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Noble Gas Surface Flux Simulations And Atmospheric Transport

Estimating Surface Flux From Underground Nuclear Explosions And Atmospheric Signatures

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Preface

This letter report is intended to summarize work supported as Contributions in Kind by the Defense Threat Reduction Agency (DTRA) and Department of State. The first part of this work presents a discussion of underground nuclear explosion (UNE) parameters, which are likely to be most influential in determining the magnitude of noble gas surface fluxes following the detonation. The surface fluxes considered here are the ones that might be typically captured by a radioxenon noble gas station located downwind from a UNE. The second part uses estimates of radioxenon surface fluxes to simulate the atmospheric signature that might be detected in the vicinity of a UNE. The detectability of near-field surface and atmospheric radioxenon signatures and their relationship to the details of a UNE are of significant interest to the CTBT monitoring and On Site Inspection communities.

Introduction

Signatures from underground nuclear explosions or UNEs are strongly influenced by the containment regime surrounding them. The degree of gas leakage from the detonation cavity to the surface obviously affects the magnitude of surface fluxes of radioxenon that might be detected during the course of a Comprehensive Test Ban Treaty On-Site Inspection. In turn, the magnitude of surface fluxes will influence the downwind detectability of the radioxenon atmospheric signature from the event. Less obvious is the influence that leakage rates have on the evolution of radioxenon isotopes in the cavity or the downwind radioisotopic measurements that might be made. The objective of this letter report is to summarize our attempt to better understand how containment conditions affect both the detection and interpretation of radioxenon signatures obtained from sampling at the ground surface near an event as well as at greater distances in the atmosphere.

In the discussion that follows, we make no attempt to consider other sources of radioactive noble gases such as natural backgrounds or atmospheric contamination and, for simplicity, only focus on detonation-produced radioxenon gases. Summarizing our simulations, they show that the decay of radioxenon isotopes (e.g., Xe-133, Xe-131m, Xe-133m and Xe-135) and their migration to the surface following a UNE means that the possibility of detecting these gases exists within a window of opportunity. In some cases, seeps or venting of detonation gases may allow significant quantities to reach the surface and be released into the atmosphere immediately following a UNE. In other release scenarios – the ones we consider here – hours to days may be required for gases to reach the surface at detectable levels. These release models are most likely more characteristic of "fully contained" events that lack prompt venting, but which still leak gas slowly across the surface for periods of months.

We briefly summarize the transport processes that determine surface fluxes and are represented in our simulations. The dependence of surface fluxes on different parameters is then discussed with examples provided by our simulations. Coupling with atmospheric simulations is next considered as well as some of the implications for detecting atmospheric signals at OSI-relevant distances from the UNE site. We end with a conclusion and suggestions for future work.

Summary of Subsurface Transport Processes Affecting Surface Fluxes

At least two different transport mechanisms or processes determine how radioactive noble gases migrate to the surface to be potentially detected during an OSI or by downwind atmospheric sampling. Our simulations indicate that each process is dominant during different periods of time following a UNE. A simulation illustrating the flux of Xenon-131m at the surface is shown in Figure 1.

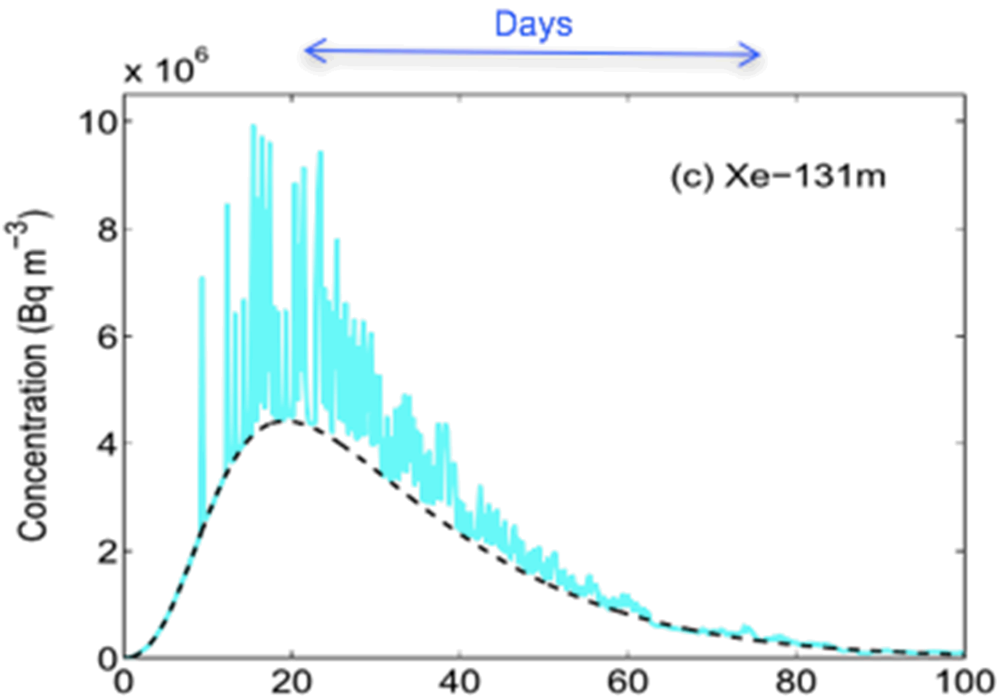

Figure 1. Predicted flux of Xenon-131m (blue) at the surface versus time following an underground nuclear explosion. The barometric component of the gas transport is the fluctuating blue line while the thermally driven component of transport is the underlying and much smoother dashed curve. Initially only the thermally driven part of migration is responsible for producing a signal at the surface. The barometric part of transport begins contributing significantly approximately 10 days after detonation according to this model.

Initially, during the first few days according to the gas-migration simulation, thermal convection and pressure-driven gas flow are responsible for moving gases upward toward the surface (Fig. 1: smooth dashed line). In cases where significant matrix permeability exists in the fracture walls, thermally driven gas migration, due to the residual heat of detonation, is responsible for "loading" the porous walls of fractures with detonation-produced noble gases as the gases flow along the network. During the early part of the flux history, the thermal and pressure drive dominate transport and are represented by the rapid and smooth rise of the flux curve as shown in Figure 1. After noble gases are loaded into the matrix, barometric pumping, which can draw gases from both the cavity and the matrix, begins to play a significant role as exemplified by the transition to rapidly fluctuating values of the flux some days after the detonation.

The results of our most complete simulations and also gas-tracer field experiments elucidating subsurface gas migration indicate that two different timings should be considered when estimating surface fluxes from a UNE. The first is the time after detonation when radioxenon arrivals are above minimum detectable levels. However, according to the logarithmic plot Fig. 1, early-time fluxes at the surface will tend to be quite weak, down orders of magnitude compared to the peak barometric-fluctuation-influenced fluxes occuring at later times. At these later times, weeks to months, when barometric influences are dominant, peak surface fluxes can be very much larger according to our simulations. Maxima during this period occur when the barometric pressure is falling. Figure 2 illustrates the affect of falling barometric pressure on surface concentrations during the period when barometric effects dominate. In the figure, atmospheric pressure is shown as a function of time with its fluctuations. The green shading superimposed over the pressure indicates gas concentrations that exceed minimum levels of detection. In the simulation, the green shading only occurs during periods of falling atmospheric pressure and gradually vanishes as the pressure rises.

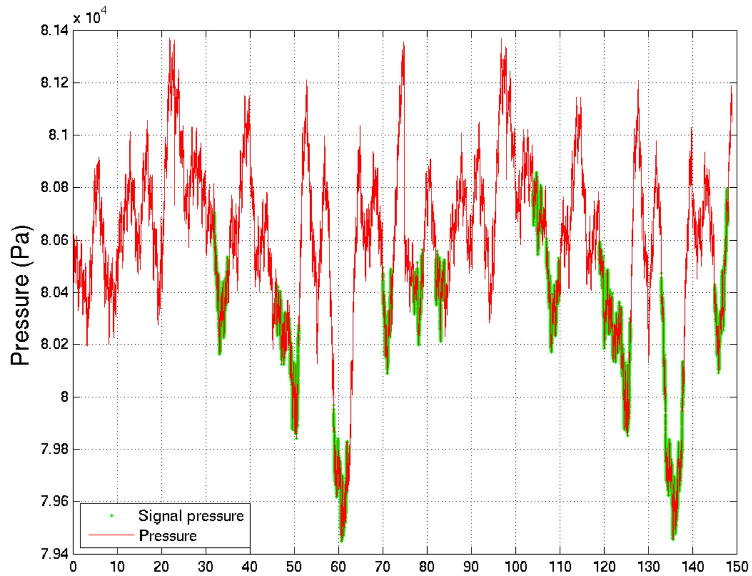

Figure 2. A subsurface gas-migration simulation showing a plot of atmospheric pressure (red line) versus time obtained from an LLNL Smart Sampler. Green points are plotted for surface pressures and times when gas concentrations are above minimum detectable levels. Note that sampling during periods of falling barometric pressure produces levels of gas at the sampling site exceeding minimum detectable levels in this simulation. However, even in the early stages of the pressure record, minimum concentrations did not reach detectable levels, as no green is present. At early times, gases are "loaded" into the matrix by the upward transport along fractures during barometric pressure fluctuation. Until the concentration in the pore space has risen to sufficient levels no signal will be detected.

Dependence of Surface Fluxes on Containment Parameters

In attempting to predict surface-flux time dependence and magnitudes, significant uncertainties exist. The geologic setting always introduces uncertainty into any gas-transport model owing to lack of information about the nature of material heterogeneities and the natural network of fractures at a site. Field experiments at different sites give us intuition and sometimes an estimate of the range of influence the geology and existing fracture network might have on gas transport from a given UNE. For attempts to either predict noble gas signatures at the detonation site or in the atmosphere , uncertainty also exists regarding the design (independent) parameters of a UNE, such as detonation depth and yield. There are also parameters (dependent) that will be determined by the UNE design, such as post-detonation temperatures in the cavity, which also influence surface flux. What follows will be a discussion of some of the independent and dependent parameters that are likely to play a significant role in the magnitude and time dependence of radioxenon surface fluxes.

Surface Flux Dependence On Yield, Detonation Depth And Permeability

Yield and detonation depth are design parameters of a planned nuclear explosion. To some extent the post-detonation permeability may be selected by using a certain geologic regime for containment. Here we consider the effects of these parameters on the surface flux which fundamentally determines whether a UNE can be detected on the ground during an On-Site Inspection or in the atmosphere. Figure 3 illustrates surface fluxes versus time from several different hypothetical detonations. Surface fluxes were simulated with the LLNL NUFT program (Nitao, 1998).

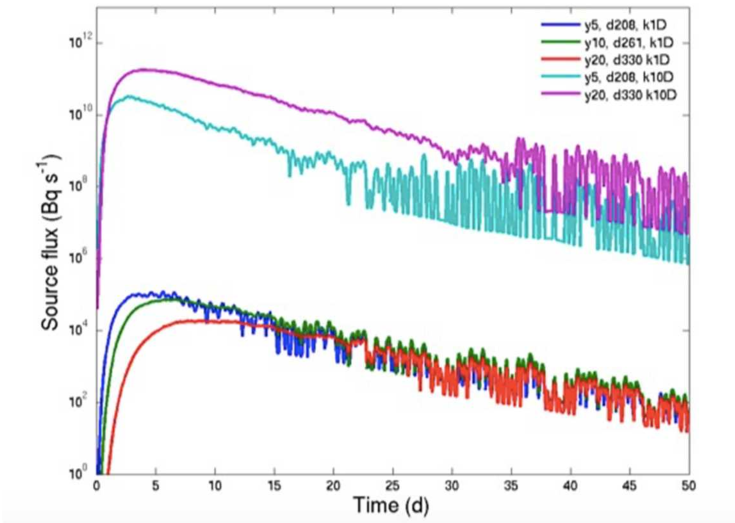

Figure 3. A plot of integrated surface flux vs time for several different yields, depths of detonation and permeabilities. Depths of detonation selected for gas transport simulations here are yield dependent where D(m) = 122 x $Y(kt)^{.33}$. Yields are 5, 10 and 20kt with bulk permeabilities of either 1 or 10 Darcy.

In the figure above, the depths simulated are not independent of yield, following the relationship D(m) = 122 x $Y(kt)^{.33}$. According to the simulations, a 5 kt event may produce surface fluxes similar to a 20 kt event having the same bulk permeability but emplaced about 50% deeper than than smaller event. Both containment regimes are assumed to have the same bulk permeability of 10 Darcy (1 Darcy = 10^{-12} m^2) which is probably a value towards the higher end of the permeability scale for a contained event considering the ~4 Darcy value obtained for the NNSS Barnwell site (Carrigan et al., 2016). It is interesting that for a permeability of 1 Darcy, the 1, 5 and 10 kt events also produce surface fluxes of comparable magnitude. Evidently, the depth-to-yield relationship effectively scales the sizes of fluxes that reach the surface. Even though one might expect fluxes and possibly concentrations in atmospheric signals to be indicative of the size of an event, this is not the case according to Figure 3 as the canonical NNSS depth relationship used here is evidently effective in offsetting most of the increase in surface flux that would otherwise result from increasing the nuclear yield of an event. Note that these LLNL simulations do include both thermally driven convection and also barometric pumping of cavity gases. The inclusion of the thermal transport effect is unique here, but is important for obtaining appropriate arrival times of gases at the surface and for the subsequent evolution of surface flux when barometric pumping becomes more important.

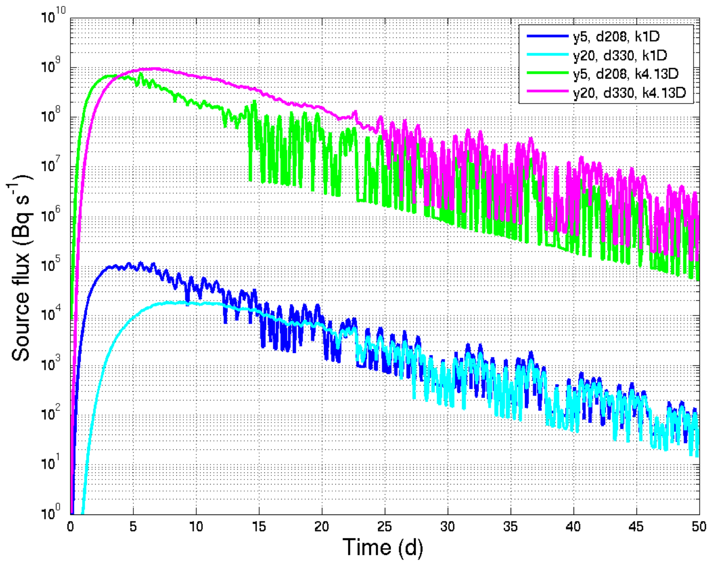

Figure 4. Plot is similar to Figure 3 but results for a more moderate 4.13 Darcy bulk permeability are plotted rather than the higher 10 Darcy permeability. Between, Figures 3 and 4, the flux from either the 5 or 20 kt events changes by orders of magnitude for factor-of-two changes in permeability.

Figure 4 illustrates the results for a more moderate value of the bulk permeability of the containment regime. This value (4.13 Darcies) corresponds to that estimated for the Barnwell event on Pahute Mesa at NNSS (Carrigan et al., 2016) and produces a value of surface flux separated by several orders of magnitude from the 1 and 10 Darcy cases. From the simulations, we find that varying the bulk permeability between 1 and 10 Darcies, a reasonable range, changes surface flux by orders of magnitude. It is clear that a significant effort to accurately estimate the permeability range of a post-detonation site is necessary if surface fluxes are to be used as an indicator of the size of an event. If magnitudes of gas release cannot be used as an indicator of characteristics like yield, it may be necessary to exploit other information, such as radioxenon isotopic ratios as used for the DPRK 2013 event (Carrigan et al., 2016).

Surface fluxes for a series of shallow events were also simulated for the same 50m depth. Most are somewhat more shallow that the depth-to-yield relationship given above. Most of these simulated events would be so shallow, according to the depth-to-yield criterion, that they might be expected to produce visible surface features, such as cratering, if they were actually carried out. Nevertheless, they may be useful for understanding how surface fluxes can vary with different design parameters. Besides yield, post detonation bulk permeability was treated as an independent variable. The results were used to produce Figures 5a and 5b which illustrate how the peak or maximum value of the total surface flux might be expected to vary with yield and permeability, respectively.

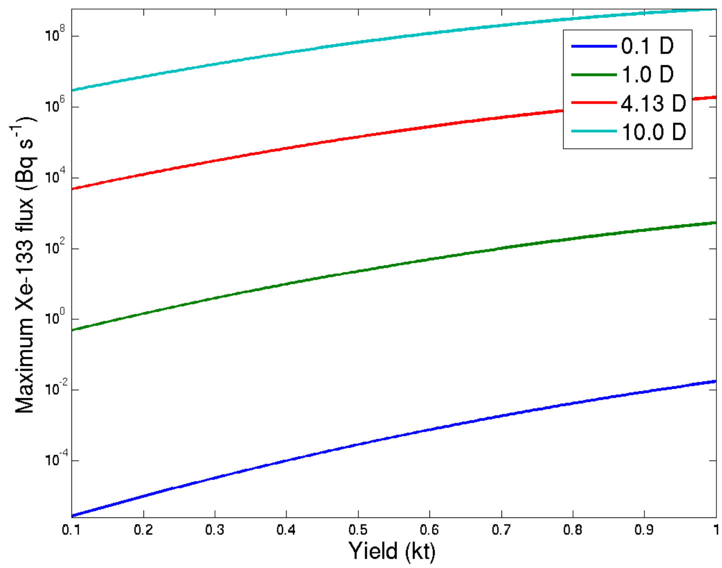

Figure 5a. The dependence of maximum or peak total (integrated) surface flux on yield is displayed for four different bulk permeabilities from 0.1 to 10 Darcies on a log-linear plot.

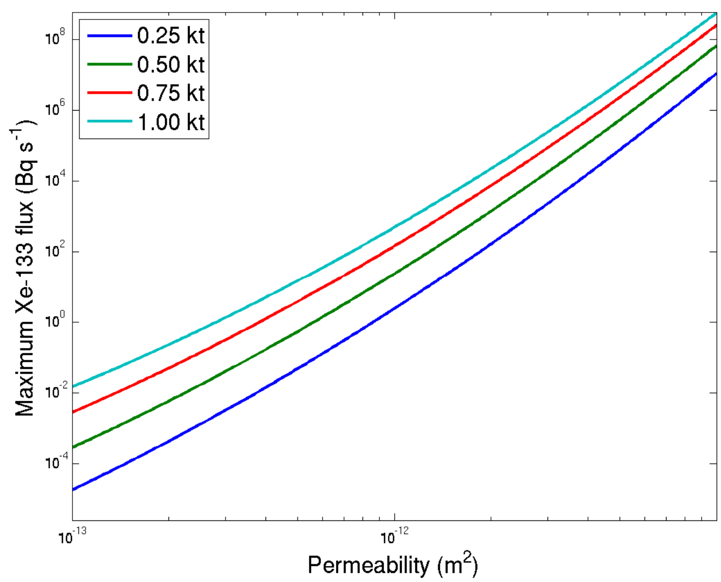

Figure 5b. The dependence of maximum or peak total (integrated) surface flux on permeability is plotted for four different yields from 0.25 to 1 kt. The peak flux to permeability relationship is displayed as log-log.

Figure 5a above suggests that an approximate factor of 2 variation in permeability may result in a ten-thousand fold difference in peak surface flux while a factor of 10 variation in permeability can produce a million-fold difference in peak surface flux for the models considered. Figure 3 shows that the million-fold surface-flux enhancement continues to exist for more deeply buried, higher yield events as illustrated by both the 5 and 20 kt cases for 1 and 10 Darcies.

Surface Flux Dependence On Post-Detonation Cavity Temperature

Some uncertainty exists regarding post-detonation cavity temperatures used in NUFT models. The models assume that cavity collapse has occurred, which will result in a cooling effect and initial temperatures are estimated to fall in the 200 to 400 C range. Figure 6 summarizes four different cases with initial temperatures varying from 100 to 400 C. The simulations indicate that an order-of-magnitude increase in surface flux might be expected for a 200 C increase in intial, post-detonation cavity temperature. Higher temperatures may be associated with detonations where collapse of the cavity has not occurred. The modeling, here, indicates that uncertainty about initial post-detonation temperatures can introduce a significant error into surface flux estimates.

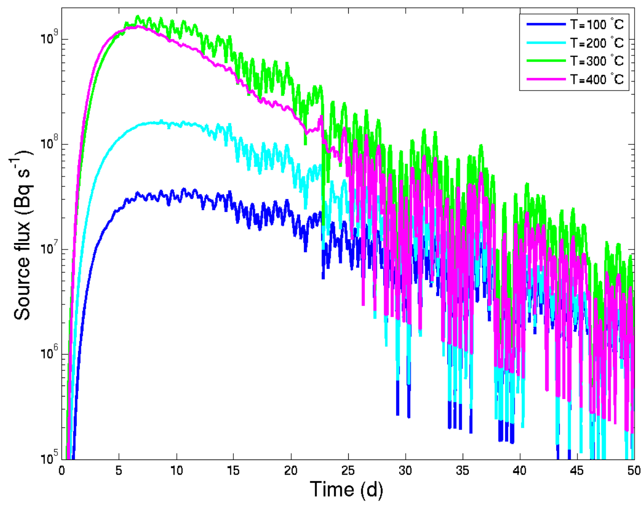

Figure 6. Effect of initial temperature on cavity/chimney regime. Four different initial temperatures were simulated. Generally, flux reaching the surface increases with increasing initial, post-detonation temperature. Why the 300 C (green) line lies higher than the 400 C (magenta) line is uncertain.

Discussion of Surface Flux Dependence Simulation Results

We have briefly investigated the effect of several UNE design parameters on influencing the magnitude of the surface flux following a UNE. A general conclusion is that lacking information, such as a depth-of-detonation estimate provided by a seismic location along with a topographic model of the test site (e.g., Zhang and Wen, 2013), it will be difficult to use surface flux estimates based on atmospheric signatures to determine nuclear yield independently from seismic estimates. At this stage of research, atmospheric ratios of radioxenon isotopes appear to be more promising for estimating nuclear yield as the dependence of ratios of radioxenon isotopes will tend to be far less sensitive to unknowns.

Atmospheric Transport Considerations

Prompt release of gases at the ground surface resulting from existing or explosively propagated vents has typically been assumed to be the only mode of transport of detonation gases from a UNE capable of giving rise to detectable levels of radioxenon gases in downwind atmospheric samples. Using the model described above for thermally and barometrically driven post-detonation transport across the broad surface of a simulated UNE site, we evaluate whether UNEs, without significant prompt vents or leaks, are potentially detectable tens of kilometers downwind with current technology. Such distances are significant for atmospheric measurements made during a Comprehensive Nuclear Test Ban Treaty (CTBT) On-Site Inspection. The potential detectability of even well contained (no prompt venting) UNEs at distances of several or more kilometers downwind would represent an excellent approach to reducing the search area during the early phases of an Comprehensive Test Ban Treaty On-Site Inspection (Carrigan, 2014) given that continuous atmospheric sampling is already strongly recommended for detecting potential contamination from legitimate radionuclide sources such as nuclear reactors and medical isotope facilities.

Based on the the first part of this report, the yield, bulk permeability of the UNE site and the depth of detonation appear to be the primary source-term parameters controlling the surface flux and therefore the distance of downwind detection from the detonation point. The following discussion is based on what might be regarded as a reasonable set of containment parameters.

Coupling Subsurface Transport With Atmospheric Transport

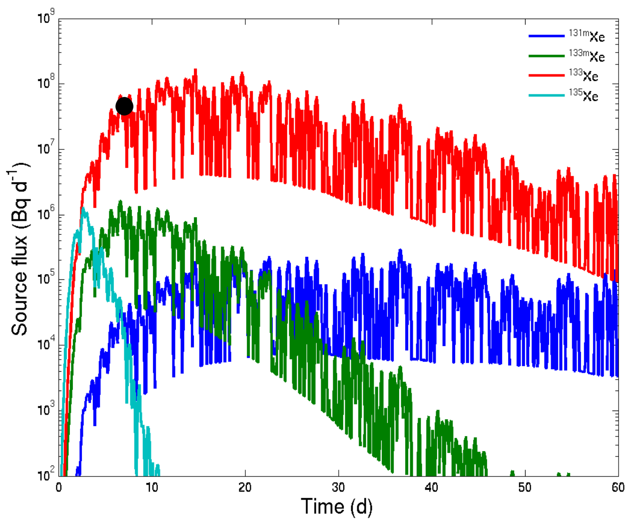

Figure 7. The model used for estimating the downwind atmospheric transport signal uses the surface flux of Xe-133 (red line) as a boundary condition for an atmospheric transport model. This simulation assumes a nuclear yield of 2.265 kt, depth of 323 m and a permeability of 3.9 Darcy which is comparable to the value obtained for the NNSS Barnwell detonation site on Pahute Mesa.

A subsurface transport model for a ~2.3 kt UNE with a detonation depth of 323 m in a containment regime having a post-detonation bulk permeability of 3.9 Darcy was selected for estimating the time-dependent containment flux at the surface. The integrated flux over the large surface for this event is of the order of 1000 Bq/s. While the integrated value may seem significant, the average value of the flux will be much less than 1 Bq/s per square meter, which would be difficult to detect using just a handheld radiation detector. Collection of gas under a tarp would yield a signal detectable by the current generation of noble gas analyzers. The black circle corresponds to the point in the time history where the integrated flux is used as a boundary condition on an atmospheric transport model (Nasstrom et al., 2007).

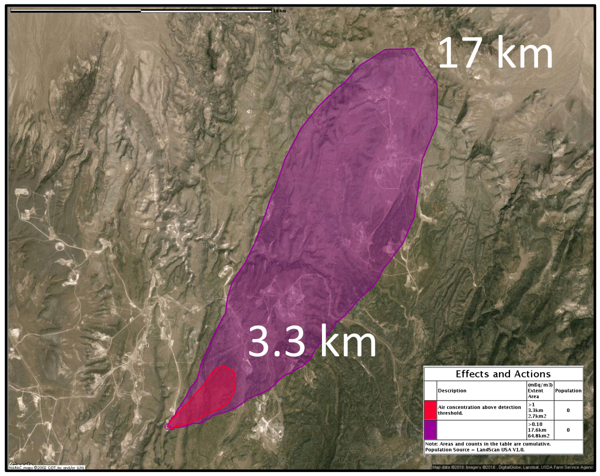

Figure 8. The plume of radionuclide gas (Xenon-133) results from the surface flux of Figure 7. at the point in the time history shown by the black circle. Two contour levels are shown here. The red contour corresponds to an activity of 1 Bq/m^3 which according to the atmospheric transport model extends to about 3.3 km. Reducing the activity to 0.1 mBq/m^3, which is still above the minimum level of detection for current technology, results in a purple contour having a length of 17 km. Note that 1 Bq/m^3 is above the worldwide average for Xe-133 in the atmosphere.

Using the flux indicated, an atmospheric transport model was used to simulate transport of Xe-133 away from the site using representative regional meteorological conditions (i.e. southwesterly winds of 3 m/s near the surface). Additionally, the transport model took into account the local topography. The simulations indicate for a minimum activity of 1 Bq/m^3 the plume would extend to a distance of about 3.3 km. Reducing the activity to 0.1 Bq/m^3 allows the plume to be detected at a distance of about 17 km from the detonation site using current technology for analyzing gas samples for radioxenon. This would seem a significant result for the On-Site Inspection component of the CTBT as it strongly suggests that gases from a contained event can be used as a means of reducing the 1000-square-kilometer inspection area to a more manageable size by monitoring for atmospheric signals and using prevailing wind direction to backtrack the detection to the source region for On-Site Inspection.

The effect of sampling at different times of day was also considered. The atmospheric boundary layer or mixing height changes as a function of temperature and time over the course of a day and the effect detection distances from the release point is illustrated in Figure 9.

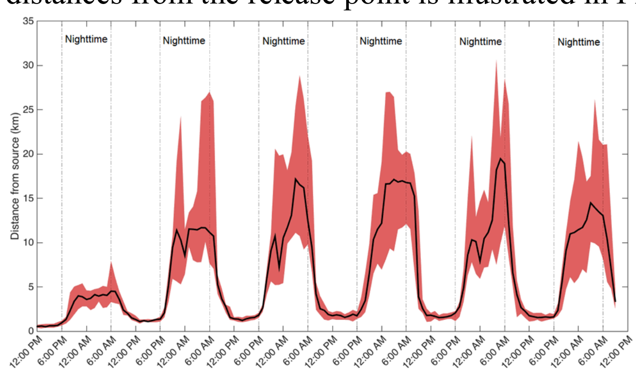

Figure 9. Downwind ^{133}Xe detection distance during the 6-day FLEXPART ensemble dispersion simulation. Black line is ensemble median detection limit while shaded region is range of ensemble values between 10th and 90th %.

A number of plume transport cases were simulated using the FLEXPART dispersion model (Stohl et al. 2005; Stohl et al. 2010) to quantify the impact of the initial state of the atmosphere uncertainty on predicted radioxenon air concentrations. Figure 9 is a plot showing the mean downwind detection distance versus time (black line) as well as the range of distances between the 10^{th} and 90^{th} percentile resulting from the ensemble of simulations (red area). What is apparent is that night-time measurements produce larger detection distance due to reduced horizontal and vertical mixing of the radioxenon atmospheric plume, other things being equal. Again, this is significant for On-Site Inspection as it suggests that the best plume detection measurements are more likely to be obtained at night.

Discussion Of Coupled Subsurface And Atmospheric Transport

A major result of this report is that even well contained underground nuclear explosions, that is, ones that do not vent promptly, can still be potentially detected by air sampling in an inspection area at distances of many kilometers from the detonation site according to our coupled subsurface transport and atmospheric simulations. This is an extremely important result for CTBT On-Site Inspection. It provides the basis for arguing that atmospheric sampling, radioxenon analysis and the atmospheric transport simulations, required for evaluation of sampling results, should be performed as part of the inspection area reduction process, which reduces the 1000-square-km inspection area to much smaller regions of interest. Additionally, the simulation of the detection distance versus time over a period of several days indicates that night time sampling of atmospheric gases may be better for detecting either very weak signals or sites at greater distances from the samplers.

Conclusion

Estimating the magnitude of the time-dependent surface flux following a UNE is necessary to predict the detectability of an event either at the surface during an OSI or downwind at a sampler in the inspection area at some distance from the UNE site. The first part of our Task 2 CiK work focused on evaluating the impact of some UNE design parameters, such as detonation depth and nuclear yield along with other model parameters such as permeability and detonation cavity/chimney temperature. We found that significant uncertainties in the any of these parameters could result in poor estimates of the surface flux, making it of questionable value for predicting parameters like nuclear yield. More likely, isotopic ratios, which are more insensitive to uncertainties in these parameters, may be more valuable for estimating UNE characteristics, such as yield (Carrigan et al., 2016). The second part dealt with evaluating the possibility of obtaining a significant atmospheric signal from a well contained event. Using our subsurface transport model surface-flux output as a boundary condition to an atmospheric transport model, we found that a well contained UNE might be detectable at a distance of almost 20 km, which is a significant distance in an OSI inspection area. Further, our simulations suggest that sampling during night time enhances detection distances, that is, the distance between the UNE site and sampling station. These simulations strongly suggest that atmospheric sampling, analysis and evaluation during an OSI can be a viable inspection-area-reduction tool.

Further work would include looking in more detail at isotopic ratios and how they can be better used to evaluate UNE design parameters. Additional field experiments, on determining post-detonation bulk permeabilities and the likely ranges of bulk permeabilities, will help in developing bounding models for estimating the magnitude of surface fluxes and distance of detection. Exploring application of a data fusion approach, relating noble gas simulations and seismic estimates of yield, is a possible means for refining noble gas transport models at sites where the geology or containment design is not known.

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