

Development and Demonstration of a Methodology to Quantitatively Assess the INL Site Ambient Air Monitoring Network

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December 2014



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ABSTRACT

This report documents a defensible methodology and modeling tool that can be used to objectively assess an air monitoring network design against established performance objectives. The methodology and tool were demonstrated by performing a preliminary assessment of the Idaho National Laboratory (INL) Site ambient air monitoring network. The methodology uses frequency of detection as the performance metric, which is defined as the fraction of “events” that result in a detection at either a single sampler or network of samplers. An “event” is defined as a release of finite duration that begins on a given day and hour of the year.

The INL Site ambient air monitoring network consists of 37 low-volume air samplers in 31 different locations. Twenty of the samplers are located on the INL Site (onsite) and 17 are located off the INL Site (offsite). Twenty-one of the samplers (mainly at onsite locations) are maintained and sampled by the INL contractor, Battelle Energy Alliance (BEA), and 16 samplers (mainly at offsite locations) are maintained and sampled by Gonzales-Stoller Surveillance for the Environmental Surveillance, Education, and Research (ESER) Program. The samplers run continuously and particulate filters are collected weekly for gross alpha and beta activity analysis and composited quarterly for specific radionuclide analysis. For this initial assessment, a nominal sampler flow rate of 2 cfm and a sampling time of 168 hours were assumed. The duration of release events varied from 1 hour up to 340 hours. Detection frequencies were calculated using both BEA and ESER-contracted laboratory minimum detectable activity (MDA) levels.

The CALPUFF Lagrangian puff dispersion model, coupled with 1 year of meteorological data, was used to calculate time-integrated concentrations at sampler locations for a 1-hour release of unit activity (1 Ci) for every hour of the year. The unit-activity time-integrated concentration (*TICu*) values were calculated at all sampler locations for releases from eight INL Site facilities. The *TICu* values were then scaled and integrated for a given release quantity and release duration. A ground-level release was simulated from each major INL Site facility at either the center of the facility or at a point where significant emissions are possible. In addition to ground-level releases, three existing stacks at the Advanced Test Reactor Complex, Idaho Nuclear Technology and Engineering Center, and Material and Fuels Complex were also modeled.

Meteorological data from the 35 stations comprising the INL Site Mesonet network, data from the Idaho Falls Regional airport, upper air data from the Boise airport, and three-dimensional gridded data from the Weather Research and Forecasting model were used for modeling. Simulations were run using an already available meteorological data set from years 2006, 2007, and 2008, but only data from year 2006 was used in the frequency of detection analysis. A comparison of annual *TICu* values calculated with CALPUFF and the National Oceanic and Atmospheric Administration MDIFFH model (currently used at INL to assess annual dose) was performed to test the validity of the CALPUFF simulation. In general, the CALPUFF simulation produced results that were comparable to those generated by MDIFFH; differences could be explained by differences in model features and capabilities. The impact of meteorological data sequences was examined by comparing *TICu* isopleths and dispersion factors at

individual sampler locations calculated with CALPUFF for each of the 3 years of meteorological data considered. Consistent results from year to year indicate a single year of data is adequate for air dispersion modeling. A validation exercise was also performed by simulating the historic release of Sb-125 from an INL Site facility in 1987 and comparing the results to annual average concentrations measured at INL samplers. The results show that CALPUFF predicted the measured concentrations more accurately than the MESODIF model (the precursor to MDIFFH) and provided dispersion estimates that were consistent with the expected uncertainty of atmospheric transport models in complex terrain environments.

For the INL Site network assessment, three representative radionuclides identified as key radionuclides in INL's annual National Emission Standards for Hazardous Air Pollutants evaluations were considered for the frequency of detection analysis: Cs-137 (beta-gamma emitter), Pu-239 (alpha emitter), and Sr-90 (beta emitter). Source-specific release quantities were calculated for each radionuclide, such that the maximum inhalation dose at any publicly accessible sampler or the National Emission Standards for Hazardous Air Pollutants maximally exposed individual location (i.e., Frenchman's Cabin) was equivalent to 0.1 mrem yr^{-1} (i.e., 1% of the 10 mrem yr^{-1} standard). Dose calculations were based on a reference individual and used the most recent dose coefficients.

Detection frequencies were calculated separately for the onsite and offsite samplers. As expected, detection frequencies were generally less for the offsite samplers compared to the onsite samplers. Overall, the monitoring network was very effective at detecting the potential releases of Cs-137 or Sr-90 from all sources/facilities using ESER MDAs and slightly less effective using BEA MDAs. For Cs-137, the maximum detection frequencies at onsite or offsite samplers were greater than 99% for all sources using ESER MDAs. Using BEA MDAs the maximum Cs-137 detection frequencies at onsite samplers were all greater than 97%, and for offsite samplers ranged from 19% to 99%. For Sr-90, the maximum detection frequencies at onsite or offsite samplers were greater than 99% for all sources using ESER MDAs. Using BEA MDAs the maximum Sr-90 detection frequencies at onsite samplers ranged from 23% to greater than 99%, and for offsite samplers from 2% to 26%. The lowest detection frequencies were associated with releases from the Idaho Nuclear Technology and Engineering Center main stack (CPP-708).

The network was less effective at detecting releases of Pu-239. Maximum detection frequencies for Pu-239 using ESER MDAs ranged from 27.4 to 100% for onsite samplers and 3 to 80% for offsite samplers. Using BEA MDAs, the maximum detection frequencies for Pu-239 ranged from 2.1 to 100% for onsite samplers and 0 to 5.9% for offsite samplers.

The methodology described in this report could be used to improve sampler placement and detection frequency, provided clear performance objectives are defined. Performance objectives would include an effective dose criterion, the likelihood of the dose criterion being exceeded, and an acceptable detection frequency.

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ACRONYMS

ATR	Advanced Test Reactor
BEA	Battelle Energy Alliance, LLC
CFA	Central Facilities Area
cfm	cubic feet per minute
CITRC	Critical Infrastructure Test Range Complex
DOE	U.S. Department of Energy
DOE-ID	U.S. Department of Energy, Idaho Operations Office
EPA	U.S. Environmental Protection Agency
ESER	Environmental Surveillance, Education, and Research (Program)
INL	Idaho National Laboratory
INTEC	Idaho Nuclear Technology and Engineering Center
MDA	minimum detectable activity
MDC	minimum detectable concentration
MEI	maximally exposed individual
MFC	Material and Fuels Complex
NESHAP	National Emission Standards for Hazardous Air Pollutants
NOAA	National Oceanic and Atmospheric Administration
NRF	Naval Reactors Facility
RDL	required detection limit
RWMC	Radioactive Waste Management Complex
SMC	Specific Manufacturing Capability
TAN	Test Area North
<i>TIC</i>	time-integrated concentration
<i>TICu</i>	time-integrated concentration for a unit (1 Ci) release
USGS	United States Geological Survey
UTM	Universal Transverse Mercator
WRF	Weather Research and Forecasting

Development and Demonstration of a Methodology to Quantitatively Assess the INL Site Ambient Air Monitoring Network

1. INTRODUCTION

This report documents a defensible methodology and modeling tool that can be used to objectively assess an air monitoring network design against established performance objectives. The methodology and tool were demonstrated by performing an assessment of the Idaho National Laboratory (INL) Site ambient air monitoring network. Airborne radionuclide emissions at the INL Site are generated from various facilities during operations, research, and scientific activities. Engineering and administrative controls are implemented to prevent, reduce, and/or eliminate these emissions from the environment. INL performs facility emissions and ambient air surveillance monitoring to assess the adequacy of these controls in protecting human health and determining environmental impacts. The basis for INL air monitoring activities is documented in the report *Technical Basis for Environmental Monitoring and Surveillance at the Idaho National Laboratory* (DOE-ID 2014a), which summarizes ambient air and other monitoring conducted at the INL Site and surrounding area to meet the requirements and criteria set forth in Department of Energy (DOE) Order 458.1, “Radiation Protection of the Public and the Environment,” (DOE 2011a) and the *Environmental Regulatory Guide for Radiological Effluent Monitoring and Environmental Surveillance* (DOE 1991), as well as address environmental risks and stakeholder concerns.

A primary component of the INL Site ambient air monitoring program is a network of low-volume air samplers that monitor atmospheric levels of radioactive particulates and radioiodine released from INL Site facilities, natural radioactivity (radon and daughters), and fallout from worldwide nuclear detonations or nuclear accidents. Samples are analyzed to determine whether radiation doses to the public are within the limits established in DOE Order 458.1 (DOE 2011a), to evaluate background and site contributions of radioactive material to the environment, and to provide documentation of ambient air concentrations in the event of a non-routine or unplanned release. The number and location of samplers that make up the ambient air monitoring network has evolved considerably since routine air monitoring began in the 1950s. Air samplers have typically been placed at facilities with significant radiological sources, at offsite locations most likely to be most impacted by emissions, background locations, and at locations chosen to help characterize ground-level concentrations between the source and populated areas. Currently, samplers are located near each major onsite facility, at locations in the predominant wind directions several miles from the facilities, and in several distant locations, including the towns of Idaho Falls, Rexburg, and Blackfoot, Idaho; Jackson, Wyoming; and Craters of the Moon National Monument west of Arco, Idaho. These sampler locations meet program goals and are based on expert judgment that includes evaluation of meteorological data, air dispersion modeling, and practical considerations such as the availability of power. DOE-ID (2014a) provides a complete description of the air monitoring program.

Although several of the current sampler locations were selected before the first guidance document (EPA 1972) was released, the INL Site ambient air monitoring network conforms to the most recent guidance (DOE 1991) and includes sampling stations beyond the minimum number required. Nevertheless, guidance documents do not provide a means for evaluating the effectiveness of a network and there is no generally accepted method for quantitatively defining and evaluating the effectiveness of a surveillance network for a single source, let alone a network that covers facilities and offsite locations distributed over a large area. This work describes a methodology for quantitatively evaluating a network and provides results of a preliminary assessment of the INL Site ambient air monitoring network.

1.1 Background

1.1.1 Previous Work

The assessment methodology used in this analysis was based on work by Ritter et al. (2003), who developed a quantitative methodology for evaluating the effectiveness of an air monitoring network. The goal of their work was to develop an objective measure of the performance (or effectiveness) of a regional network of air sampling stations as it is affected by the positions of samplers within the region relative to the positions of sources, meteorology, and air sampling/analysis parameters (i.e., flow rate, measurement sensitivity, and period for collection or compositing of sample collection media). They proposed the criterion for ‘effectiveness’ of a sampling network to be the likelihood that the activity, collected by a minimum number of samplers in the network, will exceed the minimum detectable activity (MDA) (i.e., the product of the time-integrated concentration [*TIC*] [$\text{Ci}\cdot\text{hr}/\text{m}^3$] at a sampler location and the sampler flow rate [m^3/hr], assuming the sampler operates continuously). They also proposed the “likelihood of detection” could be based on an evaluation of the “frequency of detection.” The frequency of detection is determined using a numerical air-dispersion model that utilizes multiple independent historical meteorological data sequences and simulates releases of constant activity, beginning at various times (1-hour resolution) and extending at a constant rate over various durations (1-hour increments), with each combination of release start time and duration corresponding to an equal potential *TIC* and offsite dose (actual *TICs* are dependent on actual meteorological conditions).

1.2 Purpose and Scope

The general purpose of this report is to document a quantitative assessment of the INL Site ambient air monitoring network and provide information that can be used by INL’s ambient air monitoring program to meet program goals. The specific assessment question addressed by this preliminary analysis is

What is the frequency of detection of the existing INL Site ambient air monitoring network in response to a given hypothetical radionuclide release of variable duration from INL source locations?

This question was addressed through use of an atmospheric transport model, meteorological data, source and sampler information, and a methodology to calculate frequency of detection. Frequency of detection is defined as the fraction of “events” that result in a detection at either a single sampler or network of samplers. An “event” is defined as a release of finite duration that begins on a given day and hour of the year. For example, if the release duration is 1 hour and 1 year of meteorological data are simulated, then there are 8,760 events simulated (i.e., one event for every hour of the year) and the frequency of detection is the number of hours that a detection occurred divided by 8,760 hours. A “detection” is said to occur if the amount of activity that would be collected by the sampler exceeds the MDA of the analysis method. For this assessment, detection at a single sampler constitutes detection for the network.

The atmospheric transport model was used to simulate hypothetical ground-level releases of representative radionuclides from a single “most likely” source location at each major INL Site facility, as well as releases from the major emission stacks. Representative radionuclides include a beta-gamma emitter (Cs-137), an alpha emitter (Pu-239), and a beta emitter (Sr-90). These radionuclides are identified as key radionuclides in the annual INL National Emission Standards for Hazardous Air Pollutants (NESHAP) evaluations (e.g. DOE-ID 2014b). “Most likely” source locations were determined by examining the emissions data from the most recent INL NESHAP evaluation (DOE-ID 2014b). Source locations in Idaho Falls were not considered because transport distances to real receptors are much less (about 100 m) than sources at the INL Site. Assessment of sources in Idaho Falls will be addressed subsequent to this assessment in Phase II. The model domain encompassed all samplers in the network, with the exception of the sampler in Jackson, Wyoming. The model utilized a 3-year (2006 to 2008) set of

Weather Research and Forecasting (WRF) model meteorological data and surface meteorological data from surrounding meteorological stations, as well as available upper air data from nearby airports. *TICs* were calculated by the model at each air sampler location, and the frequency of detection was calculated with a Fortran program.

This document contains a description of the INL Site ambient air monitoring network (Section 2); a description of the atmospheric transport model and meteorological data used to simulate air dispersion (Section 3); a description of the INL Site radionuclide sources and release rates (Section 4); identification of assumptions and an explanation of the methodology and equations used to calculate frequency of detection (Section 5); a presentation and discussion of the results for this preliminary assessment, including an examination of the sensitivity of the results to key assumptions and parameters (Section 6); and a summary and recommendations section (Section 7). The preliminary assessment of the current network using frequency of detection criteria as documented in this report is Phase I of II. Phase II, which will be described in a subsequent report, includes a near-field assessment of each major facility at the INL Site to identify the areas around the facilities with the potential for the highest frequency of detection, as well as a reassessment of the network with performance objectives and criteria defined through a formalized process.

2. IDAHO NATIONAL LABORATORY SITE AMBIENT AIR MONITORING NETWORK

The INL Site ambient air monitoring network presented in Table 1 and illustrated in Figure 1 consists of 37 low-volume air samplers in 31 different locations. Twenty-one samplers with the Battelle Energy Alliance (BEA) prefix are maintained and sampled by the INL Site contractor, BEA, and 16 samplers with the Environmental Surveillance, Education, and Research (ESER) prefix are maintained and sampled by Gonzales-Stoller Surveillance for the ESER Program. The network does not include miscellaneous air samplers maintained and sampled by the INL Site cleanup contractor CH2M-WG Idaho, LLC. BEA and Gonzales-Stoller Surveillance have collocated samplers at Craters of the Moon National Park, Sugar City, Blackfoot, Idaho Falls, Van Buren Avenue (near Highway 20/26), and the Experimental Field Station, which is located northeast of the Idaho Nuclear Technology and Engineering Center (INTEC). FRENCHCBN (Frenchman's Cabin) is not a sampler location, but it is included because it is the maximally exposed individual (MEI) location for the INL NESHAP analysis and it is used to determine appropriate source release quantities for this assessment (see Section 4). Table 1 indicates whether a sampler is located within the INL Site boundary and whether the sampler is publicly accessible. A publicly accessible sampler can be located within the boundaries of INL Site. For example, the BEA-REST and BEA-EBR-I samplers are located inside the INL Site boundary, but they are accessible to the public on a temporary basis.

The low-volume air samplers are configured with particulate filters for collection of particulate radionuclides and charcoal filter cartridges for collection of I-131. The samplers run continuously (24/7) and particulate filters are collected weekly and analyzed for gross-alpha and gross-beta activity. The filters are also composited quarterly (every 13 weeks) and analyzed for gamma-emitting radionuclides. Selected ESER sample composites are analyzed for Sr-90 or actinides (i.e., Pu-238, Pu-239/240, and Am-241) each quarter on a rotating basis. BEA screens for these radionuclides using gross-alpha/beta activity and gamma analyses and requests additional radionuclide specific analyses if results are anomalous. The average flow rate of the samplers between weekly collections is approximately 2 cfm.

Detection limits in terms of concentration and activity are included in Table 2 for the radionuclides of interest in this study. For this assessment, BEA's required detection limits (RDLs) were provided and used to calculate the BEA MDA values, assuming an average flow rate of 2 cfm. The ESER minimum detectable concentration (MDC) values and MDA values were provided. The reason for the large difference between the MDA values for both contractors is the ESER MDA values are based on what the analysis laboratory claims can be detected (*a priori*) and are much closer to the *a postapriori* MDA values

Table 1. INL onsite and regional air monitoring stations.

Sampler ID ^a	Location/Description	Easting ^b (m)	Northing ^b (m)	INL Onsite	Publicly Accessible?
BEA-ARA	Auxiliary Reactor Area	352512	4820236	Yes	No
BEA-BLKFT	Blackfoot	391668	4782760	No	Yes
BEA-CFA	Central Facilities Area (CFA)	342602	4821788	Yes	No
BEA-CPP	INTEC	343508	4825928	Yes	No
BEA-CRATERS	Craters of the Moon National Park	292750	4815337	No	Yes
BEA-EBR-I	Experimental Breeder Reactor-I	337858	4819578	Yes	Yes
BEA-EFS	Experimental Field Station	346110	4829754	Yes	No
BEA-GATE 4	Gate 4 entrance near Test Area North	358520	4848895	Yes	No
BEA-IF	Idaho Falls	414380	4818193	No	Yes
BEA-INTEC	INTEC	344158	4826806	Yes	No
BEA-IRC	INL Research Center (Idaho Falls)	416371	4818572	No	Yes
BEA-MFC	Materials and Fuels Complex (MFC)	366673	4828121	Yes	No
BEA-NRF	Naval Reactors Facility (NRF)	345564	4834400	Yes	No
BEA-PBF	Critical Infrastructure Test Range Complex (CITRC)	348964	4823313	Yes	No
BEA-REST	Rest Stop on Highway 20	337640	4823710	Yes	Yes
BEA-RTC	Advanced Test Reactor (ATR) Complex	341727	4828168	Yes	No
BEA-RWMC	Radioactive Waste Management Complex (RWMC)	335063	4818552	Yes	No
BEA-SMC	Specific Manufacturing Capability (SMC) Facility	360950	4857753	Yes	No
BEA-SUGAR	Sugar City, Rexburg	440759	4860651	No	Yes
BEA-TRA	ATR Complex	341316	4827516	Yes	No
BEA-VAN B	Van Buren Boulevard	339762	4822063	Yes	No
ESER-ARC	Arco	314683	4832742	No	Yes
ESER-ATO	Atomic City	353080	4811691	No	Yes
ESER-BLU	Blue Dome	352495	4881840	No	Yes
ESER-CRA	Craters of the Moon National Park	292751	4815337	No	Yes
ESER-DUB	Dubois	401640	4892296	No	Yes
ESER-EFS	Experimental Field Station	346114	4829752	Yes	No
ESER-FAA	FAA Tower near east boundary of INL	375764	4823554	Yes	Yes
ESER-HOW	Howe	340891	4849795	No	Yes
ESER-IDA	Idaho Falls	414376	4818192	No	Yes
ESER-JAC	Jackson Hole (outside domain)	519314	4813939	No	Yes
ESER-MAI	INL Main Gate	346614	4819341	Yes	No
ESER-MON	Montevue	376885	4874727	No	Yes
ESER-MOU	Mountain View Middle School, Blackfoot	391668	4782752	No	Yes
ESER-SUG	Sugar City/Rexburg	440759	4860651	No	Yes
ESER-TER	Terreton/Mud Lake	381307	4855032	No	Yes
ESER-VAN	Van Buren Boulevard	339764	4822062	Yes	No
FRENCHCBN ^c	Frenchman's Cabin (INL MEI location)	333548	4810289	No	Yes

a. Samplers with the BEA prefix are sampled and maintained by BEA. Samplers with the ESER prefix are sampled and maintained by the ESER Program.

b. Universal Transverse Mercator (UTM) coordinate system (Zone 12).

c. Frenchman's Cabin is not a sampler location, but it is the MEI location for 40 CFR 61, Subpart H (NESHAP) compliance.

Table 2. Required detection limits, minimum detectable concentrations, and minimum detectable activity values for radionuclides modeled.

Radionuclide	BEA RDL ^a ($\mu\text{Ci mL}^{-1}$)	BEA MDA ^b (pCi)	ESER MDC ^c ($\mu\text{Ci mL}^{-1}$)	ESER MDA ^c (pCi)
Cs-137	1.74E-15	12.9	1.20E-16	0.7
Pu-239	3.28E-17	0.24	3.49E-18	0.022
Sr-90	2.56E-15	19	3.41E-17	0.215

a. BEA RDL values from Table 6-5 of DOE/ID-11485.

b. BEA MDA values are based on the BEA RDL values and an average filter flow rate of 2 cfm for 13 weeks (quarterly compositing period).

c. ESER MDC and MDA values from Table 6-6 of DOE/ID-11485.

3. ATMOSPHERIC TRANSPORT MODEL

This section presents details of the atmospheric transport model, including model domain, model selection, model grid, meteorological data, terrain data, and dispersion coefficients.

3.1 Model Domain

To adequately assess the INL Site ambient air monitoring network, it was determined that the model domain must encompass the sampler locations, significant topographic features that influence airflow in the region, and primary population centers that may be impacted by INL Site releases. It was also desirable to include as many of the INL Site meteorological data stations as possible. Practical elements such as grid size and simulation run time were also considered (i.e., larger domains with finer grid resolution take longer to run).

The model domain selected (see Figure 1) is 240 km east to west and 200 km north to south for a total area of 48,000 km². This domain encompasses all sampler locations (with the exception of the sampler in Jackson, Wyoming) and all meteorological data stations that make up the INL Site Mesonet (see Section 3.4.3). It extends from the town of Carey in the west to the Idaho-Wyoming border in the east, and from 16 km south of Pocatello in the south to 20 km north of Dubois in the north. The eastern boundary includes the portion of Yellowstone National Park that lies just inside the Idaho State line. The model domain is slightly larger than the domain currently used by ESER to estimate annual population doses (see Figure 2). The ESER model was developed by the Idaho Falls National Oceanic and Atmospheric Administration (NOAA) office and uses the computer code MDIFFH.

3.2 Model Selection

Ritter et al. (2003) noted that previous evaluations of air monitoring network designs have relied on steady-state Gaussian plume models to describe dispersion conditions during radioactive releases to the atmosphere (Pelletier 1968, Waite 1972, DOE 1990). Although these models may be appropriate for network planning, they have limited applicability for modeling the range of spatial and temporal scales necessary for evaluating network performance. Thus, only non-steady-state Lagrangian puff dispersion models were considered for the regional analysis. Three models were considered: MDIFFH, HYSPLIT, and CALPUFF.

MDIFFH (Sagendorf et al. 2001) was developed by the Idaho Falls NOAA office and was designed to estimate impacts over periods of up to 1 year or more on and around the INL Site. It is used by ESER to estimate annual dispersion factors from INL Site sources that are used to calculate population doses reported in the annual INL Site annual environmental report (DOE-ID 2014c). Although MDIFFH incorporates site-specific dispersion parameters and has been validated in the near field, it does not explicitly model terrain effects, utilize upper air data for vertical wind shear, include deposition and plume depletion, or allow discrete receptors (i.e., only receptors at grid nodes are allowed). Terrain effects

are likely to be important because of the moderately complex terrain surrounding the INL Site. The INL Site is situated on the relatively flat Snake River Plain that is bordered on the west by the Lemhi, Lost River, and Pioneer mountain ranges in the west, the Beaverhead and Centennial mountain ranges in the north, and the Big Hole and Caribou mountain ranges in the east. These features result in wind channeling between the ranges and influence diurnal air flow, resulting in spatially variable wind fields within the model domain.

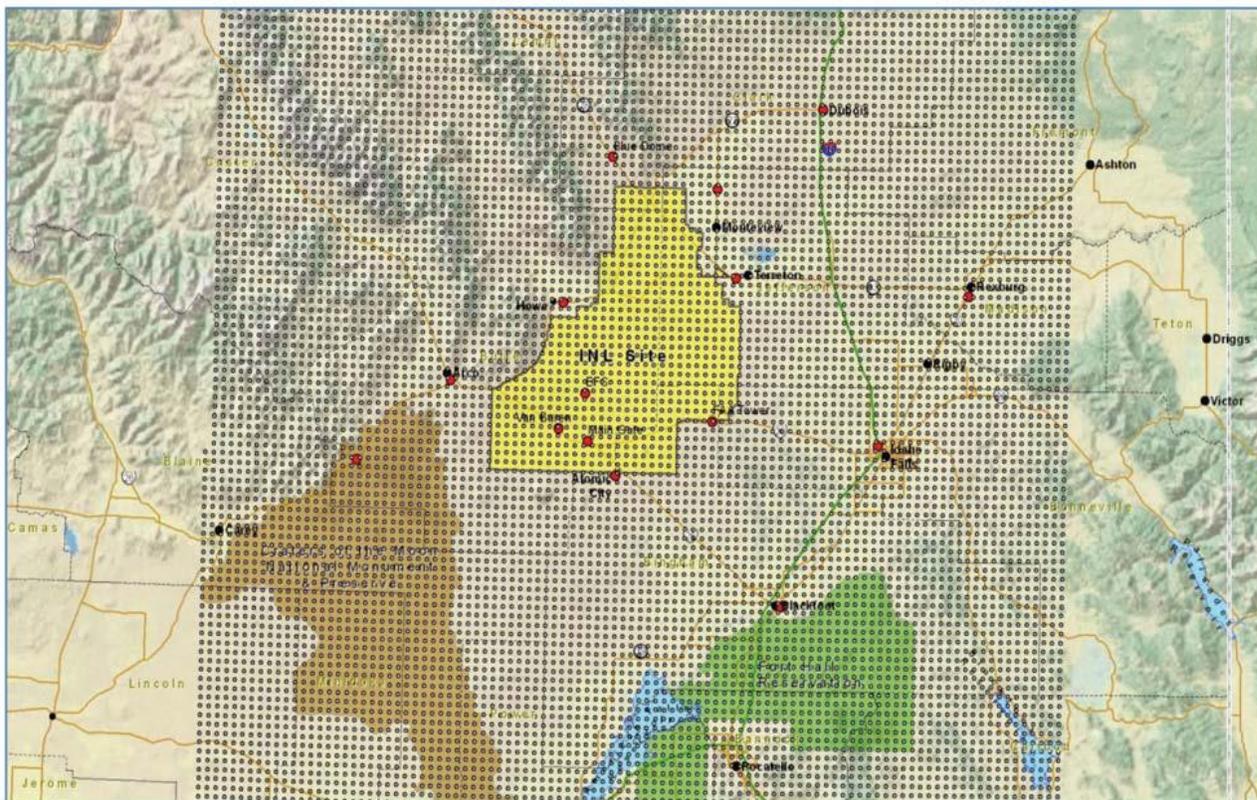


Figure 2. MDIFFH model domain showing the 2-km grid spacing and surrounding region [from DOE-ID 2014c].

The HYSPLIT (Hybrid Single-Particle Lagrangian Integrated Trajectory) model was developed by the NOAA Air Resources Laboratory (Draxler 1999; Draxler et al. 2013) for emergency response modeling. The HYSPLIT model includes terrain effects (as resolved by the meteorological data), accounts for vertical wind shear, and includes deposition. Special gridded meteorological datasets covering the entire United States at various resolutions are used as basic input to the model. However, the model is not configured off-the-shelf for incorporating site-specific surface meteorological data as collected by the NOAA.

The CALPUFF model (Scire et al. 2000a) addresses all the deficiencies of MDIFFH. It includes explicit treatment of terrain features; deposition and plume depletion; incorporation of upper air data, allowing for the effects of vertical wind shear to be modeled; and allows discrete receptors so the actual location of INL samplers are modeled instead of using the grid node nearest the sampler as was done by Ritter using MDIFFH. CALPUFF is the U.S. Environmental Protection Agency (EPA)-approved, long-range (i.e., greater than 50 km) model for evaluation of air quality impacts in Federal Class 1 areas (i.e., national parks). For these reasons, CALPUFF was the model selected for this analysis. The EPA-approved version of the model (Version 5.8, Level 130731) was used in the calculations. The CALPUFF code consists of three modules: (1) a meteorological model (CALMET), (2) a Lagrangian puff

dispersion and deposition model (CALPUFF), and (3) a post-processing program (CALPOST). Numerous preprocessing programs are also used to develop input data sets. Computations were made using an eight-core MacPro workstation running OS X Lion. The FORTRAN source code was compiled using the gfortran (GNU Project) compiler for the Mac Unix operating system.

3.3 Model Grid

The CALPUFF model domain illustrated in Figure 1 was discretized into a uniform grid of 2-km resolution, comprising 120 east-west nodes and 100 north-south nodes for a total of 12,000 nodes. Grid resolution was selected to be consistent with the current MDIFFH resolution of 2 km and to resolve the primary topographic features of the domain. The grid resolution is greater (i.e., a smaller grid spacing) than what is recommended by EPA in Fox (2009). EPA recommends a resolution of greater than or equal to 4 km, based on a tradeoff between computational efficiency and the domain size (greater than 400 km) of eastern North and South Dakota and western Minnesota, which is relatively flat. For this application, the domain size is considerably smaller and the terrain is much more pronounced, thereby justifying the use of a finer grid resolution. Vertical discretization included 10 layers. Layer heights conformed to those recommended by EPA for federal land managers (Fox 2009). The top of each layer above ground level are 20, 40, 80, 160, 320, 640, 1200, 2000, 3000, and 4000 meters.

3.4 Meteorological Data

Minimum meteorological data requirements for running CALMET are at least one surface station with estimates of cloud cover and one upper air station. Optionally, multiple surface and upper air stations can be included in a simulation, in addition to prognostic model data from weather forecasting models such as the Mesoscale Model 5 and the WRF model (<http://www.wrf-model.org/>). The use of prognostic weather forecasting model data is required by the U.S. National Park Service for CALPUFF simulations involving evaluation of air quality impacts in national parks. Because we already possess 3 years (i.e., 2006 to 2008) of WRF data across the entire United States on a 12-km grid, these 3 years were used in the model simulation. The annual variability in the 3-year data set is evaluated in Section 6.2. Each meteorological data source is discussed in the following subsections.

3.4.1 Weather Research and Forecasting Model Data

The WRF Model data were obtained from Alpine Geophysics LLC in Denver Colorado on four 1-TB portable hard drives. These data came processed through the CALWRF preprocessor and ready for acceptance into CALMET as a three-dimensional prognostic data file. Each data file contained 5 days of data. Because of the size of the data domain (i.e., the entire continental United States), a subset of the data representing the geographic region of the simulation domain was extracted first from the WRF files provided by Alpine Geophysics, and the extracted data files were then used in the CALMET simulation. The WRF data contains wind speed and direction, temperature, precipitation, and atmospheric pressure at 37 levels above the ground surface on a 12-km grid. These data were interpolated by CALMET onto the modeling grid.

3.4.2 Upper Air and Airport Surface Data

Upper air data for 2006 through 2008 was obtained for the Boise upper air station at the Boise Airport (Station Number 24141) in Boise, Idaho from the NOAA Earth Science Research Laboratory (ESRL) Radiosonde online database (<http://esrl.noaa.gov/raobs/>). These data were processed through the READ62 preprocessor (Version 5.54, Level 070627) to produce a CALMET compatible upper air data file. Other nearby upper air monitoring stations include the Salt Lake City Airport and Riverton Wyoming, but the importance of these data (as well as the Boise upper air data) is diminished because the WRF data provides three-dimensional data to the upper reaches of the atmospheric boundary layer. Therefore, only the upper air data from the Boise Airport were used.

Data from a surface station at the Idaho Falls Regional Airport (Station Number 24145) were used in the simulation. Data from years 2006 through 2008 were obtained from the National Climatic Data Center in the TD3505/CDO format (<http://www.ncdc.noaa.gov>). These data had to be converted into a form that is compatible with the input format required by the CALMET surface meteorological preprocessor, SMERGE. The SMERGE program uses various formats, including the National Climatic Data Center Card Deck 144 format (CD144). The Idaho Falls Regional Airport data was converted to CD144 format for use in SMERGE.

3.4.3 Idaho National Laboratory Site Mesonet Data

The NOAA Air Resources Laboratory Field Research Division in Idaho Falls developed and maintains the INL MESOScale meteorological monitoring NETwork (Mesonet). The network currently consists of 35 stations (Table 3 and Figure 3). Thirteen of the stations are located within the boundaries of the INL Site. The remaining stations are located at key locations on the Eastern Snake River Plain. Thirty of the stations are 15-m tall. Three of the stations on the INL Site extend to heights ranging from 46 to 76 m, with instrumentation installed at multiple levels, including at 15-m. Because of practical and aesthetic considerations, the stations at Craters of the Moon and on Big Southern Butte are only 9-m and 6-m, respectively. Wind speed and direction at the 15-m level was used in all cases except for Craters of the Moon (9 m) and Big Southern Butte (6 m). Other data included temperature at the 2 and 15-m levels (when applicable) and height insensitive data that included barometric pressure, relative humidity, and solar radiation.

Hourly meteorological data from 2006 through 2008 were received from the Idaho Falls NOAA office in the form of a large comma-delimited file. These data were parsed into separate files for each of the 35 stations and converted to CD144 format for use by the SMERGE preprocessor. Solar radiation measurements cannot be used directly in CALMET. Instead, cloud cover data are used to estimate the incoming solar radiation flux. However, direct solar radiation measurements can be used to estimate equivalent cloud cover during the daylight hours. The temperature difference at the 2-m and 10-m level, wind speed, estimates of atmospheric stability, and the Monin-Obhukov length are used to estimate cloud cover during nighttime hours. The incoming short-wave radiation is given in CALMET by Scire et al. (2000b):

$$Q_{sw} = (a_1 \sin \varphi + a_2) (1 + b_1 N^{b_2}) \quad (1)$$

where

- Q_{sw} = incoming short-wave radiation (W m^{-2})
- a_1 = net radiation constant from Holtslag and van Ulden (1983) (990 W m^{-2})
- a_2 = net radiation constant from Holtslag and van Ulden (1983) (-30 W m^{-2})
- b_1 = net radiation constant from Holtslag and van Ulden (1983) (-0.75)
- b_2 = net radiation constant from Holtslag and van Ulden (1983) (3.4)
- φ = solar elevation angle (degrees)
- N = fraction of sky covered by clouds.

Equation (1) can be solved for N during daylight hours when Q_{sw} is greater than zero:

$$N = \left(\left(\frac{Q_{sw}}{a_1 \sin \varphi + a_2} - 1 \right) / b_1 \right)^{1/b_2} \quad (2)$$

Table 3. INL and regional Mesonet stations operated by the Idaho Falls NOAA office.

Station Name	Station Identification	Onsite/Offsite of INL	Height ^a (m)	Easting ^b (m)	Northing ^b (m)
ATR Complex	ATR	Onsite	15	341065	4827623
Base of Howe Peak	BAS	Onsite	15	338297	4838013
CFA	CFA	Onsite	15	342620	4821806
CITRC	CIT	Onsite	15	348963	4823312
Dead Man Canyon	DEA	Onsite	15	333820	4832292
Grid 3/INTEC	GRI	Onsite	15	343398	4828131
Lost River Rest Area	LOS	Onsite	15	337639	4823710
MFC	MFC	Onsite	15	366673	4828121
NRF	NRF	Onsite	15	345863	4834538
RWMC	RWM	Onsite	15	334597	4818756
Rover	ROV	Onsite	15	376793	4841978
Sand Dunes	SAN	Onsite	15	358517	4848903
SMC	SMC	Onsite	15	360950	4857752
Aberdeen	ABE	Offsite	15	351174	4757425
Arco	ARC	Offsite	15	314672	4832737
Atomic City	ATO	Offsite	15	353077	4811693
Blackfoot	BLK	Offsite	15	391667	4782760
Blue Dome	BLU	Offsite	15	352501	4881852
Cox's Well	COX	Offsite	15	323055	4795792
Craters of the Moon	CRA	Offsite	9	294549	4811606
Dubois	DUB	Offsite	15	404037	4899496
Fort Hall	FOR ^b	Offsite	15	384951	4764225
Hamer	HAM	Offsite	15	400689	4873442
Howe	HOW	Offsite	15	340895	4849795
Idaho Falls	IDA	Offsite	15	415108	4817335
Kettle Butte	KET	Offsite	15	392863	4822478
Minidoka	MIN	Offsite	15	288248	4742348
Monteview	MON	Offsite	15	376890	4874726
Richfield	RIC	Offsite	15	244747	4772314
Roberts	ROB	Offsite	15	409728	4843997
Rexburg	RXB	Offsite	15	435616	4851026
Sugar City	SUG	Offsite	15	440759	4860651
Big Southern Butte	SUM	Offsite	6	336263	4806813
Taber	TAB	Offsite	15	362817	4797594
Terreton	TER	Offsite	15	385990	4855266

a. Some stations have multiple monitor heights, but data from the monitor nearest 15 m was used

b. UTM coordinate system.

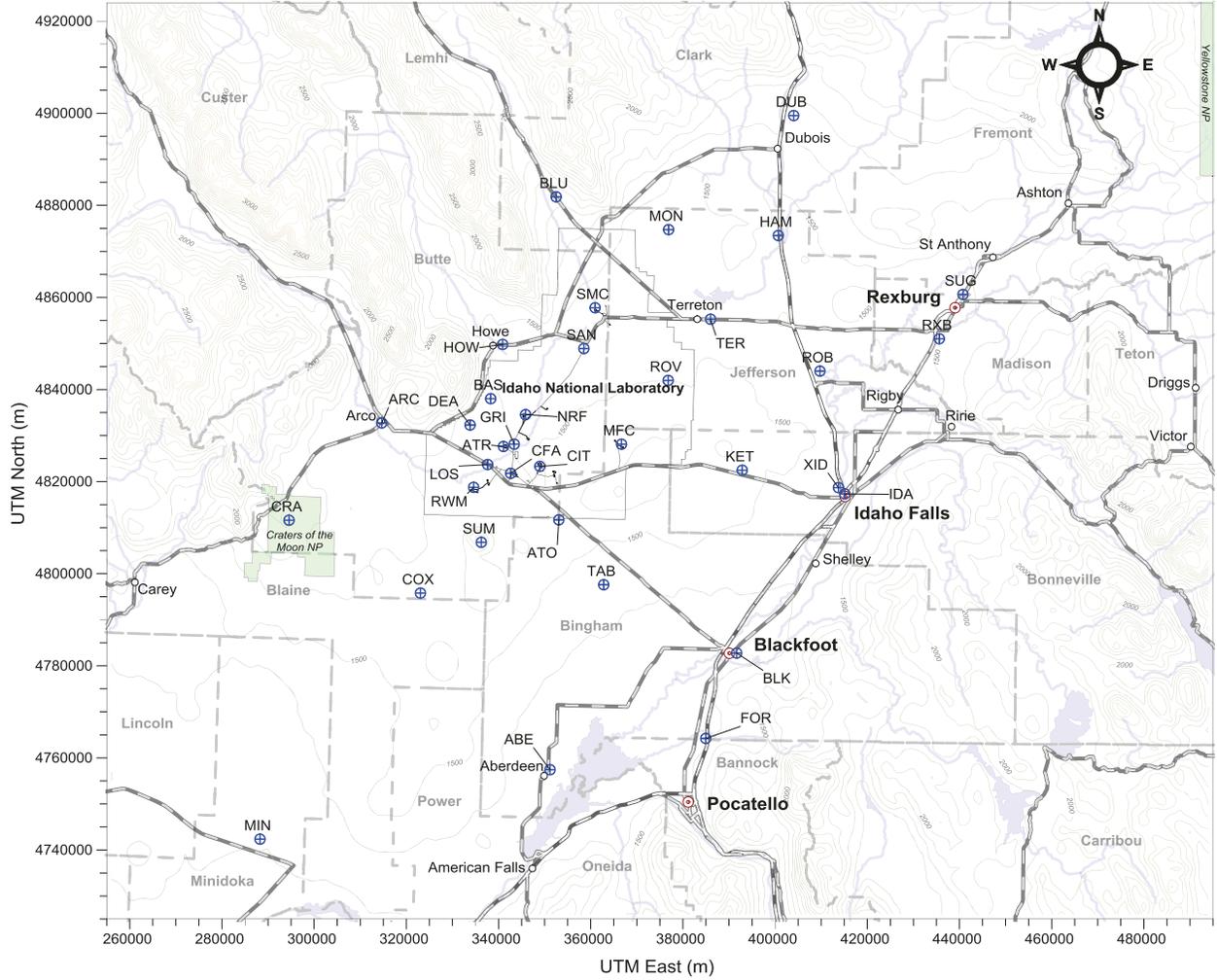


Figure 3. INL and regional Mesonet stations operated by the Idaho Falls NOAA Office.

The sine of the solar elevation angle ($\sin \phi$) was calculated using the routine in CALMET, which is based on the work of Scire et al. (1984):

$$\sin \phi = \sin r_{lat} \sin c_d + \cos r_{lat} \cos(\arcsin[\sin c_d]) \cos(0.017453 s_{ha}) \quad (3)$$

where

- r_{lat} = 0.0174533 LAT (radians)
- $\sin c_d$ = 0.39784989 $\sin(0.0174533 \sigma)$
- s_{ha} = 15(GMT - e_m) - LON (degrees)
- LAT = latitude of station (degrees)
- LON = longitude of station (degrees).

The term σ (in degrees) is given by:

$$\sigma = 279.9348 + d + 1.91482 \sin r_d - 0.079525 \cos r_d + 0.019938 \sin 2r_d - 0.00162 \cos 2r_d \quad (4)$$

where

$$d = (JD - 1)0.9856479 \text{ (degrees)}$$

$$r_d = 0.0174533 d \text{ (radians)}$$

$$JD = \text{Julian day}$$

and e_m is given by:

$$e_m = 12 + 0.12357 \sin r_d - 0.004289 \cos r_d + 0.153809 \sin 2r_d + 0.060783 \cos 2r_d. \quad (5)$$

Equation (2) was used to calculate N during daylight hours. For nighttime conditions, the 2-m and 10-m temperature differential, along with an estimate of the Monin-Obhukov length and wind speed, is used to estimate cloud cover. This method employs the Delta-T Solar Radiation stability classification scheme in EPA (2000) to first define the stability class. During nighttime conditions, stability class is defined by the following:

$$\Delta T < 0 \text{ C}^\circ \text{ and } u < 2.0 \text{ m s}^{-1}, \text{ stability class} = 5$$

$$\Delta T < 0 \text{ C}^\circ \text{ and } u \geq 2.0 \text{ m s}^{-1}, \text{ stability class} = 4$$

$$\Delta T \geq 0 \text{ C}^\circ \text{ and } u < 2.0 \text{ m s}^{-1}, \text{ stability class} = 6$$

$$\Delta T \geq 0 \text{ C}^\circ \text{ and } u \geq 2.0 \text{ m s}^{-1} \text{ and } u < 2.5 \text{ m s}^{-1}, \text{ stability class} = 5$$

$$\Delta T \geq 0 \text{ C}^\circ \text{ and } u \geq 2.5 \text{ m s}^{-1}, \text{ stability class} = 4$$

where ΔT = temperature differential (10-m temperature – 2-m temperature), and u = wind speed.

The Monin-Obhukov length can then be determined using the relationship provided in Golder (1972) that provides the inverse Monin-Obhukov length as a function of surface roughness (z_o) and stability class (Figure 4). The roughness length is determined from the land-use category provided in the U.S. Geological Survey (USGS) land-use coverage used by CALMET. For most stations, the roughness length that corresponds to rangeland ($z_o = 0.05$ m) was used.

The inverse Monin-Obhukov length was numerically determined for each hour in the meteorological period using a FORTRAN routine adapted from the RATCHET code (Ramsdell et al. 1994) that is based on the Golder (1972) graph.

The equivalent cloud cover is determined by solving Equation 16 in the AERMOD model formulation document (EPA 2004) for N :

$$N = \sqrt{\frac{1 - \frac{\theta_*}{0.09}}{0.5}} \quad (6)$$

where θ_* = the temperature scale (K) and 0.09 and 0.5 are empirical constants. The temperature scale is determined using Equation 18 in EPA (2004):

$$\theta_* = \frac{k(\theta_2 - \theta_1)}{\ln \frac{z_2}{z_1} + \beta_m \frac{(z_2 - z_1)}{L}}$$

where

$$\theta_* = \text{temperature scale (K)}$$

$$k = \text{von Karman constant (0.4)}$$

- θ_1 = temperature at 2-m (K)
- θ_2 = temperature at 10-m (K)
- z_1 = 2-m height
- z_2 = 10-m height
- L = Monin-Obhukov length (m)
- β_m = a constant (5.0).

The measured data did not include the temperature measured at the 10-m level. The temperature at this level was linearly interpolated from the 2-m and 15-m data.

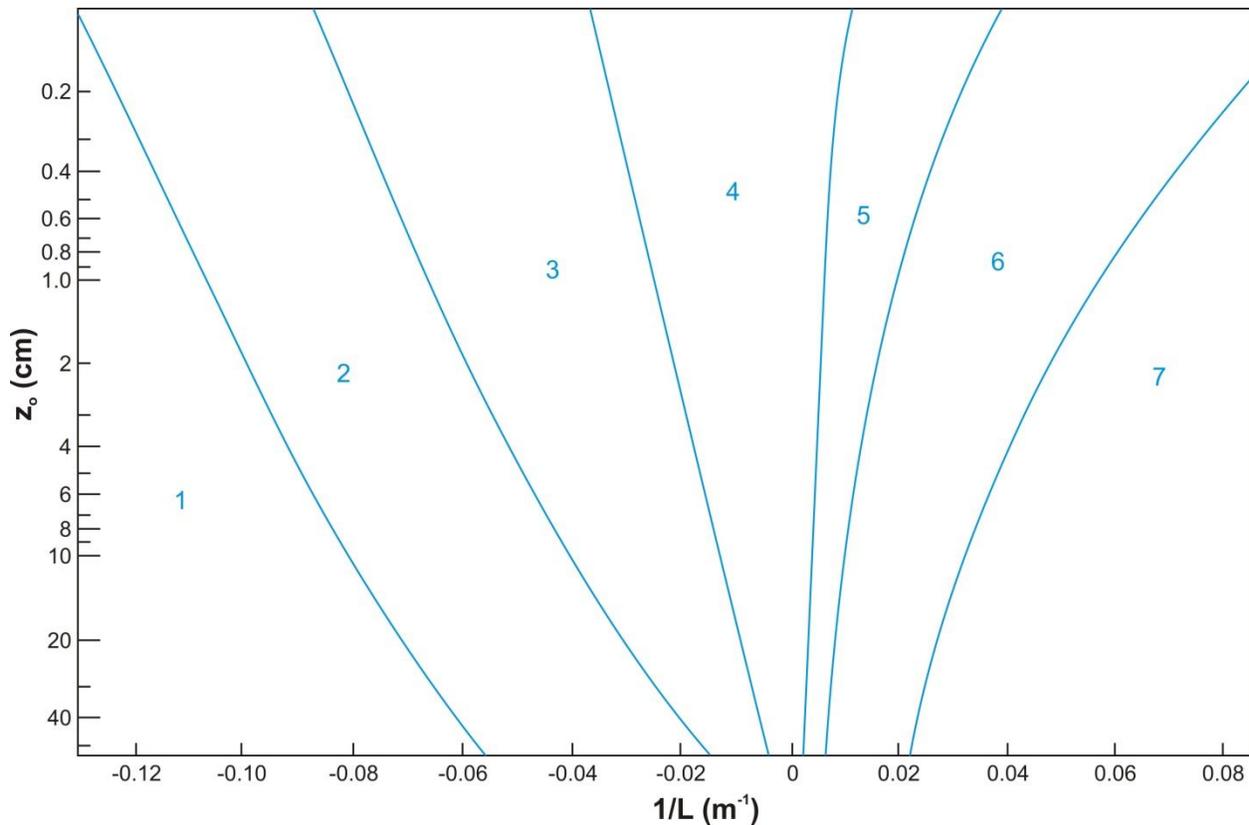


Figure 4. Inverse Monin-Obhukov ($1/L$) length as a function of surface roughness height (z_o) (redrawn from Golder 1972).

Precipitation data were also obtained from the Mesonet stations. Precipitation data are important for calculating wet deposition of particles. These data were not used in the simulation because the frequency of detection simulations did not consider dry or wet deposition (i.e., this assessment assumed the species do not decay or deposit). These data may be necessary for future simulations involving materials that deposit.

3.5 Geophysical Data

Geophysical data include terrain elevations and land use. Land use defines surface roughness height, albedo, vegetative cover, and other parameters that determine energy balance at the earth's surface. The terrain model used USGS digital elevation model data. These data are available at various resolutions and may be downloaded or ordered from the website (<http://edc.usgs.gov/products/elevation/dem.html>). For

the region encompassing the model domain, 22 one-degree digital elevation model data files were obtained (grid resolution of 90 m). The digital elevation model data were processed through the CALPUFF utility, TERREL, which averages elevation data near each grid node and generates a gridded data file for use in the MAKEGEO pre-processor. The gridded terrain elevations are contoured and plotted in Figure 1.

The digital elevation models used in this application employ the UTM coordinate system. This coordinate system is based on the distance (in meters) from a given reference point. The model domain data for this application are within UTM Zone 12. All data in this CALPUFF model simulation were represented using the UTM coordinate system.

Land use data were obtained from the USGS internet site in the Global Lambert Azimuthal for North America format. Land use and land cover types are divided into 37 categories. The raw land use data were processed through the CTGPROC utility program that produces a fractional land use value for each computational node.

Output from CTGPROC and TERREL was then processed through the MAKEGEO utility, which generated gridded land use data and terrain elevations used in CALMET. Figure 5 presents the gridded land use data for the model domain.

3.6 CALMET and CALPUFF Parameter Options

Model options for the CALMET module were generally taken from those recommended by EPA for long-range transport as described in Fox (2009), with a few exceptions. The recommended horizontal grid resolution was 2 km instead of 4 km, as discussed in Section 3.3. Fox (2009) recommends using the Lambert Conic Conformal map projection; this projection is important for large domains (greater than 400 km), but is more cumbersome to work with when producing base maps with multiple geographic layers in different UTM coordinate systems. For this reason, the CALMET default map projection of UTM was used instead. The remainder of the model parameters was the EPA-recommended default values.

In general, default input parameters for CALPUFF were used, with two exceptions: (1) the terrain adjustment algorithm and (2) the dispersion coefficient option discussed in the following subsections.

3.6.1 Terrain Adjustment

Terrain adjustment in CALPUFF is performed on a large and small (i.e., subgrid) scale. Large-scale terrain features are reflected in the wind field developed in CALMET. Puffs embedded in the CALMET wind field either rise or fall with flow along the surface or are steered by flow along the terrain. Simple adjustments to the puff dispersion are then implemented in CALPUFF on a large scale.

Small-scale features that are not resolved by the terrain grid are handled using the complex terrain algorithm for subgrid features. This algorithm accepts the flow field generated by CALMET and modifies flow and dispersion parameters to reflect the presence of a terrain feature not resolved in the terrain modeling. Features are typically a hill or other obstacle that protrudes from the overall slope of the terrain. The model domain grid spacing was sufficiently small that the complex terrain algorithm for subgrid features was not required in the CALPUFF modeling.

Simple terrain adjustment options include the simple industrial source complex-type adjustment, the CALPUFF-type of terrain adjustment, and a partial plume path adjustment (default option). In the industrial source complex-type adjustment, the plume is modeled as if the terrain above the release height were removed and placed at a level equal to the plume height. In the partial plume path adjustment, the plume elevation is adjusted to follow the terrain. The CALPUFF-type terrain adjustment uses a simplified version of the complex terrain algorithm for subgrid features. In the CALPUFF-type terrain algorithm, properties of the puff are adjusted on the basis of local strain to the flow imparted by the underlying

terrain. Based on analysis of isopleth plots of plumes in other simulations (Rood et al. 2008), the CALPUFF-type of terrain adjustment was used because it appeared to better simulate terrain effects.

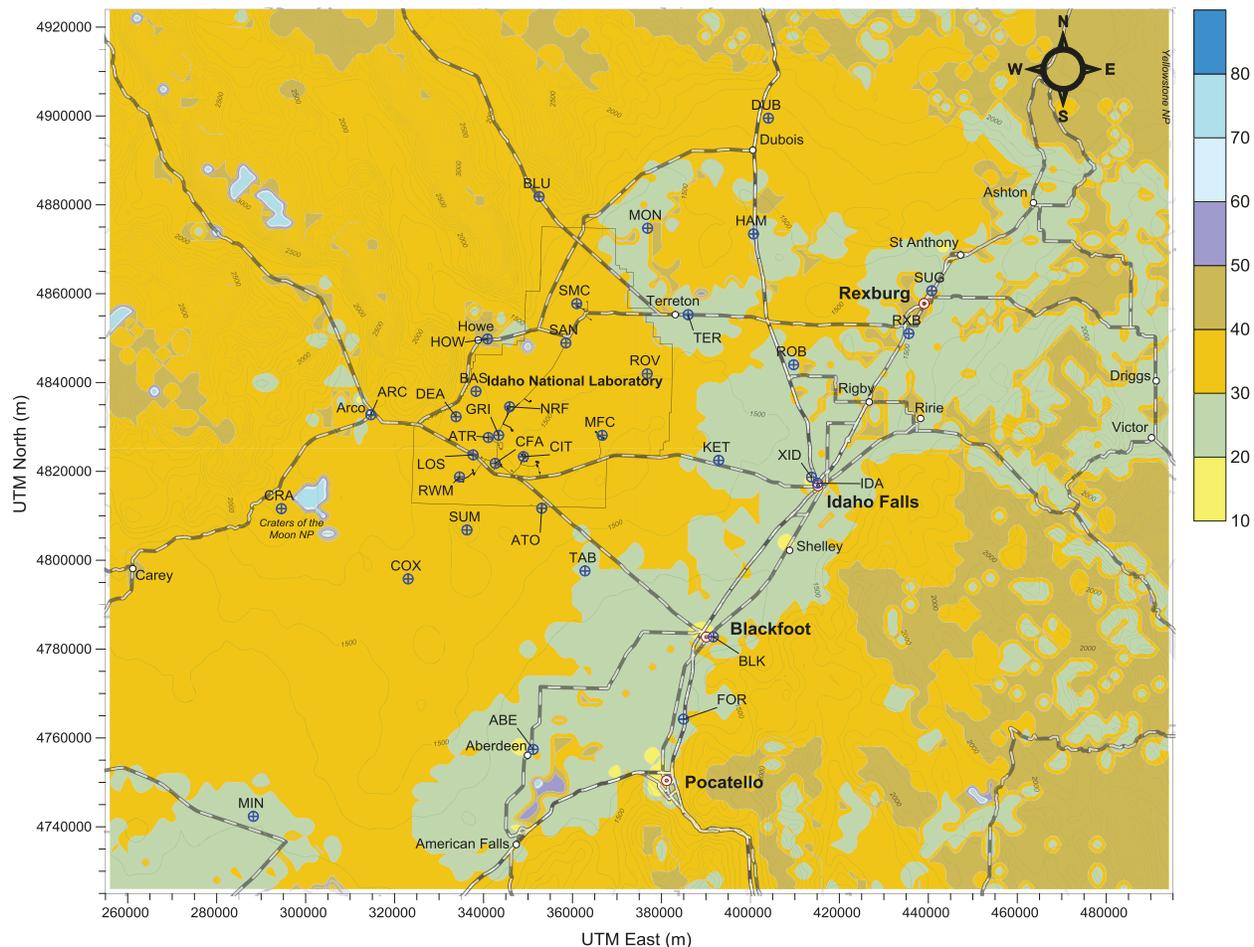


Figure 5. Land use categories in the regional model domain as defined by USGS. Land use values are as follows: 10 to 19 urban or built-up ($z_o=1.0$ m); 20 to 29 agriculture ($z_o=0.25$ m); 30 to 39 rangeland ($z_o=0.05$ m); 40 to 50 forested land ($z_o=1.0$ m); 50 to 60 water ($z_o=0.001$ m); 60 to 70 wetland ($z_o=0.2$ m); 70 to 80 barren land ($z_o=0.05$ m); and 80 to 90 tundra ($z_o=0.2$ m).

3.6.2 Dispersion Coefficients

The default dispersion coefficient option in CALPUFF is the Pasquill-Gifford Turner scheme (Dispersion Option 3) for urban and rural conditions. Other dispersion options include dispersion coefficients that are computed from micrometeorological variables and user input schemes. For these simulations, dispersion coefficients that are computed based on estimates of micrometeorological variables were chosen (Dispersion Option 2). This option calculates dispersion coefficients (σ_y and σ_z) based on an energy balance at the earth's surface. The energy balance is then related to turbulence using similarity theory. This method of dispersion coefficient estimation represents the current state-of-the-art in atmospheric dispersion modeling and is used in the AERMOD model. This dispersion option is discussed in the CALPUFF user's manual (Scire et al. 2000a; pages 2 through 25).

4. RADIONUCLIDE EMISSION SOURCES

This section presents the radionuclide emission source parameters used in this study, including locations, release parameters, and modeled release quantities.

4.1 Source Locations

For the preliminary assessment of the INL Site monitoring network, sources were defined at each of the major INL Site facilities (Table 4). The 2013 INL NESHAP evaluation (DOE-ID 2014b) reported potential radionuclide releases from more than 60 source locations at the INL Site. However, many of the sources resulted in doses that were insignificant and many sources are located relatively close together such that the sampling network response from a release would be the same for all nearby sources. Therefore, insignificant sources were not explicitly modeled and some sources were consolidated with nearby sources. The large operating stacks were modeled explicitly and included the ATR main stack (TRA-770), the INTEC main stack (CPP-708), and the Experimental Breeder Reactor-II main stack (MFC-764). The materials test reactor stack (TRA-710) was not modeled due to its close proximity to the ATR main stack and because releases from the materials test reactor stack are significantly less than the ATR stack. Stack parameters are provided in Table 5. All other releases within a facility were assigned as ground-level releases from a single location within the facility. These other releases include other non-fugitive releases from ducts and vents and fugitive releases from ponds, soil, or other. The ground-level release location for a facility was assigned to the most significant source (in terms of activity released) based on the 2013 NESHAPs evaluation (DOE-ID 2014b) or, if there were multiple significant sources, it was assigned to a location near the center of the facility. Figure 6 shows the location of all sources modeled in this study.

Table 4. Modeled source locations for the frequency of detection evaluation.

Facility	Source	Release Type	Source Description	Easting ^a (m)	Northing ^a (m)
ATR Complex	TRA-770	Stack	ATR Stack	341206	4828106
INTEC	CPP-708	Stack	INTEC Main Stack	343862	4826156
MFC	MFC-764	Stack	Experimental Breeder Reactor-II Main Stack	366326	4828209
ATR Complex	Center	Ground	Near center of ATR Complex	341401	4827855
CFA	CFA-625	Ground	Lab fume hoods (near center of CFA)	343271	4821432
CITRC	PBF-632	Ground	Waste Reduction Operations Complex Support Building Vent	349099	4823351
INTEC	CPP-1774	Ground	Three Mile Island-2 Spent Fuel Storage Installation (Near center of INTEC)	343831	4825808
MFC	MFC-774	Ground	Zero Power Physics Reactor Support Wing (South center of MFC)	366389	4828004
NRF	Center	Ground	Near center of NRF	345498	4834667
RWMC	Center	Ground	Near center of RWMC	334818	4818274
SMC/TAN	TAN-679	Ground	SMC Manufacturing and Assembly Building	360856	4857565

a. UTM coordinate system.

Table 5. Stack release parameters.

Facility	Source Stack	Stack Height (m)	Exit Diameter (m)	Exit Velocity ^a (m s ⁻¹)	Flow Rate ^a (cfm)
ATR Complex	TRA-770	76.2	1.524	10.03	38,776
INTEC	CPP-708	76.2	1.83	10.65	59,370
MFC	MFC-764	60	1.524	9.081	35,100

a. Flow rates and exit velocities based on average 2013 values.

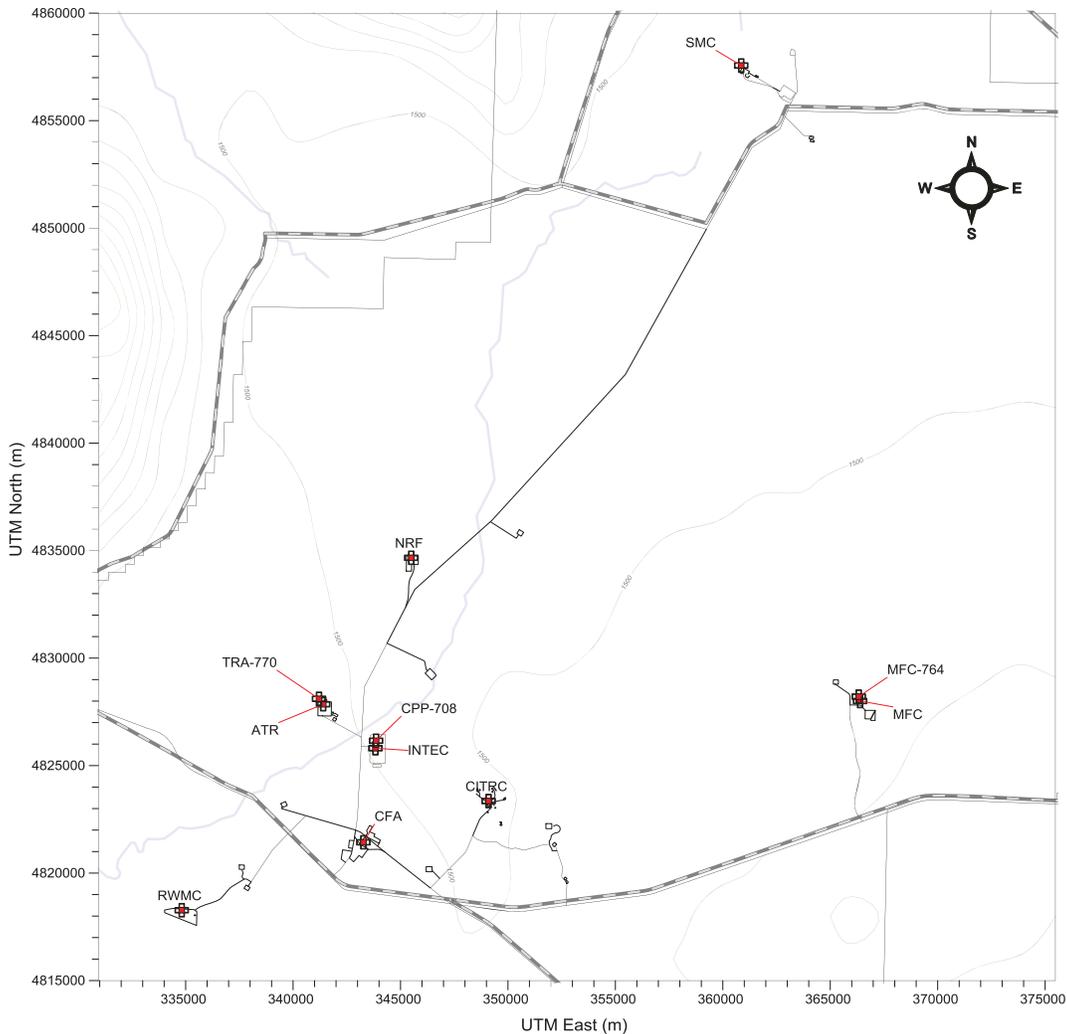


Figure 6. INL major facility source locations. TRA-770, CPP-708, and MFC-764 are stack releases. The remainder of the sources is modeled as ground-level releases.

The purpose of this preliminary assessment is to evaluate the entire monitoring network. Given the large distances between facilities and monitoring locations in the network, the assumption that all non-stack releases at each facility occur from a single location and the selection of that location is likely to influence the detection frequency only at the nearest monitoring locations (i.e., those near the boundary of the facility from which the release occurs). In other words, moving a source location a few hundred meters in any direction is not likely to influence whether or not that release is detected at monitoring locations several kilometers away. It may influence the response at the nearby monitoring location, but

that is only one or two samplers out of 37 samplers. An evaluation of monitoring locations near the facilities is planned subsequent to this assessment in Phase II.

4.2 Source Release Rates

To assess the effectiveness of the monitoring network, it is necessary to determine an appropriate release quantity that the monitoring network should be capable of detecting. In general, the significance of a release is based on the potential radiological dose consequence. The *National Emission Standards for Emissions of Radionuclides Other than Radon from Department of Energy Facilities* (40 CFR 61, Subpart H) requires that the radiological dose to any member of the public from radionuclide releases to the atmosphere be no greater than 10 mrem yr⁻¹. 40 CFR 61 Subpart H also states that air concentration measurements can be used in lieu of calculations as long as concentrations that would cause an effective dose equivalent of 1 mrem yr⁻¹ (10% of the standard) are readily detectable and distinguishable from background. For this preliminary assessment, release quantities were selected such that the maximum dose from inhalation at any publicly accessible sampler location, or the NESHAP MEI location (Frenchman’s Cabin), is no more than 0.1 mrem yr⁻¹ (1% of the standard). Publicly accessible sampler locations are shown in Table 1.

Inhalation dose was calculated using dose coefficients from the DOE *Derived Concentration Technical Standard* (DOE 2011b). DOE (2011b) uses the most recent biokinetic models and metabolic data from the International Commission on Radiological Protection and reflects the current state of knowledge and practice in radiological protection. DOE (2011b) provides dose coefficients for six age classes and a reference individual. The reference individual represents the age and gender-weighted dose coefficient. For this assessment, the dose coefficients for the reference person were used, along with an age and gender-weighted inhalation rate (18.2 m³ day⁻¹) calculated from data in Table 3 of DOE (2011b). Dose coefficients for the radionuclides considered in this study are presented in Table 6.

Table 6. Reference individual dose coefficients for radionuclides modeled (from DOE 2011b).

Radionuclide	Solubility Class	Dose Coefficient (Sv Bq ⁻¹)	Dose Coefficient (mrem pCi ⁻¹)
Cs-137	S	4.17E-08	1.54E-01
Pu-239	F	1.21E-04	4.48E-01
Sr-90	S	1.64E-07	6.07E-4

Table 7 lists the release quantities for each facility and radionuclide considered in this assessment. Release durations from 1 hour to 14 days in 1-hour increments were considered and, in all cases, the maximum dose occurred for a 1-hour release duration. Therefore, the values in Table 7 are the largest quantities of each radionuclide that could be released during any hour of 2006 (considered representative of any year) and not exceed a 0.1 mrem yr⁻¹ dose at any of the publicly accessible sampler locations. Also listed are the release type and the publicly accessible sampler location where the maximum dose occurs. To put these release quantities in perspective, the 2013 emission estimates from all INL Site sources for Cs-137, Pu-239, and Sr-90 in 2013 were 38 mCi, 0.47 mCi, and 52 mCi, respectively (Sondrup 2014, Appendix D). In other words, the 1-hour release quantities for Cs-137 in Table 7 are all greater than the total released from all INL Site sources for the entire year of 2013 (38 mCi). Six of the 11 release quantities for Sr-90 in Table 7 are greater than the 2013 INL Site total of 52 mCi. The Pu-239 releases in Table 7 are all less than the 2013 INL Site total, but the MFC-764 release (0.44 mCi) is close to the 2013 INL Site total (0.47 mCi).

Table 7. Source release quantities (activity) that produce a maximum dose of 0.1 mrem yr⁻¹ at any publicly accessible sampler location for a release duration of 1 hour.

Facility	Source	Release Type	Sampler Location of Maximum Dose	Cs-137 (mCi)	Pu-239 (mCi)	Sr-90 (mCi)
ATR Complex	TRA-770	Stack	FRENCHCBN ^b	471	0.161	120
INTEC	CPP-708	Stack	FRENCHCBN ^b	315	0.108	80
MFC	MFC-764	Stack	FRENCHCBN ^b	1,288	0.442	327
ATR Complex	Center	Ground-level	BEA-REST	168	0.0575	43
CFA	CFA-625	Ground-level	BEA-VAN B/ESER-VAN ^a	115	0.0396	29
CITRC	PBF-632	Ground-level	ESER-MAI	165	0.100	42
INTEC	CPP-1774	Ground-level	BEA-REST	99	0.0342	25
MFC	MFC-774	Ground-level	ESER-FAA	523	0.180	133
NRF	Center	Ground-level	BEA-REST	500	0.172	127
RWMC	Center	Ground-level	BEA-EBR	61	0.0210	15
SMC/TAN	TAN-679	Ground-level	BEA-GATE	553	0.190	140

a. BEA-VAN B and ESER-VAN are at the same location.

b. Frenchman's Cabin (FRENCHCBN) is not a sampler location, but is the MEI location for 40 CFR 61, Subpart H (NESHAP) compliance.

5. METHODOLOGY

This section describes the theory and methodology for calculating frequency of detection. An example calculation is also provided, as well as a description of computer codes used to implement the methodology.

5.1 Frequency of Detection Calculation

Frequency of detection is defined as the fraction of “events” that result in detection at either a single sampler or network of samplers. An “event” is defined as a release of finite duration that begins on a given day and hour of the year. Assuming a single source is emitting radionuclides into the atmosphere, frequency of detection (*FD*) is defined as:

$$FD_{r,s} = \frac{\sum_{k=1}^N f(D_{r,s,k})}{N} \quad (8)$$

where

$f(D_{r,s,k})$ = a binary function that returns 1 if the detection ($D_{r,s,k}$) is true and 0 if it is false for radionuclide r at sampler s , and event k ,

N = the number of “events.”

The number of events is the number of release periods simulated in the assessment. For example, if a 1-hr release period is considered and 1 year of meteorological data are used, then the number of events would be 365 days × 24 hrs/day × 1 event/hour = 8,760 events. A “detection” ($D_{r,s,k}$) is defined in terms of the radionuclide (r), the sampler (s), and the event (k). Detection is either true or false (i.e., either the sampler can detect the activity collected from airborne sampling or it does not). Detection is assigned a true value if the following condition is met:

$$TIC_{r,s,Q,Tr} \times F \geq MDA_r \quad (9)$$

where

$TIC_{r,s,Q,Tr}$ = time-integrated concentration for radionuclide r at sampler s for release quantity Q released over time Tr (Ci-hr m⁻³)

F = the sampler flow rate (m³ hr⁻¹)

MDA_r = minimum detectable activity for radionuclide r (Ci).

Because MDA is radionuclide specific, detections are defined in terms of sampler performance (i.e., the flow rate) and the analytical techniques used to measure a given radionuclide. Furthermore, the concentration is integrated over the time the sampler is operating to obtain the total activity accumulated on the sampler filter.

The atmospheric transport model is used to compute the $TICs$ at each of the samplers for a release quantity Q of release duration Tr and sampling time Ts . The time integrated concentration is defined by:

$$TIC_{r,s,Q,Tr} = \int_0^{Ts} C_{r,s,Q,Tr}(t) dt \quad (10)$$

where

$TIC_{r,s,Q,Tr}$ = time-integrated concentration for radionuclide r at sampler s , release quantity Q , release duration Tr , and sampling time Ts (Ci-hr m⁻³).

$C_{r,s,Q,Tr}(t)$ = concentration as a function of time for radionuclide r at sampler s , release quantity Q , and release duration Tr (Ci m⁻³).

The sampling time Ts is assumed to begin at the start of the release. This makes little difference in the results as long as the release duration is within the sampling period. For example, assume the sampling period begins on Monday at 8:00 AM and the sampling time is 168 hours. An unplanned 1-hour release starts on Saturday at 8:00 AM and persists for 24 hours (i.e., ends Sunday at 8:00 AM). In this case, the total release is encompassed in the sampling period because the sampler filter is changed out on 8:00 AM the following Monday. This example assumes that the airborne plume from the release impacts the sampler (i.e., the plume travels in the direction of the sampler from the release point). A sensitivity study is used to explore cases where the release begins a significant time into the sampling period and persists past filter change-out time (Section 6.4.2).

As a matter of practicality, $TICs$ are not calculated for each radionuclide and for all possible release durations. Instead, a unit TIC ($TICu$) is calculated for each hour of the meteorological dataset. $TICu$ is then scaled to the actual release quantity and duration to estimate the actual TIC . The $TICu$ is defined by:

$$TICu_{s,k,h} = \frac{\int_h^{\infty} Cu_s(t) dt}{Qu} \quad (11)$$

where

$TICu_{s,k,h}$ = time-integrated concentration at sampler s for a unit release rate from source k that begins at hour h (hr² m⁻³)

$Cu_s(t)$ = concentration as a function of time at sampler s for a unit release rate beginning at hour h (Ci m⁻³)

Qu = unit release rate (1.0 Ci hr⁻¹).

It is important to note that the $TICu$ values are defined for each source-sampler pair. In practice, infinity in the integrand is a finite amount of time to allow the activity emitted from the source over the 1-hour period to dissipate from the model domain. Complete dissipation occurs by either transport out of the model domain or dilution, resulting in concentrations that are negligible. The longest transport distance from any INL Site source to the edge of the model domain is about 180 km. An estimate of the transport time was made, assuming a mean wind speed of 1.0 m s⁻¹ and a straight-line trajectory:

$$T = \frac{180\text{km} \times 1000\text{m/km}}{1.0\text{ m/s} \times 3600\text{s/hr}} = 50\text{ hrs}$$

Simulations were performed to confirm this value. If the integration time is long enough for complete dissipation, then the $TICu$ value for 50 hours would be the same as the $TICu$ value for 60 hours. Using 2006 meteorological data, it was found that in most cases 50-hour integration time was sufficient for complete dissipation. However, there were some cases where the $TICu$ value for 60-hours was slightly greater than that for 50-hours. This condition would occur during (1) very light wind speeds; (2) spatially variable wind directions, resulting in curvilinear trajectories; or (3) situations where the wind direction changed significantly during transport, resulting in recirculation of the airborne activity within the model domain. For this reason, the integration time was increased to 70-hours to assure $TICu$ values captured all activity in the air observed at the sampler.

The $TICu$ values are scaled to obtain the TIC values for the actual release by the equation:

$$TIC_{r,s,Q,Tr} = \frac{\sum_{i=h}^{X+h} TICu_{s,i} \times Q}{Tr} \quad (12)$$

where X is the minimum of Tr or Ts .

Equations 8 through 12 are used to evaluate the frequency of detection at a single sampler. The frequency of detection for the entire sampling network ($FD_{r,nw}$) is evaluated by:

$$FD_{r,nw} = \frac{\sum_{k=1}^N fn(D_{r,s,k})}{N}, s \in 1..nw \quad (13)$$

where

$fn(D_{r,s,k})$ = a binary function that returns 1 if any of the samplers in the network has a detect, and 0 if no samplers in the network have a detect for radionuclide r and event k

nw = number of samplers in the network

N = the number of events.

5.1.1 Example Calculation

The general process of calculating TIC and frequency of detection values is illustrated using a simple example presented in Table 8. In this example, 20 consecutive hours of $TICu$ values (Equation 11) at a single sampler location are provided in Column 2. The BH and EH columns refer to the begin hour and end hour of the summation in Equation 12 for different release durations. This example considers release durations of 1, 2, and 3 hours. For the 1-hour release duration, each TIC is simply the $TICu$ value multiplied by the release quantity and divided by the release duration Tr (1 hr). The Q value in this example is 1 mCi (1×10^9 pCi). For the 2-hour release duration, the TIC for the first hour is the sum of the first and second-hour $TICu$ values multiplied by Q and divided by Tr (2 hrs) to yield 3.29×10^{-4} pCi-hr m⁻³. The second hour of the 2-hour release duration is the sum of the second and

third-hour $TICu$ values multiplied by Q and divided by Tr (2 hrs) to yield 3.29×10^{-4} pCi-hr m^{-3} . They are the same in this example only because the $TICu$ values for hours 1 and 3 are both zero. If a detection is true according to Equation 9, then the detect column records 1, otherwise 0 is entered. The frequency of detection is obtained by summing the number of detects and dividing by the number of events. Note that the total number of events is reduced by $Tr-1$ for release durations longer than 1-hour.

The formulations given in Equations 8 through 13 assume that the atmospheric transport model is capable of simulating a non-steady-state release because calculation of $TICu$ requires that a unit release Q is only applied to the first hour of the simulation and is zero for all other times. However, if the samplers are close to the source, then a steady-state concentration at the sampler would be achieved during the 1-hour release. A property of a Gaussian plume model is that it represents the steady-state concentration from a constant release or the time-integrated concentration from a fixed release quantity. Therefore, $TICu$ values can be estimated using a Gaussian plume model for samplers or receptors close to the source, where a steady-state concentration would be established during the 1-hour release duration. However, this is not appropriate for samplers or receptors located farther away from the source, thus the transient puff-model was used.

5.2 Methodology Implementation

The methodology for calculating frequency of detection values was implemented using Fortran codes and Perl scripts. A Fortran code was used to process the onsite meteorological data into a format compatible with the SMERGE meteorological data processor and to calculate equivalent cloud cover for INL Mesonet stations. Another Fortran code was used to convert the Idaho Falls airport data from TD3505 format to the CD144 format and extract the precipitation data into a separate CALPUFF compatible file.

A Perl script was used as a “wrapper” to set-up, execute, and post-process the CALPUFF simulations for calculating $TICu$ values (see Appendix A). The script takes the years, days, and hours that will be simulated and the source location and release parameters as input. The script then constructs a run matrix that includes (1) selecting the CALMET files that cover the meteorological period simulated, (2) writing the CALPUFF input files and executing CALPUFF, (3) post-processing results at the sampler locations using CALPOST and calculating the $TICu$, and (4) writing $TICu$ to an output file. CALPUFF does not calculate the time-integrated concentration but the average concentration for the simulation run time. For the purpose of calculating $TICu$ values, the simulation run time was always 70 hours (see discussion that follows Equation 11). The average concentration is converted to the time-integrated concentration by multiplying the average concentration by the simulation run time.

The Fortran code FREQD (Appendix B) was used to calculate frequency of detection. The FREQD code reads the $TICu$ results generated from the CALPUFF simulations and processed using the Perl script and a parameter file that identifies all samplers in the simulation, sampler flow rates, radionuclide detection limits and release quantities, whether to include the sampler in the analysis, and whether the sampler is onsite or offsite. The FREQD code produces plot files that display frequency of detection as a function of release duration that forms the basis for the evaluation.

Table 8. Example of frequency of detection calculation for a 1-hour, 2-hour, and 3-hour release duration and 20 consecutive hours of TIC_u values. Actual TIC values are based on a Q value of 1 mCi. Detections are based on a sampler flow rate of $3.398 \text{ m}^3 \text{ hr}^{-1}$ (2 cfm) and an MDA of 0.7 pCi.

Hour	TIC_u ($\text{hr}^2 \text{ m}^{-3}$)	1-hour Release Duration				2-hour Release Duration				3-hour Release Duration				
		BH ^a	EH ^a	TIC (pCi-hr m^{-3})	Detect	BH ^a	EH ^a	TIC (pCi-hr m^{-3})	Detect	BH ^a	EH ^a	TIC (pCi-hr m^{-3})	Detect	
1	0.00E+00	1	1	0.00E+00	0	1	2	3.29E-04	0	1	3	2.19E-04	0	
2	6.58E-13	2	2	6.58E-04	0	2	3	3.29E-04	0	2	4	2.24E-03	0	
3	0.00E+00	3	3	0.00E+00	0	3	4	3.03E-03	0	3	5	2.02E-03	0	
4	6.06E-12	4	4	6.06E-03	0	4	5	3.03E-03	0	4	6	2.41E-02	0	
5	0.00E+00	5	5	0.00E+00	0	5	6	3.32E-02	0	5	7	2.03E-01	0	
6	6.63E-11	6	6	6.63E-02	0	6	7	3.05E-01	1	6	8	4.49E-01	1	
7	5.44E-10	7	7	5.44E-01	1	7	8	6.41E-01	1	7	9	3.67E+00	1	
8	7.37E-10	8	8	7.37E-01	1	8	9	5.23E+00	1	8	10	4.13E+00	1	
9	9.73E-09	9	9	9.73E+00	1	9	10	5.82E+00	1	9	11	4.12E+00	1	
10	1.91E-09	10	10	1.91E+00	1	10	11	1.31E+00	1	10	12	7.41E+00	1	
11	7.11E-10	11	11	7.11E-01	1	11	12	1.02E+01	1	11	13	6.77E+00	1	
12	1.96E-08	12	12	1.96E+01	1	12	13	9.81E+00	1	12	14	6.54E+00	1	
13	0.00E+00	13	13	0.00E+00	0	13	14	1.06E-02	0	13	15	2.20E-02	0	
14	2.12E-11	14	14	2.12E-02	0	14	15	3.29E-02	0	14	16	4.65E-02	0	
15	4.47E-11	15	15	4.47E-02	0	15	16	5.92E-02	0	15	17	5.06E-02	0	
16	7.36E-11	16	16	7.36E-02	0	16	17	5.36E-02	0	16	18	3.79E-02	0	
17	3.35E-11	17	17	3.35E-02	0	17	18	2.00E-02	0	17	19	1.33E-02	0	
18	6.52E-12	18	18	6.52E-03	0	18	19	3.26E-03	0	18	20	1.49E+00	1	
19	0.00E+00	19	19	0.00E+00	0	19	20	2.24E+00	1	---	---	---	---	
20	4.48E-09	20	20	4.48E+00	1	---	---	---	---	---	---	---	---	
Number of detects					7						8			
Number of events					20						19			
Frequency of detection					0.35						0.42			

a. BH = begin hour of summation, EH = end hour of summation.

5.3 Summary of Assumptions

This section summarizes the assumptions associated with the methodology, the source term, transport and dose calculations, and sampling procedures. The assumptions, along with the section where additional information on the justification and/or impact of the assumption may be found, are as follows:

- Frequency of detection is an appropriate and objective measure of the effectiveness of an air monitoring network and represents the likelihood that a release event will be detected by a sampler or samplers in the network (Section 1.2).
- The INL Site ambient air monitoring network, as presently constituted, consists of 37 low-volume air samplers monitored by BEA and Gonzales-Stoller Surveillance for the ESER. It does not include miscellaneous air samplers maintained and sampled by the INL Site cleanup contractor CH2M-WG Idaho, LLC (Section 2). The network sampler in Jackson, Wyoming is outside the model domain and was not considered in the frequency of detection calculations.
- Stack flow rates and exit velocities were based on 2013 values and can be considered representative of future values (Section 4.1).
- Non-stack releases were modeled from a single source location at each major INL Site facility (Section 4.1).
- The quantity of radioactivity released from a source for purposes of calculating frequency of detection is the activity that would result in a maximum inhalation dose of 0.1 mrem at any of the publicly accessible sampler locations or the INL Site MEI location (Section 4.2). The probability of exceeding this dose criterion is 0% (Section 4.2 and 6.4.1). Sensitivity of dose to release duration is examined in Section 6.4.1.
- Inhalation doses were calculated for a reference individual using age and gender-weighted breathing rates and dose coefficients from DOE (2011b) (Section 4.2).
- Three representative and otherwise key radionuclides emitted at the INL Site are considered adequate for demonstrating the effectiveness of the INL Site air monitoring network for this preliminary assessment (Section 4.2).
- Releases are constant over the range of release durations considered, with 1 hour being the shortest duration (Section 4.2).
- The CALPUFF Lagrangian puff dispersion model is an appropriate model for estimating atmospheric transport and dispersion for evaluating the INL Site air monitoring network (Section 3.2).
- A horizontal grid resolution of 2 km and a vertical resolution of 10 layers are adequate for modeling dispersion in the domain of study that encompasses the INL Site air monitoring network (Section 3.3).
- The CALPUFF model of the INL monitoring network was adequately verified by comparison to MDIFFH model results and validated by comparison to data from a historic release of Sb-125 from an INL Site facility (Sections 6.1 and 6.3).
- Terrain complexities and three-dimensional wind fields are considered important features and are included in the modeling (Sections 3.4 and 3.5).
- Decay and deposition (dry or wet) were not considered in the assessment of the INL Site air monitoring network, but could be included (Section 3.4).
- Hourly meteorological data from several sources (WRF model, Idaho Falls and Boise Airports, and 35 INL Mesonet stations) provide a comprehensive and adequate meteorological dataset for the assessment of the INL Site air monitoring network (Section 3.4).

- Meteorological data from the year 2006 is representative of average conditions and demonstrated by comparisons to comparable simulations using data from 2007 and 2008 (Sections 3.4 and 6.2).
- An integration time of 70 hours is sufficient for dissipation of the release and determining a representative *TIC* value at each sampler location (Section 5.1).
- A detection for a sampler occurs if the *TIC* at the sampler location multiplied by the flow rate is greater than the minimum detectable activity (Section 5.1); a detection at any sampler in the network represents a detection for the entire network.
- Two sets of MDA values were evaluated to determine the impact of frequency of detection. The BEA MDA values were determined from contract RDLs using a sampler flow rate of 2 cfm, while ESER MDA values were provided. The ESER MDA values are close to the *a posteriori* MDA values reported by the laboratory used by ESER. The BEA MDA values are much larger than the *a posteriori* MDA values reported by the laboratory used by BEA (Section 2).
- The sampling time was 168 hours (1 week), corresponding to the sampling interval used by the monitoring program, and release durations less than 168 hours occur entirely within the sampling time (Section 5.1). Sensitivity of detection frequency to sampling time is investigated in Section 6.4.2.
- The sampler flow rate is an average value of 2 cfm, which is a typical flow rate of the low-volume samplers used by the INL network (Section 2). Sensitivity to sampler flow rate is examined in Section 6.4.3.
- The contribution from background activity was not considered for this preliminary assessment of the INL air monitoring network, but can be evaluated using the methodology. The detection frequencies are based on detecting a release from the INL Site in the absence of background activity (Section 7).

6. RESULTS

Prior to demonstrating the methodology by conducting a preliminary assessment of the INL Site ambient air monitoring network (Section 6.4), exercises were performed to verify and validate the model and evaluate variability in meteorological data. First, a verification of the CALPUFF model was performed by comparing results to MDIFFH model results in Section 6.1. The variability in the year-to-year and monthly dispersion factors and the sensitivity of the dispersion factors results to inclusion or exclusion of WRF data was evaluated and presented in Section 6.2. Section 6.3 contains the results of a model validation exercise, where model predicted concentrations were compared to measured concentrations from a release of Sb-125 in 1987. Section 6.4 contains the frequency of detection results from a preliminary assessment of the INL Site air monitoring network to demonstrate the methodology, and Section 6.5 contains an evaluation of the sensitivity of the results to input values such as release rate (Section 6.5.1), sampling time (Section 6.5.2), and sampler flow rate (Section 6.5.3).

6.1 Model Verification

To verify the CALPUFF model simulation, annual *TIC_u* values were calculated for the year 2006 and compared with those from MDIFFH published in the INL Site annual environmental report for 2006 (DOE-ID 2007). Total activity released from six facilities (i.e., CFA, INTEC, MFC, ATR Complex, RWMC, and SMC/TAN) was obtained from Table 4-2 in DOE-ID (2007). According to the methodology stated in DOE-ID (2007), the source term was the fraction of total activity from each facility times a 1 Ci hr⁻¹ release rate for the entire year (see Table 9). For the year 2006, the MEI was not at Frenchman's Cabin but about 10 km east of TAN. Table 9 shows the *TIC_u* values from each individual facility at the MEI for both CALPUFF and MDIFFH. In general, the CALPUFF *TIC_u* values were within a factor of 1.6 of the MDIFFH *TIC_u* values for ground-level releases. For stack releases, differences are as large as 2.8. The larger difference in the *TIC_u* values for stack releases is likely due to upper air data incorporated into

the CALPUFF simulation, whereas in MDIFFH, only the wind speed changes with height. The surface layer in CALPUFF extends from the ground surface to 20 m. The stack heights (60 to 76 m) would put releases into the third CALPUFF layer (40 to 80 m above ground level). Stack exit velocities for 2006 were assumed to be the same as 2013 in the CALPUFF simulation, which could also make a difference, but the difference is likely to be small compared to the impact of the upper air data.

Table 9. Activity and fraction of total activity released in 2006 and the CALPUFF and MDIFFH *TICu* values at the 2006 MEI location approximately 10 km east of TAN.

Facility	Activity		CALPUFF <i>TICu</i>	MDIFFH ^b	Type of Release ^c
	Released (Ci) ^a	Fraction	(hr ² m ⁻³)	<i>TICu</i> (hr ² m ⁻³)	
CFA	2.06	0.0003261	2.00E-08	3.24E-08	Ground-level release
INTEC	3,640	0.5761	2.38E-08	2.84E-08	Ground-level release
MFC	1,200	0.1899	2.65E-08	1.12E-08	Stack release (MFC-764)
ATR	1,400	0.2216	1.02E-08	2.82E-08	Stack release (TRA-770)
RWMC	75.7	0.01198	1.46E-08	2.74E-08	Ground-level release
TAN	0.218	0.0000345	2.31E-07	2.14E-07	Ground-level release
Totals	6,318	1.00			

a. From Table 4-2 in DOE-ID (2007).

b. From Table 8-2 in DOE-ID (2007).

c. Ground and stack releases provided by R. Eckerman, Idaho Falls NOAA office. Stack release parameters for MFC-764 and TRA-770 are those listed in Table 5.

Isopleth maps of annual *TICu* values for fractional releases from all six facilities are shown in Figure 7 for MDIFFH and Figure 8 for CALPUFF. Differences were expected because CALPUFF treats terrain effects explicitly and includes upper air meteorological data in its simulation. The effects of terrain can be seen in Figure 8, where the plume from the ATR stack impacts Big Southern Butte and the foothills of the Lemhi Mountains near Howe, resulting in higher concentrations in the elevated terrain. The 1.0 contour line from the CALPUFF simulation extends slightly farther from the INL Site compared to that of MDIFFH. Both models show terrain channeling up the Little Lost River and Willow Creek (Idaho Highway 28) drainage. The use of data from meteorological stations at Blue Dome and Howe were important to resolving the influence of terrain in the MDIFFH simulation.

The results of this verification exercise demonstrate that the CALPUFF model simulation produces results that were comparable with those of MDIFFH, and that differences can be attributed to explicit treatment of terrain, three-dimensional wind fields, and the different dispersion coefficients that are used in CALPUFF.

6.2 Meteorological Data Variability Evaluation

The frequency of detection assessment was performed using meteorological data from year 2006. To evaluate the year-to-year variability of dispersion at the INL Site, simulations of a ground-level release from INTEC were performed for 3 years (2006, 2007, and 2008) using a steady-state 1 Ci hr⁻¹ release rate. The annual *TICu* values at selected sampler locations are plotted in Figure 9. In general, there was relative consistency in the annual *TICu* values across the 3 years simulated. The mean distribution of the ratio of *TICu* for a given year and location divided by the 3-year average *TICu* value was 1.0, with a standard deviation of 0.084. The maximum difference between any 2 years was 1.5 between years 2007 and 2008 at the BEA-SUGAR sampler. Note that *TICu* values in Figure 9 are higher than what is plotted in Figure 7 and Figure 8, because the *TICu* values in Figure 9 are from a single, ground-level release at INTEC, whereas the *TICu* values plotted in Figure 7 and Figure 8 are from multiple sources, including stacks resulting in greater dilution.

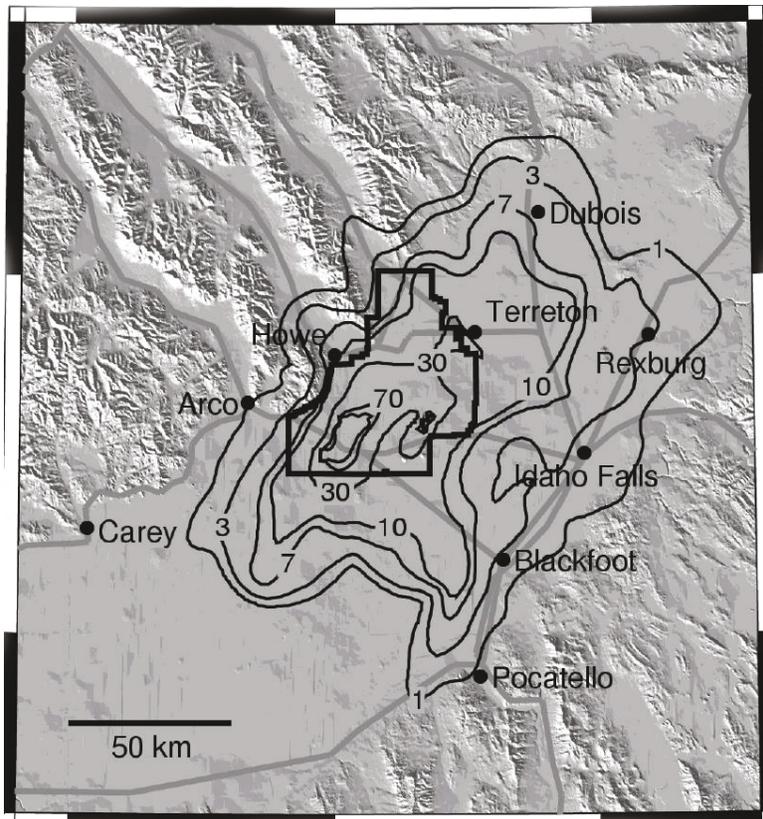


Figure 7. 2006 annual $TICu$ ($hr^2 m^{-3}$) using MDIFFH. Values are multiplied by 10^9 for plotting (figure taken from DOE-ID [2007]).

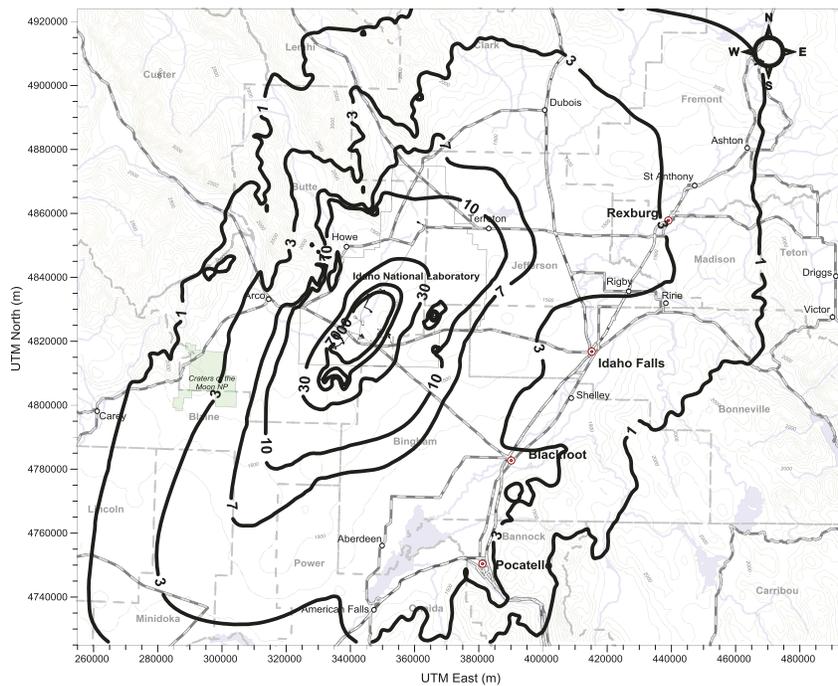


Figure 8. 2006 annual $TICu$ ($hr^2 m^{-3}$) using CALPUFF. Values are multiplied by 10^9 for plotting.

The variability can also be examined by viewing isopleth plots of the annual $TICu$ values for each year for a ground-level release at INTEC (see Figure 10). In general, there was little difference in the results, as would be expected after viewing the results in Figure 9. Also shown in Figure 10 are results for the year 2006 run without WRF data. This comparison indicates that for ground-level releases, the incorporation of WRF data makes little difference in the results. This suggests that dispersion for ground-level releases is governed primarily by surface-level meteorological data. Figure 10 also demonstrates that for ground-level releases, the CALPUFF model simulations for future years can be adequately simulated using the Mesonet surface station data and Boise upper air data.

Another presentation of the variability in meteorological conditions is illustrated in Figure 11, where the monthly-average X/Q values for a ground-level release at INTEC are plotted for all 3 years at the BEA-REST sampler located along U.S. Highway 20. The X/Q ($s\ m^{-3}$) is a more conventional representation of dispersion and is simply the concentration at the sampler location (X , $Ci\ m^{-3}$) divided by source emission rate (Q , $Ci\ s^{-1}$). Monthly average X/Q values were obtained by multiplying $TICu$ values by the ratio of $(3,600\ s\ hr^{-1})/(730\ hours)$, where 730 hours is the average number of hours in a month. In general, the highest X/Q values occur during the months of January and December and the lowest X/Q values occur during the spring and early summer months (April through June) and in November. The maximum difference between monthly X/Q values was between January 2007 and June 2008 (factor of 5.8). The maximum dose at publicly accessible sampler locations used to determine the release quantities for this study almost exclusively occurred during the months of December or January. Thus, releases during these months are more likely to be detected than releases that occur in the springtime. Furthermore, the results in Figure 11 demonstrate that dose assessments that assume a constant release over the year can be significantly under or overestimated if the release varies considerably over the course of the year.

6.3 Model Validation

A model validation exercise was performed by simulating the release and transport of a 16-Ci release of Sb-125 from the flourinel and storage stack at INTEC in 1987. Releases of Sb-125 were identified in a 1987 DOE-ID memo (Chew 1987) as an opportunity to validate the MESODIF (Start and Wendell 1974) meteorological air dispersion model. The MESODIF model was the precursor to the MDIFFH model described previously. Annual average concentrations above detection limits at 21 samplers located both on and off the INL Site (Dickson 2012) were compared with model predicted values from CALPUFF and MESODIF. Because meteorology and dispersion conditions at the site are fundamentally repeatable from year-to-year (see Section 6.2), a 3-year meteorological dataset was used (i.e., 2006, 2007, and 2008) to simulate dispersion conditions for 1987 using CALPUFF. Three-year average monthly dispersion factors, coupled with monthly Sb-125 releases from the flourinel and storage stack obtained from DOE-ID (1988), were used to calculate the annual average concentrations at the 21 samplers. Releases varied considerably from month to month, ranging from 4.59 Ci for February to 0.0018 Ci for November 1987. A detailed description of the model validation exercise, including detailed results is presented in Appendix D.

The geometric mean of the predicted-to-observed ratio for CALPUFF and MESODIF was 0.73 and 2.17, respectively, and the geometric standard deviation for CALPUFF and MESODIF was 2.22 and 3.22, respectively. The log-transformed regression coefficient (r) was 0.853 for CALPUFF and 0.739 for MESODIF (Figure 12). An F -test indicated that the linear regression for both CALPUFF and MESODIF were significant. By almost all other quantitative measures of performance, CALPUFF was judged to perform better than MESODIF. This validation exercise demonstrates that CALPUFF provides concentration estimates from INL Site releases that were within the established uncertainty of atmospheric transport models for predicting annual average concentrations in a complex-terrain environment (Miller and Hively 1987).

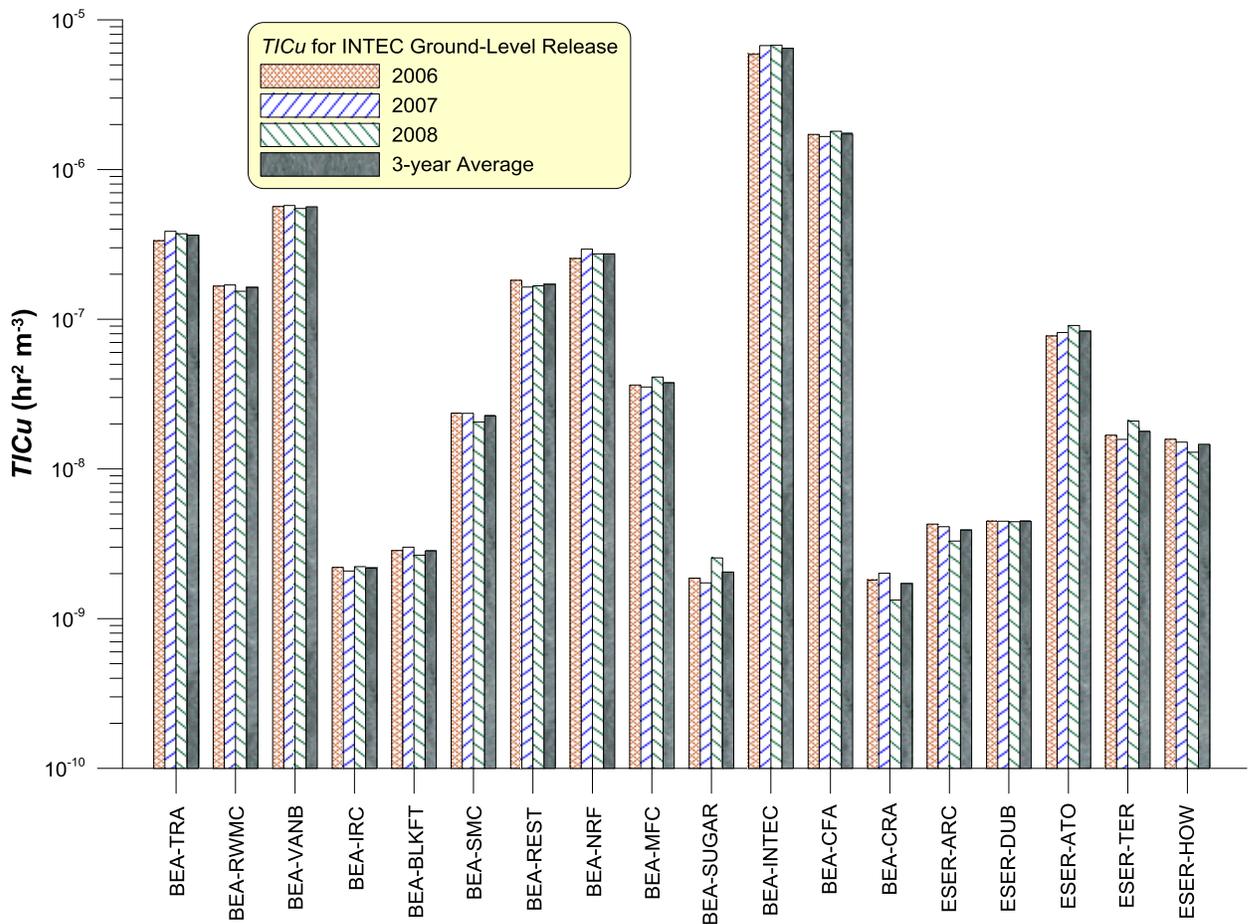


Figure 9. Annual $TICu$ values at selected samplers for 2006, 2007, 2008, and 3-year average for a ground-level release at INTEC.

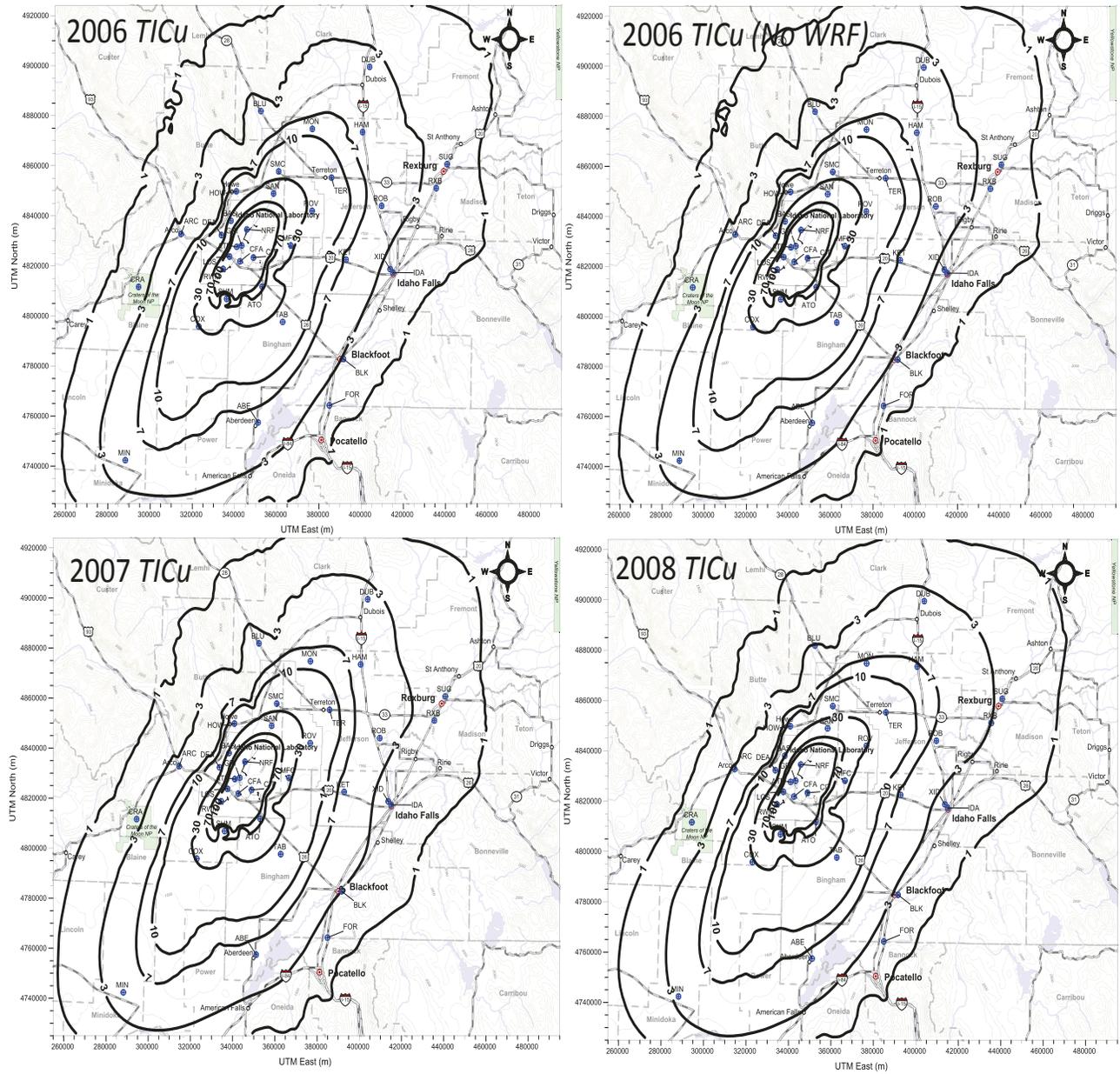


Figure 10. Annual $TICu$ isopleth maps ($h^2 m^{-3}$) for a ground-level release at INTEC using 2006, 2007, and 2008 meteorological data. The 2006 simulation includes a simulation without the WRF data (upper right pane). Mesonet meteorological stations are shown with blue symbols.

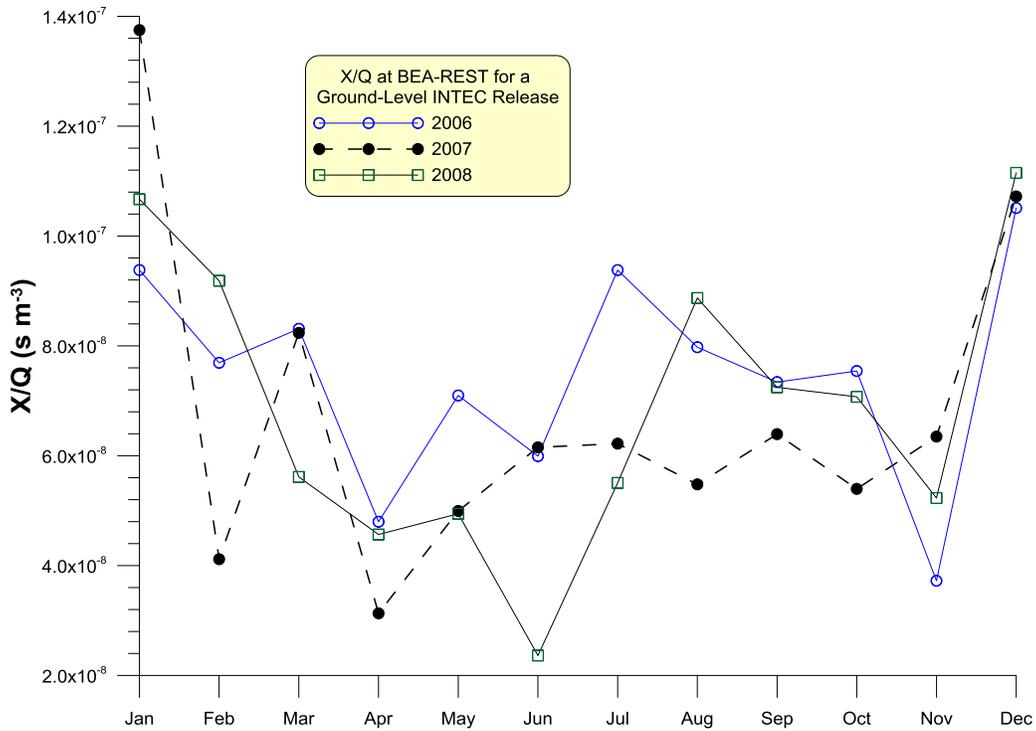


Figure 11. Monthly average X/Q ($s\ m^{-3}$) values at the BEA-REST sampler from a ground-level release at INTEC.

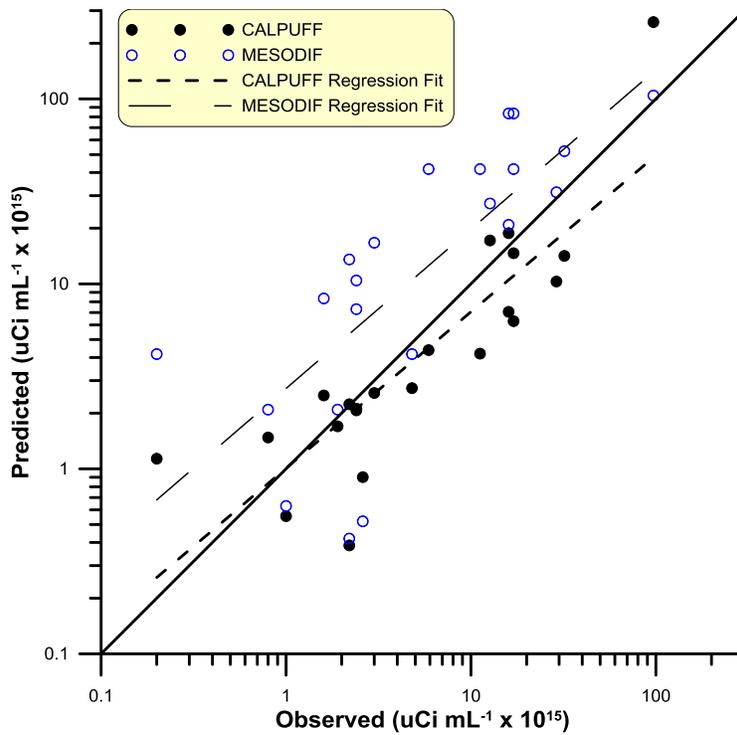


Figure 12. Scatter plot of predicted concentrations from MESODIF and CALPUFF as a function of observed concentrations. Points that lie above the perfect correlation line are over-predictions and points that lie under the line are under-predictions. Log-transformed regression lines are shown with correlation coefficients of 0.853 for CALPUFF and 0.739 for MESODIF.

6.4 Frequency of Detection Results

This section presents frequency of detection results from a preliminary assessment of the current INL Site ambient air monitoring network. Radionuclide-specific release quantities that result in a maximum effective dose of 0.1 mrem yr^{-1} at any publicly accessible sampler location (Section 4.2, Table 7) were combined with the MDA values in Table 2, a sampler flow rate of 2 cfm ($3.398 \text{ m}^3 \text{ hr}^{-1}$), and a 168-hour sampler run time to calculate the frequency of detection for release durations of 1 hour to 340 hours (about 14 days). Frequency of detection results are presented in this section for the onsite (on INL Site) and offsite (off INL Site) samplers in the network. The performance of the entire network in terms of detection frequency would not be less than the performance of either the onsite or offsite samplers, whichever is highest.

Frequency of detection results are plotted in Figures 13 through 15 as a function of release duration for three sources (i.e., the TRA-770 stack, CFA-625, and the MFC-764 stack). These three sources were chosen to display the range of variability in the results. Similar plots for all sources can be found in Appendix C. Tabulated results for all sources are also shown in Table 10 (using ESER MDAs) and Table 11 (using BEA MDAs). The tabulated results show the frequency of detection for the minimum and maximum release durations of 1 hour and 340 hours; they include the maximum frequency of detection and the release duration for which the maximum occurred. These results are also shown graphically in Figures 16 through 19.

For Cs-137 and Sr-90, frequency of detection is generally at its minimum for the 1-hour release duration, and then increases to its maximum (often greater than 95%) with increasing release duration. In some cases, frequency of detection decreases after reaching its maximum with increasing release duration. Pu-239 detection frequencies were considerably less than those of Cs-137 and Sr-90. This was because the inhalation dose coefficient for Pu-239 is a factor of 2,900 higher than Cs-137 and 738 higher than Sr-90. Thus, substantially less Pu-239 activity was required to be released to result in an inhalation dose of 0.1 mrem and the probability of detecting this smaller activity was also substantially less. The lower MDA for Pu-239 did not compensate for the smaller release quantity.

The frequency of detection for onsite samplers was nearly 100% for release durations greater than 24 hours for Cs-137 and Sr-90 using ESER MDAs. The frequency of detection values for offsite samplers using ESER MDAs were slightly less for these radionuclides, but in all cases the frequency of detection was greater than 95% for release durations greater than 30 hours. Releases from the MFC facility actually had higher detection frequencies for Cs-137 and Sr-90 in the offsite samplers compared to the onsite samplers, especially for the stack release.

For Pu-239 using ESER MDAs, the frequency of detection at onsite samplers was generally over 90% for ground-level releases of durations that exceeded about 50 hours, with the exception of CFA-625. Most stack releases exhibited substantially lower Pu-239 detection frequencies at onsite samplers. For example, the CPP-708 stack had a maximum detection frequency of 27%. In most cases, the Pu-239 detection frequencies at offsite samplers reached a maximum and then decreased with increasing release duration. This happens because as the release duration increases, so does dilution and dispersion of the released activity (which is the same for each time period assessed), resulting in the MDA threshold not being met from the activity accumulated on the sample filter during the sampling time.

Detection frequencies using BEA MDAs were noticeably less for Pu-239 and Sr-90 and only slightly less for Cs-137. The largest change in detection frequencies was noted for Pu-239. However, the BEA MDA for Pu-239 was only about a factor of 10 greater than the ESER MDA, whereas the BEA MDAs for Cs-137 and Sr-90 were 18 and 88 times greater, respectively. The Pu-239 detection frequencies decreased more than those for Sr-90 and Cs-137, because the releases quantities were substantially smaller, resulting in ambient air concentrations that were already near the ESER MDA.

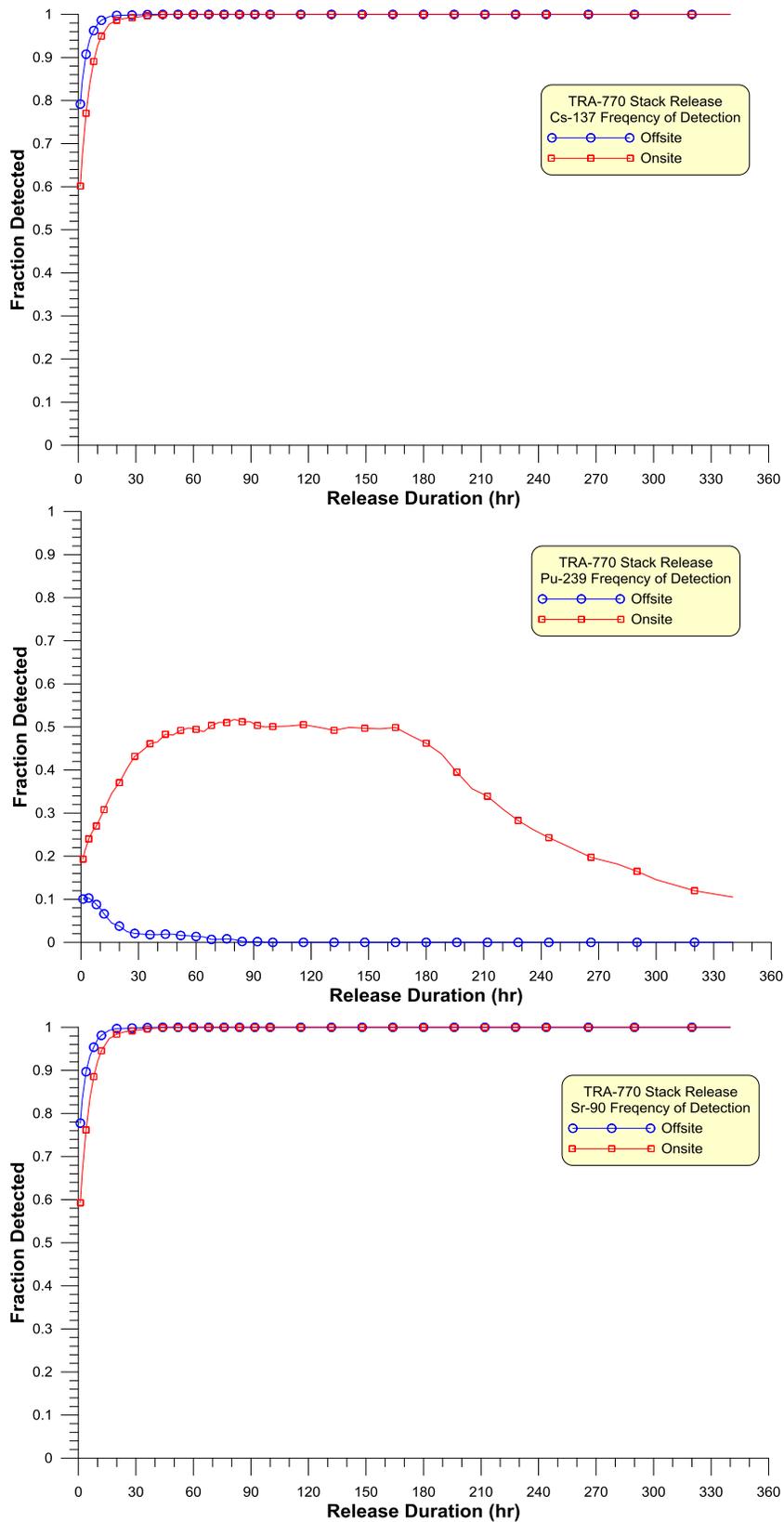


Figure 13. Frequency of detection for releases from the TRA-770 stack using ESER MDAs.

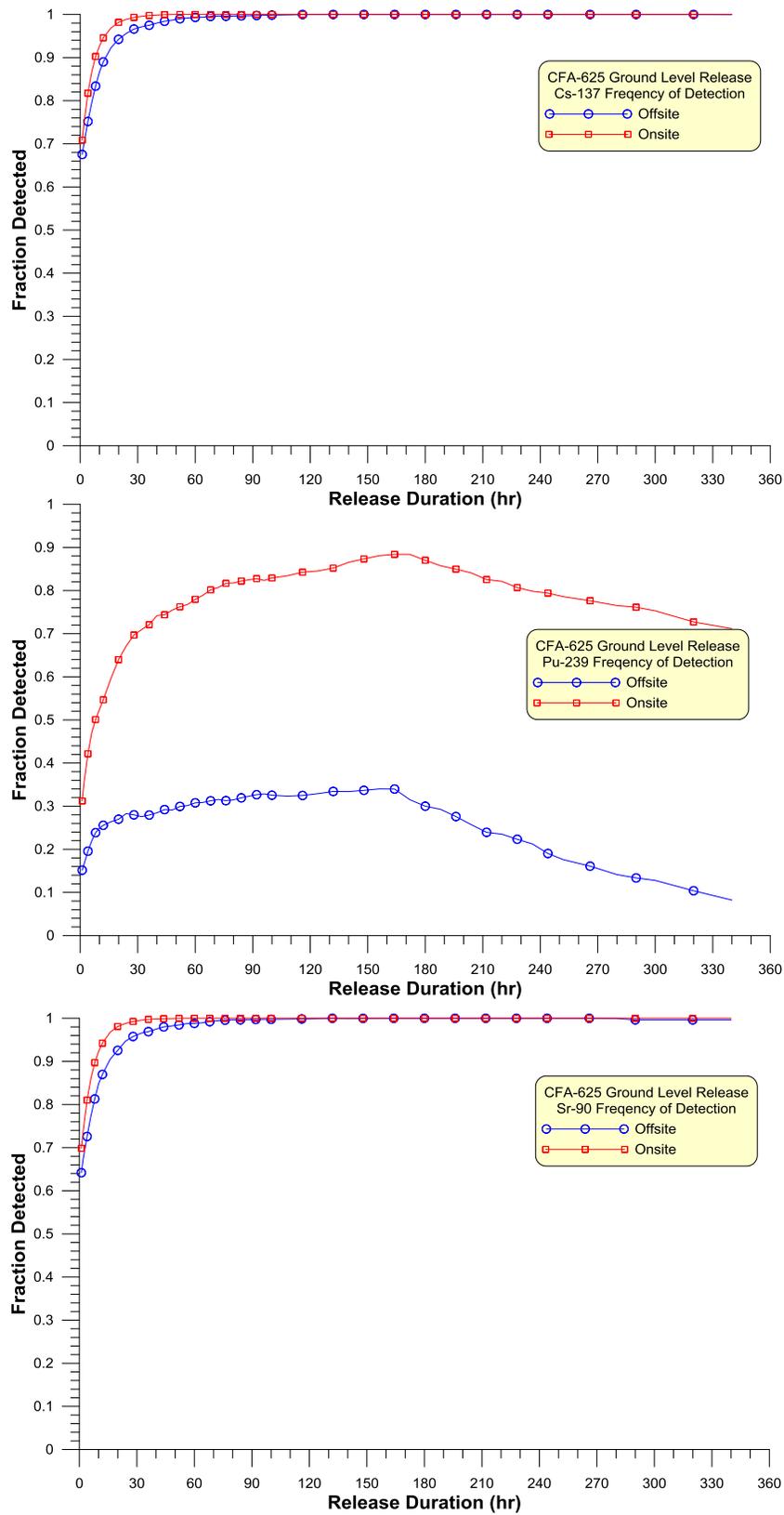


Figure 14. Frequency of detection for ground-level releases from CFA-625 using ESER MDAs.

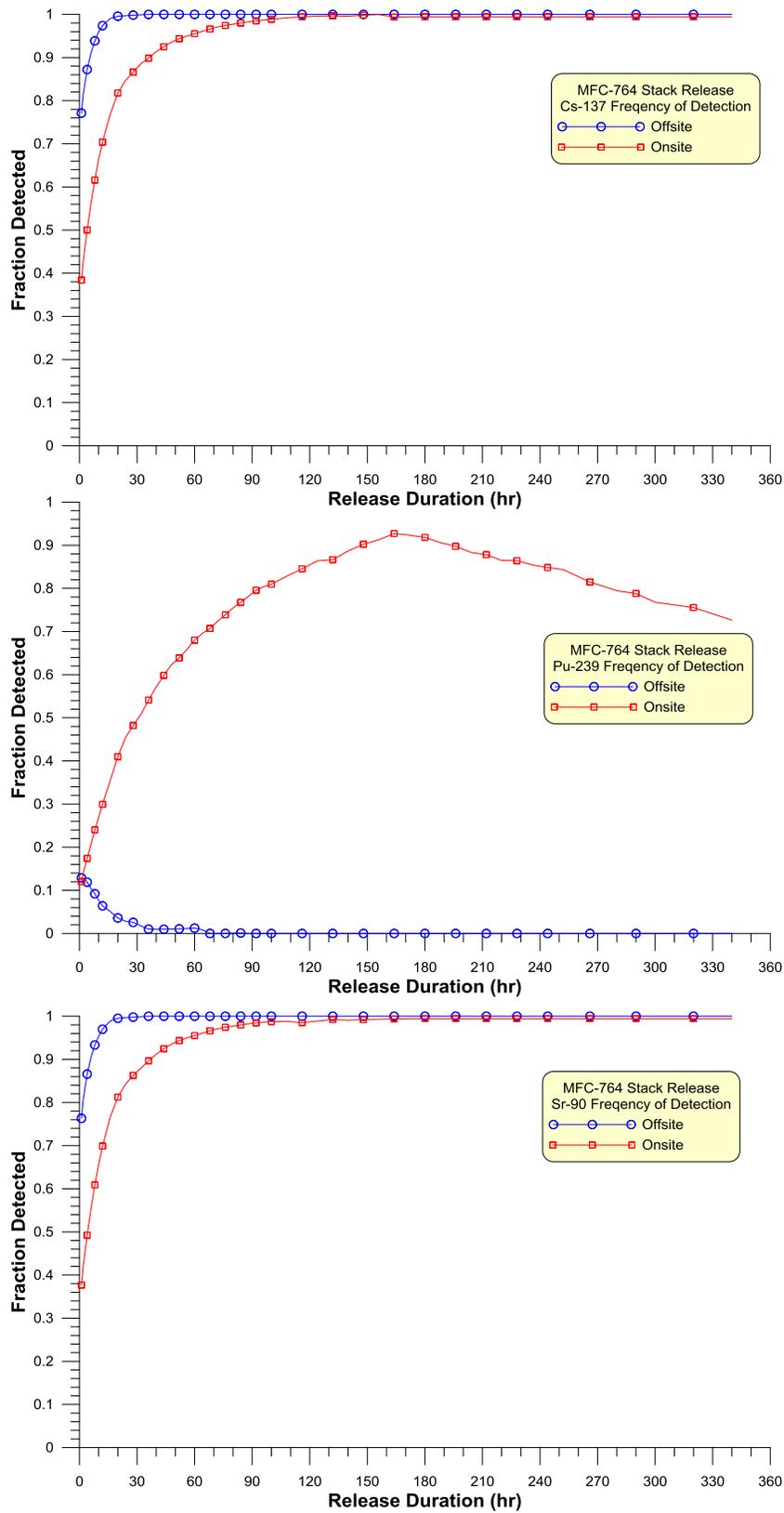


Figure 15. Frequency of detection for releases from the MFC-764 stack using ESER MDAs.

Table 10. Onsite and offsite detection frequencies using ESER MDAs and 2-cfm sampler flow rate.

Radionuclide	Source	Onsite Detection Frequency				Offsite Detection Frequency			
		1-hour Release Duration	Max	Release Duration of Maximum (hours)	340-Hour Release Duration	1-hour Release Duration	Max	Release Duration of Maximum (hours)	340-Hour Release Duration
Cs-137	ATR	0.95	1	36	1	0.83	1	60	1
	CFA-625	0.71	1	52	1	0.68	1	124	1
	CITRC	0.68	1	48	1	0.85	1	64	1
	CPP-1774	0.87	1	32	1	0.69	1	72	1
	CPP-708	0.60	1	44	1	0.70	1	140	0.98
	MFC-764	0.38	1	156	0.99	0.77	1	40	1
	MFC-774	0.69	1	48	1	0.89	1	28	1
	NRF	0.88	1	36	1	0.94	1	40	1
	RWMC	0.75	1	64	1	0.63	1	72	1
	TAN-679	0.86	1	28	1	0.93	1	28	1
TRA-770	0.60	1	48	1	0.76	1	40	1	
Pu-239	ATR	0.86	1	44	1	0.20	0.46	156	0.06
	CFA-625	0.31	0.88	164	0.71	0.15	0.34	156	0.08
	CITRC	0.35	0.99	172	0.99	0.28	0.80	164	0.43
	CPP-1774	0.57	1	84	1	0.12	0.15	8	0
	CPP-708	0.23	0.27	20	0	0.03	0.03	1	0
	MFC-764	0.12	0.93	164	0.73	0.13	0.13	1	0
	MFC-774	0.45	1	92	1	0.26	0.40	20	0.04
	NRF	0.55	1	148	1	0.27	0.49	132	0.09
	RWMC	0.58	1	76	1	0.11	0.11	2	0
	TAN-679	0.65	1	64	1	0.21	0.21	1	0
TRA-770	0.19	0.52	80	0.11	0.10	0.10	2	0	
Sr-90	ATR	0.95	1	36	1	0.81	1	64	1
	CFA-625	0.70	1	56	1	0.64	1	132	1
	CITRC	0.67	1	52	1	0.82	1	72	1
	CPP-1774	0.86	1	32	1	0.65	1	96	1
	CPP-708	0.59	1	44	1	0.67	1	148	0.95
	MFC-764	0.38	0.99	172	0.99	0.76	1	40	1
	MFC-774	0.68	1	48	1	0.88	1	36	1
	NRF	0.87	1	36	1	0.93	1	40	1
	RWMC	0.74	1	64	1	0.60	1	100	1
	TAN-679	0.86	1	28	1	0.92	1	28	1
TRA-770	0.59	1	48	1	0.74	1	44	1	

Table 11. Onsite and offsite detection frequencies using BEA MDAs and 2-cfm sampler flow rate.

Radionuclide	Source	Onsite Detection Frequency				Offsite Detection Frequency			
		1-hour Release Duration	Max	Release Duration of Maximum (hours)	340-Hour Release Duration	1-Hour Release Duration	Max	Release Duration of Maximum (hours)	340-Hour Release Duration
Cs-137	ATR	0.90	1	36	1	0.42	0.93	172	0.84
	CFA-625	0.50	1	164	0.97	0.26	0.86	172	0.64
	CITRC	0.47	1	164	1	0.46	0.98	172	0.95
	CPP-1774	0.76	1	52	1	0.26	0.69	164	0.35
	CPP-708	0.44	0.98	164	0.66	0.19	0.19	4	0
	MFC-764	0.25	0.99	164	0.98	0.42	0.60	20	0.03
	MFC-774	0.57	1	72	1	0.55	0.99	164	0.83
	NRF	0.71	1	68	1	0.57	0.96	172	0.87
	RWMC	0.66	1	68	1	0.26	0.69	148	0.15
	TAN-679	0.76	1	52	1	0.51	0.82	96	0.21
TRA-770	0.40	0.97	164	0.86	0.30	0.61	140	0.10	
Pu-239	ATR	0.69	1	48	1	0.03	0.03	1	0
	CFA-625	0.08	0.11	12	0	0.02	0.02	1	0
	CITRC	0.23	0.97	172	0.92	0.06	0.06	2	0
	CPP-1774	0.24	0.35	28	0.005	0.002	0.002	1	0
	CPP-708	0.02	0.02	1	0	0	0	NA	0
	MFC-764	0.05	0.13	10	0	0.002	0.002	1	0
	MFC-774	0.30	1	156	1	0.02	0.02	1	0
	NRF	0.33	1	164	0.98	0.03	0.03	1	0
	RWMC	0.37	0.92	164	0.26	0	0	NA	0
	TAN-679	0.45	1	124	1	0.001	0.001	1	0
TRA-770	0.05	0.05	2	0	0.001	0.001	1	0	
Sr-90	ATR	0.85	1	44	1	0.18	0.36	100	0.03
	CFA-625	0.30	0.85	164	0.63	0.14	0.30	140	0.03
	CITRC	0.34	0.99	172	0.98	0.26	0.75	164	0.34
	CPP-1774	0.55	1	108	0.99	0.11	0.13	4	0
	CPP-708	0.20	0.23	16	0	0.02	0.02	1	0
	MFC-764	0.11	0.90	164	0.67	0.11	0.11	1	0
	MFC-774	0.44	1	92	1	0.24	0.33	16	0.03
	NRF	0.53	1	148	1	0.25	0.40	44	0.05
	RWMC	0.57	1	76	1	0.09	0.09	1	0
	TAN-679	0.63	1	64	1	0.18	0.18	1	0
TRA-770	0.18	0.45	68	0.07	0.09	0.09	2	0	

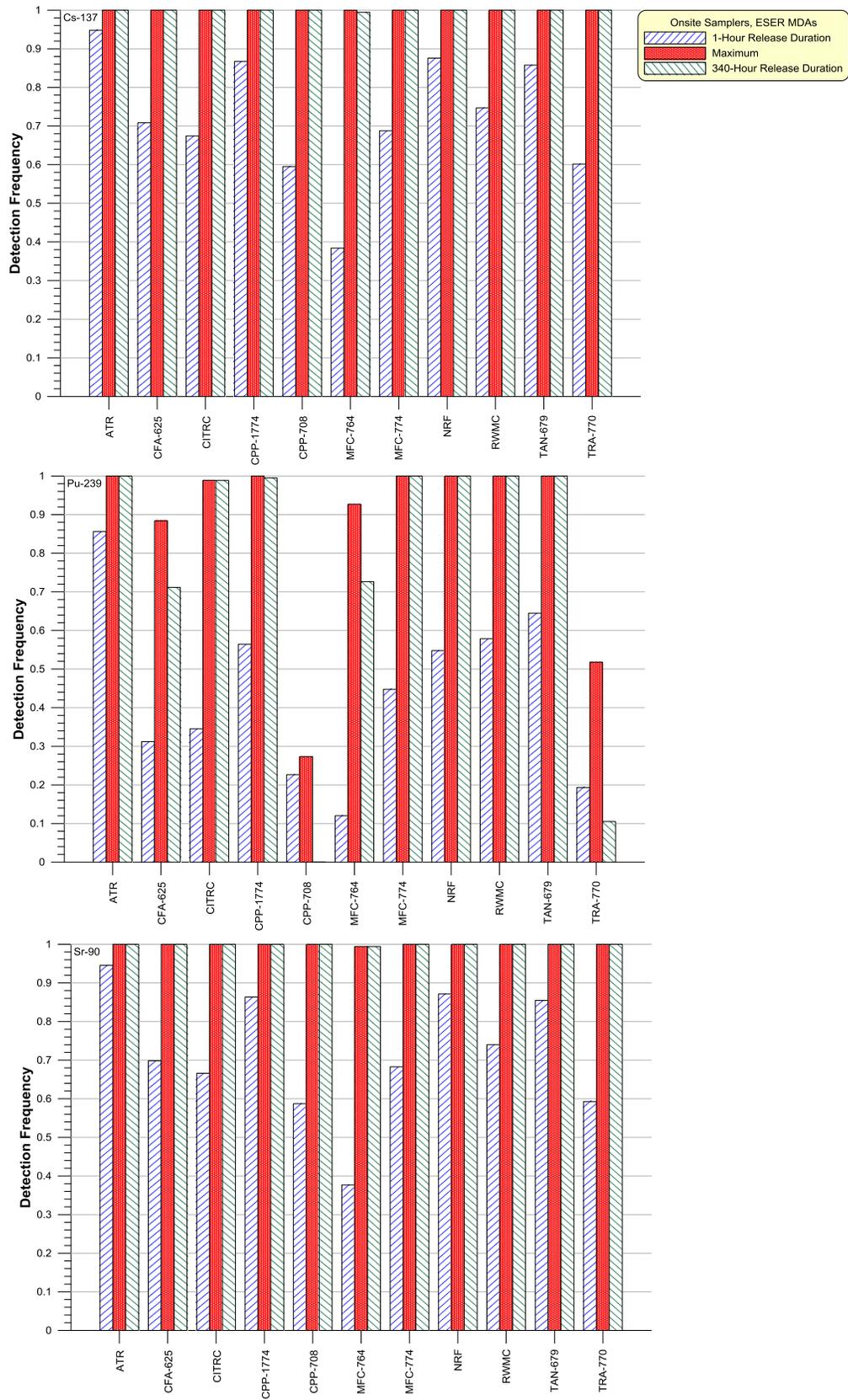


Figure 16. Detection frequency for onsite samplers using ESER MDAs.

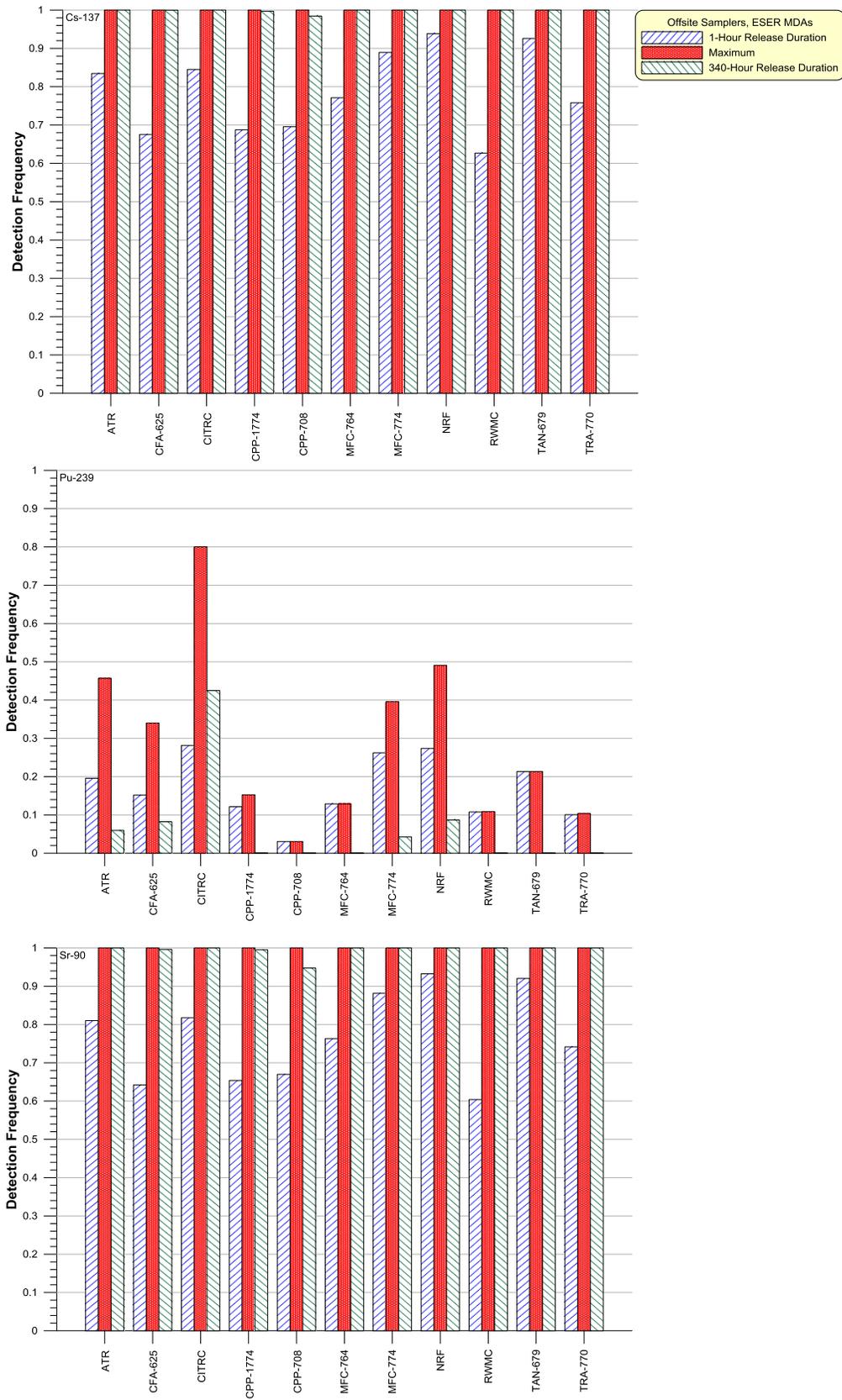


Figure 17. Detection frequency for offsite samplers using ESER MDAs.

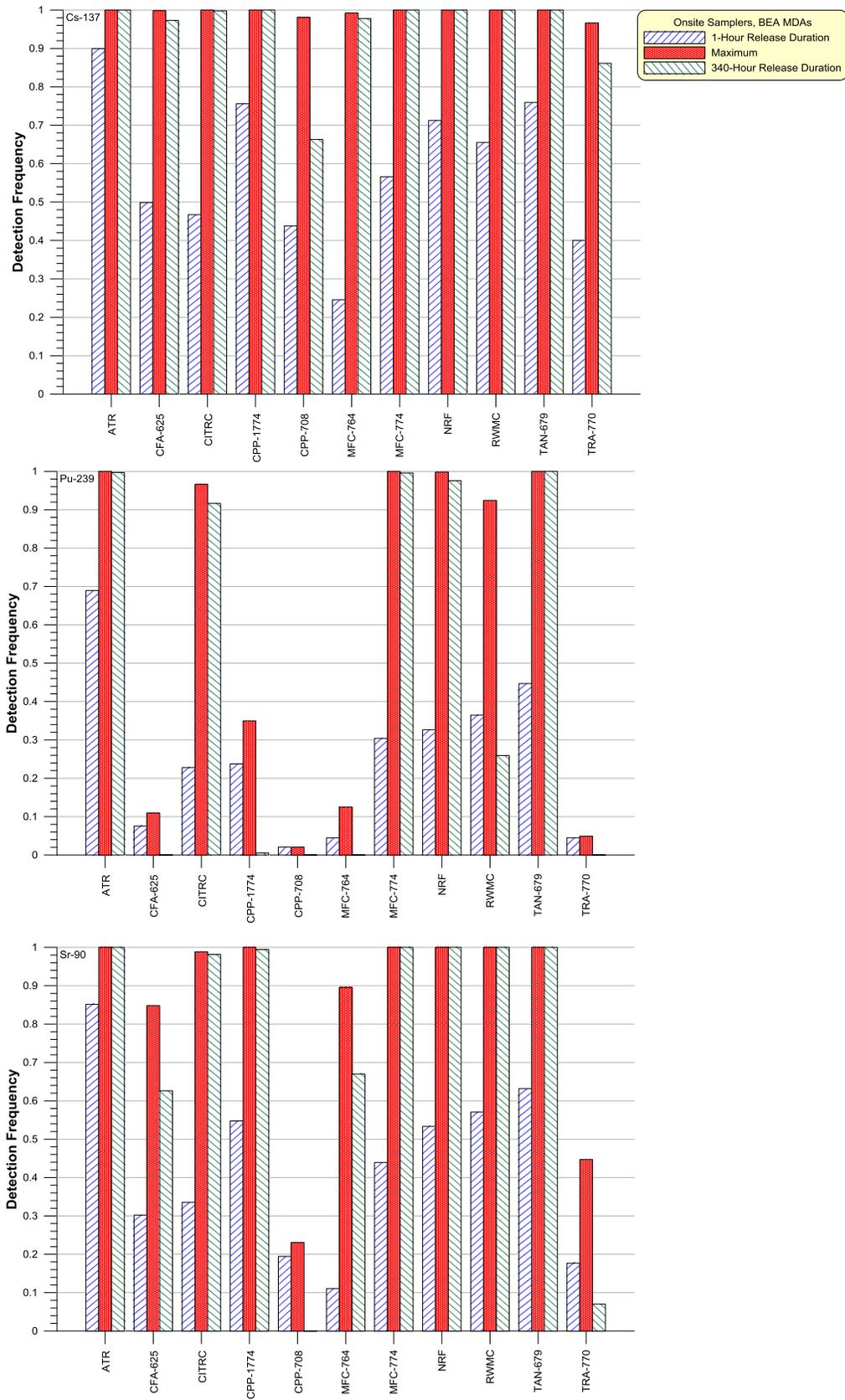


Figure 18. Detection frequency for onsite samplers using BEA MDAs.

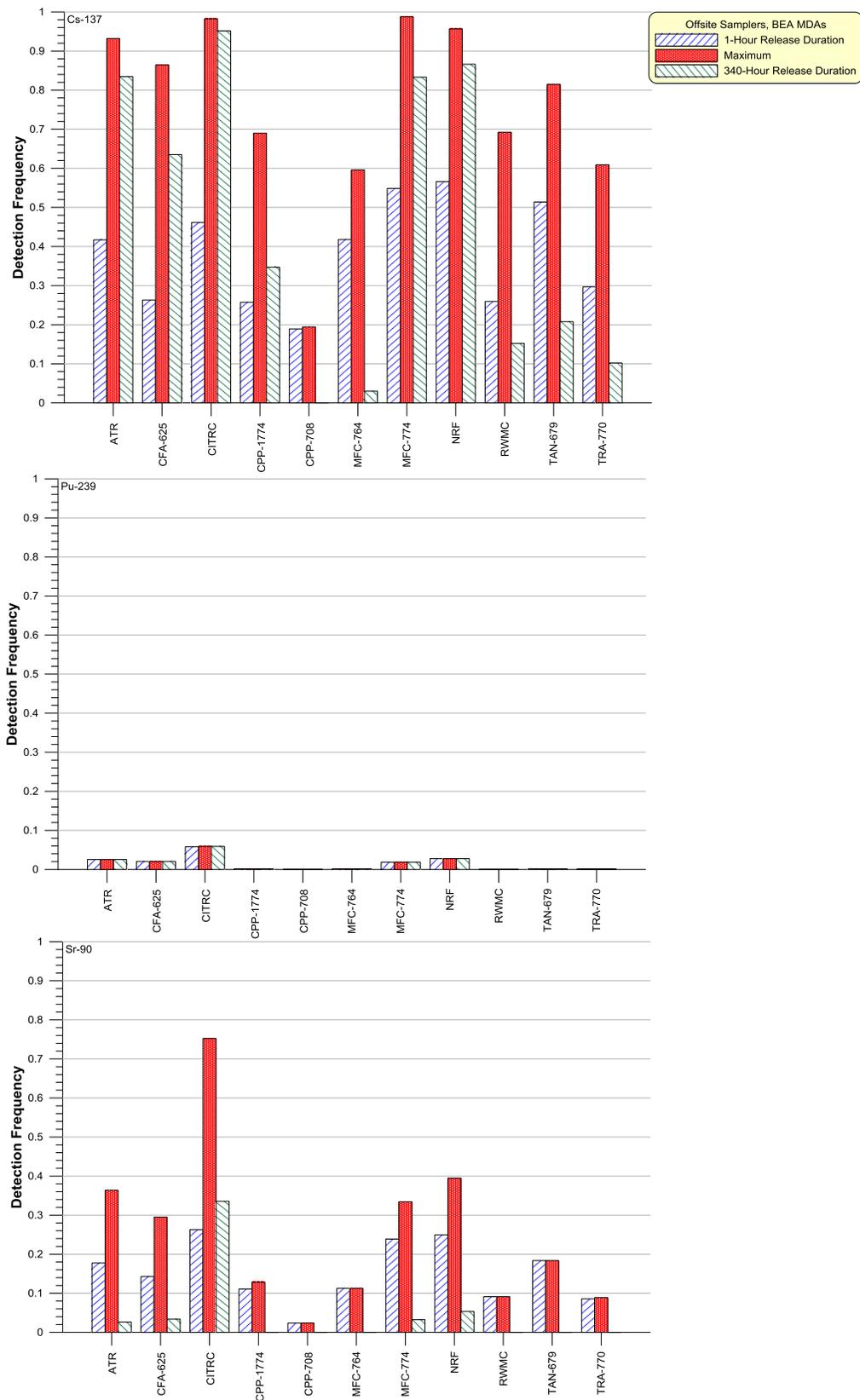


Figure 19. Detection frequency for offsite samplers using BEA MDAs.

6.5 Sensitivity Analysis

This section contains an evaluation of the sensitivity of the results to key input parameters such as release rate, sampling time, and sampler flow rate.

6.5.1 Sensitivity of Maximum Dose to Release Durations

The release quantities used for this assessment (Table 7) correspond to a maximum dose of 0.1 mrem yr^{-1} at any publicly accessible sampler location. In all cases, the 0.1-mrem yr^{-1} dose occurred for only a single hour of the modeled year and a 1-hour release duration; doses for all other release hours and release durations were substantially less (i.e., the distribution of doses across the year was highly skewed). For example, Figure 20 shows the ranked distribution of inhalation dose at the BEA-REST sampler location for a Pu-239 release of 0.0342 mCi from CPP-1774. The maximum dose at this location for this release was 0.1 mrem (again corresponding to a 1-hour release duration), but the 95th percentile dose for that same 1-hour release is 0.0014 mrem yr^{-1} , which is almost two orders of magnitude less than the 0.1-mrem criteria. If the dose criteria was the 95th percentile dose of 0.1 mrem, then detection frequencies would be based on a larger release quantity of 2.44 mCi ($0.0342 \text{ mCi} \times 0.1 \text{ mrem} / 0.0014 \text{ mrem} = 2.44 \text{ mCi}$) and the performance of the network would increase (i.e., higher detection frequencies). For example, a release of 2.44 mCi of Pu-239 from CPP-1774 would result in maximum detection frequencies of 100% for onsite samplers and 78% for offsite samplers using BEA MDAs. These detection frequencies are significantly higher than the maximum detection frequencies of 35% for onsite samplers and 0.2% for offsite samplers when using a release quantity of 0.0342 mCi and BEA MDAs.

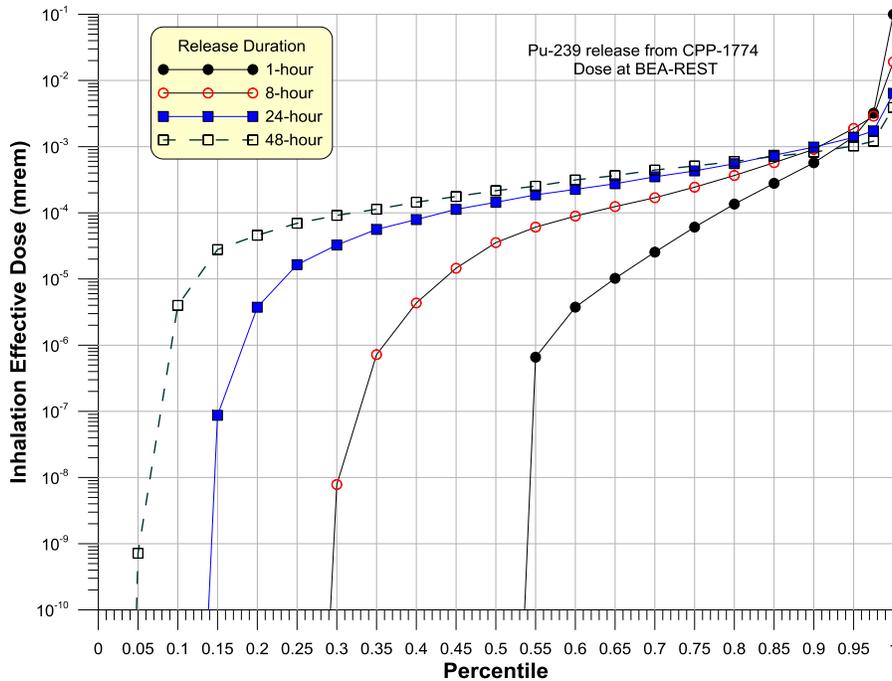


Figure 20. Distribution of inhalation doses at the BEA-REST sampler for a Pu-239 release of 0.0342 mCi from CPP-1774. Maximum dose was 0.1 mrem for a 1-hour release duration.

Another important aspect of Figure 20 is that the dose distribution becomes flatter for longer release times. Recall that all the doses are based on the same release quantity. Thus, if the same amount of activity is released over a longer period of time, then there is greater dispersion of the mass, resulting in lower doses and a more uniform dose over the affected samplers. For example, the maximum dose from a 48-hour release was about 0.005 mrem and the 50th percentile dose was about 0.0002 mrem, whereas for a 1-hour release, the maximum dose was 0.1 mrem and the 50th percentile dose was less than 1×10^{-10} mrem.

6.5.2 Sensitivity of Detection Frequency to Sampling Time

The plots in Figures 13 through 19 are based on the release being entirely captured in a 1-week (i.e., 168 hours) sampling period. However, suppose the release did not begin at the start of the sampling period, but during the sampling period. The sensitivity of the detection frequency to sampling time T_s is illustrated in Figure 21 for Sr-90 using the BEA MDA and onsite samplers. Sampling times of 168 hours, 84 hours, 48 hours, and 24 hours are plotted. The detection frequency does not change for release durations less than the sampling time. When the release duration exceeds the sampling time, only a fraction of the activity emitted to the atmosphere has the potential to be captured by the sampler, resulting in a decrease in the detection frequency. However, because sampler filters are collected and replaced each week, the fraction of the release that is not collected during the first sampling time is collected on the replacement filter during the following week. For example, according to Figure 21, the detection frequency for a 24-hr sampling time and a release duration of 150 hours is approximately 50%. That means the remaining 126 hours (150 – 24 hours) of the release will occur during the sampling time for the replacement filter and the detection frequency will be much higher (nearly 100%).

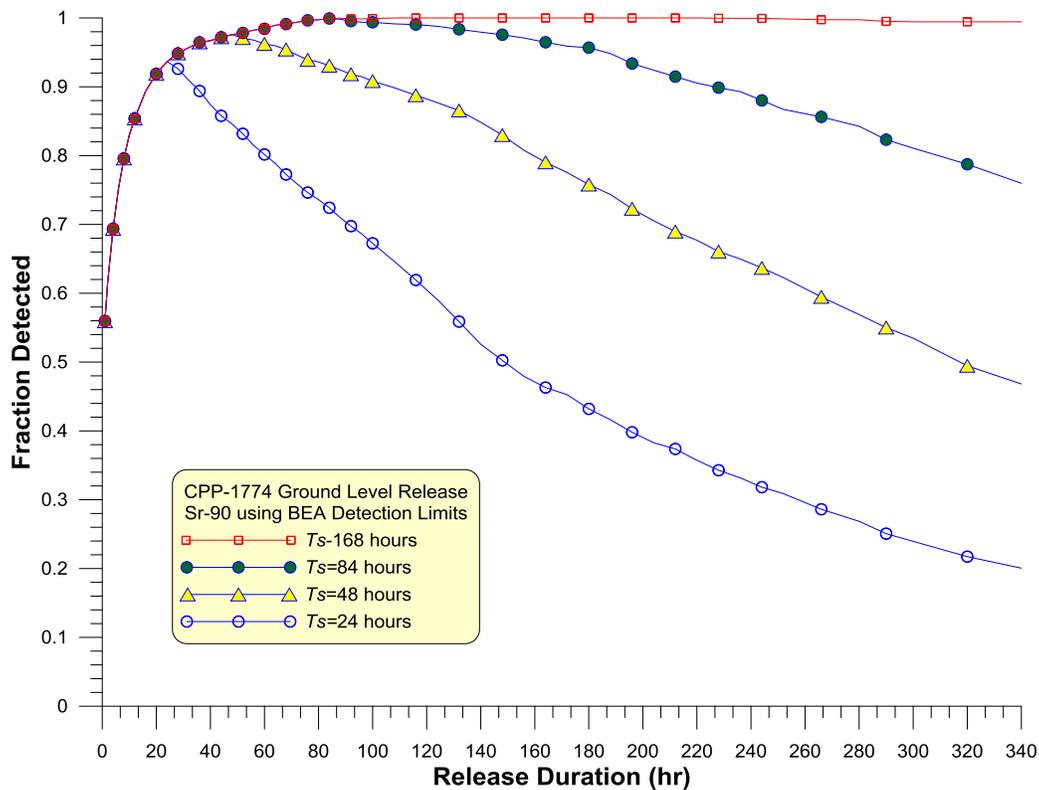


Figure 21. Detection frequency for onsite samplers as a function of release duration for different sampling times. Results are for a CPP-1774 ground-level Sr-90 release using the BEA MDA and a sampler flow rate of 2 cfm.

It should be noted that the ESER composites filters quarterly and the actual sampling time is 168 hours \times 13 weeks = 2,184 hours. The net effect of this is to increase the sensitivity of detection because more activity will be accumulated in the sample. Likewise, the MDC would decrease for a quarterly-composited filter compared to the MDC for a 1-week sample.

6.5.3 Sensitivity of Detection Frequency to Sampler Flow Rate

The amount of activity collected on the filter for a fixed sampling time is directly proportional to the sampler flow rate. Detection frequency can be improved by increasing the sampler flow rate to

compensate for a high MDA. The sampler flow rate used for this assessment was 2 cfm. However, samplers exist (i.e., high volume samplers) that are capable of much higher flow rates. The sensitivity of the detection frequency at onsite samplers to sampler flow rate is shown in Figure 22 for a Pu-239 releases from the TRA-770 stack. The top panel of Figure 22 shows the sensitivity of detection frequency to sampler flow rate for the ESER MDA and the bottom panel is for the BEA MDA. The maximum detection frequency using the ESER MDA improves from 52 to 99% by increasing the sampler flow rate from 2 to 16 cfm. The maximum detection frequency using the BEA MDA improves from 0.05 to 39% by increasing the sampler flow rate from 2 to 16 cfm.

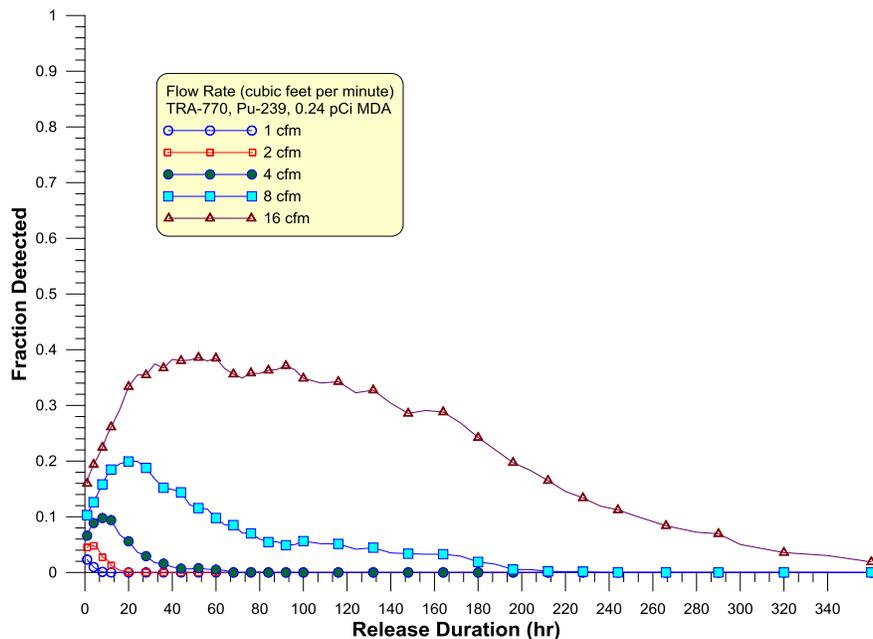
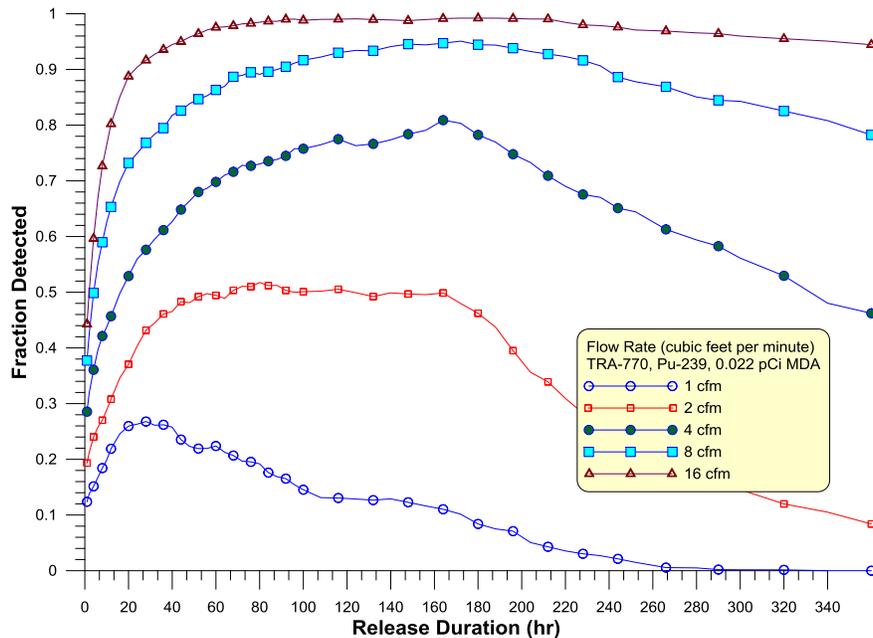


Figure 22. Detection frequency for onsite samplers as a function of release duration for various sampler flow rates. Results are for a TRA-770 stack release of Pu-239. The top panel shows the impact of the ESER MDA and the bottom panel shows the impact of the BEA MDA.

7. SUMMARY AND RECOMMENDATIONS

The frequency of detection methodology documented in this report is a viable and effective approach for quantitative evaluation of an air monitoring network. The methodology was demonstrated by performing a preliminary assessment of the INL Site ambient air monitoring network. The assessment results indicate the monitoring network is very effective at detecting potential releases of Cs-137 or Sr-90 from all sources/facilities using either the ESER or BEA MDAs, although the ESER MDAs result in a higher frequency of detection values. For Cs-137, the maximum detection frequencies at onsite or offsite samplers were greater than 97% for all sources using ESER or BEA MDAs. For Sr-90, the maximum detection frequencies at onsite or offsite samplers were greater than 99% using ESER MDAs. Using BEA MDAs, maximum values ranged from 23 to 100% for onsite samplers and 2.4 to 75% for offsite samplers. The network was less effective at detecting releases of Pu-239. Maximum detection frequencies for Pu-239 using ESER MDAs ranged from 27.4 to 100% for onsite samplers and 3 to 80% for offsite samplers. Using BEA MDAs, maximum detection frequencies for Pu-239 ranged from 2.1 to 100% for onsite samplers and 0 to 5.9% for offsite samplers.

Detection frequency is a function of the source location, release quantity, time of release (meteorological conditions), release duration, MDA, sampling time, and sampler flow rate. For this assessment, the release quantities for Cs-137, Pu-239, and Sr-90 were based on a release quantity that would result in a maximum effective dose at a publicly accessible location of 0.1 mrem. In other words, release quantities were calculated such that there is a 0% probability that a 0.1-mrem effective dose from inhalation at any publicly accessible location will be exceeded. Evaluation of the distribution of doses showed that if a 95% dose criterion (i.e., 5% probability that the 0.1-mrem effective dose would be exceeded) was used instead, then release quantities would be about a factor of 75 greater, resulting in a much-improved detection frequency.

The detection frequencies provided in this report assume a negligible background contribution. However, depending on the levels of background, the activity accumulated on the filter that would provide a positive detection could be indistinguishable from the activity accumulated on the filter from background. The effects of background on the ability of the sampling network to detect releases can be evaluated using this methodology.

The methodology described in this report could also be used to improve sampler placement and detection frequency, provided clear performance objectives are defined. Performance objectives would include an effective dose criterion, the likelihood of the dose criterion being exceeded, and the acceptable detection frequency. This study was based on a 0% probability that the effective dose criterion of 0.1 mrem will be exceeded at any of the publicly accessible sampler locations. An example alternative dose criterion might be a 5% probability that an effective dose criterion of 1 mrem will be exceeded at an actual public receptor location. An acceptable detection frequency might be 95% for a 1-hour release and 100% for an 8-hour or greater release. Given these criteria, the methodology could be used to identify optimum sampler placement, required sampler flow rates, and sampler MDAs necessary to achieve the design objectives. This will be performed in Phase II of this work.

8. REFERENCES

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Appendix A
Perl Script for Executing CALPUFF Simulations

Appendix A

Perl Script for Executing CALPUFF Simulations

This appendix contains the listing of the Perl script that is used as a wrapper for creating input files, running CALPUFF, extracting the results, and calculating the unit time-integrated concentration values. The script contained in this appendix is for ground release from the ATR Complex. To run other sources, the parameters in the "User Input" section must be changed.

```
# tics.pl
# This script sets up a matrix of runs based on a begin and end times and then sequentially marches through the time
# space by hour and calculates the time-integrated concentration (integrated from t=0 to infinity)
# at each of the INL onsite and offsite samplers. CALPOST is run and the run time averages are extracted, and then
# multiplied by the run time to convert to the TIC.
# The output is then written to a database compatible file

# Written by: Arthur S. Rood, K-Spar Inc
# July 20, 2014
# Last modified

# REQUIRES: calpuff.tmp, calpost.tmp, ptemarb.tmp
# usage perl tics
# ===== User Input =====
# $byr = begin year
# $bjd = beginning julian date
# $bhr = begin hour
# $eyr = end year
# $ejd = ending julian day
# $ehr = ending hour
# $itime = integration time (hours)

# Note: $ehr + $itime must be less than the last date of the calmet records.
# $srcname = name of source
# $xsrc, $ysrc, $zsrc = UTM geographic coordinates of source and elevation
# $srcht = height of source (m)
# $srcdia = stack diameter (m)
# $relvel = release velocity (m/s)
# reltemp = release temperature (K)
# $xyr = current year (yy)
# $xjd = current jullian date (1-365)
# $xhr = current hour
# $nyr = next year (yy)
# $njd = next jullian date (1-365)
# $nhr = next hour

# Overall time parameters
$byear=2006;
$bjd=1;
$bhr=1;
$eyear=2007;
$ejd=3;
$ehr=21;
$itime=70;

$srcname = "ATR";
$xsrc = 341.401;
$ysrc = 4827.854;
$zsrc = 1507.;
$srcht = 1.0;
$srcdia = 1.83;
$relvel = 0.1;
$reltemp = 290.0;
$qual = 1000;

@samplers = ("BEA-TRA", "BEA-CPP", "BEA-RWMC", "BEA-VAN", "BEA-IRC", "BEA-BLKFT", "BEA-SMC", "BEA-GATE", "BEA-ARA", "BEA-REST", "BEA-
IF", "BEA-NRF", "BEA-RTC", "BEA-EBR", "BEA-MFC", "BEA-SUGAR",
            "BEA-PBF", "BEA-INTEC", "BEA-CFA", "BEA-EFS", "BEA-CRATER", "ESER-VAN", "ESER-CRA", "ESER-ARC", "ESER-SUG", "ESER-IDA", "ESER-
DUB", "ESER-MON", "ESER-FAA", "ESER-MAI", "ESER-EFS", "ESER-ATO",
            "ESER-MOU", "ESER-BLU", "ESER-TER", "ESER-HOW", "FRENCHCBN");

# ===== END User Input =====
$starttime=(times)[0];
$flag=0;
$xyr=$byear;
$xjd=$bjd;
$xhr=$bhr;
$etime=$eyear+$ejd/365 +$ehr/(24*365);

# store calpuff template input file data in arrays
open(TEMPLATE,"<calpuff.tmp");

$cpuffj=0;
while ($line=<TEMPLATE>)
{
    $cpuff[$cpuffj]=$line;
    $cpuffj=$cpuffj+1;
}
}
```

```

close TMLATE;

# open output file
$outfile=$srcname ".txt";
open(OFIL,">>$outfile"); # append to current file
# open(OFIL,">$outfile"); open new file

# Utility functions, ctojd(year,month,day) ==> convert calendar day to julian day
# jdtoc(year,jdate) ==> convert julian date to calendar date
# increment(year,jdate,hours_to_add) ==> add hours to current date

print "End Time $etime\n";
while($flag==0)
{
# compute next hour
($nyr,$njd,$nhr) = increment($xyr,$xjd,$xhr,1);
# compute ending date of run
($ryr,$rjd,$rhr) = increment($xyr,$xjd,$xhr,$itime);
# compare ending date of run with overall ending date
$itime=$ryr+$rjd/365+$rhr/(24*365);
print "Current Date(yy jjj hr): $xyr $xjd $xhr\n";
if($itime>=$etime)
{
print "Last Run\n";
$flag=1;
}
}

# write ptemarb file
$temp=wptemarb();

# write calpuff file
$temp=wcaldpuff();

system "~/Codes/cpuff/calpuff/code/./calpuff.x";
system "~/Codes/cpuff/calpost/code/./calpost.x";
system "mv rank* aconc.dat";
$temp=pprocess();

# increment hour
$xhr=$nhr;
$xjd=$njd;
$xyr=$nyr;

}
close OFIL;
$endtime=(times)[0];
$runtime=$endtime-$starttime;
print "Execution time (seconds) $runtime (minutes) ";
$runtime=$runtime/60;
print "$runtime\n";

# ===== End of Main =====

sub wptemarb
{
# This subroutine write the ptemarb file - set release rate to q units per second
open(OUT,">ptemarb.dat");
printf OUT "'PTEMARB' 1 1 12 %02d%03d %d %02d%03d %d '5' 'HourRelease' %s\n" $fname2 $nsrc2 $nspec
iutm ibdat ibtim iedat ietim vrs2 lable2 \n", $xyr, $xjd, $xhr, $ryr, $rjd, $rhr;
print OUT "'TRC'";
print OUT "50.0";
printf OUT "'%-s' %7.3f %7.3f %7.3f %7.3f %7.3f 0.0 0.0" $spec1;
cid utme utmn ht dia elev
bldg_dw uflag \n", $srcname, $xsrc, $ysrc, $srccht, $srcrdia, $zsrc;
printf OUT "%02d%03d %d %02d%03d %d" $byyjjj $bhh $eyyjjj;
ehh\n", $xyr, $xjd, $xhr, $xyr, $xjd, $xhr;
printf OUT "'%-s' %7.3f %7.3f %10.3e" $cid $tempk $vexit $gemit;
\n", $srcname, $reltemp, $relvel, $sqval;
printf OUT "%02d%03d %d %02d%03d %d" $byyjjj $bhh $eyyjjj;
ehh\n", $nyr, $njd, $nhr, $ryr, $rjd, $rhr;
printf OUT "'%-s' %7.3f %7.3f 0.0" $cid $tempk $vexit $gemit;
\n", $srcname, $reltemp, $relvel;
close OUT;
return
}

sub ctojd
{
# Converts calendar day to julian day
my ($iyr, $imo, $iday) = @_;
my ($jdate, @dybfor);
@dybfor=(0,31,59,90,120,151,181,212,243,273,304,334);
$jdate=$dybfor[$imo-1]+$iday;
if($iyr%4 == 0 && $imo >= 3)
{
$jdate=$jdate+1;
}
return $jdate;
}

sub jdtoc
{
# Converts julian day to calendar day
my ($iyr, $jdate) = @_;

```

```

my ($imo,$idy,@dybfor);

# check for leap year
if($iyr%4 ==0)
{
  @dybfor=(0,31,60,91,121,152,182,213,244,274,305,335,366);
}
else
{
  @dybfor=(0,31,59,90,120,151,181,212,243,273,304,334,365);
}

if($jdate>$dybfor[12])
{
  print "Invalid Jullian Date $jdate\n";
  die;
}

for $i (1..12)
{
  if($jdate<=$dybfor[$i] && $jdate>$dybfor[$i-1])
  {
    $imo=$i;
  }
}
$idy=$jdate-$dybfor[$imo-1];
return ($imo,$idy);
}

sub increment
{
# This subroutine increments the current time by $nhrs, returns $nyr, $njd, $nhrr
my ($yr,$jd,$hr,$nadd) = @_;
local ($xyr,$xjd,$xhr,$ndays,$nhrr,$dinyr);
# determine number of days and hours to add
$ndays=int(($nadd+$hr)/24.0);
$nhrr=($hr+$nadd-24*$ndays);
if($nhrr<0) {$nhrr=$nadd+$hr;}

$xjd=$jd+$ndays;
if($yr%4 == 0)
{
  $dinyr=366;
}
else
{$dinyr=365;}

if($xjd>$dinyr)
{
  $xyr=$yr+1;
  $xjd=$xjd-$dinyr;
}
else
{$xyr=$yr;}
$xhr=$nhrr;

#   print "yr:day:hr $yr:$jd:$hr +$nadd  nhrr:$nhrr, ndays:$ndays  new yr:jd:hr $xyr:$xjd:$xhr  \n";

return ($xyr,$xjd,$xhr);
}

sub wcalpuff
{
my ($i,$icmet,$flag,@cmetfiles,@cmetjday);
@cmetfiles =
("cmet1.dat","cmet2.dat","cmet3.dat","cmet4.dat","cmet5.dat","cmet6.dat","cmet7.dat","cmet8.dat","cmet9.dat","cmet10.dat","cmet11
.dat","cmet12.dat");

open(CPUFF,">calpuff.inp");

# convert julian date to calendar date
my($mo,$day)=jdtoc($xyr,$xjd);

# determine which calmet file to use
$cmet1=".../calmet/" . $xyr . "/" . $cmetfiles[$mo-1];
# $cmet1="/Volumes/RAMDisk/" . $cmetfiles[$mo-1];  ram disk

if($mo>=12)
{
  $imo=0;
  $iyr=$xyr+1;
}
else
{
  $imo=$mo;
  $iyr=$xyr;
}
$cmet2=".../calmet/" . $iyr . "/" . $cmetfiles[$imo];
# $cmet2="/Volumes/RAMDisk/" . $cmetfiles[$mo];  ram disk

open (CPUFF,">calpuff.inp");
$i=-1;
while ($i<$cpuffj)
{
  $flag=0;

```

```

    $i=$i+1;
# -- substitute calmet files

    if ($cpuff[$i] =~ /The following CALMET.DAT filenames are processed in sequence if NMETDAT/)
    {
        print CPUFF "$cpuff[$i]";

        print CPUFF "Default Name   Type           File Nam\n";
        print CPUFF "-----\n";
        print CPUFF " none           input    !METDAT= $cmet1   ! !END!\n";
        print CPUFF " none           input    !METDAT= $cmet2   ! !END!\n";
        $i=$i+6;
        $flag=1
    }

# -- starting year
    if ($cpuff[$i] =~ /IBYR/)
    {
        print CPUFF "      Starting date:   Year (IBYR) -- No default       ! IBYR = $xyr !\n";
        $i=$i+1;
        $flag=1;
    }

# -- starting month
    if ($cpuff[$i] =~ /IBMO/)
    {
        print CPUFF "      (used only if   Month (IBMO) -- No default       ! IBMO = $mo !\n";
        $i=$i+1;
        $flag=1;
    }

# -- starting day
    if ($cpuff[$i] =~ /IBDY/)
    {
        print CPUFF "      METRUN = 0)     Day (IBDY) -- No default       ! IBDY = $day !\n";
        $i=$i+1;
        $flag=1;
    }

# -- starting hour
    if ($cpuff[$i] =~ /IBHR/)
    {
        print CPUFF "                               Hour (IBHR) -- No default       ! IBHR = $xhr !\n";
        $i=$i+1;
        $flag=1;
    }

# -- runtime
    if ($cpuff[$i] =~ /IRLG/)
    {
        print CPUFF "      Length of run (hours) (IRLG) -- No default       ! IRLG = $itime !\n";
        $i=$i+1;
        $flag=1;
    }

    if($flag==0)
    {
        print CPUFF "$cpuff[$i]";
    }

}

close CPUFF;
}

sub pprocess
{
    my ($i,$j,$line);
# This subroutine process the calpost output
    open(CPOST,"<aconc.dat");
# skip 6 lines
    for $i (1..6)
    {
        $line=<CPOST>;
    }
    for $i (0..36)
    {
        $line=<CPOST>;
        chop $line;
        $line =~ s/^[ ]+//;          # delete initial spaces
        @field = split /[ ]+/, $line; # split into fields with space or comma delimiter
        $conc[$i]=$field[2];
# convert average concentration to a tic for 1 unit per hour (h2/m3)
        $tic[$i]=$conc[$i]/3600.0/$qval * $itime;
        print "$i $samplers[$i] $conc[$i] $tic[$i] \n";
        printf OFILE "%s,%s,%d,%d,%d,%10.3e\n",$srcname,$samplers[$i],$xyr,$xjd,$xhr,$tic[$i];
    }

    close CPOST;
}
}

```


Appendix B
Documentation for the FREQD Program

Appendix B

Documentation for the FREQD Program

B-1. INTRODUCTION

This appendix contains the code documentation for the FREQD Program. Code documentation includes (1) input file structure, (2) code execution and output files, (3) software design description, (4) software configuration management, and (5) code listing. The FREQD code is written in Fortran 95 with utility subroutines written in Fortran 77. It is executed on the command line of terminal window. Input and output to the code is through ASCII files.

B-2. INPUT FILE STRUCTURE

Input to the FREQD code is through the parameter definition file and the structure of this file is provided in Table B-1. The parameter definition file is an ASCII text file that can be constructed with any text editor but should not be constructed with word processing software such as Microsoft Word. The parameter definition file is composed of records, which represent one or more lines in the file. Within each record, there are one or more fields comprising character, integer, or real data. Records and fields must be placed in the order presented in Table B-1. The parameter definition file may contain blank lines between records and any line beginning with a dollar sign (\$) in the first column is ignored and treated as a comment.

The parameter definition file references the TICu data file. Table B-2 contains the file structure for the TICu file. The TICu file contains one record that is repeated n hours \times m samplers. Thus, if 8,760 hours are simulated and 10 samplers are analyzed, then there would be 87,600 records in the file. Each record contains six fields consisting of source identification, sampler identification, year, Julian day, hour, and TICu value. The TICu value represents the 70-hour time integrated concentration for a unit release quantity (i.e., 1 Ci) released during the hour beginning the simulation. For example, a TICu record for January 10, 2006 at hour 00 would represent the time-integrated concentration from hour 00 on January 10 to hour 22 on January 12 for unit activity released during the first hour beginning the simulation (January 10, 2006, hour 0000). For unit consistency, this value is divided by the unit activity released (i.e., 1 Ci hr⁻¹) to give units of hr² m⁻³.

B-3. PROGRAM EXECUTION AND OUTPUT FILES

The program is executed on the command line by typing

[path] freqd [parameter definition file]

where the format for the parameter definition file is provided in Table B-1. If no parameter definition file is provided, then the code looks for a parameter file named freqd.par in the same directory. If that file is not found, then the program terminates.

Output files produced by FREQD are provided in Table B-3. Detailed detection frequency output is provided in the general output file. Onsite and offsite network detection frequency formatted for plotting is provided in the radionuclide plot files. A radionuclide plot file is generated for each radionuclide in the parameter file. The TIC and inhalation dose files are optional and provide the TIC and inhalation dose for each hour beginning the release in the data file. Each file represents one release duration and separate files are produced for each radionuclide.

Table B-1. Format for the FREQD parameter definition file.

Record (Field)	Code Variable	Type/Format	Units	Description
1 (1)	Title	CHAR/A80		Title of run
2 (1)	filedat	CHAR/A80		Name of <i>TICu</i> data file
2 (2)	fileout	CHAR/A80		Output file
3 (1)	nsamp	INTEGER/*		Number of samplers
Note: Record 4 is repeated nsamp times. Samplers must be in the same order as the <i>TICu</i> data file				
4 (1)	sampname	CHAR*15/*		Sampler name
4 (2)	flowr	REAL/*	m ³ hr ⁻¹	Sampler flow rate
4 (3)	rtime	REAL/*	hours	Sampler run time
4 (4)	onsite	INT/*		1 = On-site sampler, 0 = off-site sampler
4 (5)	incsamp	INT/*		1 = Include sampler, 0 =exclude sampler
5 (1)	nrad	INT/*		Number of radionuclides
5 (2)	units	CHAR*3/*		Units of measure, pCi or MBq
5 (3)	inh	REAL/*	m ³ hr ⁻¹	Inhalation rate
NOTE: Record 6 is read nrad times				
6 (1)	radname	CHAR*15/*		Radionuclide name
6 (2)	mda	REAL/*	pCi or MBq	Minimum detectable activity
6 (3)	dcf	REAL/*	mrem per pCi or Sv per Bq	Inhalation dose coefficient
7 (1)	ndur	INT/*		number of release durations
NOTE: Record 8 is read ndur times				
7 (1)	reldur	REAL/*	hours	Release duration
7 (2)	ticfiles	CHAR*80/*		Prefix for optional <i>TICu</i> output file for release duration. Enter 'NONE' for no file

Table B-2. Format of the *TICu* data file. The samplers must be in the same order as the data file and the year, Julian day, and hour must be in chronological order.

Field ^a	Code Variable	Description
1	junk	Name of source (CHAR*15)
2	junk	Name of sampler (CHAR*15)
3	year	year, yyyy (INTEGER)
4	jday	Julian day, jjj (INTEGER)
5	hr	hour, hh (INTEGER)
6	vals	<i>TICu</i> value for year, jday, hr (hr ² m ⁻³)

a. Each line (record) is composed of the six fields. There are nsamp number of records for each hour in the dataset.

Table B-3. Output files for FREQD Program.

Output File	Name	Description
General output	Defined by the user in the parameter file	General output file containing an echo of the input and detection frequency for each radionuclide, sampler, and release duration.
Radionuclide plot file	[<i>rad name</i>] _{<i>n</i>} .dat, where <i>n</i> is the sequence number of the radionuclide in the parameter file	Radionuclide plot file of detection frequency for onsite and offsite samplers as a function of release duration.
TICu and inhalation dose file	[<i>user prefix</i>]-[<i>rad name</i>].dat	This file is optional and only written if record 7, field 2 in the parameter definition file is not NONE. The TICu and inhalation dose are printed for each hour in the simulation for a given release duration. At the bottom of the file, the percentiles of the TICu and dose values are output for each sampler.
Maximum TICu and dose	MAX_tic_dose.dat	The maximum TICu and dose for each radionuclide across all release durations for each sampler and across all samplers are printed in this output file.

B-4. SOFTWARE DESIGN

The software design description depicts how the software is structured to satisfy the requirements of the software and the components and subcomponents of the software. The software requirements are stated in the main body of this report. Specifically, the software is required to implement equations in the methodology section of the report. The FREQD software is written in Fortran 95 and was developed on a Mac workstation running Mac OS X Version 10.7.5 and compiled using the gfortran compiler. Additional Fortran 77 file utility subroutines are used for reading and checking files and calculating percentiles. Each subroutine and function is described in Table B-4.

Table B-4. Description of each function subroutine and function in FREQD.

Subroutine or Function	Module	Description
main	none	Main program unit that reads the command line arguments, opens and reads the input file, calls the detection frequency function, and writes output to files and screen
readdat	funs	Subroutine reads the TICu file
integrate	funs	Subroutine integrates concentration across the sampling time for a given release duration
detect	funs	Function determines if a detection has occurred
ddose	funs	Subroutine calculates the inhalation dose
readline	fileutil.f	Subroutine reads in one line on the parameter definition file, ignoring comments and blank lines

Subroutine or Function	Module	Description
numvaline	fileutil.f	Subroutines determines the number of input values that should be present on a line
checkfile	fileutil.f	Subroutine checks two files and makes sure they are not the same name
filecase	fileutil.f	Subroutine converts all characters in a file to lowercase for file checking
fileexist	fileutil.f	Subroutine checks if a file exists
selip	Percent.f	Subroutine finds a given percentile (Copyright Numerical Recipes)
shell	Percent.f	Subroutine sorts an array for finding percentile (Copyright Numerical Recipes)

B-5. CONFIGURATION MANAGEMENT

Software configuration management provides the mechanism to identify, document, and control changes to the software. Software configuration management for FREQD is addressed within the module headers and the version date. Each module in the FREQD code contain a header that documents: (1) the name and purpose of the module, (2) the code author, (3) the date it was written, (4) a change history to the module, (5) arguments and returned values, and (5) calls to and from the module. The module header forms the basis for most of the code documentation. An example module header is shown in Figure B-1.

```

subroutine ddose(dose,tic,intval,qs,rt,dcf,inh,units)
!! =====
!! Modulal Name: ddose
!! Author: A. S. Rood
!! Date Created: 07/28/14
!! Last Modified:
!! Modifications:
!! Purpose: This subroutine calculates the tic and dose
!! Arguments:
!! dose: calculated dose value (mrem or Sv)
!! tic: time-integrated concentration (Ci-hr/m^3 or MBq-hr/m^3)
!! intval: unit time-integrated concentration integrated over the sampling time (h^2/m^3)
!! rt: release time (hours)
!! dcf: inhalation dose coefficient (Sv/Bq) or (mrem/pCi)
!! inh: inhalation rate (m^3/hr)
!! units: units of calculation (MBq or pCi)
!! Returns:
!! tic and dose
!! Called by: MAIN
!! Calls to: none

```

Figure B-1. Module header for subroutine ddose in FREQD.

Version control is primarily handled in FREQD through the version date instead of a version number. The version date can be thought of as essentially a version number and is stored in the variable *vdate* in the main program unit. The version date is an eight digit number, where the first four digits represent the year, the second two digits the month, and the last two digits the day. The version date is in the header of the general output file generated by FREQD and in all ancillary output files generated by both codes. The version date is identified as the “Level” in the ancillary output files. In this way, results from an old version of the code can be identified.

The code custodian has the responsibility of maintaining and updating the code, identifying and archiving code versions, verifying new versions of the code operate correctly, and distributing the software to end users.

B-6. CODE LISTING

```

!! FREQD.F95
!! Author: A.S. Rood
!! K-Spar Inc.
!! 4835 West Foxtrail Lane
!! Idaho Falls ID 83402
!! www.kspar.com
!! Date: September, 2014
!!
!! This program reads in time-integrated unit concentrations TICu for n samplers and for m years.
!! Each TICu represents the 70-hour time integrated concentration from a unit 1-hour release beginning
!! on a given year, jullian day, and hour. The data file must present these TICu values for each sampler
!! in chronological order. Other data are provided in a parameter definition file. These data include
!! sampler parameters (flow rate, MDA, and sampling time), number of release durations, and the release duration values.
!! Radionuclide data is also input that includes nuclide name, release quantity, and inhalation dose coefficient. The inhalation
rate is
!! also provided so that inhalation dose can also be calculated. The program then starts evaluating each release duration
!! at each sampler and computes the frequency of detection at each sampler and network-wide for onsite and offsite samplers.

```

```

module funs
contains

```

```

    subroutine readdat(vals,nsamp,year,jday,hr,nhrs,srcname,sampname,filedat)
!! =====
!! Modulal Name: readdat
!! Author: A. S. Rood
!! Date Created: 07/28/14
!! Last Modified:
!! Modifications:
!! Purpose: This subroutine reads the data file containing the TICs
!! Arguments:
!! vals(nsta,nvals): values of 1-hr unit TICs(hr^2/m^3)
!! nsamp: number of samplers
!! year(nvals): year values
!! jday(nvals): jday
!! hr(nvals): hour
!! srcname: name of source
!! sampname(nsamp): sampler name array
!! filedat: file containing tic data
!! Returns:
!! vals, srcname
!! Called By: MAIN
!! Calls to: fileexist
!! =====
    implicit none
    include 'params.inc'
    integer :: year(maxvals),jday(maxvals),hr(maxvals),nhrs
    real (kind=8) :: vals(maxsta,maxvals)
    character (len=15) srcname,sampname(maxsta),junk1,junk2
    character (len=80) filedat
    integer :: nsamp,i,j,k
    call fileexist(filedat)
    open(1,file=filedat,status='old')
    nhrs=0
10  continue
    nhrs=nhrs+1
    do i=1,nsamp
        read(1,*,end=100) junk1,junk2,year(nhrs),jday(nhrs),hr(nhrs),vals(i,nhrs)
        if(nhrs.eq.1) then
            srcname=junk1
        endif
!! check and make sure the order is correct
        if(sampname(i).ne.junk2)then
            write(*,*) 'Sampler name does not match data file ',sampname(i),junk2
            write(*,*) 'YEAR ',year(nhrs),' JDAY ',jday(nhrs),' HR ',hr(nhrs)
            stop
        endif
    enddo
    goto 10
100 close(1,status='keep')
    nhrs=nhrs-1
    write(*,*) 'Number of hours read ',nhrs
    end subroutine readdat

```

```

    subroutine integrate(vals,isamp,ihr,rtime,intval)
!! =====
!! Modulal Name: integrate
!! Author: A. S. Rood
!! Date Created: 07/28/14
!! Last Modified:
!! Modifications:
!! Purpose: This subroutine integrates the tics across the sampling time
!! Arguments:
!! vals(nsta,nvals): values of unit TICs(hr^2/m^3)
!! isamp: sampler index
!! ihr: beginning hour index

```

```

!!   rtime: number of hours to integrate over
!!   intval: itegrated value (h^2/m^3)

!! Returns:
!!   vals, srcname

!! Variables
!! Called by: MAIN
!! Calls to: none
=====
implicit none
include 'params.inc'
real (kind=8) :: vals(maxsta,maxvals),intval
integer :: isamp,ihr,rtime,i,j
intval=0.0
do i=ihr,ihr+rtime-1
  intval=intval+vals(isamp,i)
enddo

return
end subroutine integrate

integer function detect(intval,qs,rt,mda,flowr)
=====
!! Modular Name: detect
!! Author: A. S. Rood
!! Date Created: 07/28/14
!! Last Modified:
!! Modifications:

!! Purpose: This subroutine determines whether a detect or non-detect occurs
!! Arguments:
!!   intval: integrated tic value(hr^2/m^3)
!!   qs: source release (Ci or MBq)
!!   rt: release time (h)
!!   mda: minimum detectable activity (MBq or pCi)
!!   flowr: sample flow rate (m3/hr)

!! Returns:
!!   detect 1= detected, 0 = not detected
!! Called by: MAIN
!! Calls to: none
=====
implicit none
real (kind=8) :: intval,qs,rt,mda,flowr,tic
tic=intval*qs/rt*flowr

if(tic.ge.mda)then
  detect=1
else
  detect=0
endif
return

end function detect

subroutine ddose(dose,tic,intval,qs,rt,dcf,inh,units)
=====
!! Modular Name: ddose
!! Author: A. S. Rood
!! Date Created: 07/28/14
!! Last Modified:
!! Modifications:

!! Purpose: This subroutine calculates the tic and dose

!! Arguments:
!!   dose: calculated dose value (mrem or Sv)
!!   tic: time-integrated concentration (Ci-hr/m^3 or MBq-hr/m^3)
!!   intvalue: unit time-integrated concentration integrated over the sampling time (h^2/m^3)
!!   rt: release time (hours)
!!   dcf: inhalation dose coefficient (Sv/Bq) or (mrem/pCi)
!!   inh: inhalation rate (m^3/hr)
!!   units: units of calculation (MBq or pCi)

!! Returns:
!!   tic and dose
!! Called by: MAIN
!! Calls to: none
=====
implicit none
real (kind=8) :: intval,qs,rt,dcf,inh

character (len=3) :: units
real (kind=8) :: tic,dose,dcfv
tic=intval*qs/rt      !! (Activity-hr/m3)
if(units.eq.'MBq')then
  dcfv=dcf*1.0E6      !! convert to Sv/MBq
else
  dcfv=dcf
endif

dose=tic*inh*dcfv

```

```

return

end subroutine ddose

end module funs

program main
!! -----
!! This program reads in TIC values (hr^2/m^3) calculated with CALPUFF through the script tics.pl
!! for N sampler stations and M years for every hour. These data are stored in arrays that are used
!! to calculate the frequency of detection at a sampler given a release quantity, release duration,
!! and sampler MDA
!!
!! Arthur S. Rood
!! K-Spar Inc
!! 4835 W Foxtrail Lane
!! Idaho Falls ID 83401
!! www.kspar.com
!! asr@kspar.com

!! vals(nsta,nvals): time integrated concentration (hr^2/m^3)
!! frate(nsta): sampler flow rate (m3/hr)
!! mda(nsta): minimum detectable activity
!! rtime(nsta): number of hours sampler is run
!! msamp: number of samplers in data file

!! Modifications
!! 08/26/2014 - Changed loop in k+rdur.lt.nhrs TO k+rdur.le.nhrs
!! 09/12/2014 - Added percentile calculation of dose

!! Calls to: ddose, integrate, readdat, detect, readline, filecheck, numvaline
!!
!! -----
use funs
implicit none
include 'params.inc'
!! integer :: maxvals,maxyears,maxsta,maxrads,maxrdur,maxqs
!! parameter (maxsta=36,maxyears=2,maxvals=maxyears*8760,maxrads=20,maxrdur=100,maxqs=20)
integer :: year(maxvals),jday(maxvals),hr(maxvals),onsite(maxsta)
real (kind=8) :: vals(maxsta,maxvals)
character (len=80) :: filepar,filedat,fileout,fline,title,plotfile,ticfiles(maxrdur),ticfout
character (len=260) :: dline,msg
character (len=42) :: warning
character (len=3) :: units,suffix,unitstemp(3)
character (len=7) :: dunits
integer :: iline,i,j,k,ii,jj,icount,ifreq(maxsta),ijunk,idetect,incsamp(maxsta)
integer :: maxyr(maxsta),maxjd(maxsta),maxhr(maxsta),maxreld(maxsta),rank(23)
integer :: nsamp,nrad,ndur,nqs,nhrs,relldur(maxrdur),rtime(maxsta),rdur,netonsite(maxvals),netoffsite(maxvals)
character (len=15) :: sampname(maxsta),radname(maxrads),srcname,cjunk15
real (kind=8) :: frate(maxsta),mda(maxrads),qs(maxrads),intval,rfreq,rfreq1,rfreq2,inh,dcf(maxrads)
real (kind=8) :: dose,maxdose(maxsta),tic,maxtic(maxsta),maxd,mind,qtemp(3),qfact(3)
character*10 vdate,ttime,ddate
real (kind=8) :: cpu_start,cpu_end
real (kind=8) rjunk,rarr1(maxvals),rarr2(maxvals),percentile(23),pval1(maxsta,23),pval2(maxsta,23),selip
!! *****
vdate='20140826'
!! *****
!! --- Time and Date Calls
call date_and_time(ddate,ttime) !lf95
call cpu_time(cpu_start)
data percentile /0.0,0.025,0.05,0.1,0.15,0.20,0.25,0.30,0.35,0.40,0.45,0.50, &
& 0.55,0.60,0.65,0.70,0.75,0.80,0.85,0.90,0.95,0.975,1.0/
warning='Error on line: '
!! read parameter definition file
call getarg(1,filepar)
if (len(trim(filepar)).eq.0) then
filepar='freqd.par'
endif
call fileexist(filepar)
open(1,file=filepar,status='unknown')
iline=0
fline='read(dline,(a80)) title'
call readline(fline,dline,warning,1,iline)
read(dline,'(a80)') title
!! IO files
call readline(fline,dline,warning,1,iline)
read(dline,*) filedat,fileout

!! open output file and write headers
open(2,file=fileout,status='unknown')
write(2,1500) vdate
write(2, '(1x,a5,1x,a2,a1,a2,a1,a4,1x,a5,1x,a2,a1,a6)') &
'Date:',ddate(5:6), '/', ddate(7:8), '/', ddate(1:4), 'Time:', &
ttime(1:2), ':', ttime(3:4), ':', ttime(5:10)
write(2,*) 'Input File: ',filepar
write(2,1200) ('-----',j=1,7)
write(2,*) 'START OF PARAMETER DEFINITION FILE'
write(2,1200) ('-----',j=1,7)
write(2,*) title
write(2,*) 'Data File:',filedat

```

```

!! Make sure output file is not the same name as the data file
msg='Output file and data file are the same'
call checkfile(filedat,fileout,msg)

!! sampler data
fline='read(dline,*) nsamp'
call readline(fline,dline,warning,1,iline)
call numvaline(1,iline,dline)
read(dline,*) nsamp
write(2,*) dline
fline='read(dline,*) sampname(i),frate(i),rtime(i),onsite(i),incsamp(i)'
do i=1,nsamp
  call readline(fline,dline,warning,1,iline)
  call numvaline(5,iline,dline)
  read(dline,*) sampname(i),frate(i),rtime(i),onsite(i),incsamp(i)
  write(2,*) dline
enddo

!! rad data, dcf units is mrem/pCi for pCi and Sv/Bq for MBq
fline='read(dline,*) nrad,units,inh'
call readline(fline,dline,warning,1,iline)
call numvaline(3,iline,dline)
read(dline,*) nrad,units,inh
write(2,*) dline
fline='read(dline,*) radname(i),mda(i),dcf(i)'
do i=1,nrad
  call readline(fline,dline,warning,1,iline)
  call numvaline(4,iline,dline)
  read(dline,*) radname(i),mda(i),dcf(i),qs(i)
  write(2,*) dline
enddo
if(units.ne.'pCi'.and.units.ne.'MBq')then
  write(*,*) 'Units must be pCi or MBq ',units
  stop
endif
if(units.eq.'MBq') then
  dunits='Sv/yr'
  unitstemp(1)='MBq'
  qfact(1)=1.0
  unitstemp(2)='GBq'
  qfact(2)=1000.
  unitstemp(3)='PBq'
  qfact(3)=1.0e6
endif
if(units.eq.'pCi') then
  dunits='mrem/yr'
  unitstemp(1)='pCi'
  qfact(1)=1.0
  unitstemp(2)='uCi'
  qfact(2)=1e-6
  unitstemp(3)='mCi'
  qfact(3)=1.0e-9
endif

!! release durations
fline='read(dline,*) ndur'
call readline(fline,dline,warning,1,iline)
call numvaline(1,iline,dline)
read(dline,*) ndur
write(2,*) dline
fline='read(dline,*) reldur(i)'
do i=1,ndur
  call readline(fline,dline,warning,1,iline)
  call numvaline(2,iline,dline)
  read(dline,*) reldur(i),ticfiles(i)
  write(2,*) dline
enddo
close(1,status='keep')
write(2,*) 'End of Parameter Definition File'
write(2,1200) ('-----',j=1,7)

!! Read the data file
call readdat(vals,nsamp,year,jday,hr,nhrs,srcname,sampname,filedat)
write(2,*) 'Total number of hours in data file:',nhrs
write(2,*) 'Frequency of Detection'
write(2,1300) 'Radionuclide','Source Strength','(,units,)', 'Release Duration (h)', 'Sampler', 'Frequency'
write(2,1200) ('-----',j=1,9)

open(10,file='MAX_tic_dose.dat',status='unknown')          !! open tic and dose file
write(10,'(3(a4,1x),a6,1x,a11,4(1x,a10),2x,a3,2x,a7,a13,a10)') &
& 'Year','Jday','Hour','Rad','Duration(h)','Sampler','Q','TIC(hr/m3)', &
& 'Dose','units,dunits','Level Date:',vdate

!! Set up loop for computations
do jj=1,nrad
!!
do i=1,nqs          !! source strength loop
write(suffix,(i0)) jj
plotfile=trim(radname(jj)) // '_' // trim(suffix) // '.dat'
open(4,file=plotfile,status='unknown')
write(4,'(a6,2x,a6,5x,a7,2x,a2,3(1x,lpe10.3,1x,a3),a13,a10)') &
& 'RD(hr)','Onsite','Offsite','Q=',qs(jj)*qfact(1),unitstemp(1),qs(jj)*qfact(2),unitstemp(2),qs(jj)*qfact(3),unitstemp(3)
&
& ', 'Level Date:',vdate
do ii=1,nsamp
  maxdose(ii)=0.0

```

```

maxtic(ii)=0.0
enddo

do j=1,ndur          !! duration loop
write(*,*) 'Source Strength: ',qs(jj),' Release Duration ',reldur(j)
do k=1,nhrs
netonsite(k)=0
netoffsite(k)=0
enddo
if(ticfiles(j).ne.'NONE')then
ticfout=trim(ticfiles(j))//trim(radname(jj))//'.dat'
write(*,*) ticfout,radname(jj)
open(11,file=ticfout,status='unknown')
write(11,*) 'Year Jday Hr Sampler TIC(hr2/m3) TIC(trim(units),'-hr/m3) InhDose Integration Time:' &
& ,reldur(j),' Radname:',radname(jj),' Level Date: ',vdate

endif
do ii=1,nsamp          !! loop through all samplers
if(incsamp(ii).eq.1)then
icount=0
ifreq(ii)=0
rdur=min(reldur(j),rtime(ii)) ! use the minimum of the release duration or the sampling time
do k=1,nhrs          !! integrate across all hours
if(k+rdur.le.nhrs)then ! only integrate if number of hours is within the data limits
icount=icount+1
call integrate(vals,ii,k,rdur,intval)
idetct=detect(intval,qs(jj),dfloat(reldur(j)),mda(jj),frate(ii))
ifreq(ii)=ifreq(ii)+idetct
!! set the netonsite and netoffsite to 1 if at least one sampler has a detection
if(idetct.ge.1.and.onsite(ii).eq.1)then
netonsite(k)=1
endif
if(idetct.ge.1.and.onsite(ii).eq.0)then
netoffsite(k)=1
endif
endif
!! calculate tic and dose and look for max
call ddose(dose,tic,intval,qs(jj),dfloat(reldur(j)),dcf(jj),inh,units)
!! write tic and dose data to file
if(ticfiles(j).ne.'NONE')then
write(11,'(i4,1x,i3,2x,i2,1x,a10,3(1x,1pe10.3,2x))') &
& year(k),jday(k),hr(k),sampname(ii),intval,tic,dose
endif

if(dose.gt.maxdose(ii))then
maxdose(ii)=dose
maxtic(ii)=tic
maxyr(ii)=year(k)
maxjd(ii)=jday(k)
maxhr(ii)=hr(k)
maxreld(ii)=reldur(j)
endif
enddo !! end of hour loop
rfreq=dfloat(ifreq(ii))/dfloat(icount)
write(2,1400) radname(jj),qs(jj),reldur(j),sampname(ii),rfreq
endif
enddo !! end of sampler loop
rfreq1=dfloat(sum(netonsite))/dfloat(icount)
write(2,1400) radname(jj),qs(jj),reldur(j),'Onsite_Station',rfreq1
rfreq2=dfloat(sum(netoffsite))/dfloat(icount)
write(2,1400) radname(jj),qs(jj),reldur(j),'Offsite_Station',rfreq2
write(4,'(i4,2x,2(1x,1pe10.3))') reldur(j),rfreq1,rfreq2
close(11,status='keep')
enddo !! end of duration loop
close(4,status='keep')
maxd=0.0
mind=1e10
do ii=1,nsamp
if(incsamp(ii).eq.1)then
write(10,'(3(i4,1x),a6,2x,i4,7x,a8,1x,3(1x,1pe10.3))') &
& maxyr(ii),maxjd(ii),maxhr(ii),radname(jj),maxreld(ii),sampname(ii),qs(jj),maxtic(ii),maxdose(ii)
if(maxdose(ii).gt.maxd)then
maxd=maxdose(ii)
i=ii
endif
if(maxdose(ii).lt.mind)then
mind=maxdose(ii)
k=ii
endif
endif
endif
enddo

write(10,*) 'Maximum and Minimum Across all Stations'
write(10,'(3(i4,1x),a6,2x,i4,7x,a8,1x,3(1x,1pe10.3))') &
& maxyr(i),maxjd(i),maxhr(i),radname(jj),maxreld(i),sampname(i),qs(jj),maxtic(i),maxdose(i)
write(10,'(3(i4,1x),a6,2x,i4,7x,a8,1x,3(1x,1pe10.3))') &
& maxyr(k),maxjd(k),maxhr(k),radname(jj),maxreld(k),sampname(k),qs(jj),maxtic(k),maxdose(k)
write(10,*) '-----'

!! enddo !! end of q loop
enddo !! end of rad loop
close(10,status='keep')

!! calculate percentiles of dose in output files

```

```

write(*,*) 'Calculating percentiles for dose output files'
rank(1)=1
do j=1,ndur
  if(ticfiles(j).ne.'NONE')then
    do jj=1,nrad
      ticfout=trim(ticfiles(j))//trim(radname(jj))//'.dat'
      open(11,file=ticfout,status='old')
      read(11,*) dline !! read header
      read(11,'(a260)') dline !! read first line
      ii=1
      do while (ii.le.nsamp)
        if(incsamp(ii).eq.1)then
          write(*,*) radname(jj),sampname(ii)
          icount=1
          continue
20          read(dline,*) ijunk,ijunk,ijunk,cjunk15,rjunk,rarr1(icount),rarr2(icount)
          if(cjunk15.ne.sampname(ii))then
            goto 30
          endif
          read(11,'(a260)',end=35) dline
          icount=icount+1
          goto 20
          goto 30
35          read(dline,*) ijunk,ijunk,ijunk,cjunk15,rjunk,rarr1(icount),rarr2(icount)
30          do i=2,22
            rank(i)=int(percentile(i)*float(icount-1))
          enddo
          rank(23)=icount
          do i=1,23
            pval1(ii,i)=selip(rank(i),icount,rarr1)
            pval2(ii,i)=selip(rank(i),icount,rarr2)
          enddo
          endif
          ii=ii+1
        enddo
        close(11,status='keep')
        open(11,file=ticfout,status='old',position='append')
        do ii=1,nsamp
          if(incsamp(ii).eq.1)then
            write(11,*) 'Sampler: ',sampname(ii)
            write(11,*) 'Percentile TIC Dose'
            write(11,*) '-----'
            do i=1,23
              write(11,'(f5.3,7x,2(1x,1pe10.3)') percentile(i),pval1(ii,i),pval2(ii,i)
            enddo
            endif
          enddo
        close(11,status='keep')
      enddo
    endif
  enddo
enddo

```

```
1200 format(24(a10))
```

```
1300 format(1x,a12,9x,a15,a2,a3,a1,1x,a20,2x,a7,14x,a8)
```

```
1400 format(1x,a15,6x,1pe10.3,11x,i6,14x,a16,6x,1pe10.3)
```

```

1500 FORMAT(2X,' *****'&
&/,2X,' * This output was produced by the model: *'&
&/,2X,' * *'&
&/,2X,' * FREQD *'&
&/,2X,' * *'&
&/,2X,' * FREQuency of Detection program for INL sources *'&
&/,2X,' * and air monitoring network. *'&
&/,2X,' * Version date (yyyymmdd): *'&
&/,2X,' * ',a10,' *'&
&/,2X,' * Arthur S. Rood *'&
&/,2X,' * K-Spar Inc. 4835 W Foxtrail Lane *'&
&/,2X,' * Idaho Falls, ID 83402 *'&
&/,2X,' * asr@kspar.com *'&
&/,2X,' *****'&)

```

```
end program main
```

```

subroutine readline(fline,dline,warning,iunit,iline)
c =====
c Modulal Name: READLINE
c Author: A. S. Rood
c Date Created: 12/21/99
c Last Modified: 10/21/04
c Modifications:
c 10/21/04 - Added logical to skip blank lines
c Purpose: reads a line from the iunit file and either discards it
c or passes it back to the calling routine
c Arguments:
c fline: read statement
c dline: character*260 to hold values on line
c warning: waraning statement on account of an error
c iunit: the file unit to be read from
c iline: index number to read file

```

```

c Called By: MAIN, READMC
c Calls To: none
c =====
implicit none
integer iunit,iline,length,i,iflag
character*260 dline
character*80 fline
character*42 warning
10  iline=iline+1
read(iunit,'(a260)',err=99) dline
if(ichar(dline(1:1)).eq.36)then ! comment line
goto 10
endif
length=len(dline)
iflag=0
i=1
do while (i.lt.length)
if(ichar(dline(i:i)).ne.13.and.ichar(dline(i:i)).ne.32)then ! if any character other than a space
iflag=1 ! or carriage return is encountered, then
i=length
endif ! read the line
i=i+1
enddo
if(iflag.eq.0) goto 10
write(*,*) iline,fline(1:70)
write(*,*) iline,dline(1:120)
return
99 write(*,'(1x,a42,1x,i3)') WARNING,iline
write(2,'(1x,a42,1x,i3)') WARNING,iline
stop
end

subroutine numvaline(ne,iline,dline)
c =====
c Modulal Name: NUMVALINE
c Author: A. S. Rood
c Date Created: 05/05/03
c Last Modified: 05/05/03
c Modifications:

c Purpose: Finds the number of space or comma-delimited elements on a line
c and compares to the number of expected values
c Arguments:
c ne: number of expected values number of found values (returned)
c iline: line number
c dline: character string of line

c Called By: MAIN, READMC
c Calls To: none
c =====
implicit none
integer ne,iline
character*260 dline
integer na,i,nc,jj(260)
na=0
nc=len(dline)

do i=1,nc
jj(i)=ichar(dline(i:i))
enddo

i=1
do while (i.le.nc)
if(jj(i).ne.44.and.jj(i).ne.32) then
na=na+1 ! found an element
i=i+1
do while (jj(i).ne.44.and.jj(i).ne.32) ! count the number of characters in element
i=i+1
enddo
else
i=i+1 ! counting spaces and commas
endif
enddo

if(na.lt.ne)then
write(*,*) ' ERROR IN THE INPUT FILE ON LINE NUMBER: ',iline
write(*,*) ' Description: Number of values do not match the numbr
of expected values.'
write(*,*) ' Number of expected values: ',ne
write(*,*) ' Number of actual values: ',na
write(*,*) ' Error occurred on the line: ',dline
write(*,*) ' Program Halted'
stop
endif
return
end

subroutine checkfile(file1,file2,msg)
c =====
c Modulal Name: CHECKFILE
c Author: A. S. Rood
c Date Created: 01/13/04
c Last Modified: 01/13/04
c Modifications:

```

```

c Purpose:  Checks the two files (file1 and file2) and halts program
c           if they are the same case insensitive name
c Arguments:
c file1:  first file
c file2:  second file
c msg:    a warning msg printed if both files have the same case insensitive name

```

```

c Called By:  MAIN
c Calls To:  none

```

```

c =====

```

```

implicit none
character*80 file1,file2,file3,file4
character*260 msg
logical lcfiles
data lcfiles/.false./

```

```

file3=file1
file4=file2
call filcase(lcfiles,file3)
call filcase(lcfiles,file4)
if(file3.eq.file4)then
write(*,*) msg
write(*,*) trim(file1),' ',trim(file2)
write(*,*) trim(file2),' ',trim(file4)
write(*,*) ' Program Halted'
stop
endif

return
end

```

```

subroutine filcase(lcfiles,cfile)

```

```

c =====

```

```

c Modular Name:  FILECASE
c Author:  J. Scire - Modified by A.S. Rood
c Date Created: 06/10/95
c Last Modified: 01/13/04
c Modifications:

```

```

c Purpose:  Convert all characters within a file name to lower
c
c Arguments:
c lcfiles: logical - Switch indicating if all characters in the
c             filenames are to be converted to lower case
c             letters (LCFILES=T) or converted to UPPER
c             CASE letters (LCFILES=F) lcfiles is fixed as false in main
c cfiles:  char*70 - Input character string

```

```

c Called By:  MAIN
c Calls To:  none

```

```

c =====

```

```

character*70 cfile
character*1 cchar,clc(29),cuc(29)
logical lcfiles

```

```

c
data clc/'i','n','x','a','e','o','u','b','c','d','f','g','h',
1 'j','k','l','m','p','q','r','s','t','v','w','y','z','-','.',
2 '*' /
data cuc/'I','N','X','A','E','O','U','B','C','D','F','G','H',
1 'J','K','L','M','P','Q','R','S','T','V','W','Y','Z','-','.',
2 '*' /

```

```

c
if(lcfiles)then

```

```

c --- Convert file name to lower case letters

```

```

do i=1,70
cchar=cfile(i:i)
c
do j=1,29
if(cchar.eq.clc(j))then
cfile(i:i)=clc(j)
go to 52
endif
enddo
52 continue
enddo
else

```

```

c --- Convert file name to UPPER CASE letters

```

```

do i=1,70
cchar=cfile(i:i)
c
do j=1,29
if(cchar.eq.clc(j))then
cfile(i:i)=cuc(j)
go to 62
endif
enddo
62 continue
enddo
endif

```

```

c

```

```

return
end

subroutine fileexist(cfile)
c =====
c Module Name: FILEEXIST
c Author: A.S. Rood
c Date Created: 05/31/2013
c Last Modified:
c Modifications:

c Purpose: Checks whether file exists, if not terminate program
c
c Arguments:
c cfile - file name to check

c Called By: MAINF
c Calls To: none

c =====
implicit none
character*80 cfile
logical testfl
c --- Check to make sure file exists
inquire(file=cfile,exist=testfl)
if(.not.testfl) then
write(*,*) 'ERROR - the file:',cfile,' does not exist'
write(*,*) ' check for the file and try again '
stop
endif
return
end

REAL*8 FUNCTION selip(k,n,arr)
c =====
c Module Name: FUNCTION SELIP
c Created: 08/16/97
c Last Edit: 03/25/98
c (C) Copr. 1986-92 Numerical Recipes Software >v523211$.
c Purpose: Finds the kth smallest value of the array arr
c Called By: PERCENTILES
c Calls To: SHELL
c Arguments: k: kth smallest value
c n: number of simulations (array elements)
c arr: array holding values
c =====
INTEGER k,n,M
REAL*8 arr(8760*2),BIG
PARAMETER (M=64,BIG=1.E30)
CU USES shell
INTEGER i,j,jl,jm,ju,kk,mm,nlo,nxtmm,isel(M+2),indx
REAL*8 ahi,alo,sum,sel(M+2)
if(k.lt.1.or.k.gt.n.or.n.le.0) then
write(*,*) ' bad input to selip rank n ',k,n
read(*,*)
endif
kk=k
ahi=BIG
alo=-BIG
1 continue
mm=0
nlo=0
sum=0.
nxtmm=M+1
do 11 i=1,n
if(arr(i).ge.alo.and.arr(i).le.ahi)then
mm=mm+1
if(arr(i).eq.alo) nlo=nlo+1
if(mm.le.M)then
sel(mm)=arr(i)
else if(mm.eq.nxtmm)then
nxtmm=mm+mm/M
sel(1+mod(i+mm+kk,M))=arr(i)
endif
sum=sum+arr(i)
endif
11 continue
if(kk.le.nlo)then
selip=alo
return
else if(mm.le.M)then
call shell(mm,sel)
selip=sel(kk)
return
endif
sel(M+1)=sum/mm

call shell(M+1,sel)
sel(M+2)=ahi
do 12 j=1,M+2
isel(j)=0
12 continue
do 13 i=1,n
if(arr(i).ge.alo.and.arr(i).le.ahi)then
jl=0

```

```

      ju=M+2
      if(ju-jl.gt.1)then
2         jm=(ju+jl)/2
           if(arr(i).ge.sel(jm))then
             jl=jm
           else
             jm=jm
           endif
           goto 2
         endif
         isel(ju)=isel(ju)+1
       endif
13      continue
        j=1
3         if(kk.gt.isel(j))then
           alo=sel(j)
           kk=kk-isel(j)
           j=j+1
           goto 3
         endif
         ahi=sel(j)
       goto 1
     END

SUBROUTINE shell(n,a)
c =====
c   Module Name:  SHELL
c   Created:     08/16/97
c   Last Edit:  08/16/97
c (C) Copr. 1986-92 Numerical Recipes Software >v523211$.
c   Purpose:    sorts the input array
c   Called By:  SELIP
c   Calls To:   none
c   Arguments:  n: number of simulations (array elements)
c               a: array holding values
c =====
      implicit none
      INTEGER n,M
      parameter (M=64)
      REAL*8 a(M+2)
      INTEGER i,j,inc
      REAL*8 v
      inc=1
1     inc=3*inc+1
      if(inc.le.n)goto 1
2     continue
      inc=inc/3
      do 11 i=inc+1,n
        v=a(i)
        j=i
3         if(a(j-inc).gt.v)then
           a(j)=a(j-inc)
           j=j-inc
           if(j.le.inc)goto 4
         goto 3
       endif
4         a(j)=v
11      continue
      if(inc.gt.1)goto 2
      return
      END
C (C) Copr. 1986-92 Numerical Recipes Software >v523211$.

```


Appendix C
Frequency of Detection Plots

Appendix C

Frequency of Detection Plots

This appendix contains frequency of detection plots for each of the 11 sources considered (three stack and eight ground-release sources) and radionuclides considered (i.e., Cs-137, Pu-239, and Sr-90) for the onsite and offsite sampling networks. There are 20 samplers located on the INL Site (onsite) and 17 samplers located off INL (offsite). Frequency of detection results are based on a sampler flow rate of 2 cfm, a 168-hour sampling time, and two sets of MDA values. One set of MDA values is used by the Gonzales-Stoller Surveillance, who maintains and samples 16 samplers as part of the INL ESER Program. The other set of MDAs is used by the INL contractor, BEA, who maintain and sample 21 samplers. The ESER MDAs are less than the BEA MDAs, which results in frequency of detection values that are equal to or greater than those using BEA MDAs.

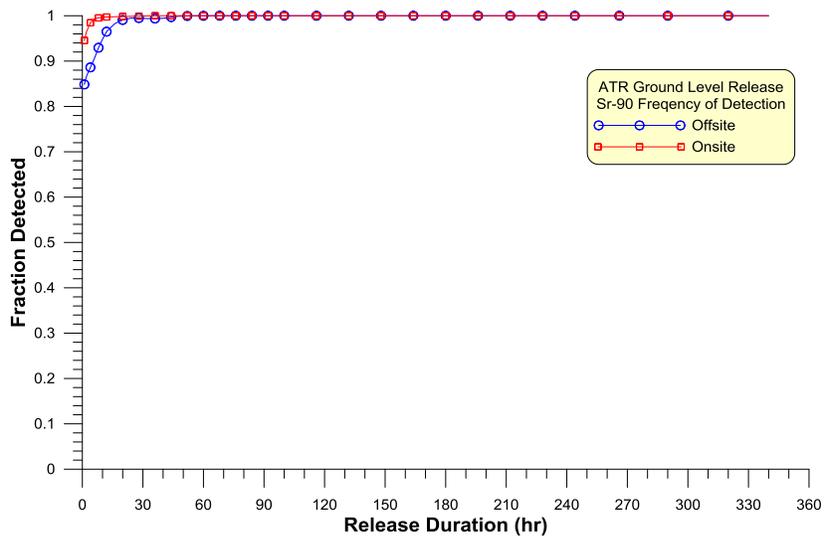
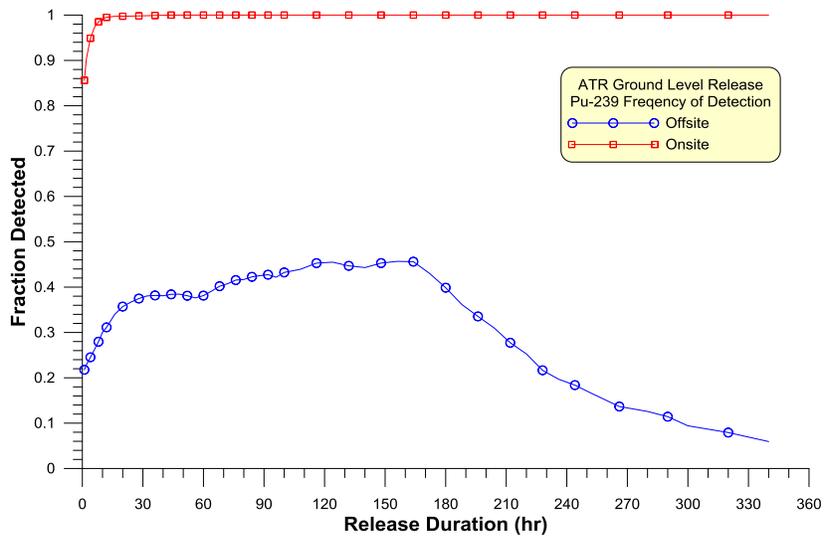
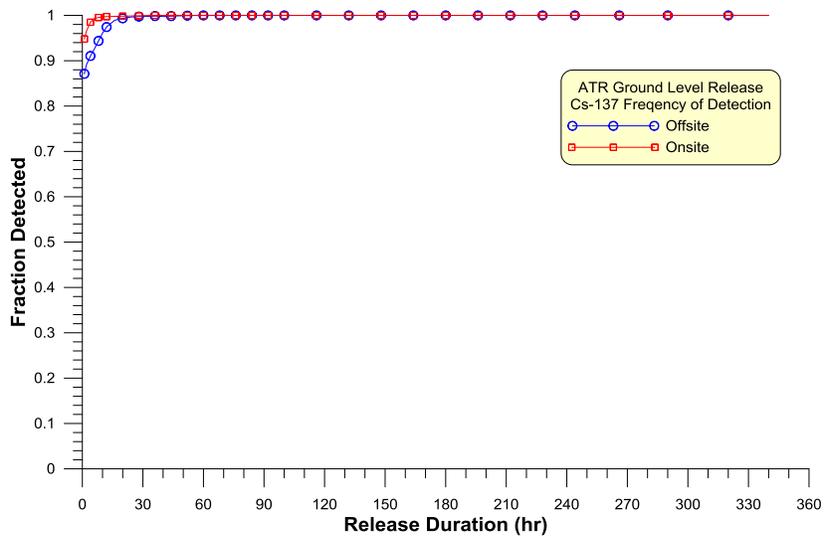


Figure C-1. Frequency of detection for ATR ground-level release using ESER MDAs.

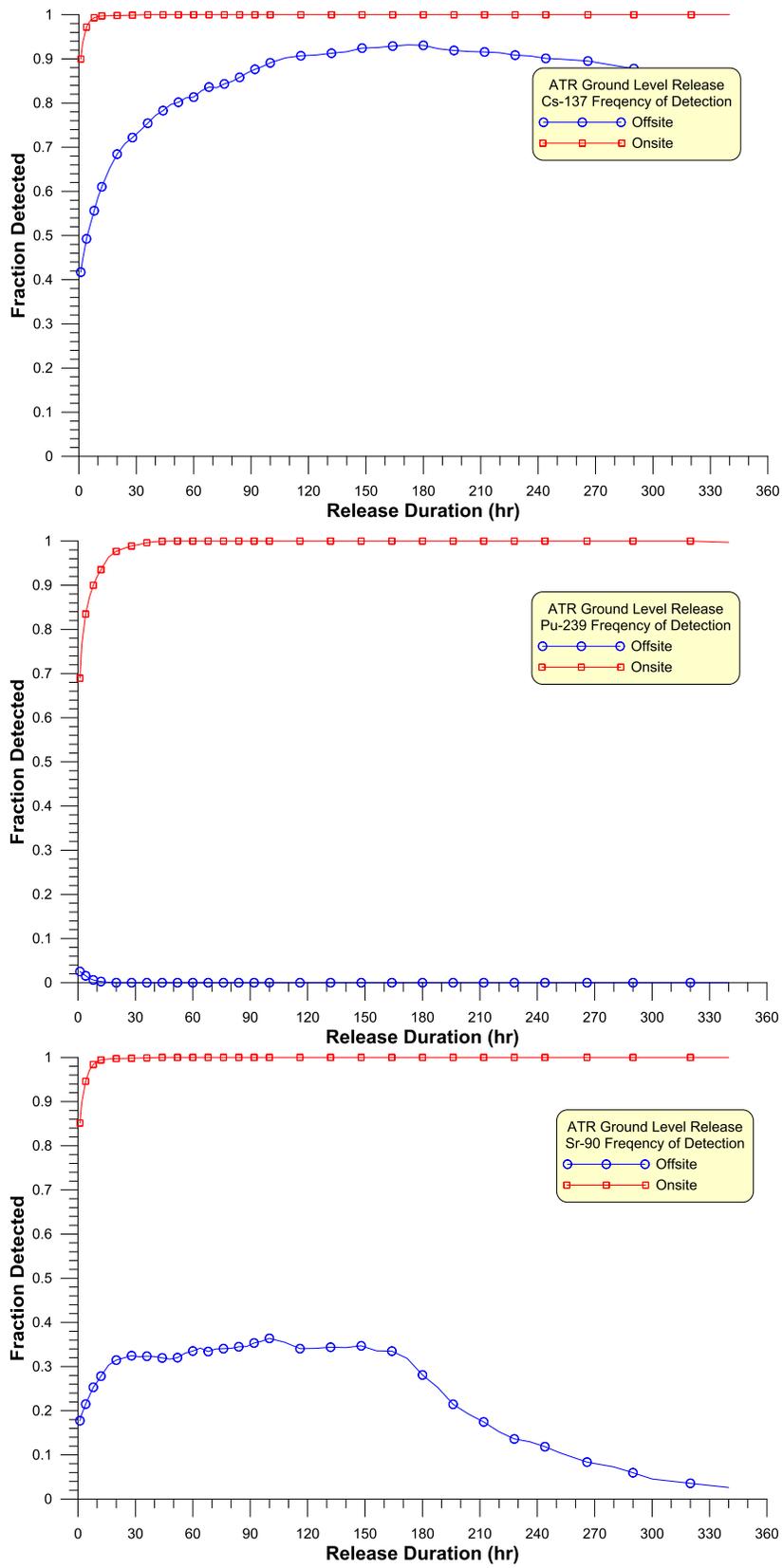


Figure C-2. Frequency of detection for ATR ground-level release using BEA MDAs.

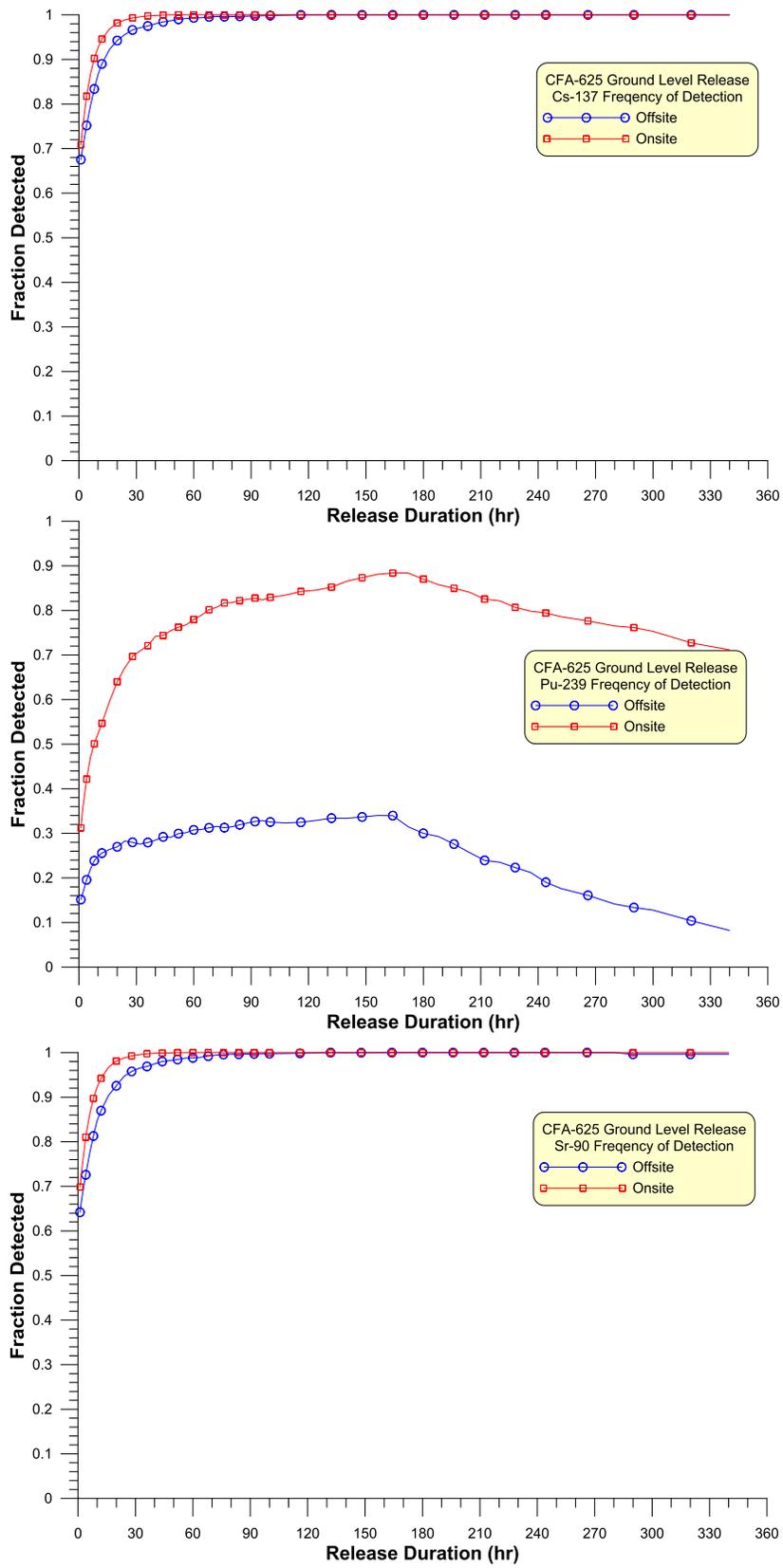


Figure C-3. Frequency of detection for CFA-625 ground-level release using ESER MDAs.

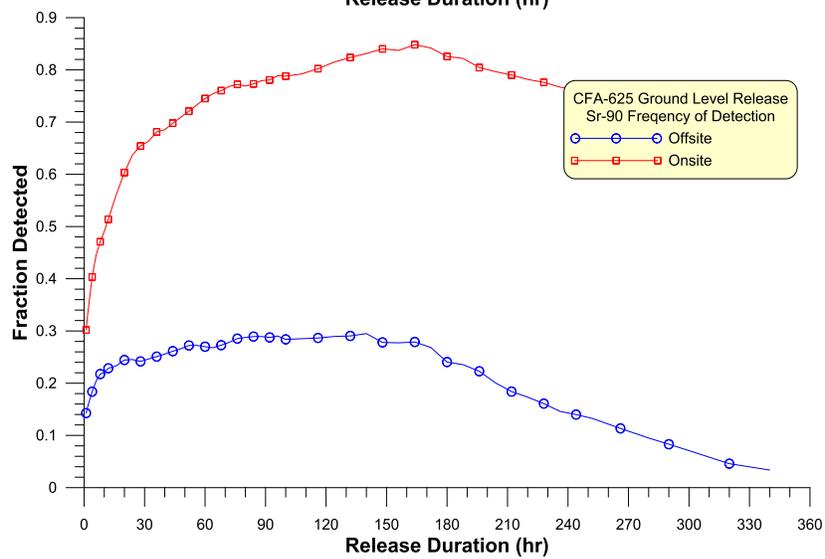
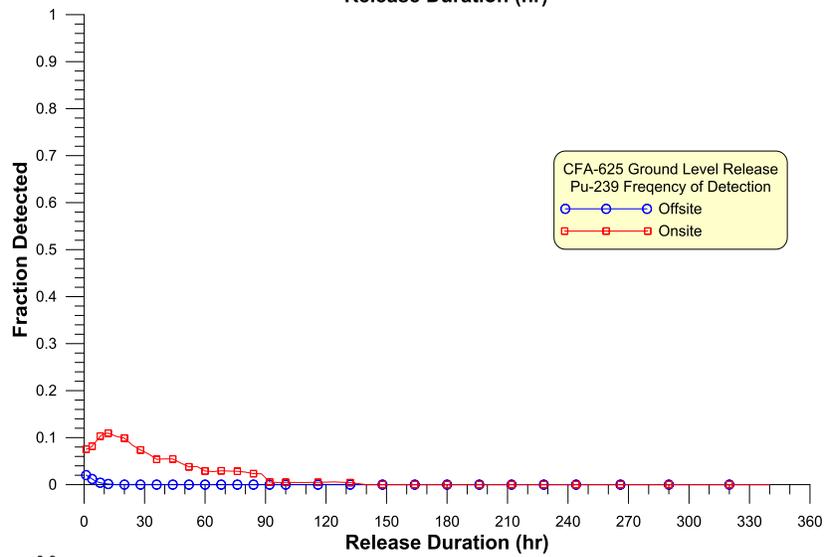
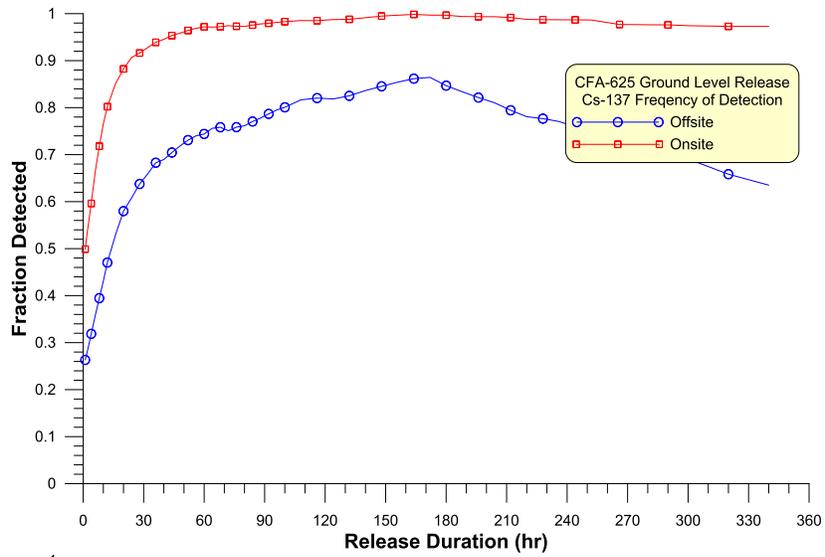


Figure C-4. Frequency of detection for CFA-625 ground-level release using BEA MDAs.

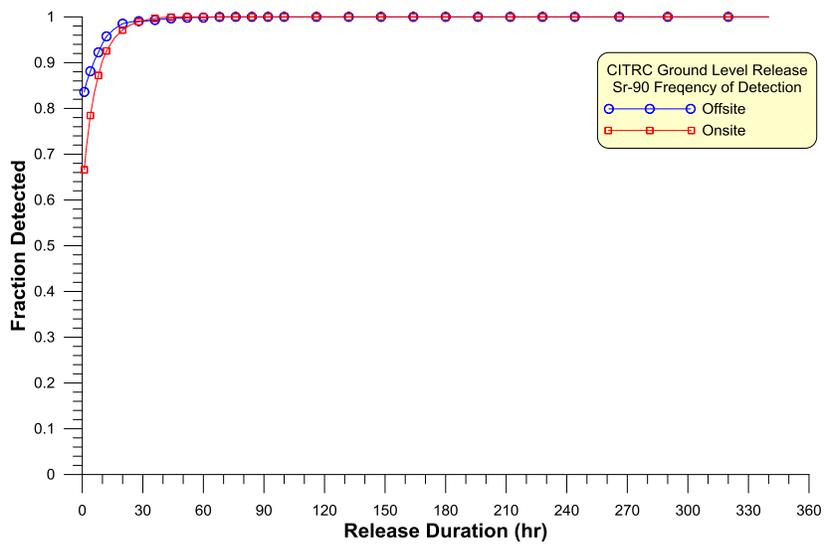
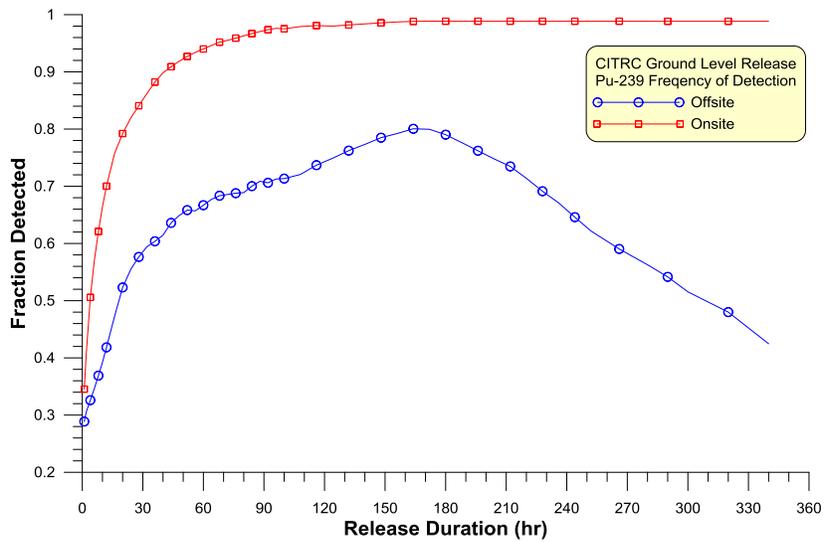
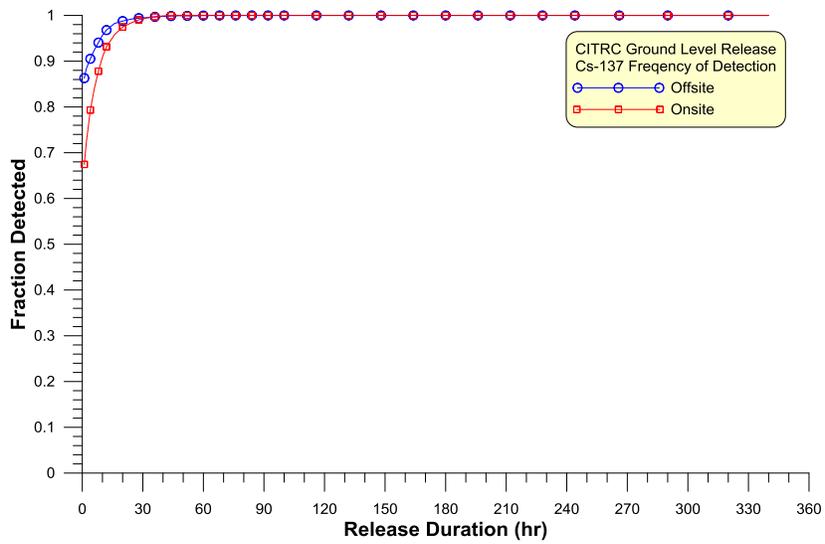


Figure C-5. Frequency of detection for CITRC ground-level release using ESER MDAs.

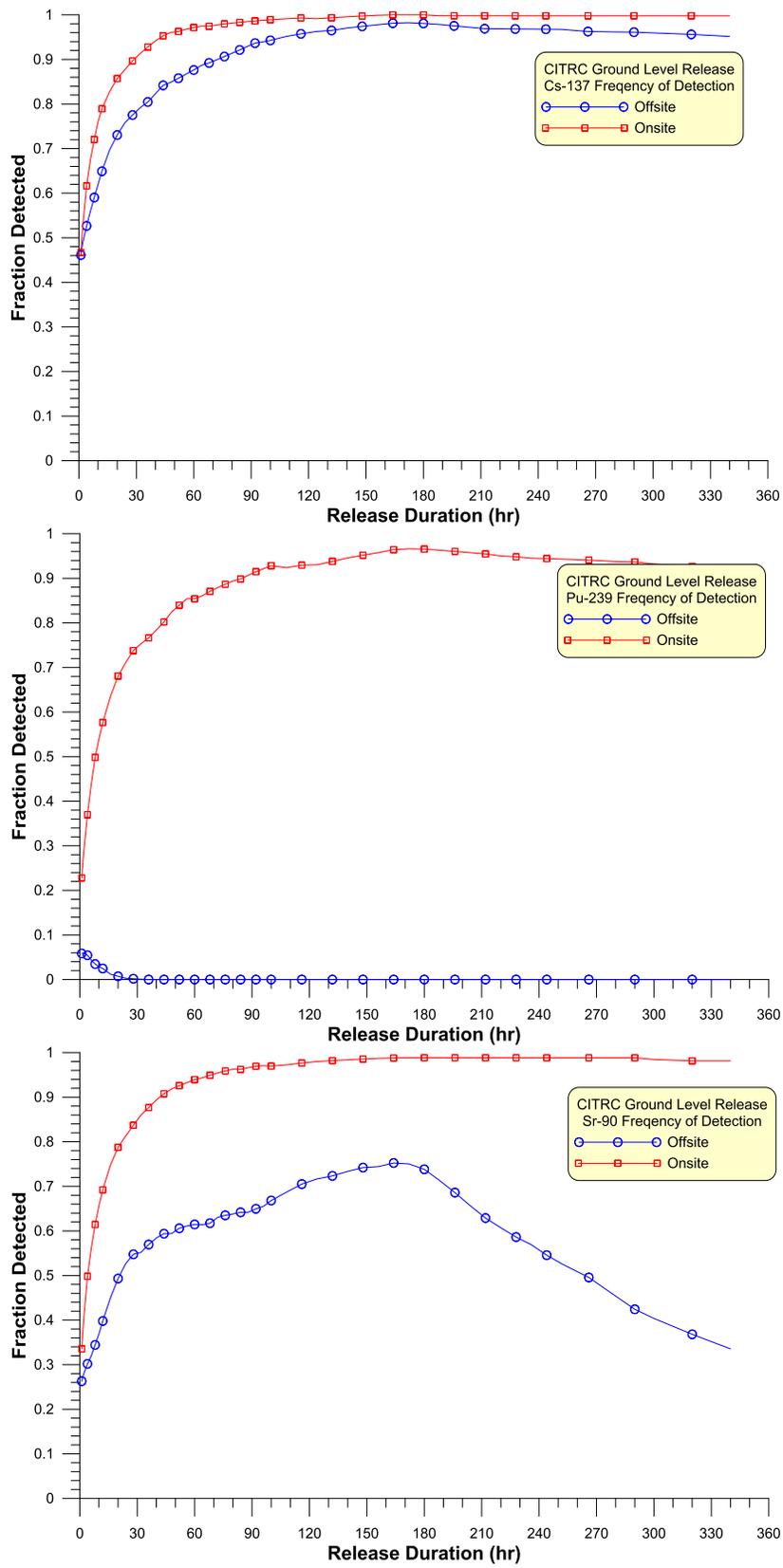


Figure C-6. Frequency of detection for CITRC ground-level release using BEA MDAs.

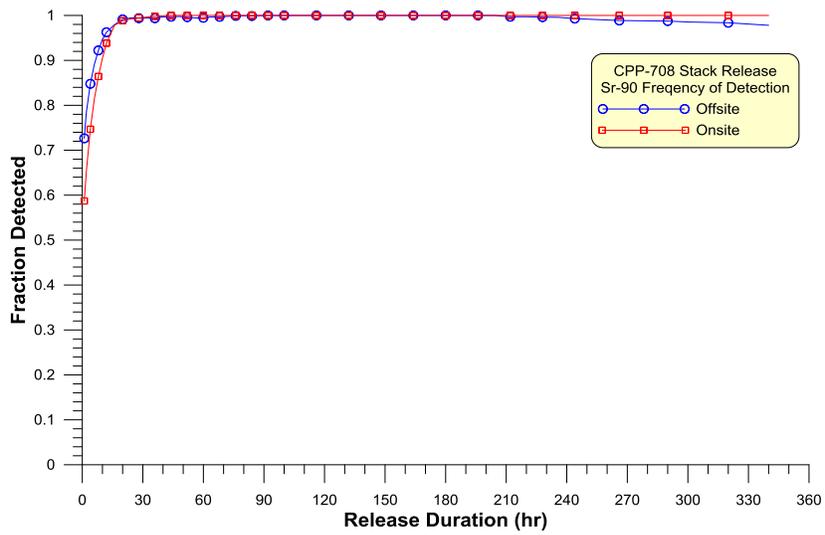
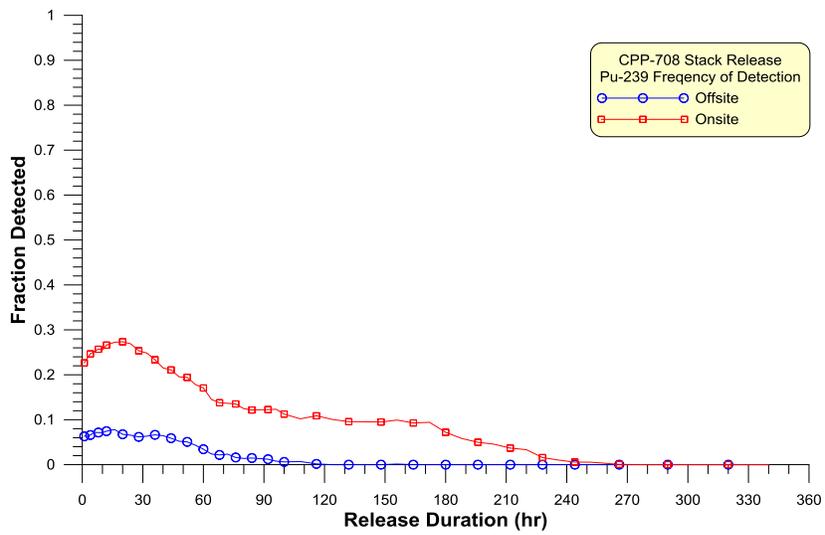
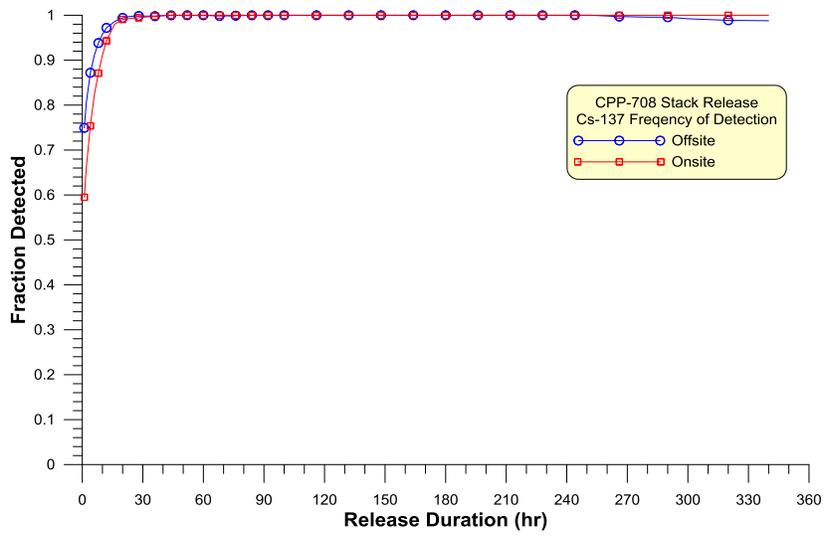


Figure C-7. Frequency of detection for CPP-708 stack release using ESER MDAs.

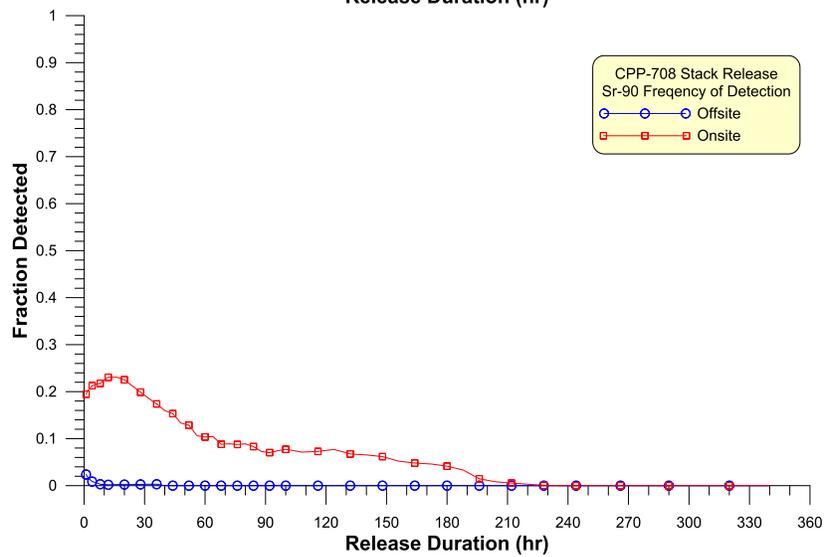
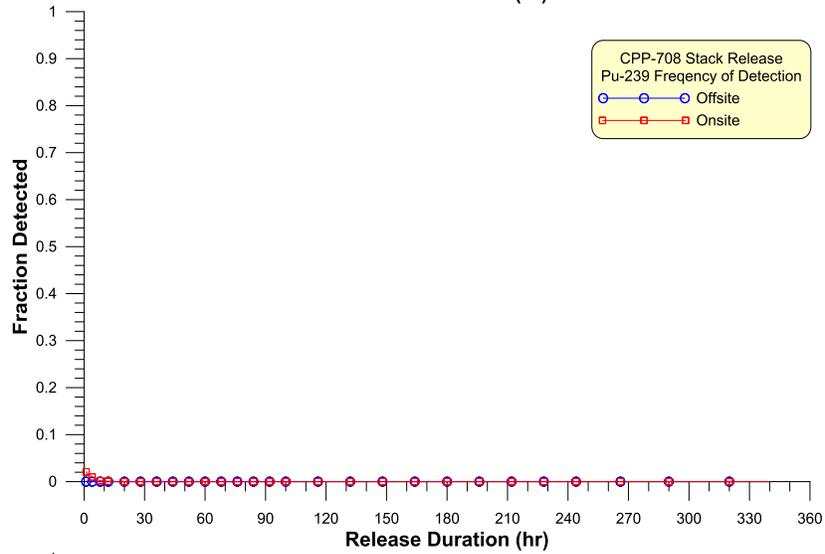
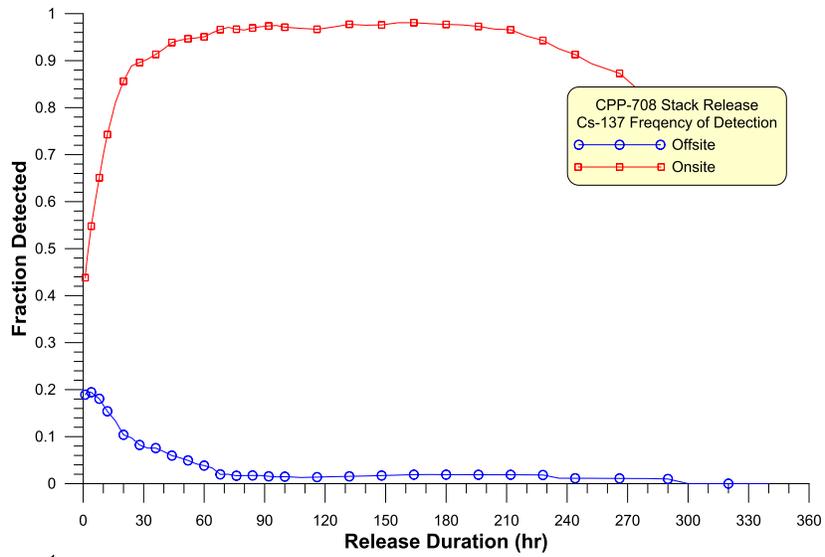


Figure C-8. Frequency of detection for CPP-708 stack release using BEA MDAs.

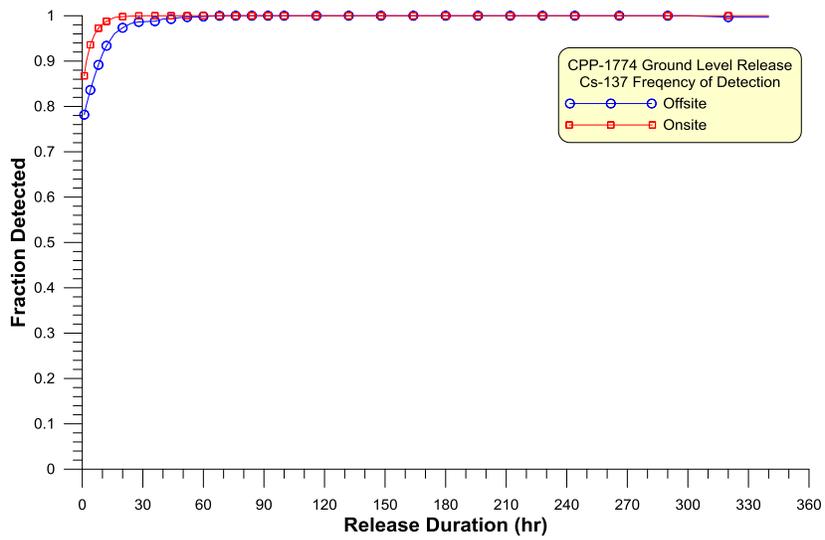
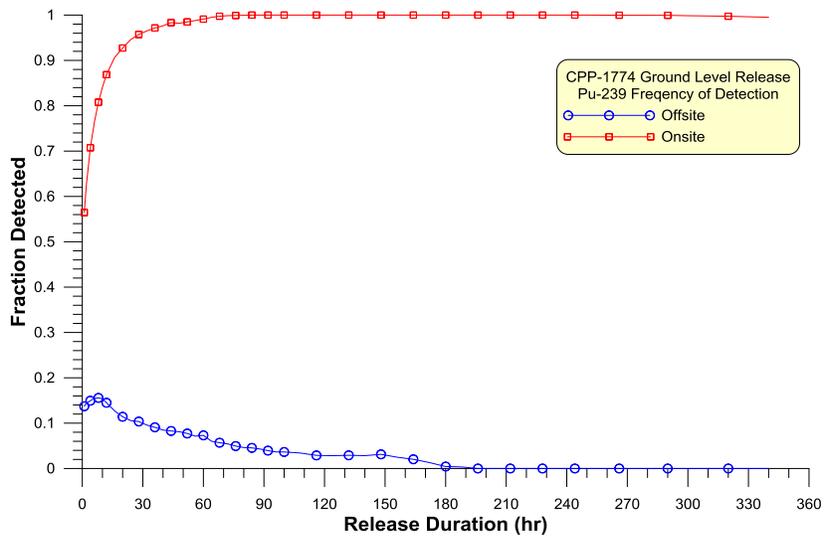
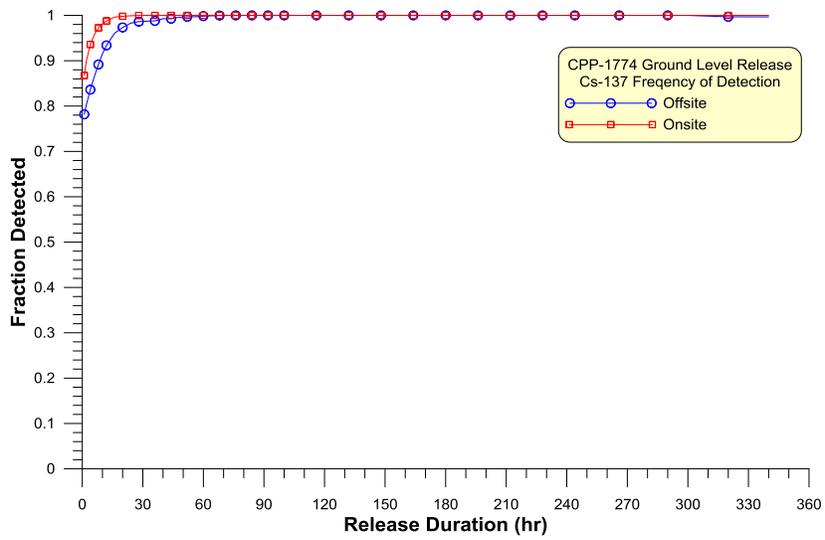


Figure C-9. Frequency of detection for CPP-1774 (INTEC) ground-level release using ESER MDAs.

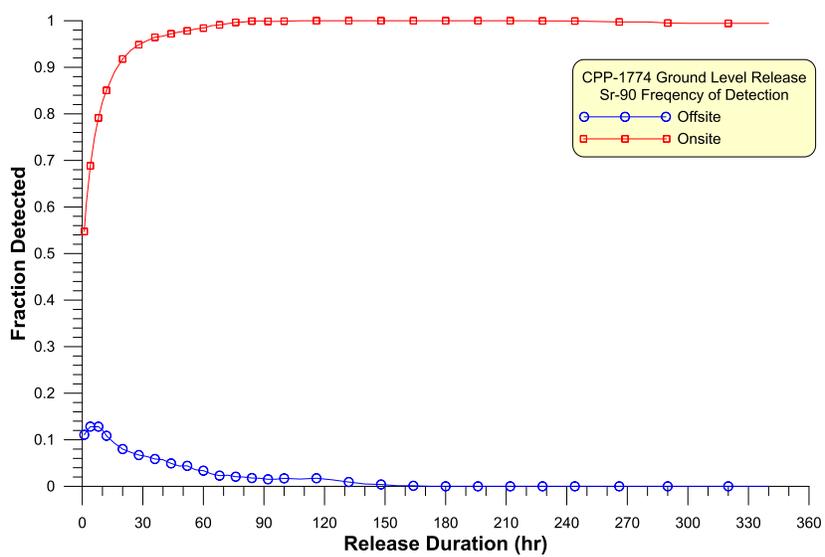
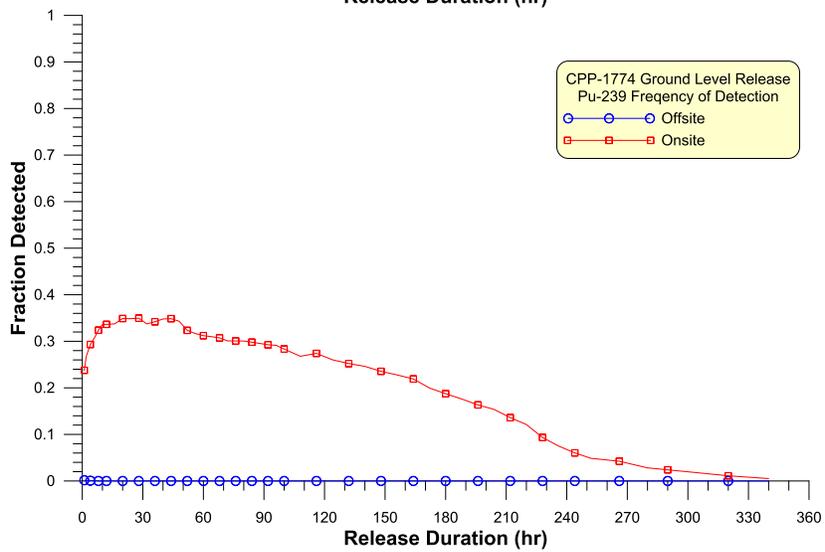
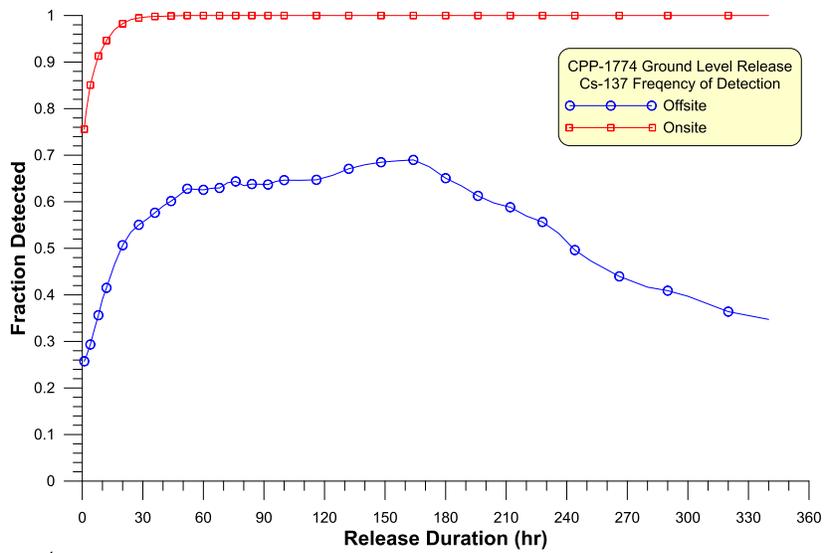


Figure C-10. Frequency of detection for CPP-1774 (INTEC) ground-level release using BEA MDAs.

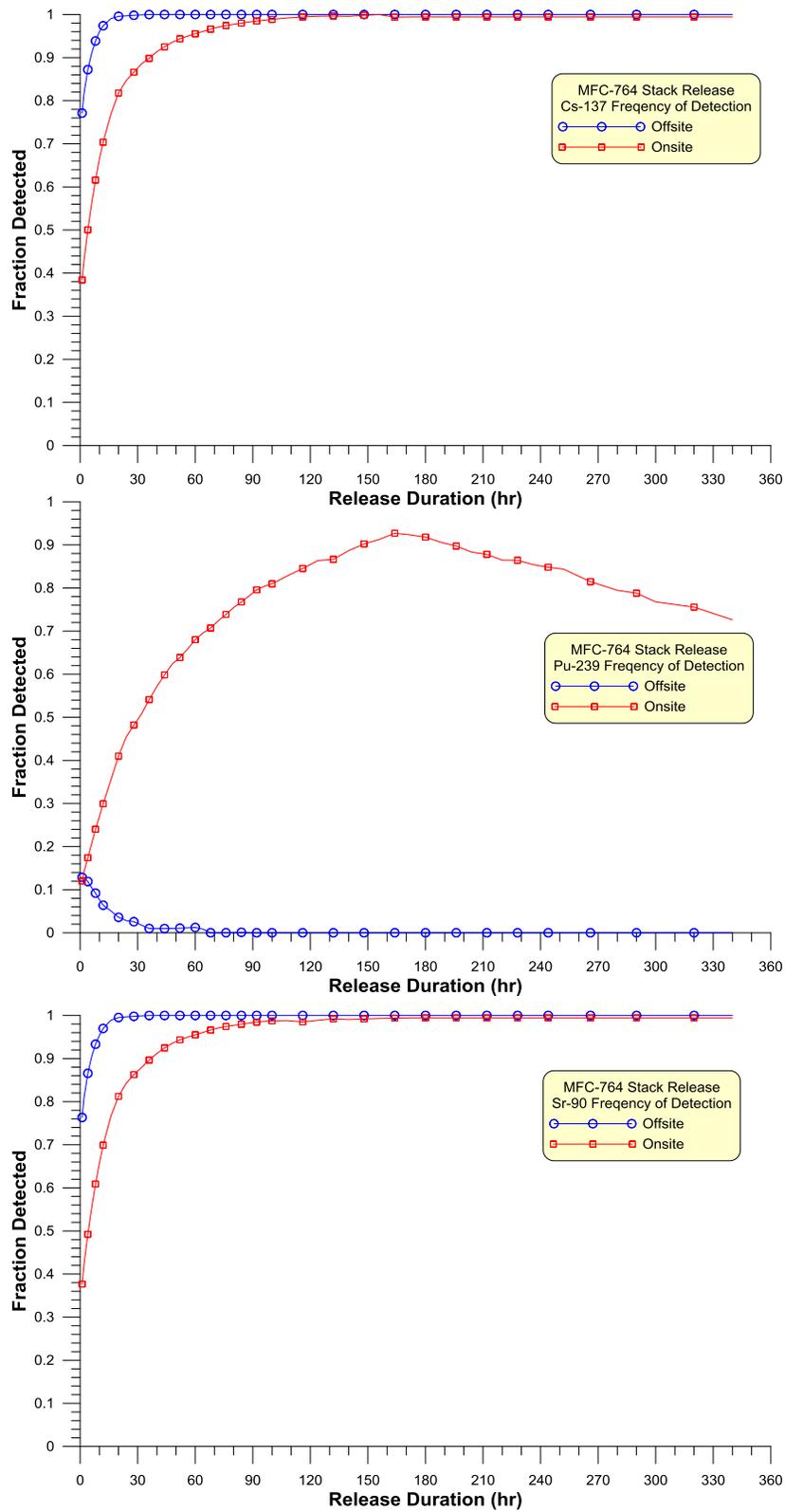


Figure C-11. Frequency of detection for MFC-764 stack release using ESER MDAs.

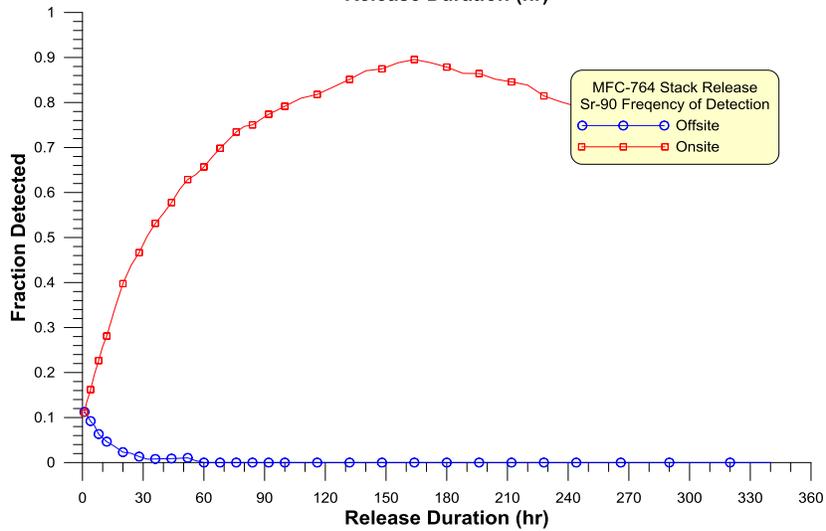
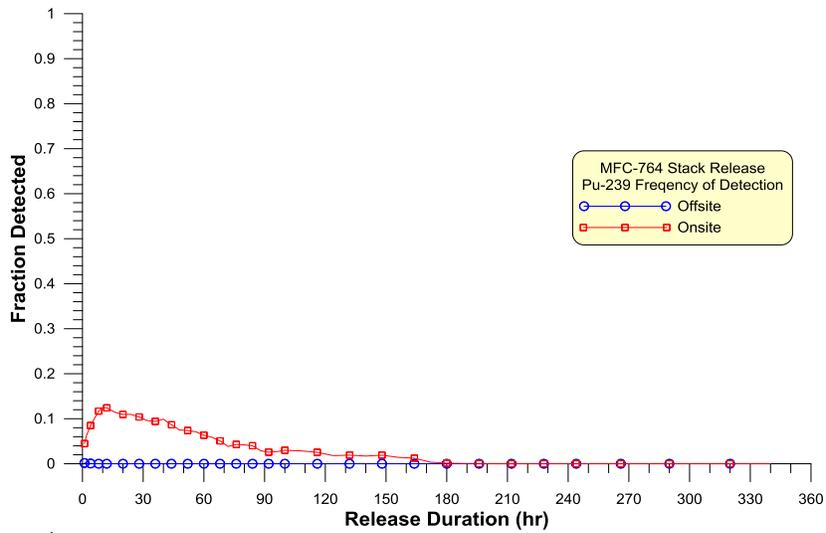
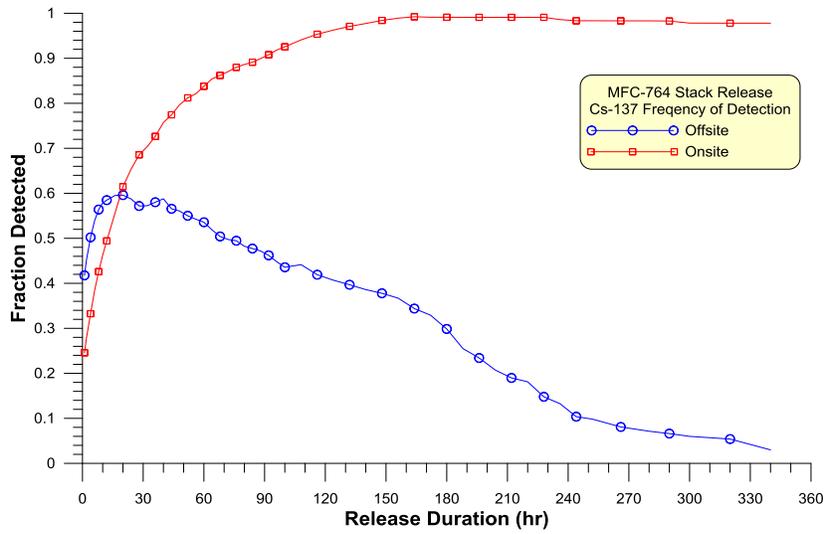


Figure C-12. Frequency of detection for MFC-764 stack release using BEA MDAs.

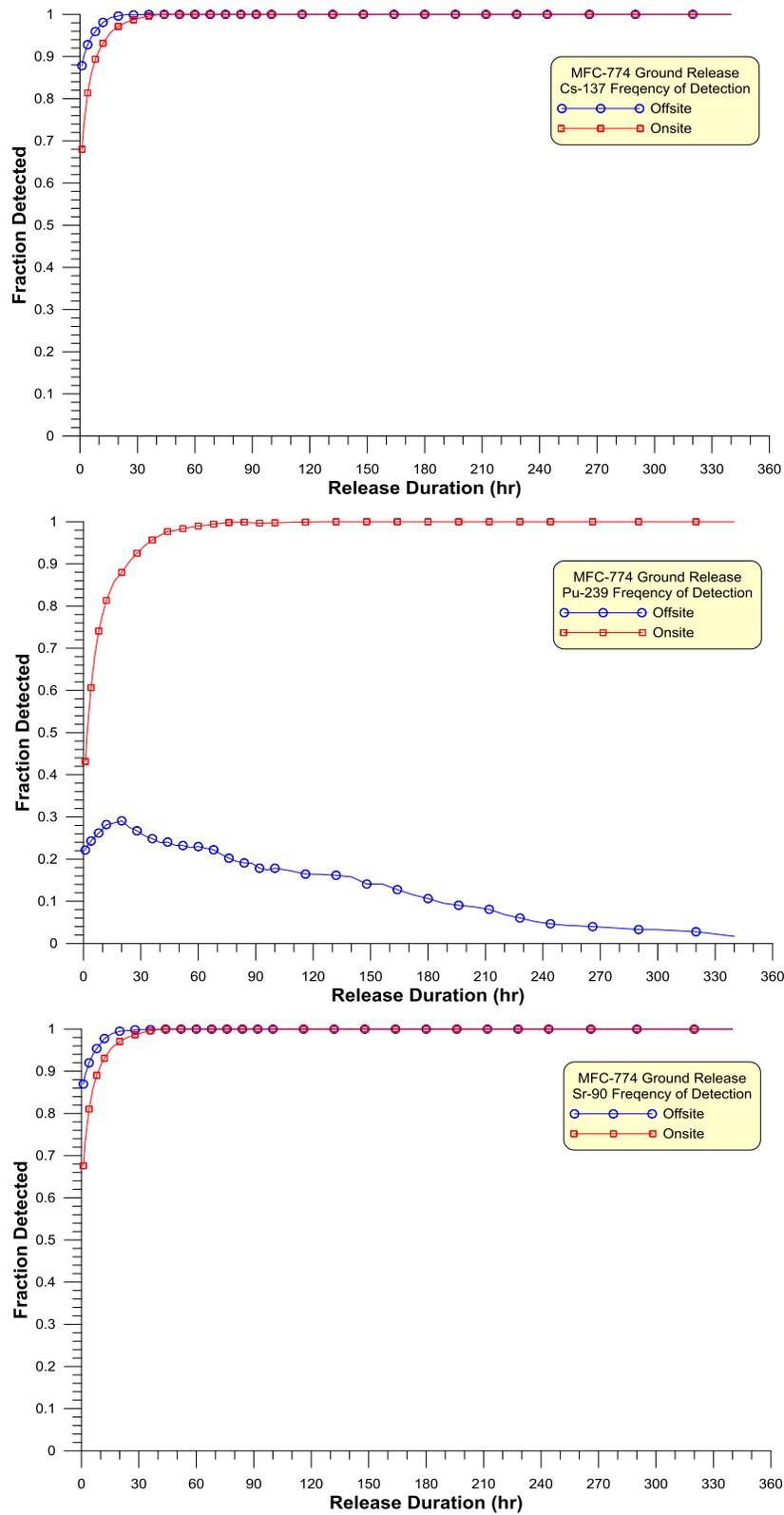


Figure C-13. Frequency of detection for MFC-774 ground-level release using ESER MDAs.

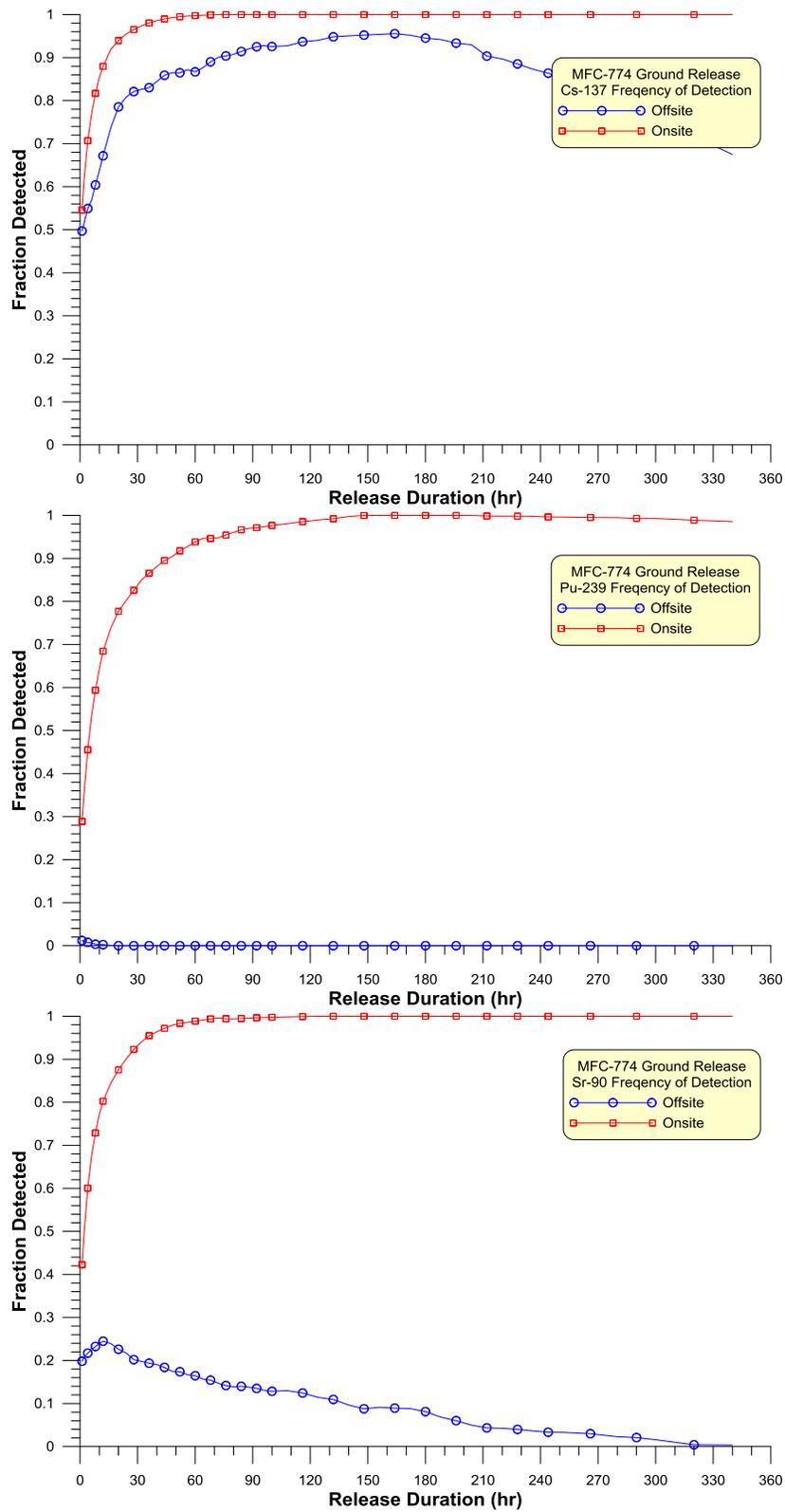


Figure C-14. Frequency of detection for MFC-774 ground-level release using BEA MDAs.

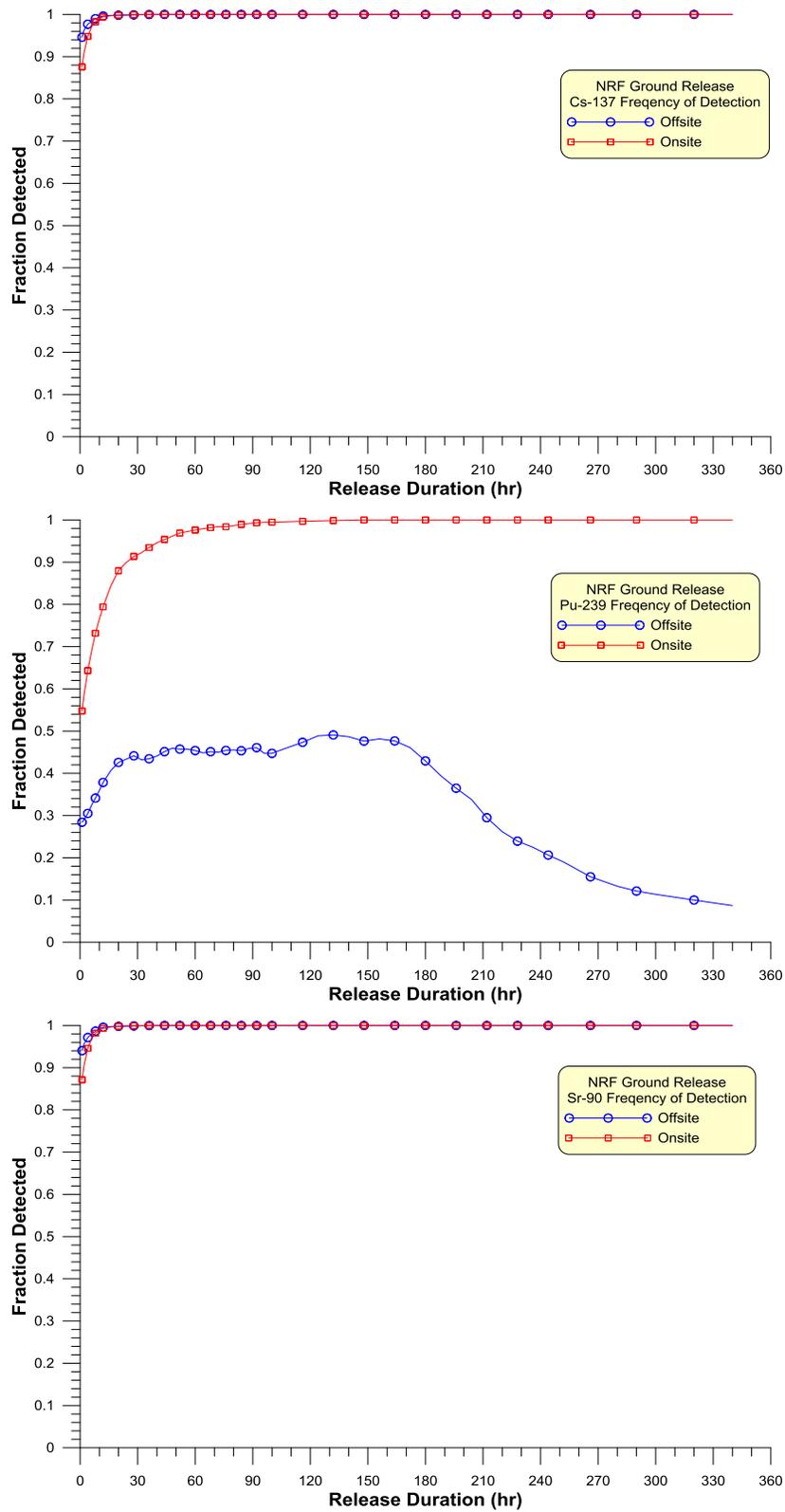


Figure C-15. Frequency of detection for NRF ground-level release using ESER MDAs.

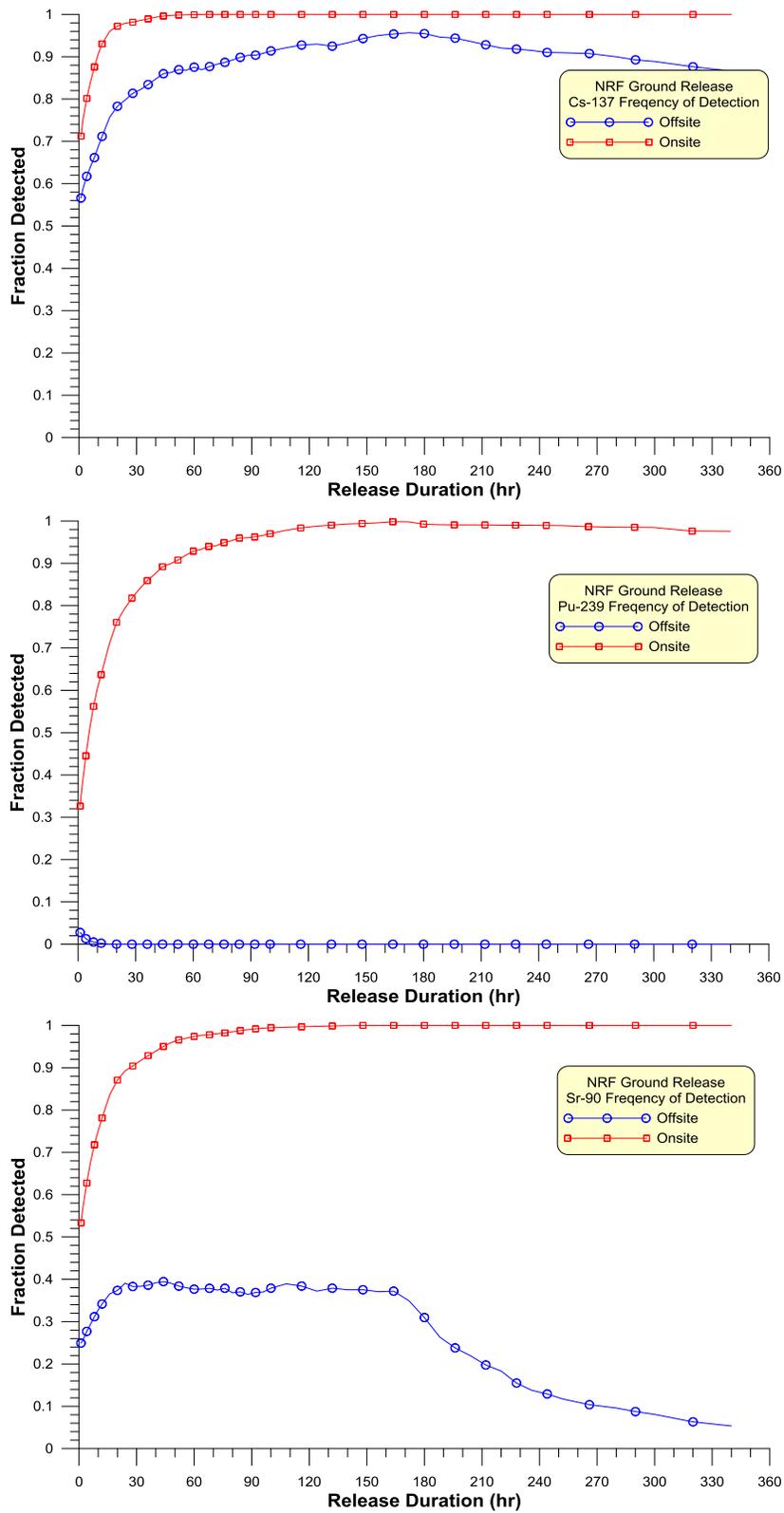


Figure C-16. Frequency of detection for NRF ground-level release using BEA MDAs.

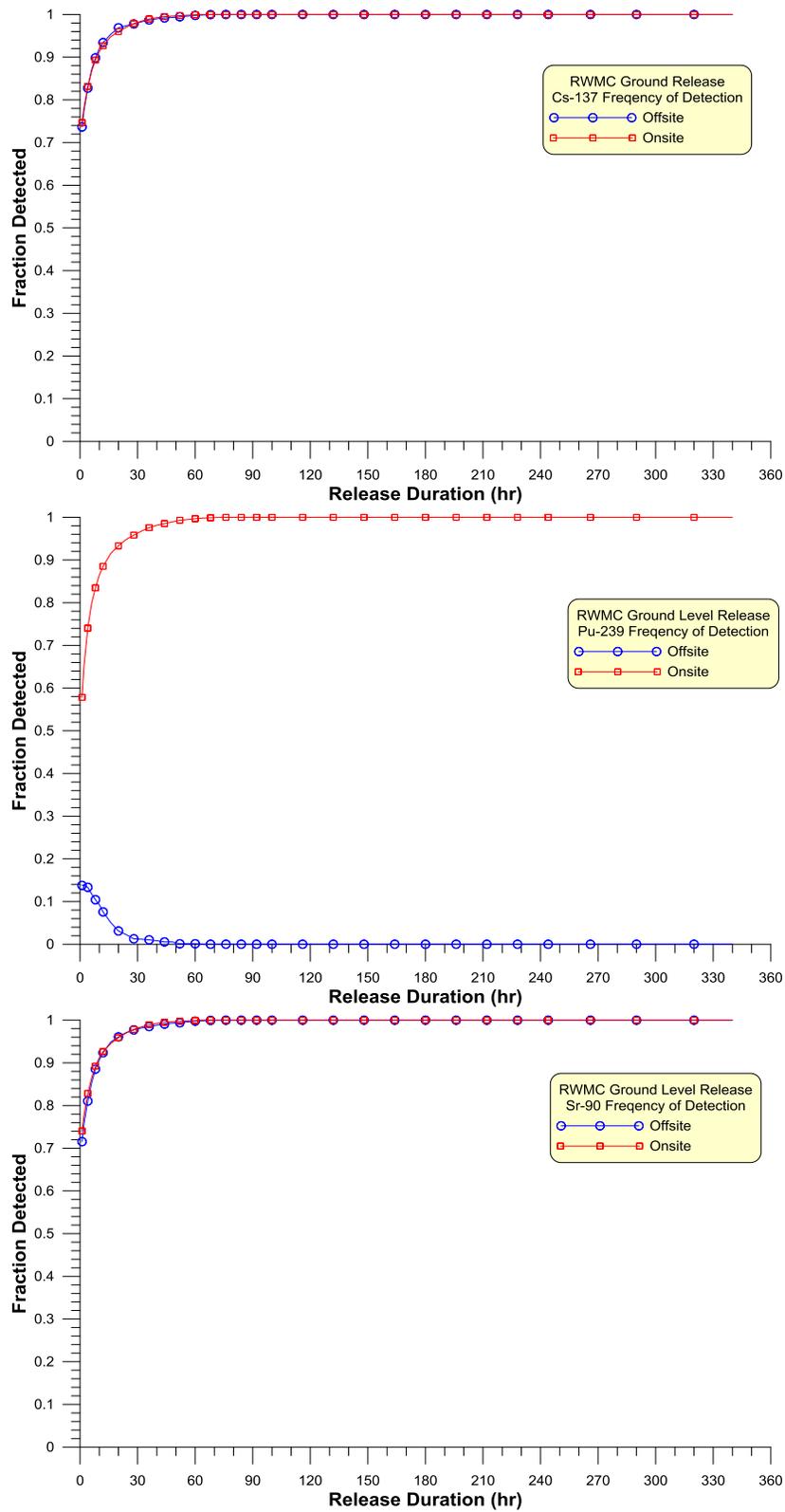


Figure C-17. Frequency of detection for RWMC ground-level release using ESER MDAs.

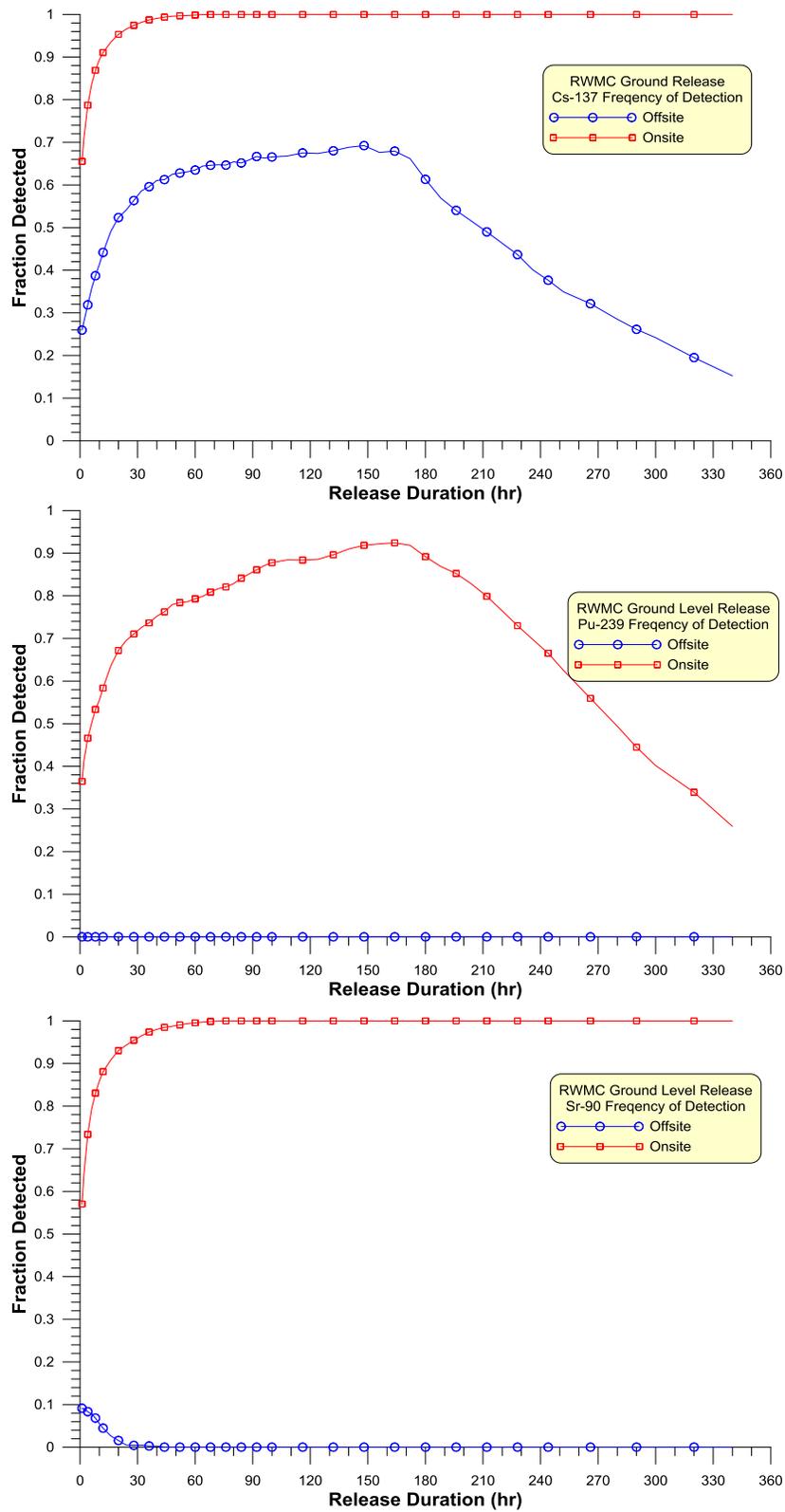


Figure C-18. Frequency of detection for RWMC ground-level release using BEA MDAs.

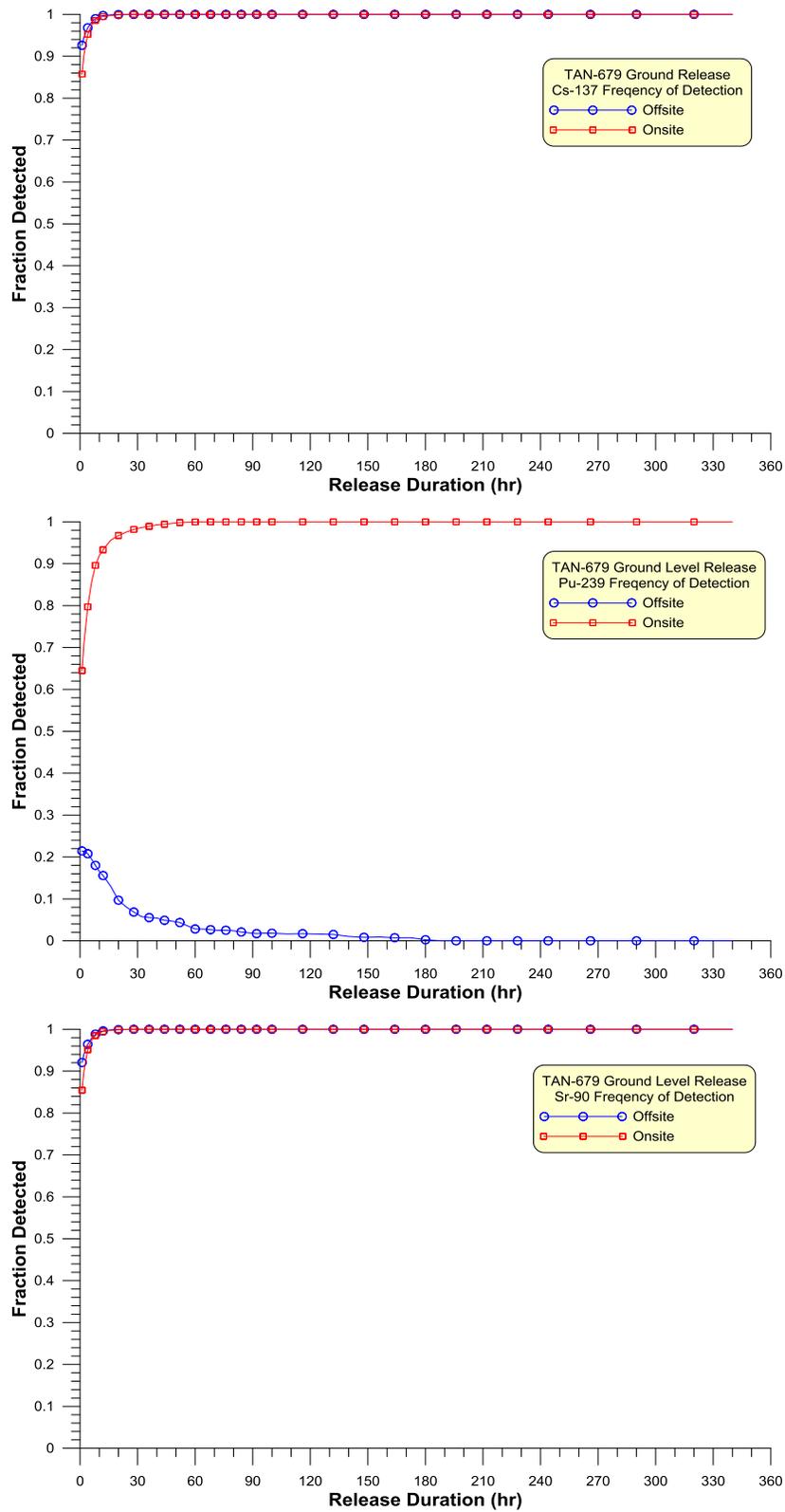


Figure C-19. Frequency of detection for TAN-679 (SMC/TAN) ground-level release using ESER MDAs.

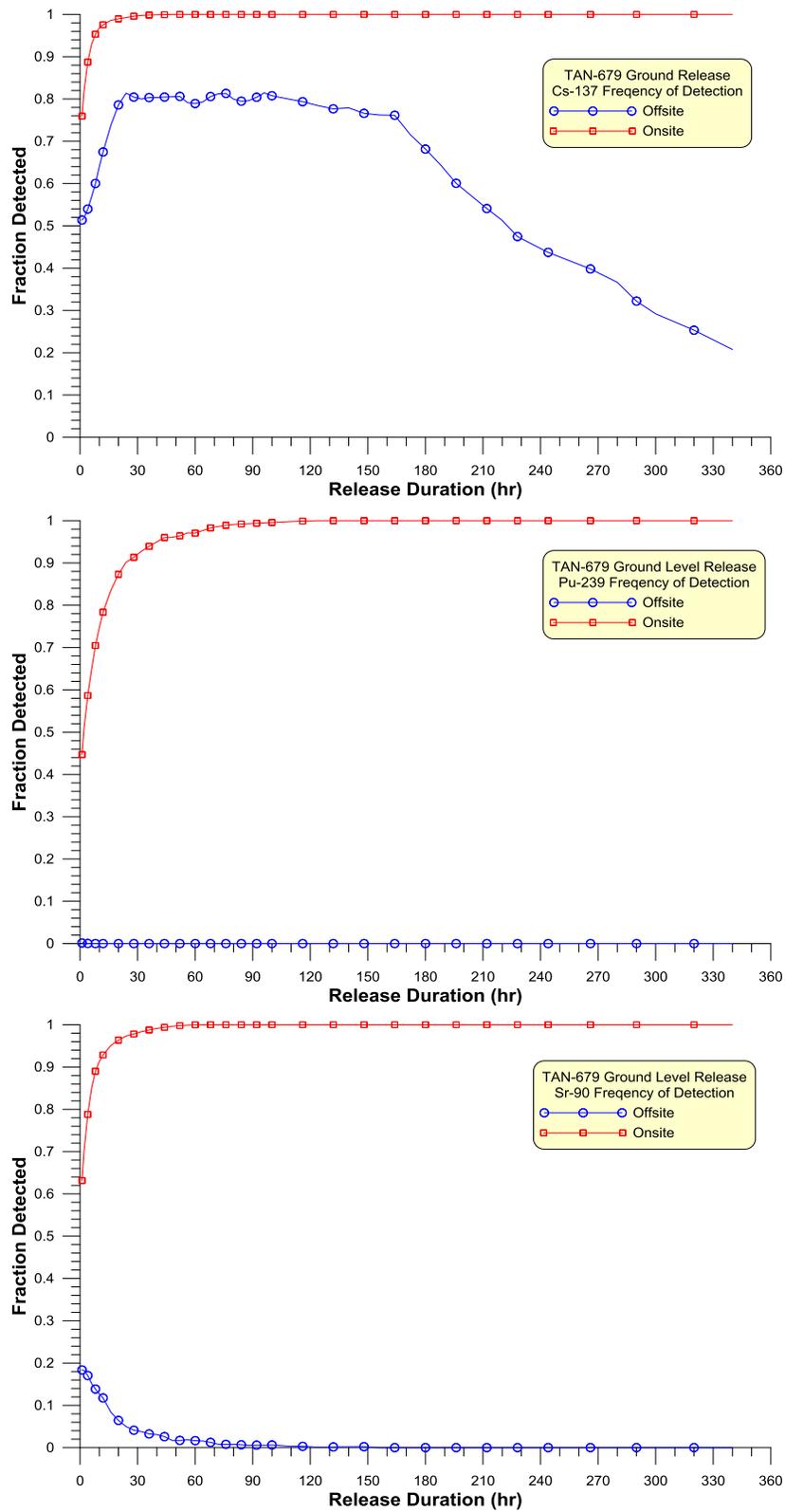


Figure C-20. Frequency of detection for TAN-679 (SMC/TAN) ground-level release using BEA MDAs.

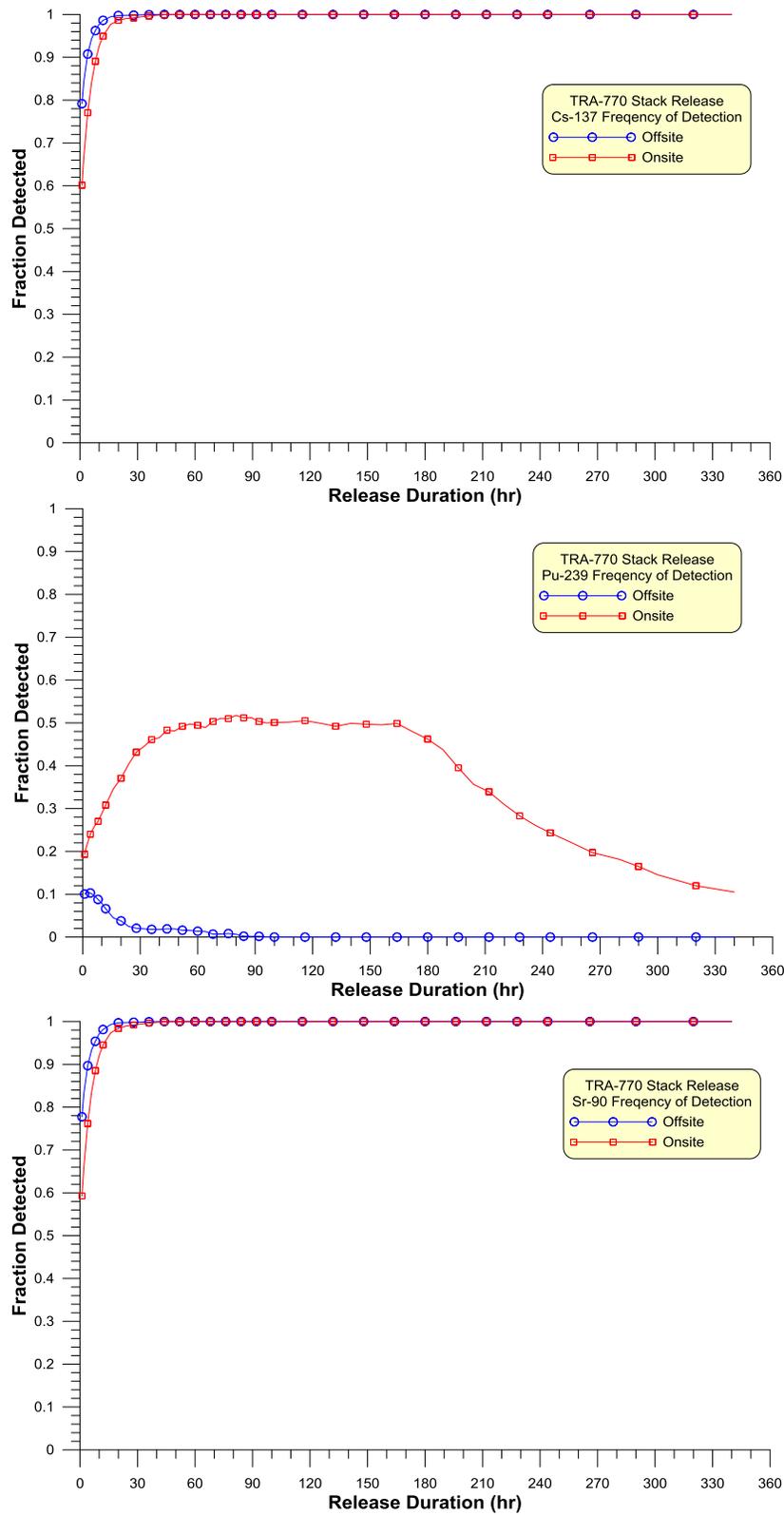


Figure C-21. Frequency of detection for TRA-770 (ATR) stack release using ESER MDAs.

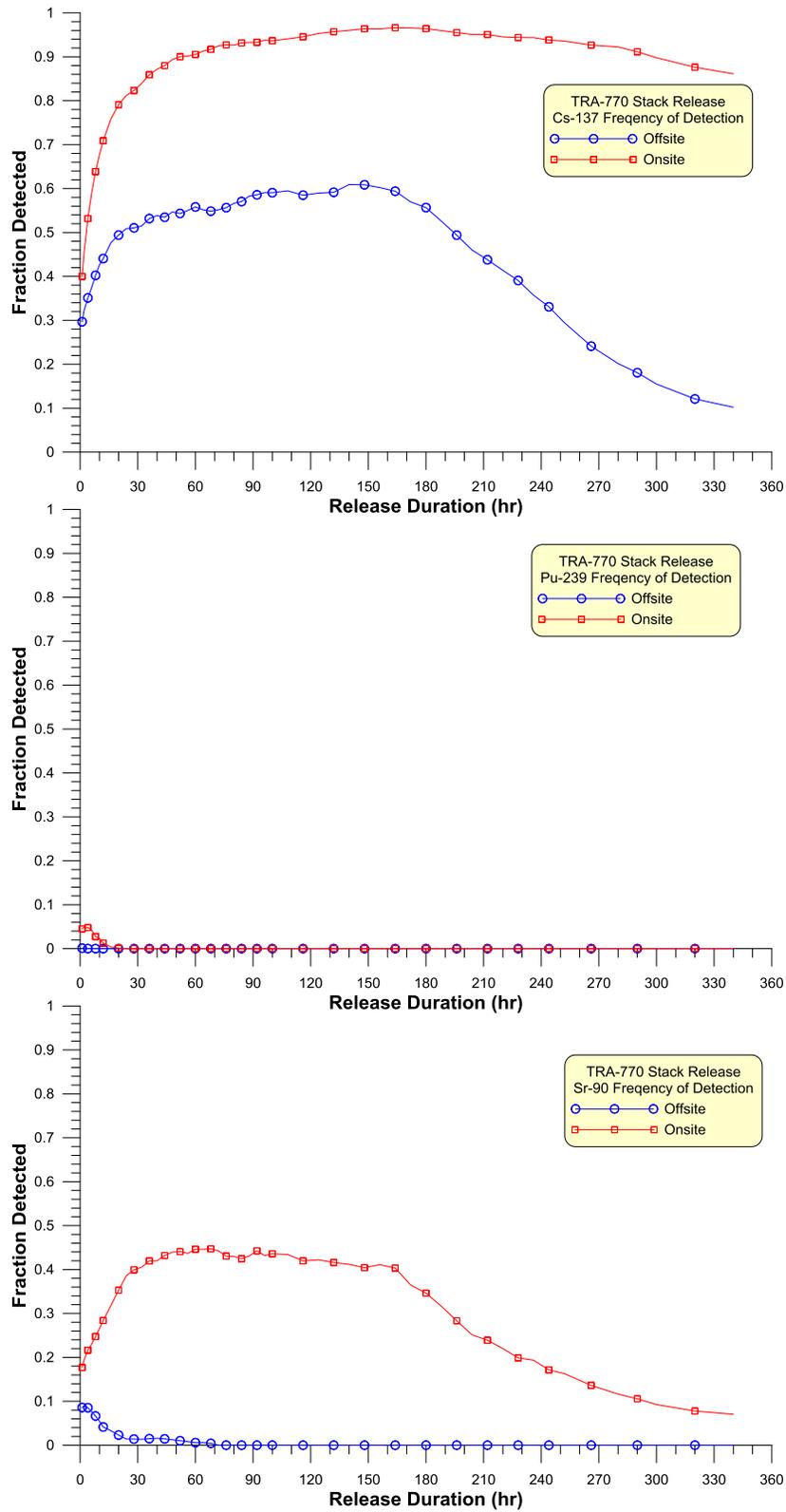


Figure C-22. Frequency of detection for TRA-770 (ATR) stack release using BEA MDAs.

Appendix D

Model Validation

Appendix D

Validation of the CALPUFF Model

D-1. INTRODUCTION

This appendix contains a description of an exercise to validate the CALPUFF model using gaseous Sb-125 releases from the Flourinel and Storage (FAST) stack during fuel reprocessing at INTEC in 1987. Releases of Sb-125 were identified in a 1987 DOE-ID memo (Chew 1987) as an opportunity to validate the meteorological air dispersion model used at the time, MESODIF (Start and Wendell 1974). The MESODIF model was developed at INL by NOAA and is the predecessor for the current NOAA model MDIFF (Sagendorf et al. 2001), which was used to simulate accidental gaseous releases and assess annual dose at INL. The MESODIF simulation results and 1987 annual average measured concentrations of Sb-125 at INL samplers were obtained in a letter from Richard L. Dickson, DOE-ID to Lynn E. Rockhold, BEA March 7, 2012 (Dickson 2012).

D-2. CALPUFF MODELING

The CALPUFF model described in the main body of the report was used in this model validation exercise. The domain size, grid spacing, terrain, and land use characteristics were identical to that used in the frequency of detection analysis.

D-2.1 Meteorological Data

Sb-125 releases at INTEC occurred from 1980 to 1990 as a result of fuel reprocessing operations. The year of highest Sb-125 releases occurred in 1987. Because meteorological data for 1987 were not obtained nor processed for use in the CALPUFF simulation, a composite meteorological data set from 2006 to 2008 was used to estimate Sb-125 concentrations at sampler locations in 1987. The composite meteorological dataset included data from the INL Mesonet stations, surface data from the Idaho Falls Regional Airport, upper air data from the Boise Airport, and three-dimensional gridded data from the WRF model. Approximating 1987 meteorological data with the 2006 through 2008 composite data set are considered appropriate for this validation exercise based on the evaluation of meteorological data variability in Section 6.2 of the main body of this report. Three-year average monthly dispersion factors (X/Q) were output from the CALPUFF model (Table D-1) and used to calculate annual average concentrations at the sampler locations.

Table D-1. Monthly-average dispersion factors (X/Q in $s\ m^{-3}$) at network samplers calculated with CALPUFF using a 3-year meteorological data set from 2006 to 2008.

Sampler	Jan	Feb	Mar	Apr	May	Jun	Jul	Aug	Sep	Oct	Nov	Dec
BLCK	1.14E-09	1.75E-09	1.16E-09	1.03E-09	1.30E-09	6.47E-10	9.02E-10	6.54E-10	1.08E-09	1.49E-09	1.42E-09	1.71E-09
CRAT	1.62E-09	6.01E-10	9.90E-10	7.73E-10	5.31E-10	9.02E-10	7.05E-10	8.85E-10	6.64E-10	7.19E-10	7.89E-10	7.51E-10
IF	1.41E-09	1.58E-09	8.71E-10	6.37E-10	8.04E-10	1.21E-09	9.58E-10	7.38E-10	9.11E-10	9.13E-10	1.14E-09	1.67E-09
REXB	2.26E-09	2.06E-09	1.33E-09	6.73E-10	6.50E-10	6.34E-10	5.89E-10	5.32E-10	6.21E-10	1.12E-09	1.71E-09	2.45E-09
ARCO	3.50E-09	1.95E-09	2.16E-09	1.62E-09	1.57E-09	7.68E-10	1.33E-09	1.16E-09	1.93E-09	2.12E-09	1.57E-09	1.97E-09
ATOM	3.50E-09	1.95E-09	2.16E-09	1.62E-09	1.57E-09	7.68E-10	1.33E-09	1.16E-09	1.93E-09	2.12E-09	1.57E-09	1.97E-09
FAA	2.30E-09	2.23E-09	1.66E-09	1.85E-09	1.77E-09	2.10E-09	2.81E-09	2.19E-09	3.08E-09	1.85E-09	2.02E-09	3.45E-09
HOWE	1.28E-08	6.20E-09	5.19E-09	7.61E-09	2.19E-09	1.76E-09	3.08E-09	3.67E-09	5.19E-09	6.04E-09	6.80E-09	1.05E-08
MONT	3.19E-09	3.47E-09	2.81E-09	3.00E-09	1.74E-09	1.70E-09	1.80E-09	2.40E-09	3.69E-09	2.97E-09	5.19E-09	4.42E-09
MUDL	4.62E-09	4.32E-09	5.23E-09	4.15E-09	3.55E-09	4.20E-09	2.94E-09	3.64E-09	4.11E-09	5.27E-09	5.74E-09	5.74E-09
RENO	5.20E-09	4.57E-09	3.99E-09	3.92E-09	1.09E-09	1.16E-09	1.19E-09	2.62E-09	2.79E-09	4.37E-09	7.99E-09	6.84E-09
ANL	4.27E-09	3.56E-09	3.49E-09	3.53E-09	2.69E-09	4.12E-09	5.31E-09	4.05E-09	6.11E-09	3.44E-09	3.46E-09	6.86E-09
ARA	4.87E-09	6.21E-09	3.97E-09	3.81E-09	4.24E-09	3.43E-09	6.10E-09	3.34E-09	6.47E-09	5.04E-09	4.13E-09	6.02E-09

Sampler	Jan	Feb	Mar	Apr	May	Jun	Jul	Aug	Sep	Oct	Nov	Dec
CFA	2.83E-08	3.35E-08	2.74E-08	1.48E-08	2.76E-08	1.56E-08	3.24E-08	3.16E-08	3.41E-08	3.53E-08	2.49E-08	2.86E-08
EBR	2.29E-08	1.72E-08	1.83E-08	1.70E-08	1.88E-08	1.91E-08	2.50E-08	2.51E-08	2.51E-08	2.50E-08	2.32E-08	2.57E-08
EFS	3.81E-08	3.59E-08	3.24E-08	4.15E-08	3.44E-08	3.28E-08	3.07E-08	3.54E-08	4.37E-08	5.19E-08	6.57E-08	6.09E-08
ICPP	4.22E-07	3.30E-07	4.42E-07	3.35E-07	5.77E-07	5.94E-07	8.24E-07	6.42E-07	7.77E-07	6.77E-07	4.81E-07	3.65E-07
NRF	9.81E-09	8.60E-09	5.15E-09	9.57E-09	6.41E-09	7.47E-09	8.13E-09	1.13E-08	9.32E-09	1.24E-08	1.25E-08	1.84E-08
PBF	7.66E-09	1.20E-08	7.14E-09	6.69E-09	7.24E-09	5.00E-09	7.92E-09	4.28E-09	8.18E-09	7.54E-09	7.16E-09	9.59E-09
RWMC	1.61E-08	1.31E-08	1.26E-08	1.06E-08	1.26E-08	1.08E-08	1.94E-08	1.48E-08	1.69E-08	1.75E-08	1.71E-08	1.66E-08
TAN	8.03E-09	4.59E-09	4.84E-09	5.23E-09	2.43E-09	2.73E-09	3.11E-09	5.97E-09	6.27E-09	6.45E-09	9.15E-09	1.01E-08
TRA	1.05E-08	1.33E-08	7.52E-09	8.60E-09	9.06E-09	1.20E-08	1.66E-08	1.25E-08	1.62E-08	1.58E-08	1.25E-08	1.61E-08
VANB	3.05E-08	2.46E-08	2.26E-08	2.20E-08	2.81E-08	2.41E-08	3.53E-08	3.15E-08	3.69E-08	3.58E-08	3.28E-08	3.31E-08

D-2.2 Source Term

Dickson (2012) reported the annual Sb-125 releases from 1980 to 1990 (Table D-2). Releases were a result of fuel reprocessing with most of the release emitted from the FAST stack (Table D-3). The release for 1987 was reported as 16 Ci and was reported to vary from month-to-month. Fuel reprocessing for 1987 ceased from the middle of October to the middle of December. Although releases were also reported to occur in short bursts of about 8-hours in duration, the MESODIF model assumed a uniform release over the year of 1987.

Table D-2. Sb-125 source term as provided in Dickson (2012).

Year	Sb-125 Release (Ci)	Year	Sb-125 Release (Ci)
1980	1.34	1986	0.93
1981	0.19	1987	16
1982	0.0079	1988	7.4
1983	<0.0031	1989	0.00039
1984	0.019	1990	0.00021
1985	0.0062	Total	25.9

To provide better temporal resolution of the Sb-125 source term, the original monthly release data as reported in the INL Radiological Waste Management Information System for 1987 (DOE-ID 1988) was obtained. Most of the Sb-125 release was from the FAST stack (15.85 Ci) and only a small amount (0.00616 Ci) was attributed to the main stack (CPP-708) (Table D-3). The reported releases from the FAST stack varied significantly by month, with February having the highest release (4.59 Ci) and November the smallest release (0.00188 Ci). The total release was apparently rounded by Dickson to 16 Ci. For modeling purposes, only releases from the FAST stack were considered because it accounted for over 99.6% of the release. Stack parameters for the FAST stack are provided in Table D-4.

D-3. PERFORMANCE MEASURES

Several simplified measures were used to evaluate model performance (Cox and Tikvart 1990; Weil et al. 1992). These measures were the fractional bias (*FB*) and normalized mean square error (*NMSE*). *FB* is given by

$$FB = \frac{2(\bar{C}_o - \bar{C}_p)}{\bar{C}_o + \bar{C}_p} \quad (1)$$

where C_p and C_o are the predicted and observed concentrations, respectively. Overbars indicate averages over the sample. NMSE is given by

$$NMSE = \frac{\overline{(C_o - C_p)^2}}{\overline{C_o} \overline{C_p}} \quad (2)$$

Table D-3. Monthly releases of Sb-125 in 1987 from the INTEC FAST and main stacks (CPP-708) (from DOE-ID 1988, page CPP-32, 33, 43, and 45).

Month	FAST (Ci)	CPP-708 (Ci)	Total (Ci)
January	7.590E-01	2.800E-07	7.590E-01
February	4.590E+00	2.700E-05	4.590E+00
March	1.450E+00	5.390E-06	1.450E+00
April	1.497E+00	8.180E-06	1.497E+00
May	9.560E-01	3.300E-05	9.560E-01
June	1.160E+00	5.170E-03	1.165E+00
July	9.380E-01	1.540E-04	9.382E-01
August	1.480E+00	1.470E-05	1.480E+00
September	2.400E+00	3.770E-04	2.400E+00
October	5.500E-01	3.520E-04	5.504E-01
November	1.880E-03	9.460E-06	1.889E-03
December	7.230E-02	4.490E-06	7.230E-02
Totals	1.585E+01	6.156E-03	1.586E+01

Table D-4. Location and release parameters for the FAST stack (from DOE-ID 1997).

Parameter	Value
Location (UTM east, UTM north) (m)	343725, 4826050
Stack height (m)	48.8
Exit diameter (m)	1.65
Exit velocity (m/s)	11.04
Gas temperature (assumed ambient) (K)	293

The FB is a measure of mean bias. A FB of 0.6 is equivalent to model under-prediction by about a factor of two. A negative value indicates model over-prediction. The NMSE is a measure of variance; a value of 1.0 indicates that a typical difference between predictions and observations is approximately equal to the mean. The NMSE and FB are appropriate when the typical difference between the predictions and observations are approximately a factor of two (Hanna et al. 1991) and the range of predictions and observations in the dataset is small (i.e., less than a factor of two). This was not the case in this study, where ratios of model predictions to observations ranged from 0.1 to 20, and within a data set, the predicted and observed concentrations ranged from the near zero to about $100 \mu\text{Ci m}^{-3} \times 10^{15}$. In these cases a log-transformed measure of model bias and variance is more appropriate because it provides a more balanced approach (Hanna et al. 1991) in terms of evaluating performance in the entire range of concentrations (the FB and NMSE will be strongly influenced by high model predictions or observations). The log-transformed measures described in Hanna et al. (1991) are the geometric mean bias (MG) and the geometric mean variance (VG) and are defined by

$$MG = \exp(\overline{\ln C_o} - \overline{\ln C_p}) = \exp\left(\overline{\ln \frac{C_o}{C_p}}\right) \quad (3)$$

$$VG = \exp\left[\overline{(\ln C_o - \ln C_p)^2}\right] \quad (4)$$

Geometric mean bias values of 0.5 and 2.0 indicate a factor of two over-prediction and under-prediction, respectively. A *VG* value of 1.6 indicates about a factor of two difference between predicted and observed data pairs.

Another simple log-transformed performance measure that is easily understood is the geometric mean and geometric standard deviation of the distribution of the predicted-to-observed ratios. A scatter plot of the predicted and observed concentrations and the linear regression coefficient between the predicted and observed pairs were also included as performance measures.

Confidence intervals were calculated for the FB, NMSE, MG, and VG performance measures using bootstrap resampling as implemented in the BOOT software (Hanna et al. 1991).

D-4. RESULTS

Annual average air concentrations of Sb-125 for year 1987 as predicted by CALPUFF are shown in Figure D-1. A comparison of predicted air concentration values from MESODIF and CALPUFF and observed (measured) values are presented for each sampler in Table D-5. The sampler identified as RENO is not in the current INL air monitoring network, and was located where the road from Howe to Dubois crosses the northern INL boundary (see Figure D-1). For the performance measure calculations, measured data less than zero were omitted from the dataset, thus the dataset consisted of 21 predicted-observed pairs. Performance measures for MESODIF and CALPUFF are presented in Table D-6.

In general, the CALPUFF performance measures were closer to their optimum value compared to those of MESODIF, with the exception of the NMSE. However, the confidence interval for the CALPUFF NMSE encompassed its optimum value. In fact, for all the CALPUFF performance measures, where confidence intervals were calculated, only the VG did not encompass the optimum value. For the MESODIF model, only the NMSE encompassed its optimum value. Both the FB and MG performance measures for MESODIF indicated a positive bias and the confidence intervals did not include 0 and 1.0, respectively. The CALPUFF FB value indicated positive bias and was mainly driven by the over-prediction of the highest concentration at the ICPP sampler. However, using log-transformed performance measures (MG and GM), CALPUFF showed a slight negative bias, but confidence intervals on the MG included the optimum value 1.0.

An *F* test was used to evaluate the quality of the regression. The critical *F*-value for *n*-1 degrees of freedom (*F*_{1,21}) was 4.3 for $\alpha = 0.05$ and 8.0 for $\alpha = 0.01$. The calculate *F*-values for MESODIF and CALPUFF were 26 and 120 respectively. Thus, since the calculated *F*-value exceeded the critical *F*-value for both models, the regression was judged to be significant (i.e., reject the null hypothesis of a random scatter of points with a slope of zero).

Table D-5. Predicted and observed (measured) annual-average Sb-125 air concentrations for 1987.

Sampler ID	MESODIF ($\mu\text{Ci mL}^{-1} \times 10^{15}$)	CALPUFF ($\mu\text{Ci mL}^{-1} \times 10^{15}$)	Measured ($\mu\text{Ci mL}^{-1} \times 10^{15}$)
BLCK	0.21	0.62	-0.4
CRAT	0.42	0.39	2.2
IF	0.63	0.55	1
REXB	0.21	0.60	-0.3

Sampler ID	MESODIF ($\mu\text{Ci mL}^{-1} \times 10^{15}$)	CALPUFF ($\mu\text{Ci mL}^{-1} \times 10^{15}$)	Measured ($\mu\text{Ci mL}^{-1} \times 10^{15}$)
ARCO	0.52	0.90	2.6
ATOM	13.56	0.90	2.2
FAA	4.17	1.14	0.2
HOWE	4.17	2.73	4.8
MONT	2.09	1.48	0.8
MUDL	7.30	2.12	2.4
RENO	2.09	1.70	1.9
ANL	10.43	2.07	2.4
ARA	16.69	2.57	3
CFA	83.44	14.65	17
EBR	31.29	10.29	29
EFS	83.44	18.8	16
ICPP	104.3	260.1	97
NRF	41.72	4.39	5.9
PBF	41.72	4.19	11.2
RWMC	20.86	7.06	16
TAN	8.34	2.49	1.6
TRA	41.72	6.28	17
VANB	52.15	14.16	32

Table D-6. Performance measures for the Sb-125 comparison with CALPUFF and MESODIF.

Performance Measure	Optimum Value	CALPUFF	MESODIF
Fractional Bias (<i>FB</i>)	0.0	-0.297	-0.728
Normalized Mean Square Error (<i>NMSE</i>)	0.0	6.05	1.76
% within a factor of 2	100	52.4	33.3
Geometric Mean Bias (<i>MG</i>)	1.0	1.36	0.460
Geometric Mean Variance (<i>VG</i>)	1.0	2.02	6.73
Geometric Mean P/O ratio (<i>GM</i>)	1.0	0.73	2.17
Geometric Standard Deviation (<i>GSD</i>)	1.0	2.22	3.22
Regression Coefficient (<i>r</i>)	1.0	0.929	0.758

Shaded/bold values indicate 95% confidence intervals calculated with the BOOT software that encompassed the optimum value of the performance measure.

A scatter plot of the predicted concentration as a function of the observed concentration for both MESODIF and CALPUFF is presented in Figure D-2. It is clear from Figure D-2 that CALPUFF performs best when predicting concentrations between 2 and 20 $\mu\text{Ci mL}^{-1} \times 10^{15}$. The MESODIF model predicts the highest concentration quite well, while CALPUFF over-predicts the value by more than a factor of 2. The highest concentration was observed at the ICPP sampler located approximately 200 m west of the FAST stack. The MESODIF model does not represent this exact location, but is instead at the node nearest the location, whereas the CALPUFF model used the exact location of the sampler as represented by a discrete receptor location. It is uncertain whether MESODIF would have also

over-predicted the concentration had the exact sampler location been used. Using the 3-year meteorological data set instead of the 1987 meteorological data does not appear to have significantly impacted the predicted annual average concentrations.

Based on the performance measures, CALPUFF was judged to perform better than MESODIF. Some of this improvement may be attributed to differences in the CALPUFF and MESODIF model formulations (i.e., CALPUFF uses three-dimensional wind fields and explicit treatment of terrain). However, overall the MESODIF model also performed quite well in this exercise in terms of estimating concentrations. The results from both models are within the established uncertainty of atmospheric transport models for predicting annual average concentrations in a complex-terrain environment (Miller and Hively 1987). Other factors may have also contributed to the better performance of CALPUFF. Namely, that the source term was discretized by month instead of a steady-state value for the entire year as was done in MESODIF.

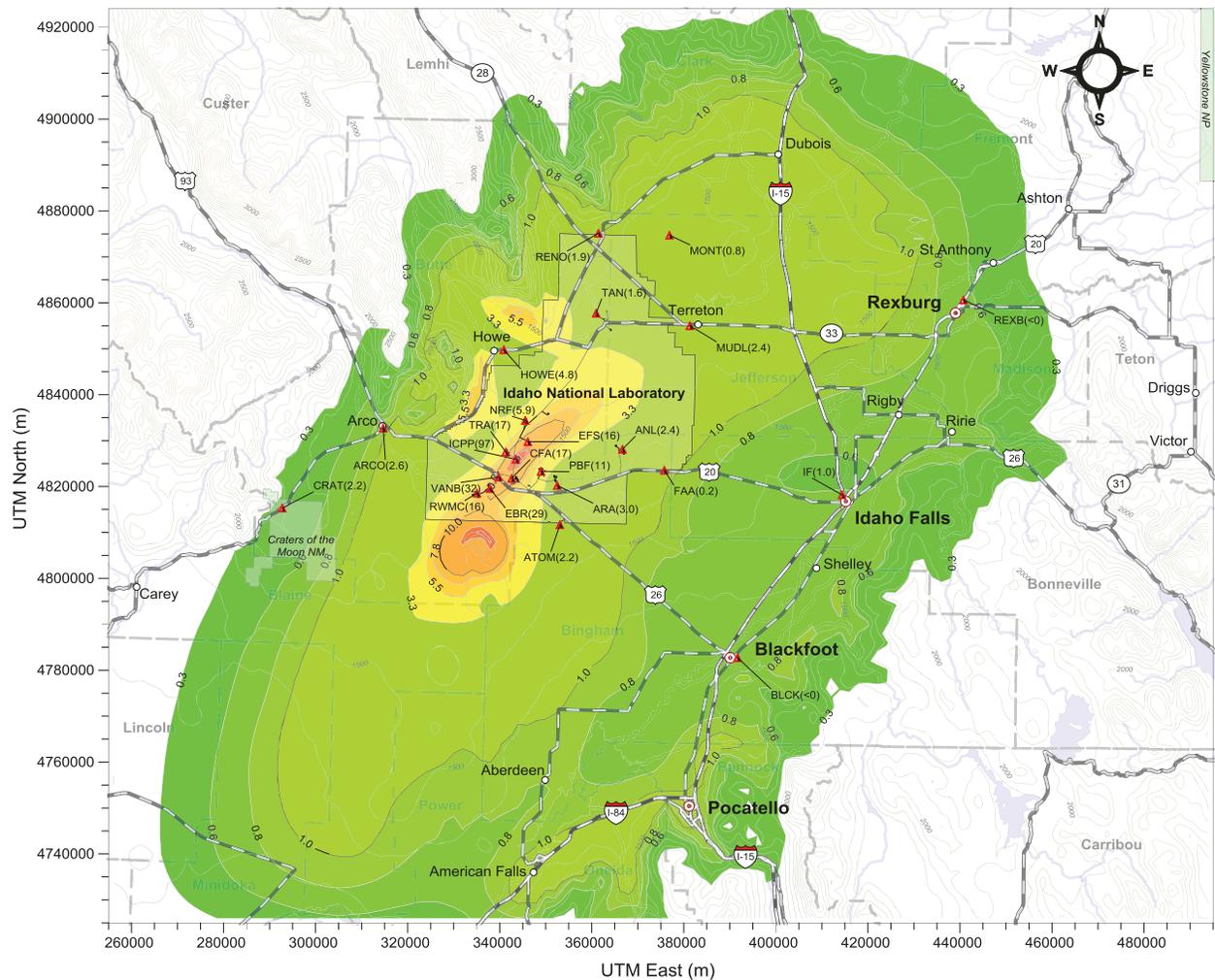


Figure D-1. Annual average air concentration isopleths of Sb-125 ($\mu\text{Ci mL}^{-1} \times 10^{15}$) calculated with the CALPUFF model using a 3-year meteorological data set. Measured values are shown next to the sampler IDs (names) in parentheses.

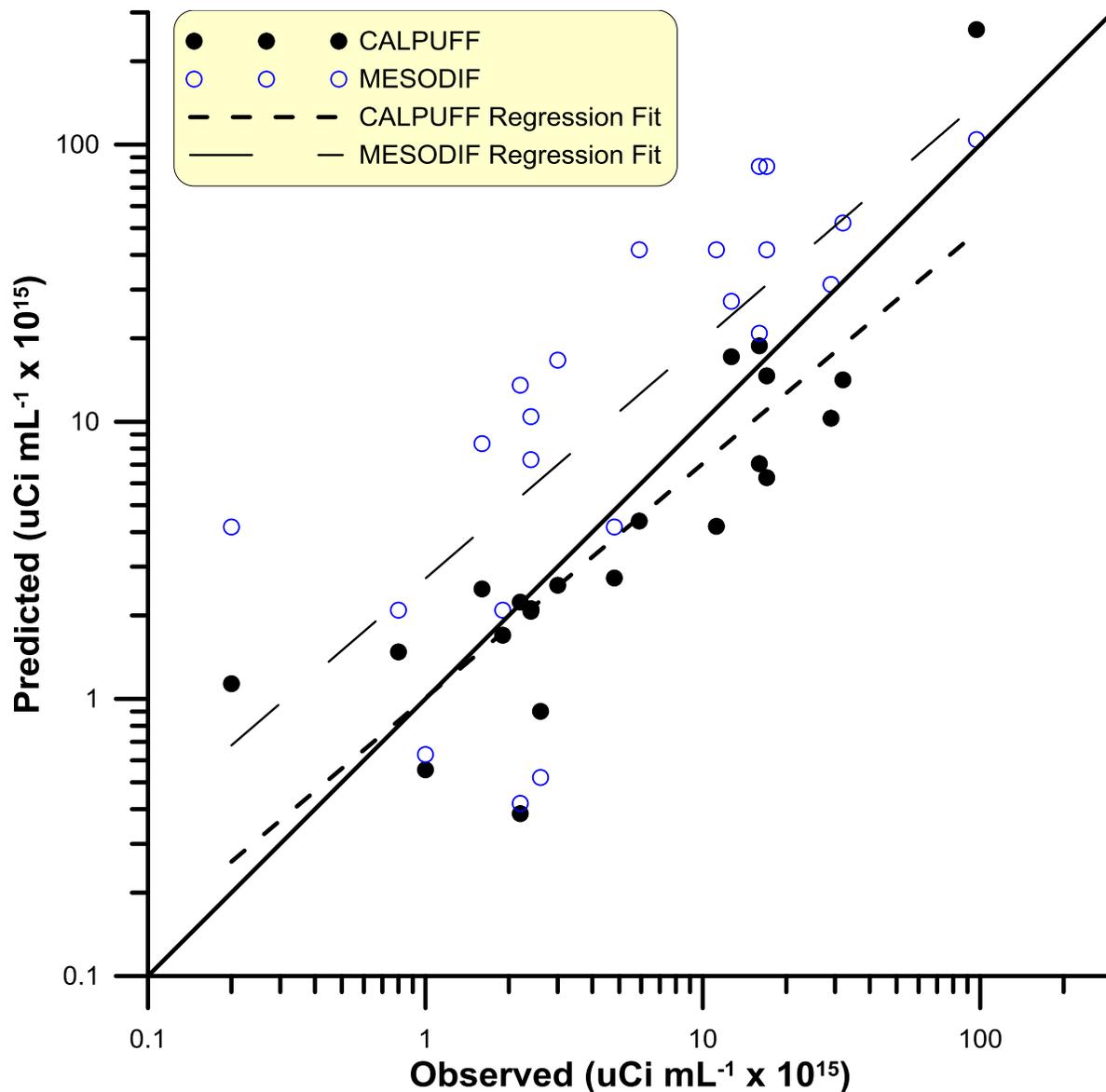


Figure D-2. Scatter plot of predicted and observed concentrations for MESODIF and CALPUFF. Points that lie above the perfect correlation line are over-predictions; points that lie under the line are under-predictions.

D-5. REFERENCES

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