditions, especially when the complexity of the region is of utmost importance for decision making when compared to the CFD approach.

[14,19,20] made comparisons of Gaussian models with the use of computational fluid dynamics and concluded that CFD, although requiring greater computational effort, is more appropriate for situations involving complex topographies.

The uncertainties and errors attributed to CFD simulations that cause results to be close to or within their actual or exact values can be reduced by using control procedures to prevent propagation. For example, by running multiple simulations with a variety of turbulence models and seeing how modeling affects the results, we can better determine uncertainty through sensitivity and uncertainty analysis.

In this work we used three k-ε turbulence models (standard, realizable and RNG) and type A uncertainty estimates using the equation below:

$$u_n = \delta/\sqrt{n}$$ (1)
2. Utilization of CTBTO International Monitoring System and computational fluid dynamics simulation to improve measurements

In this paper, we will use the data available from CTBTO International Monitoring System (IMS) and FLEXPART to solve by the data inversion method and seek to reconstruct the emission of radionuclide $^{137}$Cs from Fukushima and thus use CFD techniques to simulate the dispersion of this radionuclide within a terrain approximately one mile away. To evaluate the measurements generated by FLEXPART and CFD and the impact, they may have on the determination of dose levels.

3. Methodology

Initially, a search was made on the measurements of atmospheric activity concentrations of radionuclides from Fukushima through bibliographic searches and the references show a very large field of information about $^{131}$I, $^{133}$Xe and $^{137}$Cs. Thus, the field of study was focused on the atmospheric dispersion of $^{137}$Cs. And the sources are listed in the table below:

| Station Name   | Longitude | Latitude | Num RN | Data Source |
|----------------|-----------|----------|--------|-------------|
| Okinawa        | 127.9     | 26.5     | 37     | CTBTO       |
| Takasaki       | 139.0     | 36.3     | 38     | CTBTO       |
| Guam           | 144.9     | 13.6     | 80     | CTBTO       |
| New Hanover    | 150.8     | -2.6     | 51     |             |

a. The Okinawa Station uses RASA technology, with an estimated 3-10% error associated with acquisition time and presents the following calibration data:

| ID:                 | 7300030339 |
|---------------------|------------|
| Energy Units:        | keV        |
| Calibration Updated: | YES        |
| Calibration Creation Date: | 2007-11-24 12:09:53.89 |
| Equation Channel Energy formula: | $E(c) = -0.132 + 0.3302c$ |
| Equation Resolution Energy formula: | $FWHM(E) = 0.69 + 0.03358\sqrt{E}$ |
| Equation Resolution Energy formula: | $L(E) = \ln(947.9/E)$ |
| $e(E) = e^{-3.485+0.7744l-0.1272l^2-0.07285l^3+0.1033l^4-0.03746l^5}$ |

$c =$ channel; $E =$ energy; $e =$ efficiency (counts/gamma).  

b. Takasaki Station uses SAUNA technology, with an estimated 3-10% acquisition time error and has the following calibration data:
Table 3. Beta Energy to Channel Calibration equation.

| ID: | EN-B-4851729 |
|-----|--------------|
| Energy Units: | keV |
| Calibration Updated: | YES |
| Calibration Creation Date: | 2007-02-22 12:09:53.89 |
| Equation formula: | \( C(E) = t_0 + t_1 E + t_2 E^2 \) |
| Equation coefficients: | [-6.56097913, 0.37012004, -6.971E-5] |

Table 4. Gamma Energy to Channel Calibration equation.

| ID: | EN-G-4857339 |
|-----|--------------|
| Energy Units: | keV |
| Calibration Updated: | YES |
| Calibration Creation Date: | 2007-11-24 12:09:53.89 |
| Equation formula: | \( C(E) = t_0 + t_1 E + t_2 E^2 \) |
| Equation coefficients: | [0.19391035, 0.37240597, -3.988E-5] |

According to [5, 9, 11, 25] it is estimated that the quantity of \(^{137}\text{Cs}\) released in the period from 12 to 22 March 2011 was in the order of \(10^{14}\text{Bq} / \text{s}\) listed in the table below.

Table 5. Release fractions and estimated released activities from some sources.

| Source | \(^{137}\text{Cs}\) (PBq) |
|--------|----------------|
| STOHL  | 36.6 |
| MELCOR (Gauntt et al., 2001) | 16.4 |
| ZAMG   | 66  |
| ISRN   | 30  |

And after inversion, we get to \(17 \times 10^{14}\text{Bq} / \text{s}\) using FLEXPART which is the model used by CTBTO for verification purposes. Therefore and with the release source determined we started the CFD simulation as we benchmarked before validating the setup in Ansys.

Thus, to validate the work performed, we reproduced the simulation of [3] by the CFD tool through the Discrete Phase Model (DPM) model.

Using ANSYS SpaceClaim for 3D and 2D geometry modeling of a rough representation of the Fukushima Daichi nuclear plant, illustrated in Figures 3 and 4, the ANSYS-Mesh for the discretization of the mesh, illustrated in Figures 5 and 6, ANSYS- Fluent, for the physical definition and solution of the problem through the law of conservation given by equation 1, below:

\[
\frac{\partial \rho \phi}{\partial t} + \frac{\partial \rho u_i \phi}{\partial x_i} = \frac{\partial}{\partial x_i} \left( \Gamma \frac{\partial \phi}{\partial x_i} \right) + [S] \phi
\]  

(2)

On what:
- I represents the accumulation term or the rate of change of magnitude \(\phi\), over time which is maintained when the analysis is transient and is nullified in the stationary analysis;;
- II represents the advective transport term;
- III represents the term diffusive transport
- IV represents the term source;
- \(\rho\) is the specific mass;
- \(t\) is the time;
• $x_i$ generically represents the Cartesian direction;
• $u_i$ represents the velocity vector component along the $i$ direction;
• $\phi_i$ is the quantity to be conserved;
• $\Gamma$ is the diffusividade da grandeza conservada no meio;
• $S^d$ it is the diffusivity of the greatness conserved in the middle;

Figure 3. Geometry 3D Fukushima Daichi Unit 1.

Figure 4. Geometry 2D.

The model in the Eulerian approach for the continuous phase and the Lagrangian approach for the dispersion phase establishing the DPM for particle evaluation and dispersion. The turbulence was resolved using a $k-\varepsilon$ RANS approach in the presence of obstacles to observing the recirculation effects generated around the obstacles that are not considered by the CTBTO model.
The dose obtained due to air inhalation ($E_{inh}$) and the dose due to radioactive cloud immersion ($E_{im}$) for the $^{137}$Cs was calculated using the equations below:

$$ E = \sum_i E_{inh} + E_{im} $$

On what

$$ E_{inh} = C_A R_{inh} DF_{inh} $$

$$ E_{im} = C_A DF_{im} O_f $$

Where:

The dose due to inhalation ($E_{inh}$) and radioactive cloud immersion ($E_{im}$) is measured in Sv, the concentration of $^{137}$Cs in air is measured in Bq/m$^3$ and the inhalation rate ($R_{inh}$) is given in m$^3$ / year and the Inhalation ($DF_{inh}$) and Immersion ($DF_{im}$) coefficients are measured Sv/Bq and $e O_f$ is the fraction of the year in which the critical group is exposed. And it was calculated from March 13 to 18, 2011 period adopted for inversion of data collected at the radionuclide station.

4. Discussions and Results

The use of FLEXPART returned a measurement estimate of 46% below that found by [25], 24.8% below found by [5] and 56.6% below found by [11] however very close to that found, according to the temporal form of MELCOR [9].
With the emission source determined and after validating the simulation, it was decided to conduct the other simulations in the 2D model to reduce the computational effort, for example the 3D model has about 57 times more elements than the 2D model.

Since for concentration profile analysis, near-obstacle recirculation zone analysis and dose calculation and others along the plane have no impact on the results.

After release into the atmosphere, radionuclides undergo downwind (advection) and mixing (turbulent diffusion) processes. Radioactive material will also be removed from the atmosphere by wet and dry soil deposition and radioactive decay illustrated in Figures 7 and 8.

**Figure 7.** The most important processes affecting the transport of radionuclides released to the Atmosphere [1].

**Figure 8.** Air flow velocity around a building, showing the vortex zone.

And the presence of buildings and / or other obstacles will disturb airflow through the three zones around the building / obstacles illustrated in figures 9 and 10 below.
Figure 9. Air flow around a building, showing the three main zones of flow: displacement zone, wake zone and cavity zone [1].

Figure 10. Air flow velocity around a building, showing the recirculation zone.

The concentration of the radioactive cloud from the launch point to the distance of 1.6 km is illustrated in figure 11. It represents well the advection and diffusion stages until the moment of its deposition in the ground.
At the end of the simulation, a line was drawn at a height of 30 m, as shown in Figure 11, to calculate the cumulative dose ($E$) from air inhalation ($E_{inh}$) and radioactive cloud immersion ($E_{im}$) for $^{137}\text{Cs}$. Illustrated in Figures 12 and 13.

Thus the dose level decreases as the distance from the emission source. Being the highest dose characterized by the adult (133 Sv) and (21 Sv) that is close to the reactor emission source.

For the determination of the source variable by the inversion method and consequently the levels of radiological cloud concentration, dispersion velocity and dose were taken into account the uncertainties estimates in table 6 below:
Table 6. Uncertainty Estimate type A.

| Source | Concentração Nuvem | Velocity | Dose for adults | Dose for infants |
|--------|--------------------|----------|----------------|-----------------|
| 1,28x10^{13} | 0,02               | 0,03     | 0,19           | 0,16            |

5. Conclusion
The estimate found for the $^{137}$Cs release rate in FLEXPART may have been below the values referenced in Table 2. Due to the non-consideration of important information such as Japan's complex topography, radionuclide emission time correction during the blast phase reactors and the low number of stations studied for the collection of measurements, perhaps needing to implement in the setup reducing the previous simplifying hypotheses. And improving its accuracy in determining emissions is a very important and key point for CFD simulations to return measurements closer to the real.

The use of computational fluid dynamics for the calculation of atmospheric dispersion was an additional tool that allowed a more realistic simulation of terrain conditions and showed the ability of this tool to model radionuclide atmospheric dispersion problems. Providing with better accuracy the level of concentration, deposition, dose, temperature, and others across the terrain, unlike Gaussian models.

Future implementations of this work will follow the analysis line with other turbulence models and the insertion of radionuclide transport over the water surface.

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