CTBTO_WMO_SEA Software Requirements Specification

This document defines the requirements for the CTBTO_WMO_SEA software development. These requirements will be used as the basis for design and acceptance testing. Both functional and non-functional requirements are defined. The functional requirements define the tasks the software shall perform; its interaction with other systems; and its capability to protect data. The non-functional requirements define the required level of performance; the resources that may be used; ease of use; ease of maintenance; and its capability to run in different environments.

Summary

CTBTO_WMO_SEA is a software package that covers all functionalities required to support the efficient operation of the CTBTO_WMO response system in particular in context of special analysis of interesting events with known geo-temporal references as derived from the various seismic and infra-sound event bulletins available to the PTS.

The capabilities of the software package address two major purposes: (i) to conveniently initialize and conduct forward ATM calculations to predict the evolution of the plume that would result from a release at the configurable release point including the diagnosis of the related synthetic nuclear measurement scenario in the IMS network, and (ii) to allow for automated and operational collection, inter-comparison, source location analysis and web reporting of the backtracking calculation data received from external meteorological centres on basis of the CTBTO-WMO response system.

In dependence of the event regarded, the software addresses many CTBT relevant use cases alike the performance of expert technical analysis on request of a member state, special event analysis for known CTBT relevant events (alike DPRK1 and DPRK2), CTBTO-WMO response system and National Data Centres Preparedness exercises, and the validation of the PTS ATM software.
Document history

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<th>Version</th>
<th>Date</th>
<th>Author</th>
<th>Description</th>
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<tr>
<td>1.0</td>
<td>23 Sep 2009</td>
<td>Andreas Becker</td>
<td>Version 1.0 attached to the RFP</td>
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1. SCOPE

1.1. Identification

This document applies to the CTBTO_WMO_SEA software Version 1.0.

1.2. Rationale

The CTBTO_WMO_SEA software development project is performed in order to cover for two major requirements:

1. Improve PTS capabilities in forward atmospheric transport modelling for special event analysis (SEA) or Expert Technical Analysis (ETA) kind of activities of the PTS (e.g. those post DPRK1 and DPRK2 events)\(^1\).
   - Events that qualify for this can be identified by the PTS for its own purposes (e.g. forward modelling of event with known geo-temporal references alike DPRK1/2 or volcanic eruptions) but also at any time by member states in context of an ETA or NDC preparedness exercise (NPE), the latter being pursued at least once a year.
   - Current ATM tools available are scientifically sound (state-of-the-art) but need substantially enhanced integration in operational workflows, in order to minimize the demand on human resources during their operation.
   - The tools need improved pre- and post-processing capabilities, so forward ATM exercises can be conveniently operated via a web page hosted graphical user interface and results alike synthetic RN detection scenarios can be parsed for further processing, for example to trigger the CTBTO-WMO response system or for integration in standard mapping tools alike GoogleEarth or the PTS interactive (batch mode) analysis tool WEB-GRAPE (SRS2KML).

2. Enhance and consolidate PTS in-house software in use for the CTBTO-WMO response system and data fusion exercises alike NPE’s
   - The current software applications in use require substantial human resources interaction and attention in order to collect and analyse data received from WMO centres during utilization of the response system, e.g. during NPE’s or for every Level 5 categorized RN detection.
   - The PTS software currently in use to create reporting web-pages is in an ad hoc status, with very limited maintainability and portability.
   - There is no integration of the ad hoc reporting web page for CTBTO-WMO exercises into the IDC products web-page.

In total all the above listed deficiencies lead to an unacceptable demand on PTS human resources during SEA or SEA like PTS activities on qualified events alike DPRK1 and DPRK2 or the annual NPE’s in view of the possibility to rationalize the effort by SW based support.

The rationale of this project is thus (i) to provide software for an web page GUI controlled forward radionuclide plume scenario generator and (ii) to enhance and consolidate the CTBTO-WMO response system software.

\(^1\) DPRK1 & 2: October 2006 and May 2009 events announced by the Democratic People’s Republic of Korea
1.3. System overview

1.3.1. The four layer workflow of the PTS ATM system

The four-layered ATM software system of the PTS is rather a layered than modular structured one as the data flow is always directed towards the next higher numbered layer. The modularity, however, is in place with regard to the capability of the system to exchange tools covering functionality of one of the four layers. The layers have the following functionality assignment (with the name of IDC SW tools currently in charge given in brackets):

- **Layer 1**: Pre-Processing: Retrieval of appropriate wind-field and other input data required. (NCEPDATA, ECMWFDATA).
- **Layer 2**: Receptor oriented transport simulation (FLEXPART_5.1, HYSPLIT_4.9) with the so-called source-receptor sensitivity (SRS) fields as final result. This is covered by the SRSM-MODEL Version 1.0 package [4] that will undergo a substantial upgrade to Version 2.0 by upgrading FLEXPART to Version 8.1 by the start of this SW development project.
- **Layer 3**: Post-Processing based on the SRS fields. In doing so products pertaining to the radionuclide samples taken are calculated. This includes the several Field of Regard (SRS2FOR, processing part of plotFOR_2.1 [7]) and possible source region (PSR) products. The belonging layer 3 executables have been implemented also into the interactive analysis tool WEB-GRAPE [11].
- **Layer 4**: Visualization of the layer 3 output in both, batch mode (SRS2FOR, SRS2KML plotting part of plotFOR_2.1) and interactive mode. The latter is also covered by the interactive analysis tool WEB-GRAPE.

All these layers (see also Error! Reference source not found.) run in batch mode. Layers 3 and 4 comprise the post-processing of the core ATM results, the source-receptor sensitivity (SRS) fields being available after completion of Layer 2. The SRS fields contain almost all information required to backtrack the radionuclide (RN) measurements taken every day in the global IMS RN network to their Fields-of-Regard (FOR) and Possible Source Regions (PSR).

![Diagram of the four-layer workflow](image)

**Figure 1**: Illustration of the 4-layer workflow in the field of atmospheric transport modelling as implemented at the PTS. (Figure adopted from Fig.5 of Kalinowski et al. 2008 [2]). The final analysis tool WEB-GRAPE is also capable to export any visualization into zipped kml (=kmz) files for import into Google Earth. The SRS2KML
1.3.2. The source-receptor sensitivity (SRS) data format

Within its daily operational schedule the SRSM-MODEL package calculates for a configurable number of RN samples (Annex A) taken at one of the 79 already defined stations of the International Monitoring System the pertaining SRS fields. Each SRS field file is thus RN sample specific and consists of one header line and a number of data lines as follows:

**Header line:**

Longitude of station / latitude of station/ measurement (collection) start time / Measurement stop time [UTC] / Total mass [Bq] released in backward model / Maximum number of hours backward / Output frequency [hours] / averaging time [hours] / resolution of output grid in longitude / latitude [degrees] / station identifier [as specified in notification mail message]

**Data lines:**

Latitude of grid point / longitude of grid point / backward time step number / value of source-receptor sensitivity [identical to retro-plume concentration; Bq/m³]

**Example:**

```
-12.33 -37.00 20030131 00 20030201 00 0.13E+16 144 3 3 1.00 1.00 "RN068"
-38.00 -14.00 1 0.6063586E+00
-38.00 -13.00 1 0.1569079E+02
-38.00 -12.00 1 0.1637941E+01
-37.00 -12.00 1 0.1625708E+01
-38.00 -15.00 2 0.1696579E-01
-37.00 -15.00 2 0.1694598E-01
-38.00 -14.00 2 0.5807510E+01
-37.00 -14.00 2 0.5745895E+01
-38.00 -13.00 2 0.4009043E+02
```

Note: To yield the source-receptor sensitivities [1/m³], the values need to be divided by the total mass releases (seventh entry in the header record).

1.3.2.1. Naming conventions for SRS fields calculated in-house PTS:

Depending on the transport model that was utilized the SRS files are named as follows:

- `RNxxx.fp.YYYYMMDDhh.f5.srm.gz` (if calculated with FLEXPART)
- `RNxxx.hy.YYYYMMDDhh.h4.srm.gz` (if calculated with HYSPLIT)

So the clear text ASCII files are compressed with gzip. With RNxxx being the station ID as defined in the so-called ‘gard.dat’ configuration file (Annex A), YYYYMMDDhh the date of collection stop as assumed in the model run. In the above example, the file is named as follows:

`RN068.fp.2003020100.f5.srm.gz`

1.3.2.2. Naming conventions for comparison exercises (e.g. with WMO centres)
Depending on the meteorological centre (supplier) of the data the SRS files are named as follows:

\[ \text{RN}xxx.YYYYMMDDhh.<mcid>.txt.gz \]

Whereby the \(<\text{mcid}>\) denotes the 4-digit meteorological centre identifier. For the PTS results the \(<\text{mcid}>\) is ‘CTBT’ so the above example would be named as follows:

\[ \text{RN068.2003020100.CTBT.txt.gz} \]

### 1.3.3. The source-receptor sensitivity (SRS) data format, forward (PLUME) mode

The SRS data format can also be used to encode results from forward modelling (e.g. surface level plume concentration). The rules for the data lines are the same, therefore negative numbers are counted up in temporal forward direction.

**Header line:**

Longitude of source location / latitude of source location / release start time / release stop time [UTC] / Total mass [Bq] released in forward model / Maximum number of hours forward / Output frequency [hours] / averaging time [hours] / resolution of output grid in longitude / latitude [degrees] / station identifier [as specified in notification mail message]

**Data lines:**

Latitude of grid point / longitude of grid point / backward time step number / value of plume concentration Bq/m³

**Example:**

```
-12.33 -37.00 20030131 00 20030201 00 0.13E+16 168 3 3 1.00 1.00 "X7D22"
-38.00 -14.00 -1 0.6063586E+00
-37.00 -14.00 -1 0.6299873E+00
-38.00 -13.00 -1 0.1569079E+02
-37.00 -13.00 -1 0.1574570E+02
-38.00 -12.00 -1 0.1637941E+01
-37.00 -12.00 -1 0.1625708E+01
-38.00 -15.00 -2 0.1694598E-01
-37.00 -15.00 -2 0.1696597E-01
-38.00 -14.00 -2 0.5807510E+01
-37.00 -14.00 -2 0.5745895E+01
-38.00 -13.00 -2 0.4009043E+02
```

**Note:** If the PLUME SRS data values (fourth column) stem from a pure tracer concentration run, they can be generalized by dividing them by the total mass released yielding source-receptor sensitivity values in terms of reciprocal dilution volumes. These values can be then scaled against any assumption on the amount (activity in Bq) released during the simulated release period.

### 1.4. Document overview

This document defines solely the CTBTO_WMO_SEA Version 1.0 software requirements. These requirements will be used as the basis for design and acceptance testing.

Both functional and non-functional requirements are defined. The functional requirements define the tasks the software shall perform; its interaction with other systems; and its capability to protect data. The non-functional requirements define the required level of...
performance; the resources that may be used; ease of use; ease of maintenance; and its capability to run in different environments.

Each mandatory, testable requirement is stated using the word shall. Therefore, each shall in this document should be traceable to a documented test. Each mandatory, non-testable requirement is stated using the word will. Each recommended requirement is stated using the word should. A permissible course of action is stated using the word may. This convention is used in [12207].

This document is compliant with the Software Requirements Specification described in [DSTD].
## 2. REFERENCES

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<th>Number/Author</th>
<th>Title</th>
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<td>CTBTO/PTS</td>
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<td>9126</td>
<td>ISO/IEC 9126</td>
<td>Information technology - Software product evaluation - Quality characteristics and guidelines for their use</td>
<td>ISO/IEC</td>
<td>1991(E)</td>
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<td>2</td>
<td>Kalinowski, Becker, Saey, Tuma, Wotawa</td>
<td>The Complexity of CTBT Verification. Taking Noble Gas Monitoring as an Example</td>
<td>Complexity</td>
<td>26 March 2008</td>
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<td>3</td>
<td>Eckhardt, Stohl, Sodemann, Frank, Seibert and Wotawa</td>
<td>The Lagrangian particle dispersion model FLEXPART version 8.0</td>
<td>NILO, Norway</td>
<td>July 2009</td>
</tr>
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<td>4</td>
<td>Wotawa</td>
<td>New ATM Software layer 2; Software package SRSM-MODEL Version 1.0; Short User Guide</td>
<td>CTBTO/SRS M-MODEL/</td>
<td>10 Feb 2003</td>
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<td>5</td>
<td>AWST-TR-06/03</td>
<td>ATM Software Requirements Specification</td>
<td>IDC/ATM/S RS</td>
<td>2 July 2007</td>
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<td>Wotawa</td>
<td>New ATM Software layer 4; Automated ATM product (Field of Regard) generation and attachment to Reviewed Radionuclide Reports (RRR); Software package plot-FOR Version 2.1; Short User Guide</td>
<td>CTBT/plot-FOR V 2.1/</td>
<td>8 November 2008</td>
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<tr>
<td>8</td>
<td>PTS</td>
<td>IDC Data Base Scheme</td>
<td>IDC5.1.1 Rev5</td>
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3. FUNCTIONAL REQUIREMENTS

1. Web page GUI controlled forward plume and radionuclide scenario predictor

1.1. There shall be a web based software application that provides the GUI to initialize, configure and post-process the forward radionuclide (RN) scenario generator conveniently and in all relevant aspects.

1.1.1. As detailed with requirements 1.2 to 1.5 the GUI shall allow for configuration of all parameters essential to determine any interesting kind of forward ATM, (e.g. particle number, number of levels in output, down-scaling range for the FLEXPART receptor_conc output, etc.)

1.1.2. As a general approach the web tool shall write configuration files for the ATM forward runs with FLEXPART.

1.1.2.1. For FLEXPART there is an example web-based tool [6] described in http://zardoz.nilu.no/~andreas/publications/web_based_tool.pdf. It runs at NILO (Norwegian Institute for Air Research, Instituttveien 18, 2027 Kjeller, Norway). It is capable to post-process and visualize runs made with the Lagrangian Particle Dispersion Modelling (LPDM) FLEXPART for scientific projects and covers therefore a row of the Task 1 requirements of this TOR.

1.1.2.2. A more comprehensive example implementation, can be visited on http://www.ready.noaa.gov/ready/hysplit4.html, however for the LPDM HYSPLIT [see first section titled ‘HYSPLIT-WEB (Internet-based)’].

1.1.3. The run itself is committed by a call to a running deck script alike ‘RUNA-EVENT_ECM.csh’ (Annex B) controlling PTS implementation of FLEXPART Version 5.1

1.1.3.1. For the forward RN scenario generator to be developed for this project a new script is to be developed, that supports all modelling and visualization configurations detailed in the following requirements 1.2 to 1.4

1.2. The software shall provide for a FLEXPART forward run user interface comprising

1.2.1. A source (event) definition GUI (section) writing into the ‘RELEASES’ (see Appendix A3.4 of [3]) and ‘SPECIES’ (A3.6 of [3]) configuration files

1.2.1.1. For the source initialization the GUI of the tool shall offer configurable choices of seismic and infra-sound event lists alike SEL1,2,3, REB, SSEB, or infra/volcano events from the IDC data base.

1.2.1.1.1. Suitable scripts to retrieve these lists from the IDC data base into clear text ASCII files can be provided by the Commission.

1.2.1.2. An automatic update mode shall be possible, restarting the model when the same seismic or infra-sound event is re-analysed. (e.g. SEL1 -> SEL3 -> REB) by tracking of the information related to the unique EventID.

1.2.1.2.1. To fulfil requirement 1.2.1.2 the event lists of requirement 1.2.1.1 should also feature the EventID in addition to the OriginID.

1.2.1.3. Alternatively the tool shall allow for forward runs from user-selectable locations.

1.2.1.3.1. The select process for the geo-temporal source location shall be supported via a mapping tool.

1.2.1.3.1.1. FLEXPART allows for application of simple source geometries by provision of the coordinates required to describe a point, line,
1.2.1.3.1.2. The mapping tool should facilitate provision of these source object edge coordinates as follows

1.2.1.3.1.2.1. For a point source a left click on the map shall immediately define the coordinates, whereby a right click on a map shall open a dialogue for the user where the calculated horizontal coordinates (latitude; longitude) can be adjusted (fine tuned) and confirmed

1.2.1.3.1.2.2. For line source the same as for requirement 1.2.1.3.1.2.1 shall happen, after a line as been defined via the mapping tool

1.2.1.3.1.2.3. For an area the same as for requirement 1.2.1.3.1.2.1 shall happen, despite the fact that now the SW and NE corners of the box are defined in two records by dragging and dropping.

1.2.1.3.1.2.4. The user shall be offered a check-box to assign in addition also a vertical range to the area chosen, yielding a volume source definition. Again an editing step shall be available, in between to confirm the calculated volume source borders (SW, NE corner, lowest and highest elevation)

1.2.1.3.1.2.5. The resulting figures including the number of particles to be used for the forward run shall be parsed into the belonging FLEXPART configuration file ‘RELEASES’.

1.2.1.4. There shall be a GUI (section) to configure the emission scenario (temporal course of the emission) and the species (half-life time) and all further source related settings configurable within the limits offered by the most recent version of FLEXAPRT 8.x, comprising standard and user-defined emission scenarios.

1.2.1.4.1. The section shall have two levels of complexity exposed to the user

1.2.1.4.1.1. In the first level there shall be only the possibility to specify the nuclide, and to switch on/off dry and/or wet deposition

1.2.1.4.1.1.1. For the nuclide it shall be possible to enter the nuclide symbol name explicitly (e.g. Xe-133). The name will be translated into the nuclide specific half-life time (via a lookup table offered by the commission). If ‘Tracer’ is given, a zero half-life time shall be applied (indicated by a ‘999.9’ in the configuration file ‘SPECIES’)

1.2.1.4.1.1.2. For dry and wet deposition binary switches (check boxes) shall be offered. If they are checked, reasonable default values for radionuclides shall be applied.

1.2.1.4.1.2. On the second level, the user shall be exposed to the entire SPECIES_nnn file(s) to be examined. The file shall contain already the settings made in level one and start from reasonable default values.

1.2.1.4.1.3. The user is expected to make educated decisions, while directly editing into the SPECIES draft file via a text editor in the GUI section.

1.2.2. A GUI (section) to configure the topology of the output grids writing into the ‘OUTGRID’ configuration file (see Appendix A3.2 of [3])
1.2.2.1. As for the source configuration, (requirements 1.2.1.3) the grid topology selection process shall be supported via a mapping tool.

1.2.2.2. The user shall be allowed to define mother and nested grids. For the mother grid there shall be always the option to select a global grid.

1.2.2.3. The grid section selection shall work similar as for the area source definition described in requirement 1.2.1.3.1.2.3

1.2.3. **A GUI (section) to define the active receptor locations being written into the RECEPTORS configuration file** along with the requirements of FLEXPART (see A3.3 in [3]).

1.2.3.1. There shall be a Network Definition GUI where the user can configure the receptor locations, he/she likes to examine during the forward run.

1.2.3.1.1. The Network Definition GUI shall make use of a clear text file comprising the so-called ‘gard.dat’ configuration file for PTS ATM Layer 2 calculations. (Example file will be provided by the PTS).

1.2.3.1.2. If the forward model is started, the RECEPTOR file shall be updated according to the latest version of the gard.dat file. An example script ‘update_receptors.csh’ (reprinted in Annex C) can be provided.

1.2.4. **A GUI (section) to configure the AGECLASS configuration**

1.2.4.1. It shall be possible to edit the AGECLASS configuration file (see A3.5 in [3]) by a click on a link to this file placed on the GUI.

1.2.5. **A runtime configuration GUI (section) re-writing and committing the COMMAND configuration file**

1.2.5.1. The GUI shall open the COMMAND file for direct editing by clicking on a respective link called ‘Edit configuration file COMMAND’. Settings are to be made according to the documentation in Appendix A3.1 in [3]

1.2.5.2. When opening the COMMAND file, settings for the beginning data and time of the simulations shall already be adjusted to the earliest source listed in the RELEASES file.

1.2.5.2.1. In doing so the beginning date shall be the nearest date & time prior to the earliest beginning date & time in the RELEASES file.

1.2.5.3. All settings of the COMMAND file shall be editable via a text edit box in the GUI section. When committing a forward run, the latest version of the COMMAND configuration file will be examined.

1.2.6. **An input meteorological field data configuration GUI (section).**

1.2.6.1. In this section the user shall be able to determine which kind of wind field (and therefore which FLEXPART executable) shall be utilized.

1.2.6.2. It shall be possible to edit the configuration file ‘pathnames’ via the GUI.

1.2.6.3. Upon completion of the edits the ‘AVAILABLE’ file shall be updated to fit to the most recent input data availability.

1.2.6.4. For the users convenience the software shall be capable to easily switch between two separate wind fields without making any further changes.

1.2.7. **Upon completion of all settings there shall be a ‘COMMIT’ button to parse all information into the FLEXPART configuration files**.

1.2.7.1. All relevant configuration files, being located under $FLEXPART-EXEDIR/options, i.e. AGECLASSES, COMMAND, RELEASES, OUTGRID, RECEPTORS, */SPECIES, shall be updated upon commitment of a forward run.

1.3. The software shall provide for a FLEXPART forward run post-processing interface.
1.3.1. The post-processing tool flexout2srs in use for post-processing FLEXPART binary output shall be integrated and generalized to allow also for storage of vertical levels other than surface level.

1.3.2. The software shall allow for post processing of the virtual RN station measurements

1.3.2.1. The virtual measurements stored by FLEXPART in extra receptor files, shall be post-processed yielding virtual sample concentrations (described in requirement 1.3.2.1.3) that can be utilized as pseudo Level 5 detections to trigger the CTBTO-WMO response system.

1.3.2.1.1. In doing so the contractor can consolidate the flexout2alertmail and flexout2notmail FORTRAN routines currently in use to develop own software to evaluate the receptor_conc output files of FLEXPART.

1.3.2.1.2. An example output of these routines looks like this

1.3.2.1.3. Files suitable to trigger the WMO-CTBTO response system are issued once per day and rather look like this

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<tr>
<th>RN-Station</th>
<th>Col-Start</th>
<th>Col-Stop</th>
<th>SampleCon[mBq/m³]</th>
<th>UTC of arrival</th>
<th>Minimum Importtime (hours)</th>
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1.3.2.2. In addition the software shall feature a forward run concentration predictor that operates directly from the grid cell values stored in the SRS data format for co-located RN stations (Export concentrations as ASCII/Excel file, automatic visualization) that operates directly from the grid cell values.

1.3.2.2.1. The PTS software utility SRS2POINTS offers this functionality and could be integrated, notwithstanding that any independent software development addressing this requirement is welcome too.

1.3.2.3. There shall be a switch to determine from which of the two above approaches virtual sample concentrations are transformed into the input files for the notification Email messages in use for the CTBTO-WMO response systems, described in requirement specification 1.3.2.1.3

1.3.3. Links to all past forward runs that are stored on a flat file systems shall also stored in a forward run data base, to facilitate identification and retrieval of past runs of users’ interest via a DB query.

1.3.3.1. The table to be defined for this purpose shall be compatible with the IDC RN data base scheme described in [8]

1.3.3.2. The table shall allow for querying past runs according to the EventID.

1.4. The software shall provide for a FLEXPART forward run visualization interface
1.4.1. The software shall be capable of plotting and storage of standard visualizations of forward runs in standard bitmap formats (png, jpg, animated gif, mpeg) on basis of the FLEXPART output in SRS format as described in requirement 1.3.1

1.4.1.1. The software shall be capable to inter-operate with the plotFOR Version 2.1 software package [7] that allows for automated generation of contour maps of the plumes in two different vector formats (postscript, or the NCARGraphics gmeta format).

1.4.1.2. plotFOR Version 2.1 makes use of the NCAR Graphics Version 4.4.1 and the ImageMagick OSS libraries, the latter for the conversion of the postscript graphs into bitmaps formats, png, jpeg and/or (animated) gif and mpeg.

1.4.1.3. The contractor is invited to utilize any other plotting library if it can be operated without any additional licenses.

1.4.2. The software shall be capable to interoperate with SRS2KML (in the -FOR PLUME mode) allowing for batch mode utilization of WEB-GRAPE functionalities.

1.4.3. The software shall be capable to parse the relevant information on the FLEXPART configuration (e.g. receptor listing file, gard.dat) into the configuration files of the plotting tools. (e.g. the gard.dat information of FLEXPART into the gard.plu file listing source and station locations considered by WEB-GRAPE/SRS2KML when plotting a FLEXPART run in PLUME mode).

1.4.4. The software shall be capable to enhance the forward ATM post-processing in order to view particle clouds in Google Earth from particle cloud dumps (particle position output FLEXPART normally utilized for the warm-start option, see Chapter 11.3 of [3])

1.4.4.1. The PARTICLE2KMZ tool to be developed for that purpose shall be capable to interoperate with the files partposit_<date> and partposit_end, FLEXPART can output if appropriate settings for the variables IPIN and MQUASILAG are made in the configuration file COMMAND (see requirements 1.2.5)

1.5. The software shall provide for a forward ATM web page reporting tool

1.5.1. The web based reporting tool shall host the daily forward scenarios after a possible nuclear test or any other special event analysis (SEA) comprising GUI section for the following purposes

1.5.1.1. Standardized display of plumes
1.5.1.2. Display of predicted concentrations at RN stations
1.5.1.3. Display of measured concentrations, if any
1.5.1.4. Version tracking and update possibility
1.5.1.5. Inter-comparison between ECMWF and NCEP-based results
1.5.1.6. Inter-comparison between forecasts from different days

2 Automated reporting tool for the CTBTO-WMO response system

2.1. Enhance software for WMO response system event notifications sent to the participating meteorological centres of the WMO response system

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2 NCAR Graphics is available for free from [http://ngwww.ucar.edu/](http://ngwww.ucar.edu/)

3 Imagemagick is available for download from [http://www.imagemagick.org/script/download.php](http://www.imagemagick.org/script/download.php)
2.1.1. Enhance PTS software that creates notifications for level-5 events to take multiple station/day events into account

2.1.2. Enhance PTS software to create notifications also for noble gas scenarios in batch mode

2.1.3. Facilitate conduction of exercises by automated creation of notification messages from forward ATM based RN scenario predictions made for exercise/test scenarios

2.2. Enhance web based scenario reporting tools for exercises and special event analysis

2.2.1. Allow for a joint reporting and post-processing of multiple RN particulate (e.g. Level 5 category samples) and noble gas radionuclide detections in one scenario (i.e. RN detections from multiple locations/times where it is possible that they originate from one EVENT)

2.2.2. The software shall monitor the automated collection of the data received in response to the request

2.2.3. The web tool shall be capable to generate WMO Centres response statistics providing a book keeping function with regard to the response rates and times of the different participating centres

2.2.4. The web tool shall be capable to generate WMO Centre comparison statistics: Consolidation of auto-reporting on the web page of the exercise, including plot generation, and integration of the standard display of MMFORs inter-comparison statistics published in [9].

2.2.4.1. Example implementations are available at

2.2.4.1.1. http://fts.ctbto.org/atm/WMO-Cooperation/Reports/SPT1-2005/

2.2.4.1.2. http://fts.ctbto.org/atm/WMO-Cooperation/Reports/exp2005/

2.2.4.2. Again the usage or integration of available tools alike SRS2KML [10] or WEB-GRAPE [11] is encouraged.

2.2.5. Integration of notification procedures with PTS forward ATM calculations (in exercise mode)

2.2.6. Integration of the information gathered into a data fusion bulleting prototype web page

2.2.6.1. Example implementations are available at

2.2.6.1.1. https://www2.ctbto.org/CTBTO-WMO_data_fusion_2008/data_fusion.html

2.2.6.1.2. https://www2.ctbto.org/CTBTO-WMO_experiment/ctbto-wmo.html

2.2.7. The software shall finally support setting of links to the Reviewed Radionuclide Reports (RRR’s) into web based report, for both the particulate and the noble gas samples that were analysed to be relevant for the source location and data fusion exercise reported.

3 Runtime Environment:

3.1. The CTBTO_WMO_SEA software shall run under UNIX/LINUX while making use of the native C and FORTRAN compiler package gcc running at the PTS.

3.1.1. The current Version of gcc is 4.1.2 20080704 (Red Hat 4.1.2-44)

4 Supported operating systems

4.1. Intel/AMD x86 32bit Linux, Kernel version 2.6.x

4.2. Intel/AMD x86_64 64bit Linux, Kernel version 2.6.x

5 Hardware requirements
5.1. The software shall be capable to execute, completely meeting all requirements besides accelerated navigation and animation, on a 2.0 GHz AMD Opteron or higher with 2048 Mb of RAM, running the Linux OS.

4. ACCEPTANCE TESTING REQUIREMENTS

6. The software will be tested in Phases 2, 4 and 5 of the project at CTBTO against the requirements as described in the updated SRS.

5. DOCUMENTATION REQUIREMENTS

7. All documentation will be written in English in MS Word format
10. New Software Installation Plan (SIP) document describing installation and configuration of the software.
11. New Software User guide, describing usage of the functionality of the software.
12. Source code will be documented in the code according to suitable standards.
13. There shall be a help function implemented that is called with a click on a ‘Help’ link located on the top left corner of the web page GUI option and upon any users’ choice of options that are non-compliant with the required syntax or inconsistent to the capabilities of the software driven by the settings of the respective configuration file.

6. SECURITY REQUIREMENTS

14. There are no specific security requirements for this software despite the normal ones applicable for any software application running at the IDC.
14.1. The software shall be capable to run under a normal PTS user account without requiring su privileges during runtime
14.2. Utilization of the software application shall not interfere with the normal automated processing of the PTS
14.3. The web page GUI is expected to run from an intranet based web server only.
14.4. Any population of results on the reporting web tool to the IDC products web page will require privileges of the web page administrator.

7. PORTABILITY REQUIREMENTS

15. The CTBTO_WMO_SEA software package shall be available as a download kit.
16. The new software can alternatively make use of other software libraries if they are Open Source and if they are shipped with the delivery.

8. PERFORMANCE REQUIREMENTS

17. Utilization of PTS forward ATM software tool FLEXPART via the web page GUI of CTBTO_WMO_SEA instead of running it from command line shall not deteriorate the performance. Hence the FLEXPART runs shall require only the same time as if they would have been started and controlled from command line based tools.
18. Acceptance requirement is the software’s capability to perform
18.1. All functional requirements stipulated in Chapter 3 of this SRS document
18.2. The forward plume calculations shall be identical to the ones calculated with command line based scripts.

18.3. Version 1 shall be capable to run from standard web browsers like Firefox Version 3.5.x or higher or Konqueror Version 3.3.x or higher available on Linux OS.

18.4. A full daily update of the reporting web page shall not take longer than 12 hours per 10x10 SRS data request examined.

10 TERMINOLOGY

Glossary

Accuracy Capability of the software product to provide the right or agreed results or effects. ISO/IEC 9126.

Adaptability Capability of the software product to be adapted for different specified environments without applying actions or means other than those provided for this purpose for the software considered. ISO/IEC 9126.

Analysability Capability of the software product to be diagnosed for deficiencies or causes of failures in the software, or for the parts to be modified to be identified. ISO/IEC 9126.

ATM layer 1 Pre-processing. Retrieval of appropriate wind-field and other input data required (NCEPDATA, ECMWFDATA).

ATM layer 2 Receptor oriented transport simulation (FLEXPART_3.2, HYSPLIT_4.6) with the SRS fields as final result.

ATM layer 3 Post-Processing based on the SRS fields. In doing so products pertaining to the radionuclide samples taken are calculated. This includes the several FOR and PSR products. The belonging layer 3 executables shall be easily accessible and utilized by WEB_GRAPE.

ATM layer 4 Visualisation of the layer 3 output in both, batch mode and interactive mode. The latter shall be covered by WEB_GRAPE.

Changeability Capability of the software product to enable a specified modification to be implemented. ISO/IEC 9126.

Coexistence Capability of the software product to coexist with other independent software in a common environment sharing common resources. ISO/IEC 9126.

Efficiency Capability of the software product to provide appropriate performance, relative to the amount of resources used, under stated conditions. ISO/IEC 9126.

Fault tolerance Capability of the software product to maintain a specified level of performance in cases of software faults or of infringement of its specified interface. ISO/IEC 9126.

Functionality Capability of the software product to provide functions which meet stated and implied needs when the software is used under specified conditions. ISO/IEC 9126.

Installability Capability of the software product to be installed in a specified environment. ISO/IEC 9126.

Interoperability Capability of the software product to interact with one or more specified systems. ISO/IEC 9126.
<table>
<thead>
<tr>
<th>Learnability</th>
<th>Capability of the software product to enable the user to learn its application. ISO/IEC 9126.</th>
</tr>
</thead>
<tbody>
<tr>
<td>Maintainability</td>
<td>Capability of the software product to be modified. Modifications may include corrections, improvements or adaptation of the software to changes in environment, and in requirements and functional specifications. ISO/IEC 9126.</td>
</tr>
<tr>
<td>Maturity</td>
<td>Capability of the software product to avoid failure as a result of faults in the software. ISO/IEC 9126.</td>
</tr>
<tr>
<td>Operability</td>
<td>Capability of the software product to enable the user to operate and control it. ISO/IEC 9126.</td>
</tr>
<tr>
<td>Portability</td>
<td>Capability of the software product to be transferred from one environment to another. ISO/IEC 9126.</td>
</tr>
<tr>
<td>Recoverability</td>
<td>Capability of the software product to re-establish a specified level of performance and recover the data directly affected in the case of a failure. ISO/IEC 9126.</td>
</tr>
<tr>
<td>Reliability</td>
<td>Capability of the software product to maintain a specified level of performance when used under specified conditions. ISO/IEC 9126.</td>
</tr>
<tr>
<td>Replaceability</td>
<td>Capability of the software product to be used in place of another specified software product for the same purpose in the same environment. ISO/IEC 9126.</td>
</tr>
<tr>
<td>Resource behaviour</td>
<td>Capability of the software product to use appropriate amounts and types of resources when the software performs its function under stated conditions. ISO/IEC 9126.</td>
</tr>
<tr>
<td>Security</td>
<td>Capability of the software product to protect information and data so that unauthorized persons or systems cannot read or modify them and authorized persons or systems are not denied access to them. ISO/IEC 9126.</td>
</tr>
<tr>
<td>Stability</td>
<td>Capability of the software product to avoid unexpected effects from modifications of the software. ISO/IEC 9126.</td>
</tr>
<tr>
<td>Stakeholder</td>
<td>Individual or organization that is affected by the system or whose input is needed in order to develop the system. Examples of stakeholders include management, project sponsor, domain area experts, technology experts, system developers, testers, users and lawyers. Robertson and Robertson (1999).</td>
</tr>
<tr>
<td>Suitability</td>
<td>Capability of the software product to provide an appropriate set of functions for specified tasks and user objectives. ISO/IEC 9126.</td>
</tr>
<tr>
<td>Testability</td>
<td>Capability of the software product to enable modified software to be validated. ISO/IEC 9126.</td>
</tr>
<tr>
<td>Time behaviour</td>
<td>Capability of the software product to provide appropriate response and processing times and throughput rates when performing its function, under stated conditions. ISO/IEC 9126.</td>
</tr>
<tr>
<td>Understandability</td>
<td>Capability of the software product to enable the user to understand whether the software is suitable, and how it can be used for particular tasks and conditions of use. ISO/IEC 9126.</td>
</tr>
<tr>
<td>Usability</td>
<td>Capability of the software product to be understood learned, used and attractive to the user, when used under specified conditions. ISO/IEC 9126.</td>
</tr>
<tr>
<td>Use case</td>
<td>A collection of possible scenarios related to a particular goal. The scenarios describe the interaction between a user and the system. Use cases were first proposed by Jacobson I. et al (1992).</td>
</tr>
<tr>
<td>Abbreviations</td>
<td>Descriptions</td>
</tr>
<tr>
<td>------------------------</td>
<td>-----------------------------------------------------------------------------</td>
</tr>
<tr>
<td>ANSI</td>
<td>American National Standards Institute</td>
</tr>
<tr>
<td>API</td>
<td>Application Programming Interface</td>
</tr>
<tr>
<td>ARR</td>
<td>Automated Radionuclide Report</td>
</tr>
<tr>
<td>ASCII</td>
<td>American National Standard Code for Information Interchange</td>
</tr>
<tr>
<td>ATM</td>
<td>Atmospheric Transport Modelling</td>
</tr>
<tr>
<td>bmp</td>
<td>Bitmap</td>
</tr>
<tr>
<td>COG</td>
<td>Centre of Gravity</td>
</tr>
<tr>
<td>CTBTO</td>
<td>Comprehensive Nuclear-Test-Ban Treaty Organization</td>
</tr>
<tr>
<td>DBF</td>
<td>Differential binary FOR</td>
</tr>
<tr>
<td>ECAL</td>
<td>SRS based forward Event Calculator</td>
</tr>
<tr>
<td>ECMWF</td>
<td>European Centre for Medium-Range Weather Forecasts</td>
</tr>
<tr>
<td>ECMWFDATA</td>
<td>ECMWF data retrieval program</td>
</tr>
<tr>
<td>eps</td>
<td>Encapsulated Postscript</td>
</tr>
<tr>
<td>FOR</td>
<td>Field of Regard</td>
</tr>
<tr>
<td>GIF</td>
<td>Graphics Interchange Format</td>
</tr>
<tr>
<td>GNU</td>
<td>GNU is not Unix</td>
</tr>
<tr>
<td>GRIB</td>
<td>Gridded Binary</td>
</tr>
<tr>
<td>GPSI</td>
<td>Global Point Source Indicator</td>
</tr>
<tr>
<td>GUI</td>
<td>Graphical User Interface</td>
</tr>
<tr>
<td>HTTP</td>
<td>Hypertext Transfer Protocol</td>
</tr>
<tr>
<td>https</td>
<td>HTTP over SSL</td>
</tr>
<tr>
<td>IDC</td>
<td>International Data Centre</td>
</tr>
<tr>
<td>IMS</td>
<td>International Monitoring System</td>
</tr>
<tr>
<td>IEC</td>
<td>International Electrotechnical Commission</td>
</tr>
<tr>
<td>IFs</td>
<td>Integral FORs</td>
</tr>
<tr>
<td>ISO</td>
<td>International Organization for Standardization</td>
</tr>
<tr>
<td>jpeg</td>
<td>Joint Photographic Experts Group</td>
</tr>
<tr>
<td>lat</td>
<td>Latitude</td>
</tr>
<tr>
<td>long</td>
<td>Longitude</td>
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<tr>
<td>NCEP</td>
<td>United States National Center for Environmental Prediction</td>
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<td>NCEPDATA</td>
<td>NCEP data retrieval program</td>
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<td>NDC</td>
<td>National Data Centre</td>
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<tr>
<td>MHz</td>
<td>Megahertz</td>
</tr>
</tbody>
</table>
ANNEX A: Example configuration files gard.dat, gard.dat.special, RELEASEINFO.DAT and RUNINFO.DAT

Configuration file gard.dat:

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<th>Latitude</th>
<th>Longitude</th>
<th>Station</th>
<th>Col. Stop</th>
<th>Rad.</th>
<th>Station name</th>
<th>Collection stop time: hhmm [UTC]</th>
<th>Radioactive decay: s [-999.9: infinite]</th>
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Configuration file **RELEASINFO.DAT**:

8 ! Number of operational Stations for daily runs
560000 ! Number of particles per station
0.0 150.0 ! Release height [m] (from - to)
1.3000E15 ! Release strength [Bq]

# Gards station file
../runspec/gard.dat
# Directory where RELEASES file is written to:
../options/

# Sites: specify collection stop time in Gards station file

Configuration files **RUNINFO.DAT(.SPECIAL)**:

# File with Release timing information
../createrelase/minmaxtime

336 ! Number of hours backward
3 ! Source-receptor (concentration) output every ??? hours

# Directory where COMMAND file is written to:
../options/
ANNEX B: Script for daily forward mode run of FLEXPART ‘RUNA-EVENT_ECM.csh’

#!/bin/csh

# SCRIPT FOR WMO Experiment FORWARD SCENARIO MODEL RUN ON THE IDC DVL LAN
#
# Automate the ATM calculations for Special Event Analysis (SEA)
#
if ($#argv == 1) then
  set eventnum=$argv[1]
else
  # Default Date: Today 0 UTC
  
  echo 'Need to define event day number (1,2,...)'
  exit
endif

#source $HOME/.cshrc

PATHNAMES - CHANGE IF NECESSARY

set RUNID = "DPRK2-GL100"

set fnameflex = "$ATMFORSEC"/flexpart51.ecmwf.forward/forward-"$RUNID"

set RELID = "X7D$eventnum"

# DON'T TOUCH ANYTHING BELOW THIS LINE
#
# synchronize RECEPTOR settings
#
# cd $ATMFORSEC/forward_scenario
# update_receptors.csh 82
#
# echo RUNA$RUNID > runNG
# echo 'started at' >> runNG
# date '+%Y%m%d %H%M%S' >> runNG
# date '+%Y%m%d' > runstamp
# echo '20090525' > runstamp
# echo $argv[1] > runstamp
# ./calcdates
# set gribend = `cat ./today+07`
# set flexana = `cat ./today`
# echo "20"$flexana >./runstamp
# CREATE AN UPDATED RELEASES FILE FOR FLEXPART
# cd $ATMFORSEC/forward_scenario/createreleaseV5
# save original RELEASEINFO.DAT file
# cp SCENARIO-SELECT.TXT SCENARIO-SELECT.BAK
# cp "$RUNID".TXT SCENARIO-SELECT.TXT
# cp "$RUNID"_X7D$eventnum”.txt SCENARIO-SELECT.TXT
# cp RELEASEINFO.DAT RELEASEINFO.BAK
# cp RELEASEINFO."$RELID"_ANA RELEASEINFO.DAT
a.out
#cp RELEASEINFO.BAK RELEASEINFO.DAT
#cp SCENARIO-SELECT.BAK SCENARIO-SELECT.TXT
cp flexdate="cat flexdatestamp"
cp RELEASES_RELEASES "$RELID"_of_$flexdate
cp collectdate="cat colstop"
set flexdate
set collectdate
#
# CREATE AN UPDATED COMMAND FILE FOR FLEXPART
cd $ATMFORSEC/forward_scenario/createcommandV5
cp CONTROL CONTROL.SAV
cp CONTROL."$RELID" CONTROL
a.out
cp CONTROL.SAV CONTROL
# EXECUTE FLEXPART
cd $fnameflex
./FLEXPART
cd $ATMFORSEC/flexpart51.ecmwf.forward/flexout2srmV5
cp CONTROL CONTROL.SAV
cp CONTROL.$RUNID CONTROL
a.out
cp CONTROL.SAV CONTROL
mkdir "/dvlscratch/ATM/PLUME_SRS_ARCHIVE/"$flexdate
mkdir "/dvlscratch/ATM/PLUME_SRS_ARCHIVE/"$flexdate/flexpart.ecmwf.ll
gzip -f -c "$RELID"*"$flexdate"srm > 
"/dvlscratch/ATM/PLUME_SRS_ARCHIVE/"$flexdate"/flexpart.ecmwf.ll/"$RELID".fp."$flex
date"00.f5.srm.gz"
# prepare receptor_conc file for plotting
cd $fnameflex/output
cp receptor_conc /tmp/receptor_conc_plot
## Calculate REC-MAILMESSAGE files with RELEASE disclosure
cd $ATMFORSEC/forward_scenario/flexrec2notmailV5
cp CONTROL.$RELID CONTROL
echo "1" > FW-success
a.out
#
# prepare send resuling receptor sample conc to email list
rm -f *0mail
cat LOCAL_REL01 >EVENTmail
cat "$RELID"_* >>EVENTmail
#
mkdir $ATMFORSEC/forward_scenario/flexrec2notmailV5/"$RELID""$flexdate
mv *.l $RELID"$flexdate
## Calculate REC-MAILMESSAGE files without RELEASE disclosure
cd $ATMFORSEC/forward_scenario/flexrec2alertmailV5
a.out
## send resuling receptor sample conc to members of email list
cat REL01_* >REL01mail
#
mkdir $fnameflex/forward_scenario/flexrec2alertmailV5/"$RELID""$flexdate
mv *.l $RELID"$flexdate
#
cd $ATMFORSEC/forward_scenario/flexrec2gmtV5
a.out
#
cd $ATMFORSEC/forward_scenario/flexrec2gmtV5/wgb_rnstat
rm -f REL*
cd $ATMFORSEC/flexpart51.ecmwf.forward/flexout2srmV5
set srsmfile = `ls -t "$RELID"*.fp.$flexdate*.srm`
set lastsrsmfile = $srsmfile
if(-e /tmp/EVENT.srm) then
rm /tmp/EVENT.srm
endif

cp $lastsrmfile /tmp/EVENT.srm
gzip -f $lastsrmfile
mv $lastsrmfile*.gz ./save

cd $ATMFORSEC/srsmplot-forward
if (-e gmeta1.ps) then
rm gmeta1.ps
endif
a.out
convert -delay 50 -trim -resize 700x700 gmetal.ps /tmp/file.gif
cp gmetal.ps /tmp/Scenario"$RELID"-ECM.$(flexdate).ps
mv /tmp/file.gif /tmp/Scenario"$RELID"-ECM.$(flexdate).gif

# Read in general configuration options
echo 'cd mailist'
cd $ATMFORSEC/configs
set maillist1 = `cat config.maila`
echo 'maillist finished'
uuencode /tmp/Scenario"$RELID"-ECM.$(flexdate).gif Scenario"$RELID"-ECM.$(flexdate).gif >EVENT_movie.u
echo "DPRK2 Event - "$RELID" - Post-Analysis Run with ECMWF wind field" >./hfa
cat ./hfa ../forward_scenario/flexrec2notmailV5/EVENTmail EVENT_movie.u >EVENT.u
set helpvar = "MAIN"
if ($helpvar == "MAIN") then mailx -s "DPRK2 Event: ECMWF based Post-Analysis Run, $RELID at $(flexdate)" $email <EVENT.uend
rm -f *.u

# Store Scenario Plot
cd $ATMFORSEC/srsmplot-forward
mv /tmp/Scenario"$RELID"-ECM.$(flexdate).ps Scenario"$RELID"-ECM.$(flexdate).ps
mv /tmp/Scenario"$RELID"-ECM.$(flexdate).gif Scenario"$RELID"-ECM.$(flexdate).gif
gzip -f Scenario"$RELID"-ECM.$(flexdate).gif

# Archive FLEXPART output
cd $fnameflex/output
if (-e /dvlscratch/ATM/forward-$RUNID) then
mkdir /dvlscratch/ATM/forward-$RUNID/ECMoutput/$flexdate
else
mkdir /dvlscratch/ATM/forward-$RUNID
if (-e /dvlscratch/ATM/forward-$RUNID/ECMoutput) then
mkdir /dvlscratch/ATM/forward-$RUNID/ECMoutput/$flexdate
else
mkdir /dvlscratch/ATM/forward-$RUNID/ECMoutput
mkdir /dvlscratch/ATM/forward-$RUNID/ECMoutput/$flexdate
endif
endif
mv grid_conc* /dvlscratch/ATM/forward-$RUNID/ECMoutput/$flexdate
mv dates /dvlscratch/ATM/forward-$RUNID/ECMoutput/$flexdate
mv header /dvlscratch/ATM/forward-$RUNID/ECMoutput/$flexdate
mv receptor_conc /dvlscratch/ATM/forward-$RUNID/ECMoutput/receptor_conc.$RUNID.$flexdate
#gzip -f /dvlscratch/ATM/forward-$RUNID/ECMoutput/receptor_conc.$RUNID.$flexdate/

# rm running file
rm -f $ATMFORSEC/forward_scenario/runNG
exit
ANNEX C: Script update_receptors.csh to update configuration of receptors (virtual RN stations) being active forward mode runs

```csh
#!/bin/csh

# This routine shall be called before the ATM production pipeline is started.
# It reads in the Gards station file and produces the needed files that control
# the model runs:
#
#    - File RECEPTORS

set gardfile = "$ATMFORSEC/gard.dat"
set gardfile = "./gardf.dat"
set receptorsfile = "$ATMFORSEC/flexpart51.ecmwf.forward/options/RECEPTORS"
set colstop_file = "$ATMFORSEC/forward_scenario/colstop_gard.dat"

set numstat = `head -1 $gardfile`
if($#argv == 0) then
    set numstat1 = $numstat
else
    set numstat1 = $argv[1]
endif

set xlonlist = `tail -$numstat $gardfile | awk '{print $1}'`
set ylatlist = `tail -$numstat $gardfile | awk '{print $2}'`
set statidlist = `tail -$numstat $gardfile | awk '{ print $3}'`
set colstoplist = `tail -$numstat $gardfile | awk '{print $4}'`
set sampltimelist = `tail -$numstat $gardfile | awk '{print $8}'`

# Read in 7-line header of RECEPTORS file
head -7 $receptorsfile > /tmp/RECEPTORS.$user
echo $numstat1 > /tmp/colstop_file.$user

set ind1 = 0
foreach statid ($statidlist)
    @ ind1=$ind1 + 1
    if($numstat1 >= $ind1) then
        echo "1.  ----------------  4X,A16" >> /tmp/RECEPTORS.$user
        printf "%9s
" $statidlist[$ind1] >> /tmp/RECEPTORS.$user
        echo "    RECEPTORNAME" >> /tmp/RECEPTORS.$user
        echo " " >> /tmp/RECEPTORS.$user
        echo "2.  ------.----       4X,F11.4" >> /tmp/RECEPTORS.$user
        printf "%15.4f
" $xlonlist[$ind1] >> /tmp/RECEPTORS.$user
        echo "    XRECEPTOR" >> /tmp/RECEPTORS.$user
        echo " " >> /tmp/RECEPTORS.$user
        echo "3.  ------.----       4X,F11.4" >> /tmp/RECEPTORS.$user
        printf "%15.4f
" $ylatlist[$ind1] >> /tmp/RECEPTORS.$user
        echo "    YRECEPTOR" >> /tmp/RECEPTORS.$user
        echo "=========================================== =========== " >> /tmp/RECEPTORS.$user
        set idum1 = 0
        set idum1=`echo $colstoplist[$ind1] | cut -b 1-2`
        echo $idum1 $sampltimelist[$ind1] $statidlist[$ind1] >> /tmp/colstop_file.$user
    endif
end

cp /tmp/RECEPTORS.$user $receptorsfile
cp /tmp/colstop_file.$user $colstop_file

echo "Finished"
```