

## Application of CHARM<sup>®</sup> for studying chemical dispersion due to accidental release

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### Abstract

The EPA risk management program (RMP, Rule 112r) requires hazard assessment and emergency response programs. To assure that you have adequate resources and that plans are well organized for any contingency, you need to plan for emergency response. Should such an accident occur, you need real time data to guide the response activities (CHARM – *Software, when realism counts*, [www.charmmodel.com](http://www.charmmodel.com)). An example given in this paper helps the planner to understand how dispersion modelling can help to guide response activities. There are two versions of CHARM; the first deals with a flat terrain and second deals with a complex terrain. Both use different types of algorithms. In a flat terrain, release is simulated as it simulates a series of puffs, while in a complex terrain, release is determined by the fundamental equations of Navier-Stokes. The CHARM<sup>®</sup> software is an application that calculates the movement and concentration of airborne plumes from released chemicals; thermal radiation impacts from fires; and overpressures from mechanical and vapour cloud explosions. In this paper the complex terrain version of CHARM is being used and instantaneous release of 50 kg Chlorine is being considered to explain the simulation process. It is worth mentioning that hazard assessment could be done in a cost effective manner using data mostly available free of cost, like satellite images, digital elevation model, digital surface model, chemical properties of released chemicals, surface roughness data and meteorological parameters.

*Keywords:* CHARM, Complex Hazardous Air Release Model, dispersion model, hazard assessment, chemical release, accidental release, complex terrain, Chlorine.



## 1 Introduction

It is always a matter of concern for strategic planners as well as those involved in emergency response planning that what will be the extent of any potential release for specific period of time. Sometimes they require monitoring the actual scenario to guide the response activities. People involved in disaster management also like to see visual impact on map for rescue operations and evacuation plans through identification of potential hazard zone so that priority areas for their operation could be marked. There are several models available which can be used to address the answer such type of questions and CHARM<sup>®</sup> is one of them. CHARM<sup>®</sup> (Complex Hazardous Air Release Model) is sophisticated modelling software and it requires several sets of data to perform effective simulation and using resource mostly available free of cost how it would be done is main aim of this paper.

## 2 Materials

### 2.1 Satellite base map

A base map of any point of interest can be downloaded through Google Earth<sup>®</sup>. This is the requirement to visualize the scenario and to see the extent of dispersion. Other software like Bing<sup>®</sup> and Yahoo maps<sup>®</sup> may be used. Depending upon the requirement of the task free available images can fulfil the most of the requirements. If someone needs very high resolution images then are available on cost for almost entire World. Downloaded maps through Google Earth or through any other free resources are normally in the form of JPEG and hence not geo-referenced. To make them geo-referenced CHARM<sup>®</sup> provides CharmEd (as a part of its installations files) for geo-referencing. Under 'map definition' option user can define point, scale, map location and release location.

Alternatively, a mapping program CHARMInetMaps can be used. This mapping software can be downloaded from CHARM website as a freeware. Maps downloaded through CHARMInetMaps are geo-referenced by default. CHARMInetMaps facilitates to download satellite images either from Google, Yahoo and Bing with several scales of spatial resolutions to fit in user requirement. The saved maps can be opened directly into CharmEd or in CHARM<sup>®</sup> main program.

### 2.2 DEM (digital elevation model)

DEM is used in the model to depict actual terrain information to have factual picture about the land. It can be downloaded from mapping resource sites. DEM with 30 meter resolution is available free of cost in the format which is compatible with latest version of CHARM and can be downloaded from the GDDEM website [4].



### 2.3 Google sketchup file

Google sketchup<sup>®</sup> software can be used to draw 3D buildings. Alternatively several sketchup models are available to download from Google Trimble data warehouse [5]. The Google Sketchup community is uploading 3D buildings constantly from round the globe and anyone may find them for their own area of interest. Google building maker software can also be used to draw 3D buildings but unfortunately it will be retired June 1, 2013 [6]. In this paper, DEM is being considered while sketchup files are not being used.

### 2.4 Surface roughness data

Surface roughness is a measure of the interaction between the wind and the surface [7]. It affects wind speed with altitude. A single file for Surface Roughness for the entire world can be downloaded from the USGS website [8]. This is called GLCC (global land cover characterization) data. Some examples of surface roughness are mentioned in Table 1.

Table 1: Surface roughness examples [9].

Surface	Roughness (cm)
Smooth mud flats; ice	0.001
Smooth snow	0.005
Smooth sea	0.02
Level desert	0.03
Snow surface; lawn to 1cm high	0.1
Lawn, grass to 5 cm	1–2
Lawn, grass to 60 cm	4–9
Fully grown root crops	14
Parkland, bushes	50
Large obstacle; suburb, forest	50–100

### 2.5 Meteorological parameters

CHARM<sup>®</sup> requires meteorological information like ambient temperature, pressure, wind direction, wind speed and stability class. This information of any station can be entered in several ways. It can be either entered manually in main CHARM data input screen. Once data is entered it can be saved as met file with .met extension and saved met file can be opened next time. Meteorological data can be acquired through other sources like Portable Meteorological station and through National Weather Services (NWS) website [10]. NWS weather information hourly basis and CHARM update its plume too whenever meteorological information changes. But to excess NWS data directly from CHARM there is a need to have meteorological interface software MetInter but

this is not free of cost. On the other hand manual entry of meteorological information can be used as a substitute.

## 2.6 Chemical parameters

Physical properties of chemicals as well as physico-chemical properties play a key role to simulate the release. Fortunately CHARM is available with required properties of 200+ chemicals. These properties include mol. weight, boiling point, melting point, triple point temp. and pressure, critical temp., pressure and volume, heat of vaporization, surface tension of liquid phase, liquid density, vapour heat capacity etc. A minimum amount of chemical data is required to perform a simulation. If more data is provided, other impacts such as fires and explosions can also be calculated.

## 3 Methods

### 3.1 Acute exposure guideline levels

The AEGL (acute exposure guideline levels) are needed to be set first. The NAC (National Advisory Committee), USA developed AEGL for high priority toxic chemicals [11]. The three AEGLs for Chlorine are given in Table 2. These levels can be set through Isopleth concentration within CHARM.

Table 2: AEGL for Chlorine.

Guideline	Threat type	Quantity in ppm against exposure time				
		10 min	30 min	1 hr	4 hrs	8 hrs
AEGL-1	Discomfort, non disabling	0.5	0.5	0.5	0.5	0.5
AEGL-2	Irreversible long lasting	2.8	2.8	2.0	1.0	0.71
AEGL-3	Life threat or death	50	28	20	10	7.1

### 3.2 Base map

CHARMInetMaps is being used to download map for selected area. As already discussed that map downloaded through CHARMInetMaps are geo-referenced by default. Figure 1 is a ready to use map downloaded through CHARMInetMaps and it is geo-referenced. Map is now opened in CharmEd for further processing.

### 3.3 DEM

DEM (digital elevation model) of 30m resolution was downloaded from GDEM website and then viewed under grid option within CharmEd. It is noted that the



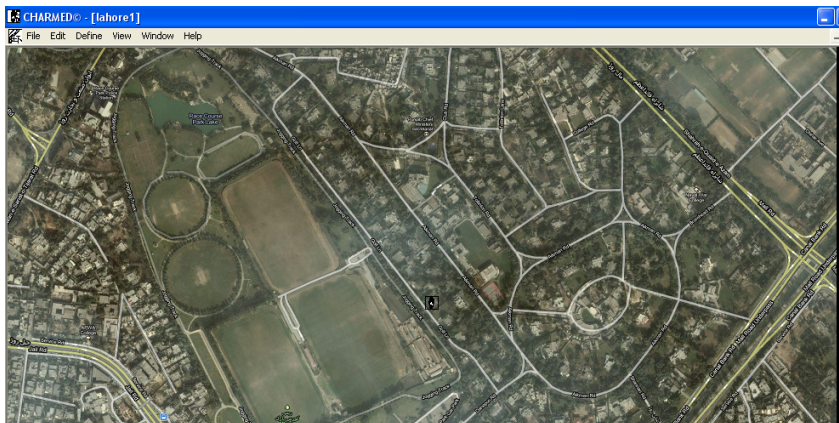


Figure 1: Map of selected area downloaded through CHARMInetMaps.



Figure 2: Each grid showing DEM (digital elevation model) projection.

map has been divided in block as each block represent single value of elevation in Figure 2. Grid size is adjustable and can be customized.

### 3.4 Surface roughness data

Surface roughness data can be entered by simply selected GLCC data file within CharmEd. It is noted that each grid represents surface roughness value similar to the DEM value. Now both DEM and surface roughness can be viewed by selecting relevant option. By double clicking on any grid user can see detail analysis of surface roughness. This option is also available with screen showing DEM.



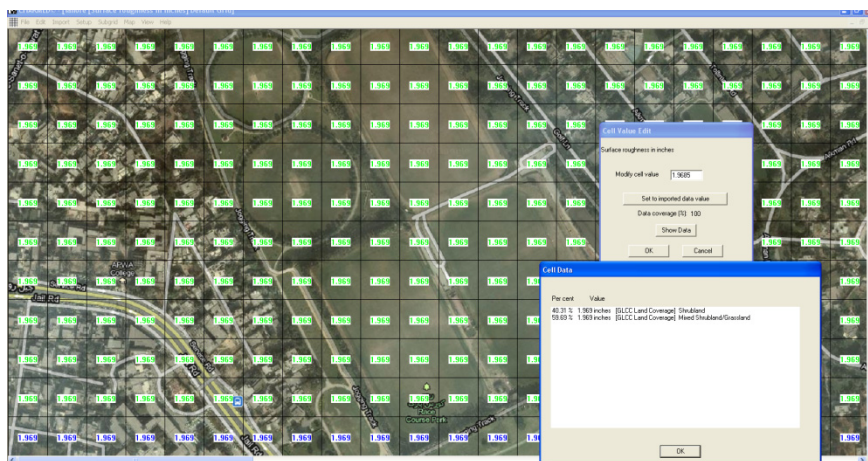


Figure 3: Each grid represents surface roughness value.

### 3.5 3D view

Just to check the grid, DEM and map adjustment before actual simulation run we may use 3D view option of CharmEd. We may increase Z-scale to zoom elevations.



Figure 4: 3D view to show DEM impact.

## 3.6 Main CHARM application

### 3.6.1 Data input screen

CharmEd is used for mapping, geo-referencing, release location, DEM and surface roughness views and edits. Final output file then saved in .grd format which would be ready to use file for main CHARM application for simulation.

Main CHARM requires some data input related to release like chemical to be release, release type for e.g. instantaneous release, response output, amount of release, location, isopleth conc., release height, initial emission rate, source

diameter etc. and other site related info. It is noted that Lat. Long information in is also required which can be set by selecting map file which is already geo-referenced or could be entered manually in CHARM data input screen mentioned in Figure 5. CHARM requires .grd file or DEM and surface roughness data while meteorological information is also required. Using all these data mentioned CHARM performs simulation.

```

Version 11.3.0.29
Title: Standard CHARM Run - Chlorine
Species: Chlorine
Species Surface Deposition Efficiency: 0
Release Type: User Specified After-Release Conditions
Emergency response output: Plume
Location: 55° 54.2672' N, 3° 9.3497' W
Isoleth Concentrations (ppm): 0.5 , 2 , 20
Release Height Above Ground 0 ft
Instantaneous Release
Amount Released: 500 pounds
No particle distribution defined
Exit Temperature assumed to be ambient or boiling pt.
Source Diameter: 10 ft
Emission moving opposite of wind direction
Vertical Angle of Release: 90°
Exit Speed (Calculated): 0 m/s
Exit state assumed vapor
Droplet Mass Fraction: 0
Molar Water Vapor Fraction: 0
Molar Air Fraction: 0
*****
Additional Release Data
None
*****
Grid Data
Title: Default Grid
Min Altitude: 23 ft, Max Altitude: 49 ft
Min Roughness: 0.01811 in, Max Roughness: 7.87402 in
Hx = 59, Hy = 34, HZ = 15
Dx = 100 ft, Dy = 100 ft, Dz = 10 ft
SW Corner at 55° 53.8627' N, 3° 9.7194' W
Subgrids
None
*****
Chemical Reactions
None
*****
Additional Met Site Data
None
*****
Met Data
Title: Standard CHARM Met

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Figure 5: Main CHARM window with all entered parameters.

### 3.6.2 Plume output

CHARM output shows dispersion pattern considering all factors including DEM and surface roughness. After performing scenario calculations for after one hour of instantaneous release is give in Figure 6 and 3D in Figure 7. Due to the prevailing wind the release move away in downwind direction from release location. One can see the entire area which has been affected during the accidental release even the dispersion has moved away and this support activity for those interested in emergency response and evacuation, hazard assessment, and prophylaxis measure. Figure 8 shows integrated affected area and its 3D version in Figure 9.

Figure 6 is an example view to understand the importance of spatio-temporal information of release which not only supports those involves in response plan but also for those who would like to estimate the impact of disaster. Movement of release in downwind direction showing importance of Terrain as well as surface roughness which depict picture close to real situation. CHARM can display information for each second or minutes. Green area is representing for AEGL-1, Yellow for AEGL-2 and Red for AEGL-3. Figure 7 shows a graphical representation showing maximum distance graph for all three types of conc. after 30 minutes of runtime.



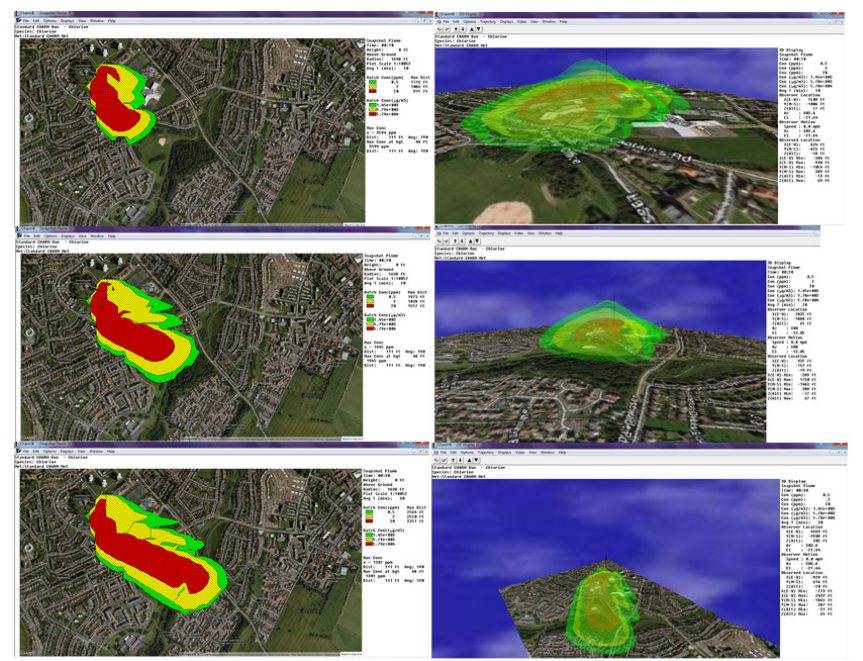


Figure 6: 2D and 3D views of instantaneous release of 500 pounds of Chlorine after 10 min, 20 min and 30 min of release. Shaded area showing AEGL limit values for 1 hour as given in Table 2.

## 4 Discussion

Maximum distance covered by Chlorine release after 30 minutes is shown in figure 8 is 636 m for AEGL-3 (20 ppm for 1 hour of release), for particular set of meteorological parameters, terrain and surface roughness. Definitely the release distance would be different for different sets of meteorology, DEM and surface roughness. Hence CHARM is a good support tool for response plan and activities. Many online resources mentioned here to explain that CHARM is cost effective and easy to implement system to see impact of hazardous chemical release. Through dispersion software CHARM<sup>®</sup> and acquisition of several layers of data one can visualize on one click the extent of release and able to notify relevant authorities. The CHARM<sup>®</sup> software can be downloaded from for trial period. MetInter is meteorological software and this is not free software alternatively meteorological parameters can be entered manually through CHARM main data input screen under Met parameter section. Met parameter



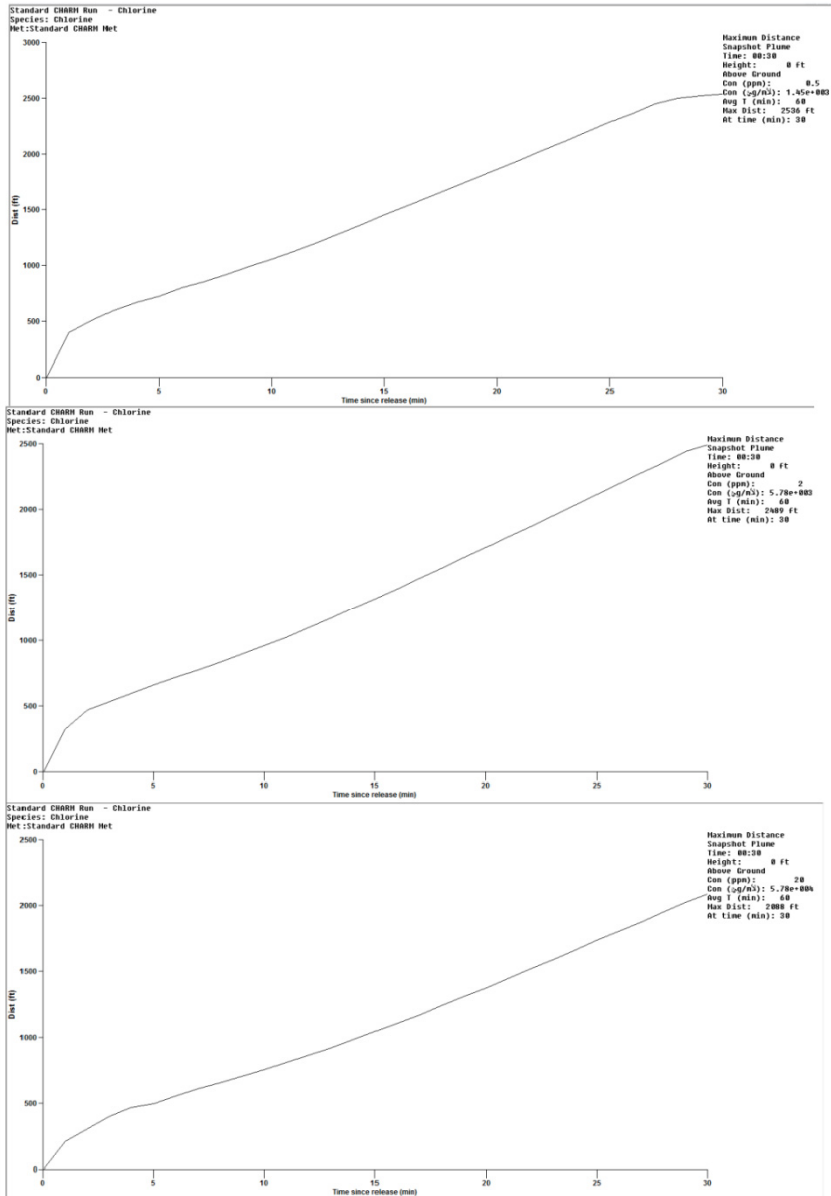


Figure 7: Maximum distance graph for 0.2, 2.0 and 20 ppm of inst. release of Cl.



Standard CHARM Run - Chlorine			Standard CHARM Run - Chlorine		
Species: Chlorine			Species: Chlorine		
Met:Standard CHARM Met			Met:Standard CHARM Met		
Maximum Distance Table			Maximum Distance Table		
Snapshot Plume			Snapshot Plume		
Time: 00:30	Height:	0 ft	Time: 00:30	Height:	0 ft
Above Ground			Above Ground		
Conc(ppm):	0.5	Conc(ug/ml): 1.45e+003	Conc(ppm):	2	Conc(ug/ml): 5.78e+003
Avg T (min):	60		Avg T (min):	60	

Time (min)	Distance	Distance	Time (min)	Distance	Distance
1	396 ft	121 m	1	321 ft	98 m
2	508 ft	155 m	2	468 ft	142 m
3	598 ft	182 m	3	532 ft	162 m
4	671 ft	205 m	4	593 ft	181 m
5	725 ft	221 m	5	656 ft	200 m
6	801 ft	244 m	6	717 ft	219 m
7	856 ft	261 m	7	770 ft	235 m
8	918 ft	280 m	8	832 ft	254 m
9	989 ft	301 m	9	892 ft	272 m
10	1056 ft	322 m	10	956 ft	292 m
11	1126 ft	343 m	11	1023 ft	312 m
12	1203 ft	367 m	12	1092 ft	333 m
13	1283 ft	391 m	13	1167 ft	356 m
14	1367 ft	417 m	14	1242 ft	379 m
15	1451 ft	442 m	15	1318 ft	402 m
16	1534 ft	468 m	16	1394 ft	425 m
17	1617 ft	493 m	17	1474 ft	449 m
18	1699 ft	518 m	18	1554 ft	474 m
19	1781 ft	543 m	19	1632 ft	497 m
20	1864 ft	568 m	20	1710 ft	521 m
21	1946 ft	593 m	21	1790 ft	546 m
22	2030 ft	619 m	22	1870 ft	570 m
23	2113 ft	644 m	23	1953 ft	595 m
24	2200 ft	670 m	24	2033 ft	620 m
25	2286 ft	697 m	25	2112 ft	644 m
26	2363 ft	720 m	26	2196 ft	669 m
27	2449 ft	746 m	27	2279 ft	695 m
28	2499 ft	762 m	28	2356 ft	718 m
29	2524 ft	769 m	29	2439 ft	743 m
30	2536 ft	773 m	30	2489 ft	759 m
30	2536 ft	773 m [MAX]	30	2489 ft	759 m [MAX]

Standard CHARM Run - Chlorine		
Species: Chlorine		
Met:Standard CHARM Met		
Maximum Distance Table		
Snapshot Plume		
Time: 00:30	Height:	0 ft
Above Ground		
Conc(ppm):	20	Conc(ug/ml): 5.78e+004
Avg T (min):	60	

Time (min)	Distance	Distance
1	210 ft	64 m
2	304 ft	93 m
3	398 ft	121 m
4	467 ft	142 m
5	496 ft	151 m
6	552 ft	168 m
7	607 ft	185 m
8	656 ft	200 m
9	705 ft	215 m
10	754 ft	230 m
11	809 ft	247 m
12	863 ft	263 m
13	914 ft	279 m
14	980 ft	299 m
15	1043 ft	318 m
16	1105 ft	337 m
17	1170 ft	357 m
18	1241 ft	378 m
19	1310 ft	399 m
20	1375 ft	419 m
21	1448 ft	441 m
22	1522 ft	464 m
23	1589 ft	484 m
24	1660 ft	506 m
25	1737 ft	529 m
26	1807 ft	551 m
27	1872 ft	571 m
28	1951 ft	595 m
29	2022 ft	616 m
30	2088 ft	636 m
30	2088 ft	636 m [MAX]

Figure 8: Tabular view shows maximum distance table for 0.2, 2.0 and 20 ppm.



once entered can be saved and recalled. Average met. Parameters for a day or a month round a year can be noted down from any meteorological website. Climatic data (30 years averages) monthly averages can also be used for approximation as most of the time average values could be used as projected weather except in those days when weather behaves abruptly. If meteorological parameters keep changing then it is better to get real-time data to see the dispersion effect with changing weather conditions. For this purpose Meteorological data from NWS (National Weather Service) can be imported directly into CHARM through software MetInter (meteorological interface). This data update on hourly basis and update the plume consequently. The CHARM comes up with required parameters of 200+ chemicals of industrial use. DEM of 30m was downloaded from Aster GDEM website. Also downloaded 1km surface roughness data GLCC (Global Land Coverage Classification) from GLCC website. Satellite images served as backdrop were downloaded through Google Earth® or through CHARMInetMaps. CHARMInetMaps is provided by CHARM Inc. Google Earth® images are readily available for use without cost for such scholarly and not for profit purposes (including educational activities or scholarly publication) through the 'fair use' clause of the Google permission guidelines, provided that appropriate attribution is given by reprinting the copyright attribution text and Google logo [12]. Another consideration is that Google Earth imagery is not updated in real-time and the imagery may or may not represent all physical features and construction if done after the date mentioned within Google Earth imagery. The geo-referencing of images is required which can be done through ArcGIS or Erdas Imagine. CHARMInetMaps is free software and can be downloaded from CHARM website to get imageries of any area of interest. The software has an option to get imageries from any of the resources like Google, Bing and Yahoo. The other benefit is that these imageries are already geo-referenced for CHARM and no need to geo-reference them.

The maps with dispersion pattern provide reality picture and minute information for refuge operations, disaster management authorities and planners to intervene the situation with cost effective and efficient manner. The final product i.e. maps showing dispersion pattern can be export in the format compatible of Google Earth so that viewer can view visual impact of scenario on Google Earth. It is noted that both 2D and 3D of impact can be saved in CHARM so that viewer can visualize both type of impacts.

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