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Modeling Noble Gas Transport and Detection for The Comprehensive Nuclear-Test-Ban Treaty

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1 Modeling Noble Gas Transport and Detection for The 2 Comprehensive Nuclear-Test-Ban Treaty

3 YUNWEI SUN¹ and CHARLES R. CARRIGAN¹

4 *Abstract* – Detonation gases released by an underground nuclear test include trace amounts
5 of ¹³³Xe and ³⁷Ar. In the context of the Comprehensive Nuclear Test Ban Treaty (CTBT) On
6 Site Inspection protocol, such gases released from or sampled at the soil surface could be used to
7 indicate the occurrence of an explosion in violation of the Treaty. To better estimate the levels
8 of detectability from an underground nuclear test(UNE), we developed mathematical models to
9 evaluate the processes of ¹³³Xe and ³⁷Ar transport in fractured rock. Two models are developed
10 respectively for above-boiling and below-boiling tests. When the temperature is below the boiling
11 point and the subsurface system is sufficiently dry, the system is described using a single-gas-phase
12 transport model and the barometric pumping becomes the major driving force to deliver ¹³³Xe and
13 ³⁷Ar to ground surface. A above-boiling test is simulated using a two-phase and multi-component
14 transport model. In the model, steam production and bubble expansion are the major processes
15 driving noble gas components to ground surface. After the temperature in the chimney drops below
16 boiling, barometric pumping takes over the role as the major transport process.

17 **Keywords:** Noble gas, transport, CTBT, detection, modeling

18 1. Introduction

19 Noble gas isotopes, such as ¹³³Xe and ³⁷Ar, have been studied for detection of nuclear
20 explosions for the Comprehensive nuclear-Test-Ban Treaty (CTBT, Bowyer et al., 2002).
21 Because of their short half-lives, the ambient background concentrations for those gas com-
22 ponents are extremely low (Dresel and Waichler, 2004). The International Monitoring Sys-
23 tem (IMS) has developed the measurement sensitivity for ¹³³Xe better than 1 mBq m⁻³.
24 However, in addition to nuclear explosions, radioxenon isotopes may be produced and re-
25 leased from civil events. To better understand under what geohydrologic conditions the Xe
26 and Ar signals will reach the surface in detectable amounts and to better estimate the value
27 of subsurface noble gas sampling during an On Site Inspection, the transport mechanisms
28 from a underground nuclear test to ground surface have to be studied.

29 Gas-phase transport has been studied for various purposes (Webb, 1996; Wu et al., 1998;
30 Tidwell 2006; Pruess 2006). The barometric-pumping phenomenon has been identified as a
31 driving force for gas-phase transport in the subsurface system (Nilson et al., 1991; Lindstrom
32 et al., 1994; Wyatt et al., 1995; Carrigan et al., 1996; Auer et al., 1996; Martinez and
33 Nilson 1999; Neeper 2001; 2002; Rossabi, 2006). The gas-phase advection in response to the
34 pressure oscillation at ground surface behaves as cyclical “breathing” or push-pull gas flow
35 through the permeable alluvia or fractures. Diffusive exchange between fractures and rock
36 matrix dampens and delays the signature of gas concentrations at ground surface (Carrigan
37 et al., 1996).

38 In addition to these breathing processes that have been studied, we developed a single-gas
39 transport model and two-phase multi-component transport model to study a below-boiling
40 test and a above-boiling test, respectively. In the single-gas model, we quantitatively studied
41 the detectability and how the overburden alluvia affect the concentration signal at ground

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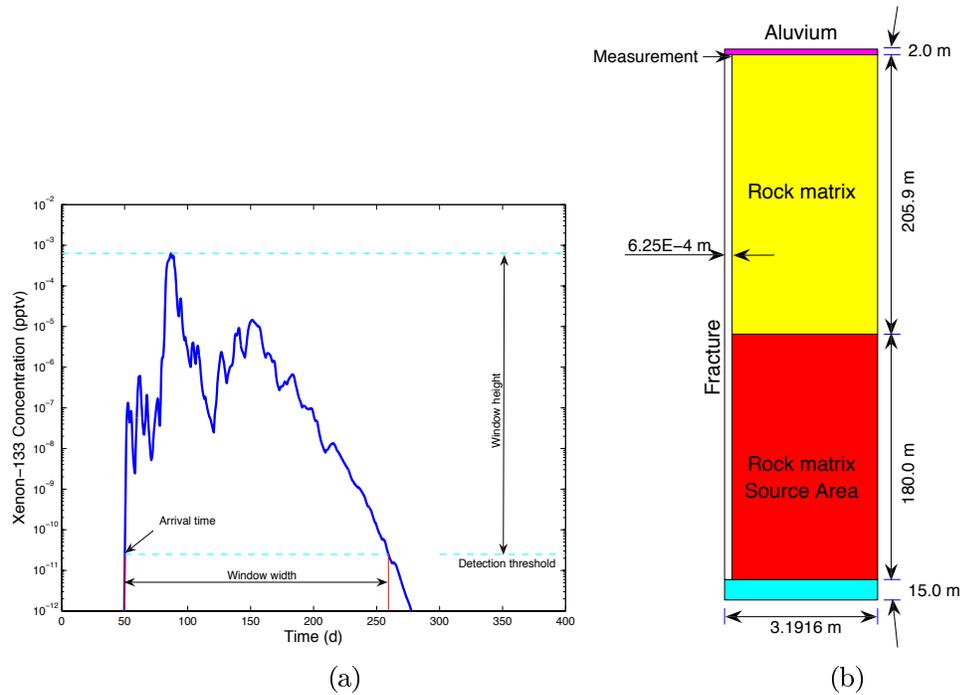
42 surface. In the above-boiling model, we demonstrated how the phase change and heat-pipe
43 phenomena affect the gas-phase transport and how to capture the concentration signal at
44 or near ground surface.

45 **2. Physical Systems**

46 The physical processes that control noble gas migration from the working point of a nu-
47 clear detonation to ground surface are complex and interdependent. In an underground
48 nuclear explosion, vaporization and compression of geologic media will create and expand
49 an open, approximately spherical cavity surrounding the working point. The cavity reaches
50 its full size within a fraction of a second after detonation. The cavity radius is a function
51 of the energy of the detonation, its depth of burial, and the strength of overlying geologic
52 units (Carle et al., 2008). A steam bubble, together with radionuclides including noble gas
53 isotopes, is formed and initially well contained within the cavity because of the highly com-
54 pressed and impermeable cavity wall. Afterwards, steam-driven fractures (hydro-fractures)
55 may be propagated from the cavity into the surrounding area and significantly reduce the
56 cavity pressure. When the pressure within the cavity drops below the pressure resulting
57 from the overburden rock, the cavity may collapse into the cavity creating a rubblez chimney,
58 where radioactive gases are re-distributed over the void volume of the chimney. Under
59 the conditions of thermally driven convection from the working point and barometric pres-
60 sure oscillation at the ground surface, noble gas nuclides migrate upward toward the ground
61 surface and make detection possible.

62 **2.1. Definition of Detectability**

63 The success of noble gas detection from an underground nuclear test depends on the gas
64 transport in the geological system. The geological structure, as well as many physical and
65 chemical properties, controls the concentration profile of gas nuclides at and near ground
66 surface. Taking the geological model of Carrigan et al. (1996) as an example, if the detection
67 sensitivity (threshold) for xenon-133 is 1 mBq m^{-3} (Auer et al., 2004; 2010; Saey et al.,
68 2009), as shown in Figure 1, the detectability can be characterized by (1) arrival time;
69 (2) detection window width; and (3) detection window height (above the threshold). The
70 arrival time, which is mainly determined by diffusivity of gas nuclides in the rock matrix
71 and permeability in fractures, is defined as the time when the concentration of the noble
72 gas component of the soil gas reaches its detection threshold. The detection window width
73 is the time duration between the arrival time and the time when the concentration drops
74 below the threshold. The window height is measured as the order of magnitude of the peak
75 concentration exceeding the threshold. For a given radionuclide with a specific half-life (e.g.,
76 5.24 days of ^{133}Xe), monitoring is expected to be conducted within its detection window.



77 (a)
 78 (b)
Figure 1. Study domain of single-gas-phase transport for the Non-Proliferation Experiment. (a)
 79 An example of xenon-133 concentration history at the outlet of the fracture. (b) Geometry of study
 80 domain. Note that the horizontal dimension is exaggerated.

79 2.2. Non-Proliferation Experiment

80 The Non-Proliferation Experiment (NPE) detonated on September 22 in 1993, was a low-
 81 yield chemical explosion (Carrigan et al., 1996). The NPE was conducted the south-central
 82 N-Tunnel below the surface of Rainier Mesa. Gas components, ^3He and sulfur hexafluoride
 83 (SF_6) were released at the source (433.4 m depth) and monitored over approximately 500
 84 days. The experimental data suggested that ^{133}Xe and ^{37}Ar would have been detectable
 85 after the detonation (Carrigan et al., 1996). A discrete fracture model was developed to
 86 describe the transport of ^3H and SF_6 . In this study, we replace stable gas components, ^3H
 87 and SF_6 with decaying isotopes, ^{133}Xe and ^{37}Ar , in the numerical model and investigate the
 88 detectability.

89 2.3. Rainier Test

90 The Rainier test, which was conducted on September 19, 1957, is considered as the first
 91 fully contained underground test (Tompson et al., 2010). In the years following the test,
 92 extensive reentry mining and drilling operations were undertaken to characterize the cavity
 93 and altered environment.

94 The Non-Proliferation Experiment, which was detonated near the Rainier test, was con-
 95 ducted to study the transport of gas-phase components in the fractured rock. Although both
 96 the Rainier and the NPE tests were conducted in the same bedded tuff system, they are
 97 considered as above-boiling and below-boiling tests. In the above-boiling test the residual
 98 heat produced by a nuclear detonation alters the themohydrological condition, which in turn
 99 becomes the dominant driving force for gas-phase transport. Without considering the test-
 100 induced heat, the barometric pumping on the ground surface is the only driving force for the

101 NPE chemical test. A full-scale Rainier-test model is developed to understand (1) the phys-
102 ical processes that affect the gas-phase radionuclide redistribution under transient pressure
103 and temperature conditions; (2) the effects of variably saturated conditions on gas-phase
104 radionuclide transport under thermal conditions; (3) the role of fracture-matrix interactions
105 and matrix diffusion; and (4) the role of barometric pumping on noble gas detection.

106 3. Conceptual Models

107 Two conceptual models are presented in this section. The Non-Proliferation Experiment
108 for ^{133}Xe transport is described as an isothermal and single-gas-phase transport in rock
109 matrix with a discrete fracture. The Rainier Test is described using a two-phase and four-
110 component (water, air, ^{133}Xe , and ^{37}Ar) transport under thermal conditions in a dual-
111 permeability domain.

112 3.1. Conceptual Model of NPE

113 As shown in Figure 1(b), a single vertical fracture penetrates the rock matrix. The frac-
114 ture aperture size is based on the mean value of estimated aperture size and matrix block
115 size (i.e., distance between fractures) is estimated using the fracture frequency. An allu-
116 vial layer of 2 m is overlain on the top of fractured rock. It is assumed that both heat and
117 radionuclides are distributed over the rock-matrix source area and the thermal effect on gas-
118 phase transport remains minimal. The liquid saturation is assumed to be constant between
119 the working point and ground surface and does not affect gas-phase permeability. There-
120 fore, the physical system is conceptualized as a single gas-phase transport under isothermal
121 condition. Detailed description about rock properties, initial and boundary conditions, and
122 model grids is referred to Carrigan et al. (1996). Three uncertain parameters, aperture size
123 of fracture, permeability in alluvium, and gas diffusivity in rock matrix are considered to
124 characterize the detectability indices, arrival time and detection window size.

125 3.2. Conceptual Model of Rainier Test

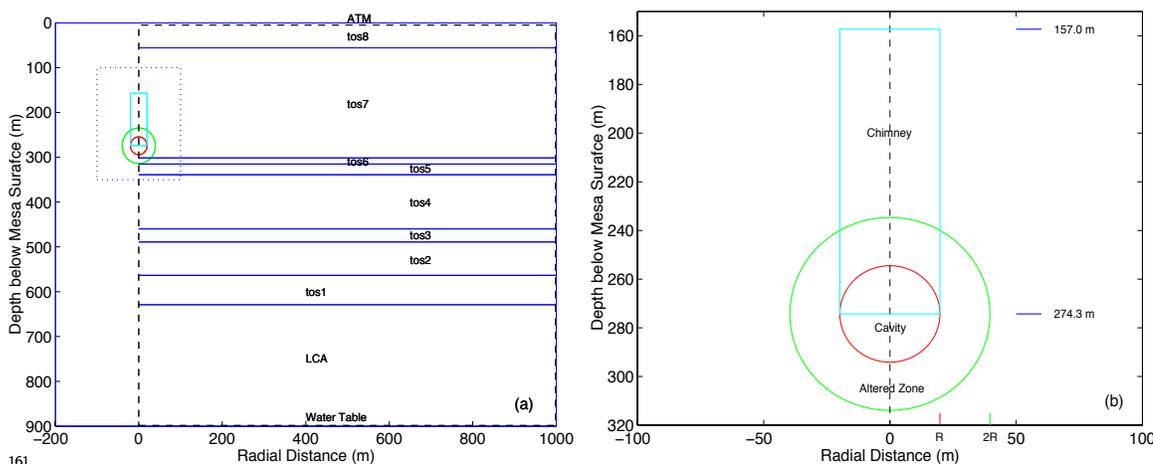
126 The Rainier-test is simulated using a sequence of separate yet continuous models that
127 represent multiple-phase flow under thermal conditions in the fractured rock environment
128 surrounding the test cavity and chimney. The models are developed in a two-dimensional,
129 radial symmetric geometry and are based on a modeling domain extending from the ground
130 surface to the water table and extending a significant distance away radially (1000 m) from
131 the vertical axis passing through the working point. Then, the assumption of the ambient
132 thermal and hydrologic condition is justified at the outer boundary.

133 The use of distinct model stages for the Rainier test allows important aspects of the
134 thermohydrologic dynamics and evolution to be addressed over periods (1) before deto-
135 nation, (2) after detonation and before chimney collapse, and (3) after chimney collapse.
136 Transition between the stages involves the changing material domains and the mapping of
137 initial conditions. The pre-test model is used to produce the ambient thermal and hydrologic
138 conditions, under which internally consistent and steady-state saturation, pressure, and tem-
139 perature conditions are simulated for one million years within an unaltered system before
140 detonation to reach equilibrium. The pre-test model is considered as the conversion from a
141 boundary-value problem to a steady-state condition. The test model is designed to present
142 the processes after the detonation and before the chimney collapse. A spherical cavity, which
143 holds explosively produced thermal energy, pressure, and radionuclides, is imbedded in the
144 model grids. The post-collapse model is designed to examine the longer-term gas-phase
145 transport. The collapse causes reassignment of rock materials in the chimney domain and
146 physical property alteration in the surrounding zone.

147 Differently from the NPE model, all models of Rainier test are based upon a non-
 148 isothermal, two-phase flow formulation involving water and air as principal components,
 149 and specifically considering xenon-133 and argon-37 as minor components in determining
 150 their migration and redistribution for quantifying the detectability. The fractured rock sys-
 151 tem is conceptualized as a dual continuum medium (fracture and matrix, DKM, Ho, 1997;
 152 Sun et al., 2010) and simulations were conducted using the NUFT code (Nitao, 1998).

153 3.3. Study Domain and Grids of Rainier Test Model

154 The study domain is composed of 17 geologic units, covers the entire unsaturated zone
 155 from ground surface to the water table, and includes the detailed geometry of the cavi-
 156 tity, chimney, and altered zone, which were produced by the Rainier detonation. Grid-
 157 block sizes range from a few tens of centimeters around the chimney to tens of meters
 158 in the far field. As shown in Figure 2, the physical system is discretized in a radially-
 159 symmetric (cylindrical) coordinate system. The conceptual model is based on a dual-
 160 permeability presentation of overlapping fracture and matrix continua (Sun et al., 2010).



161 **Figure 2.** Study domain of the Rainier test model. (a) Vertical cross-section of the Rainier test
 162 model. “tos1”, “tos2”, ..., and “LCA” are geologic units where tos7 is subdivided into 9 subunits.
 The dashed line defines the study domain. (b) Local geometry of the cavity, chimney, and altered
 zone. The detonation location is at (0, 274.3), the cavity radius is 19.81 m, and the chimney height
 is 117.3 m between the depth of 157.0 m and the working point.

163 3.4. Physical Properties

164 Physical properties include component, phase, and rock properties. Rock properties
 165 include permeability, porosity, thermal conductivity, specific heat, and the van Genuchten
 166 parameters α , m , and residual saturation, to specify saturation-dependent gas and liquid
 167 permeability and capillary pressure (Sun et al., 2010).

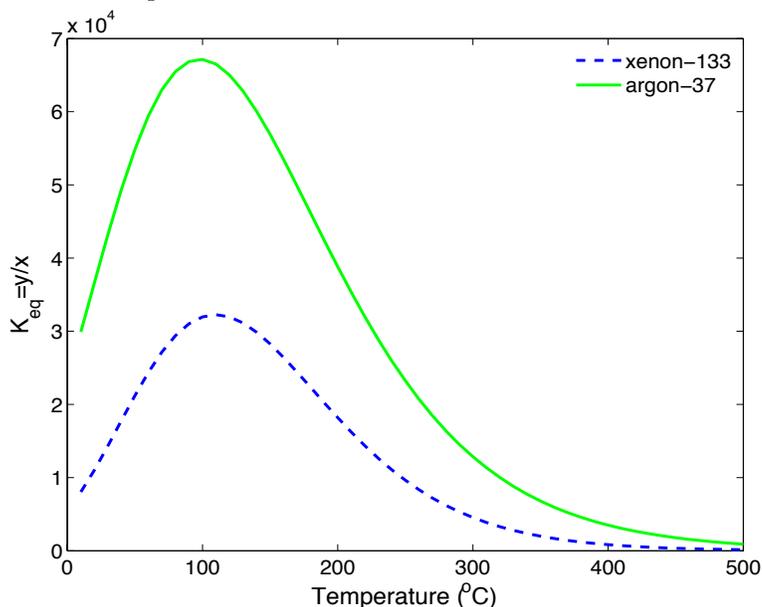
168 **3.4.1. Phase and Component Properties.** The phase-equilibrium partitioning coef-
 169 ficient, K_{eq} , for a dissolved component in adjoining gas and liquid phases is defined as the
 170 ratio of its mole fractions in the gas phase, y , to its mole fraction in the liquid phase, x .
 171 A Clever gas solubility model (Clever, 1979; 1980) is applied to the gas phase-equilibrium
 172 relations for xenon-133 and argon-37 such that

$$173 \quad K_{eq} = \frac{y}{x} = \frac{p_g^r}{S p_g} \quad (1)$$

174 where S is the mole fraction (solubility) of component xenon-133 or argon-37 dissolved in
 175 the liquid phase measured at the reference gas pressure, p_g^r , and p_g is the gas-phase pressure.
 176 The solubility is determined using experimental data as a function of temperature (Ekwurzel,
 177 2004)

$$178 \quad \ln S = A + \frac{B}{T_n} + C \ln T_n + FT_n \quad (2)$$

179 where A , B , C , and F are model parameters specific to xenon and argon, and T_n is the
 180 temperature in Kelvin divided by 100. The dependence of K_{eq} on temperature for xenon
 181 and argon is shown in Figure 3.



182 **Figure 3.** Phase-equilibrium coefficient of xenon-133 and argon-37 as a function temperature.

183 The free molecular diffusion coefficients in gas and liquid phases, D_g and D_l , can be
 184 modeled as a function of temperature, T_k (degrees Kelvin), and gas-phase pressure, p_g (Pa)

$$185 \quad D_g = D_g^0 \frac{p_g^r}{p_g} \left(\frac{T_k}{273.15} \right)^{n_g}, \quad D_l = D_l^0 \left(\frac{T_k}{273.15} \right)^{n_l}. \quad (3)$$

186 The diffusion model parameters, D_g^0 , D_l^0 , n_g , and n_l should be fitted to experimental data.
 187 Because of the lack of experimental data for xenon and argon diffusion in gas phase, we
 188 estimate the D_g^0 accordingly to molecular mass of gas-phase components and assume n_g
 189 to be zero. This assumption may result in an underestimation of the gas-phase transport
 190 in the high temperature zone. The diffusivity model in liquid phase was fitted using the
 191 experimental data of Holocher et al. (2002). Equilibrium partitioning and free molecular
 192 diffusivity model parameters for noble gases are given in Table 2.

Table 1. Equilibrium partitioning and free molecular diffusivity model parameters for xenon and argon.

Component	A	B	C	F	D_g^0 ($10^{-5}\text{m}^2\text{s}^{-1}$)	n_g	D_l^0 ($10^{-9}\text{m}^2\text{s}^{-1}$)	n_l
Ar	-57.67	74.76	20.14	0.0	2.00	0.0	1.44	7.22
Xe	-74.74	105.21	27.47	0.0	1.24	0.0	0.66	9.25

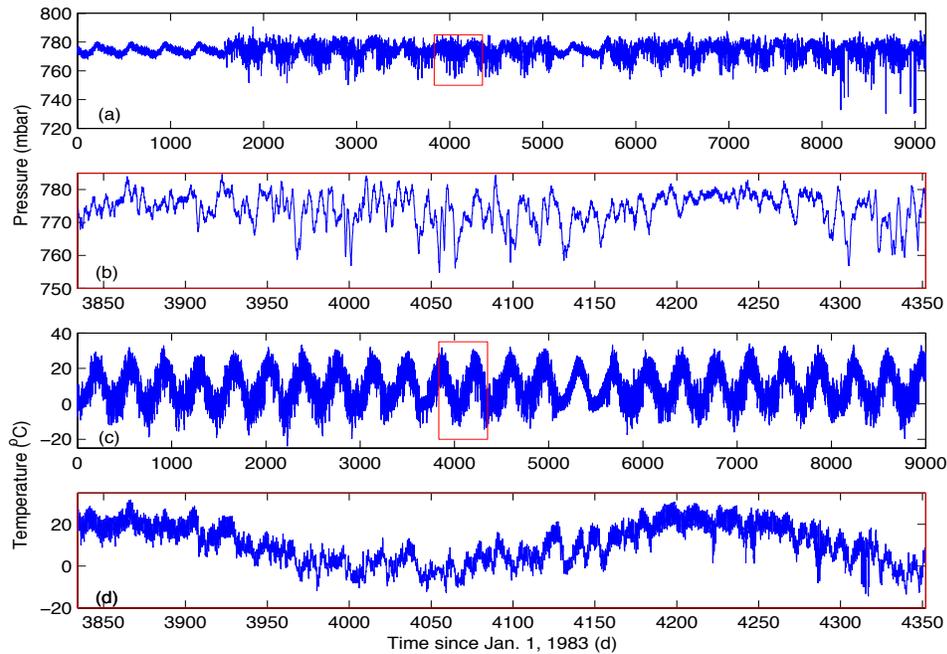
193 **3.4.2. Rock Properties.** DKM rock properties are further categorized as medium-
 194 dependent hydrologic and thermal properties and partitioned physical properties (Buscheck
 195 et al., 2002). The hydrologic properties include relative permeability, porosity, van
 196 Genuchten α and m , residual saturation, and transition saturation (Sun et al., 2010). The
 197 maximum saturation of all materials is assumed to be 1.0. For the fracture medium, three
 198 additional parameters, fracture connectivity, fracture frequency, and specific interaction area
 199 between fracture and matrix media, are included. Single-continuum materials, such as allu-
 200 vium, use the same properties in fracture and matrix.

201 Appropriate values for the tortuosity factor are selected for the matrix and fracture
 202 continuum on the basis of the parameter range given by de Marsily (1986), which ranges
 203 from a value of 0.1 for clays to 0.7 for sands. A value of 0.2 is estimated for the matrix
 204 continuum because the pore sizes for the matrix are closer to that of clays than to that
 205 of sands. A value of 0.7 is assumed for the fracture continuum because the effective pore
 206 sizes for fractures are similar to those of sands. Tortuosity factors are also estimated with
 207 a Millington model using residual saturation from the van Genuchten parameters (Nitao,
 208 1998). The effective diffusion coefficient for gas-phase components is a linear function of the
 209 tortuosity factor,

$$210 \quad D_e = \tau\phi(1 - S_l)D_g \quad (4)$$

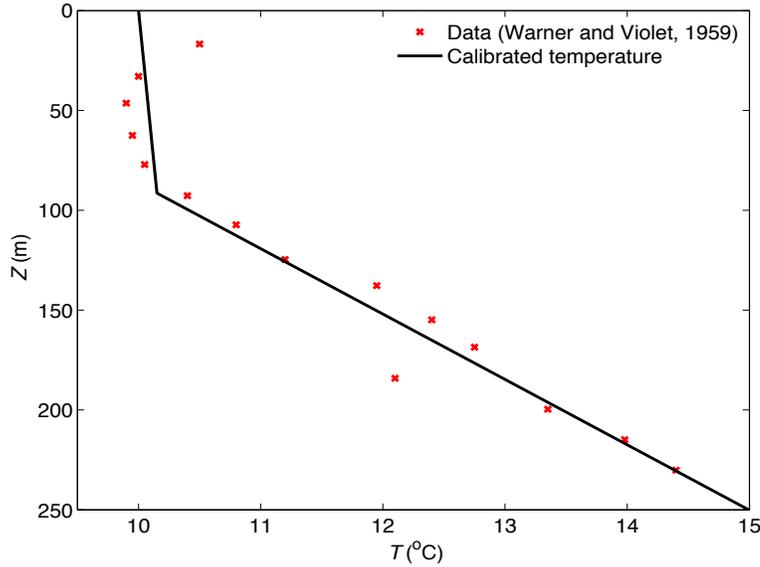
211 where τ is the tortuosity factor, ϕ is the porosity, S_l is the liquid saturation, and D_g is the
 212 diffusion coefficient defined in (3).

213 **3.4.3. Boundary/Initial Conditions.** The ground surface and water table are con-
 214 sidered to be the upper and lower boundaries of the Rainier Test models. At the ground
 215 surface boundary, gas-phase conditions are specified by the air composition and the liquid-
 216 phase saturation is fixed to be zero. At the water table boundary, liquid-phase conditions are
 217 specified based on ground water compositions with a full liquid saturation. Initial conditions
 218 between ground surface and water table are obtained by running the pre-test model using
 219 the specified boundary conditions, physical properties, and stratigraphy. Figure 4 shows a
 220 time series of the measured pressure and temperature at Rainier Mesa over 9,130-day period
 221 between January 1, 1983 and December 31, 2007. The data show the diurnal, annual, and
 222 daily variations. Pre-calibration exercise indicates that the variation of temperature does
 223 not significantly affect gas-phase flow while the daily variation of surface pressure signif-
 224 icantly drives the push-pull processes between fractures and rock matrix. Therefore, the
 225 mean value of temperature over the NPE monitoring period (517 days), 9.98 °C is assumed
 226 as a constant temperature boundary at the surface.



227 **Figure 4.** Barometric and temperature boundary conditions at ground surface. (a) Hourly pressure data from January 1, 1983 to December 31, 2007 (Tompson et al., 2010). (b) Hourly pressure data used in the NPE experiment (Carrigan et al., 1996). (c) Hourly temperature data from January 1, 1983 to December 31, 2007 (Tompson et al., 2010). (d) Hourly temperature data during the NPE experiment.

228 Two sets of temperature data are available for estimating thermal conductivities of 17
 229 stratigraphic layers at the locations underneath Rainier Mesa. At shallow depth, tempera-
 230 ture was measured from ground surface to the working point (274.3 m depth) in well UCRL-3
 231 before the detonation (Warner and Violet, 1959). A more current measurement of 29.86 °C
 232 was obtained at the water table in nearby well ER-12-3 (Tompson et al., 2010). Taking
 233 9.98 °C and 29.86 °C as boundary temperatures at the surface and water table respectively
 234 and assuming a constant vertical heat flux of 0.033 Watts, the thermal conductivities of
 235 those 17 layers are identified.



236 **Figure 5.** Vertical temperature profile. The temperature was measured in well UCRL-3 on August
 13, 1957 (Warner and Violet, 1959).

237 4. Modeling Results and Analyses

238 4.1. Model Results of Non-Proliferation Experiment

239 In the NPE model, the barometric pumping is the only driving force for gas-phase convec-
 240 tion in fractures. Among many other parameters, component diffusivity, fracture aperture
 241 size, and permeability and thickness of alluvium (if there is any) dominate the detection
 242 indices (arrival time, detection window width and height). The model of Carrigan et al.
 243 (1996) is modified using USNT module (Nitao, 1998) with and without alluvium coverage.
 244 Two sets of 100 UNST models are developed for (1) possible combinations of the diffusiv-
 245 ity and aperture size without the alluvium coverage, and (2) possible combinations of the
 246 diffusivity and alluvium permeability with the coverage. Model samples are produced using
 247 the LPTAU method in the PSUADE code (Tong, 2005).

248 **4.1.1. Effect of Effective Diffusivity and Fracture Aperture Size.** The effective
 249 (intraparticle) diffusivity is defined as the product of free diffusivity and tortuosity. In the
 250 below-boiling test, the barometric pumping of surface pressure is the only driving force for
 251 gas component release through ground surface. Figure 6 shows the concentration histories
 252 for ^{133}Xe and SF_6 at the mouth of the fracture. Pure diffusion without considering the
 253 barometric pumping never delivers ^{133}Xe to ground surface at the detection level.

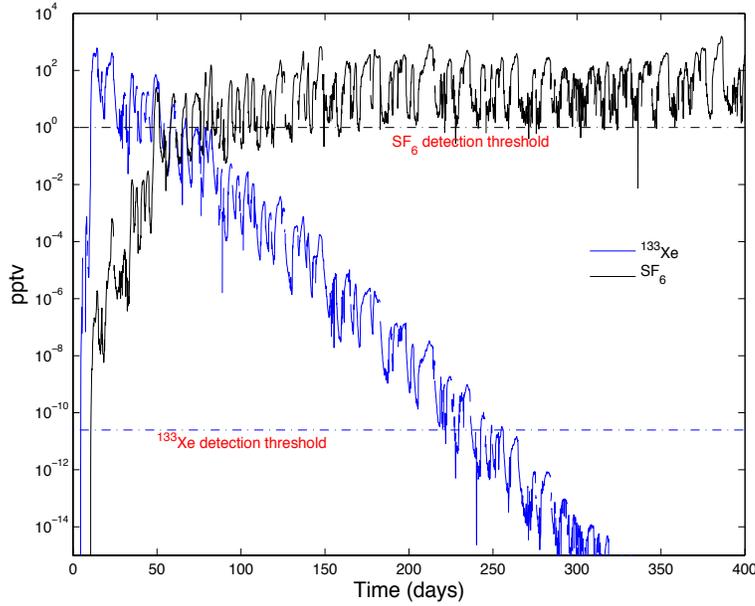


Figure 6. Concentration histories for ^{133}Xe and SF_6 at the outlet of the fracture (Figure 1b).
 254 Diffusivities for ^{133}Xe and SF_6 are respectively, $3.16 \cdot 10^{-7}$ and $7.60 \cdot 10^{-6}$. The half aperture size is
 255 $7.50 \cdot 10^{-4}$.

256 Taking 1 mBq m^{-3} (equivalent to $2.48 \cdot 10^{-11}$ pptv in air) as the measurement threshold
 257 for ^{133}Xe , the response surface of the arrival time is constructed using the PSUADE code
 258 (Tong, 2005). The first arrival time of the threshold concentration is proportional to the
 259 diffusivity in rock matrix and inversely proportional to the fracture aperture size when the
 260 permeability in alluvium takes the logarithmic mean value. As shown in Figure 7, the
 effective diffusivity appears more sensitive than aperture size to the arrival time.

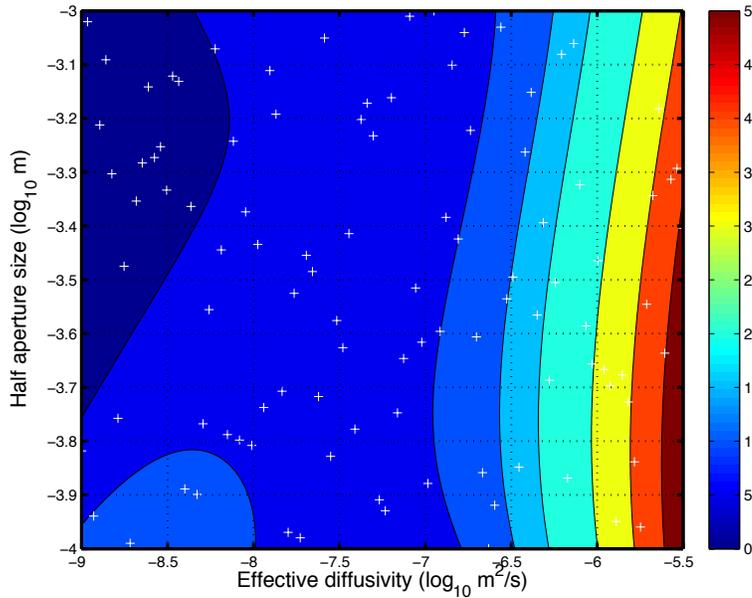


Figure 7. Arrival time (days) of ^{133}Xe as a function of effective diffusivity and half-aperture size of fracture. Note that the white “+” indicates sample locations in the space of matrix diffusivity and half-aperture size.

The detection window width is also examined as a function of the diffusivity and half-aperture size (Figures 8). These two figures 7 and 8 can be used for detecting other gas components with specific diffusivity ranges.

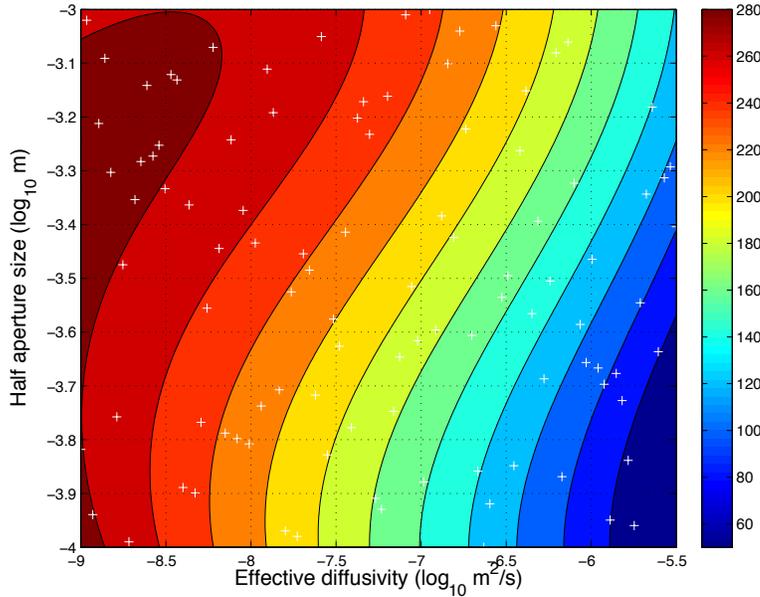
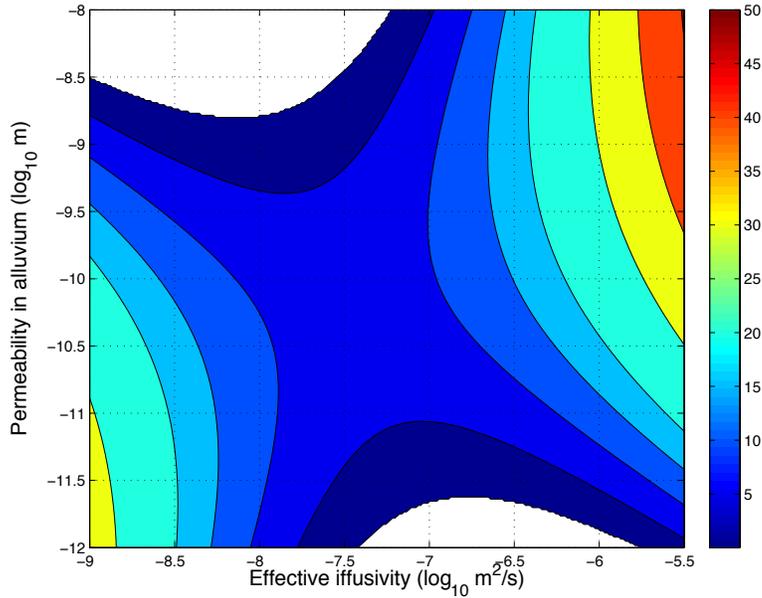


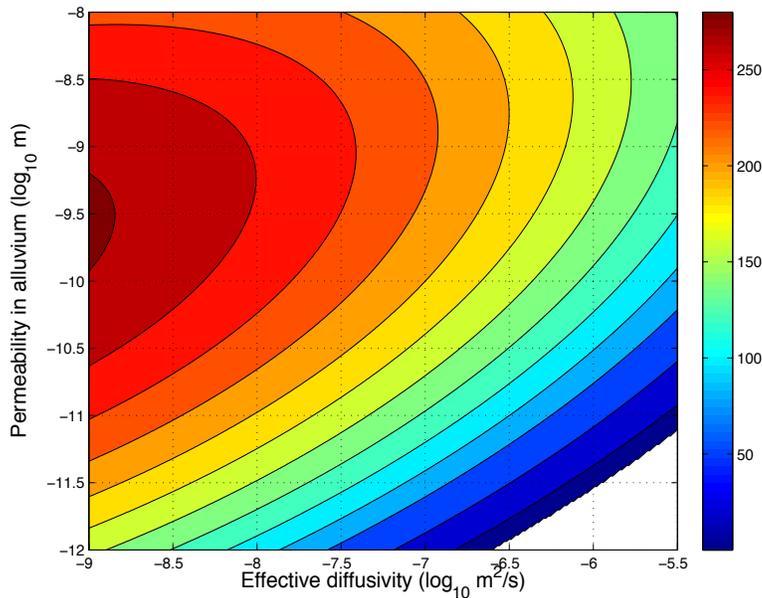
Figure 8. Detection window width (days) of ^{133}Xe as a function of effective diffusivity and half-aperture size.

4.1.2. Effect of Diffusivity and Alluvium Permeability. When the fracture aperture size is fixed with the logarithmic mean value, the detectability is evaluated in terms of matrix diffusivity and alluvium permeability. Alluvial layers or low-permeability rock on the top of the study domain reduce the effect of barometric pumping on gas-phase advection, dampen the magnitude of concentration signal, and cause a delay (phase shift) of the cyclic concentration history. Using the PSUADE code (Tong, 2005), a sensitivity analysis of detection characteristics is conducted in terms of the diffusivity and permeability.

Figures 9 and 10, show the arrival time and detection window width respectively, as functions of ^{133}Xe diffusivity and the permeability in alluvium. The white area in those figures indicates the non-detectable zone. The concentration history of ^{133}Xe on ground surface may never reach the detection threshold for high diffusivity in rock matrix and low permeability in alluvium. Although the alluvium thickness is fixed (2.0 m) in the model, it is expected that the non-detectable area grows monotonically with the thickness.



279 **Figure 9.** Arrival time (days) as a function of effective diffusivity and permeability in alluvium.



280 **Figure 10.** Detection window width (days) as a function of effective diffusivity and permeability
281 in alluvium..

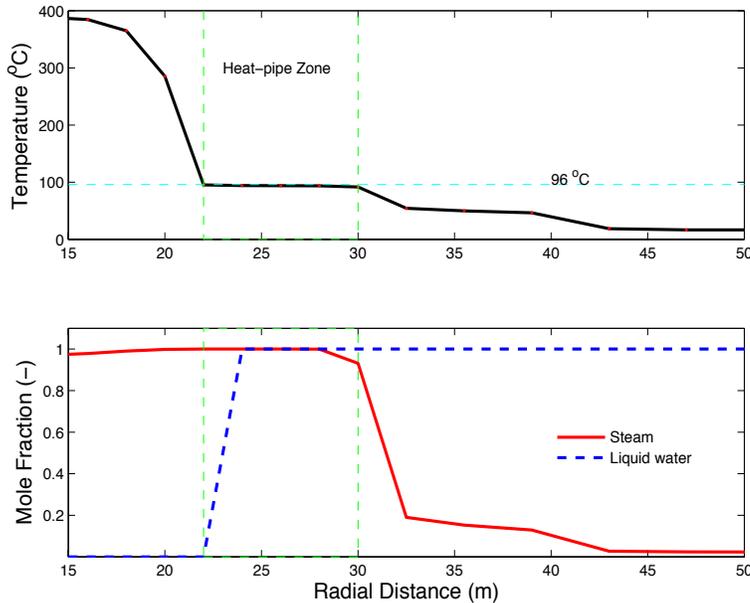
281 4.2. Model Results of Rainier Test

282 In Rainier Test model, we consider two-phase, four-component transport in a dual-
283 permeability medium under thermal conditions. The main transport mechanisms include
284 gas- and liquid-phase advection, dispersion and diffusion, and vapor-liquid partitioning.
285 Test residual heat maintains the working point and surrounding area above boiling point
286 for about two years. The countercurrent flow of steam and liquid water is formed between
287 the boiling and condensation zones when the vapor and liquid fluxes are of sufficient mag-

288 nitude. Because of the high efficiency of latent heat transport, the temperature gradient in
 289 the heat-pipe zone is minimal, resulting in nearly isothermal conditions (Sun et al., 2010).
 290 Capillary pressures play an important role in determining gas-phase flux from the hot end
 291 to the cool end of the heat pipe, and liquid-phase flux back to the hot side.

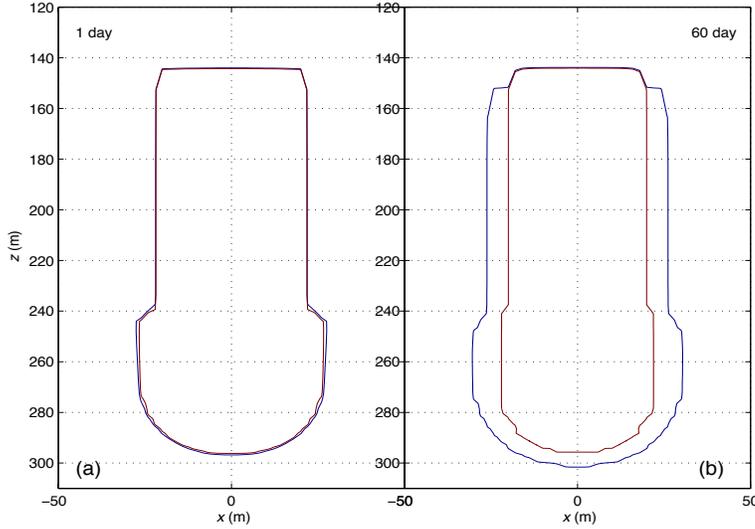
292 **4.2.1. Steam Expansion and Heat-Pipe Phenomenon.** Prior to the chimney col-
 293 lapse, the total water mass is estimated using the initial saturation, porosity, and melted
 294 volume of rock within the cavity (equivalent to the puddle glass volume). The steam bubble
 295 is formed by the test heat and well contained in the cavity by the compressed and imper-
 296 meable cavity wall. Immediately after cavity collapse, the steam bubble expands, under
 297 thermally induced pressure gradient, to the chimney and crushed zones (within two cavity
 298 radii). Temperature profile drops rapidly with the radial distance from the cavity. There-
 299 fore, most water outside the cavity after detonation will initially be in the liquid phase. The
 300 puddle zone temperature, however, will be much higher than the boiling point.

301 As shown in Figure 11, a geologic heat pipe is formed by the countercurrent flow of steam
 302 in fractures and liquid water in matrix between the boiling and condensation zones. The
 303 8-meter-wide plateau on temperature profile results from the gas-phase flux from the hot
 304 end to the cool end of the heat pipe and the liquid-phase flux toward to the working point.
 305 The steam bubble grows from the working point and shrinks after reaching the maximum
 306 size. As liquid water supplies to the chimney zone, the steam production results in high
 307 pressure and drives xenon and argon away from the chimney.



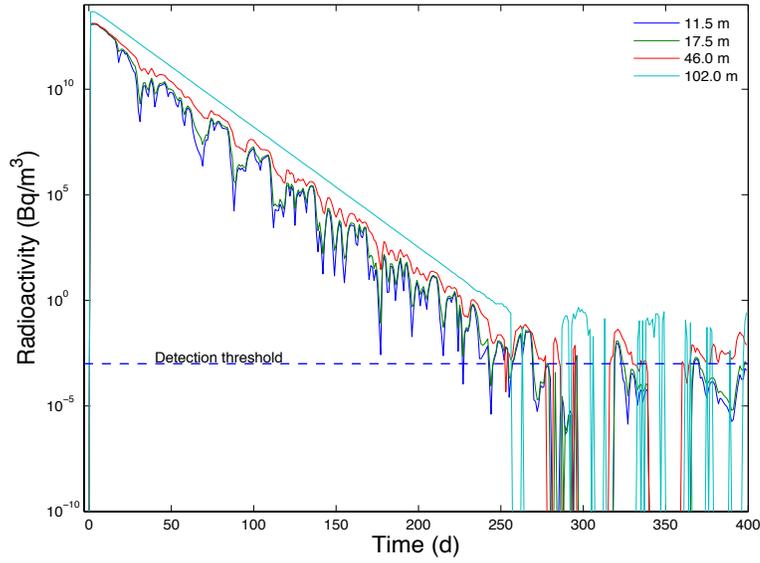
308 **Figure 11.** Temperature profile for $z = 274.3$ m and $t = 60$ d. The dashed green box represents
 the heat-pipe zone, in which gas phase flows from left to right in fractures and liquid phase flows
 from right to left in matrix by capillary pressure. The temperature in the heat-pipe zone remains
 constant.

309 Figure 12 shows the heat-pipe zone defined between the the boiling front (red line) and
 310 condensation front. The heat-pipe zone develops at 1 day (Figure 12a) and reaches 8 meter
 311 wide (at $z=274.3$ m) at 60 days. The inner line bounds the steam zone while the outer line
 312 holds the liquid water.

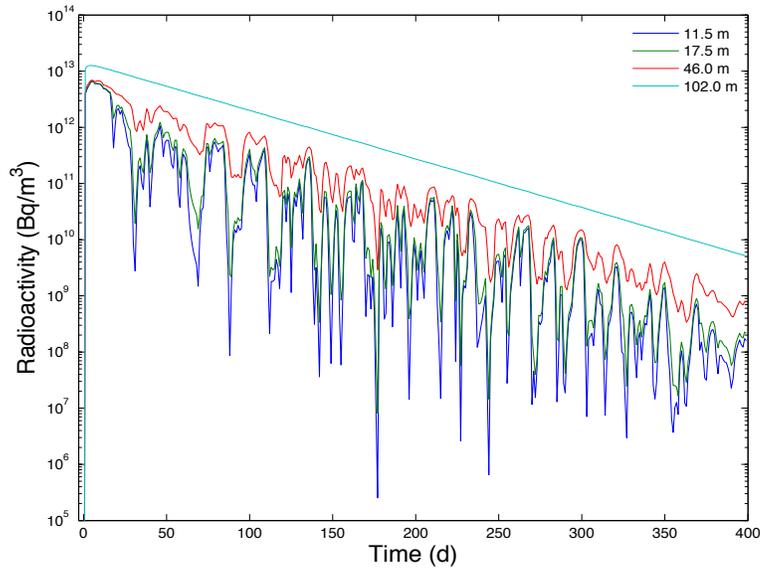


313 **Figure 12.** Heat pipe zone at 1 day (a) and 60 days (b). The heat pipe zone is defined between
the boiling front (red line) and condensation front (blue line).

314 **4.2.2. Sample Concentrations.** Radioactivities of ^{133}Xe and ^{37}Ar and mole fractions
315 of water and air are measured at depth of 11.5, 17.5, 46, and 102 m on the vertical central
316 line ($x=0$, Figure 1). As shown in Figures 13 and 14, both ^{133}Xe and ^{37}Ar reach their
317 peak concentrations within a few hours and then decay accordingly to their half-lives. The
318 detection window width for ^{133}Xe is about 260 days. The concentration history of ^{133}Xe at
319 those points (at depth of 11.5, 17.5, 46, and 102 m) is dominated by the barometric boundary
320 condition at low concentration magnitudes. Figure 13 shows the different mechanisms before
321 and after 260 days. The thermally driven advection and the first-order reaction control
322 ^{133}Xe concentration histories in the first 260 days. When the concentration drops to a
323 certain magnitude near threshold level, the effect of barometric-pumping boundary with
324 concentration of 1.0×10^{-30} (mole fraction) becomes more apparent. For this reason, ^{133}Xe
325 concentration after 260 days fluctuates with the boundary pressure. However, because of
326 the longer half-life of ^{37}Ar , its concentration magnitude is much higher than the boundary
327 concentration and the surface-boundary effect does not dominate the concentration history
328 of ^{37}Ar with the simulation time (500 days).

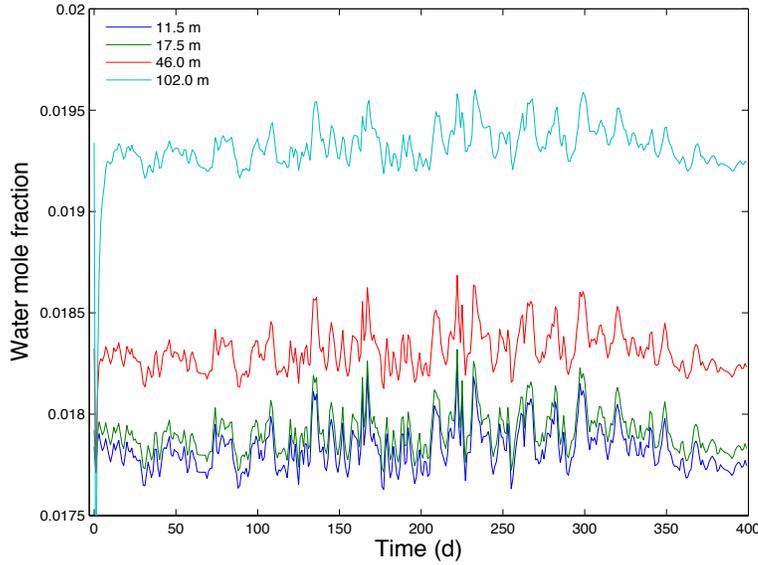


329 **Figure 13.** Concentration histories of xenon-133 at depth of 11.5, 17.5, 46, and 102 m.

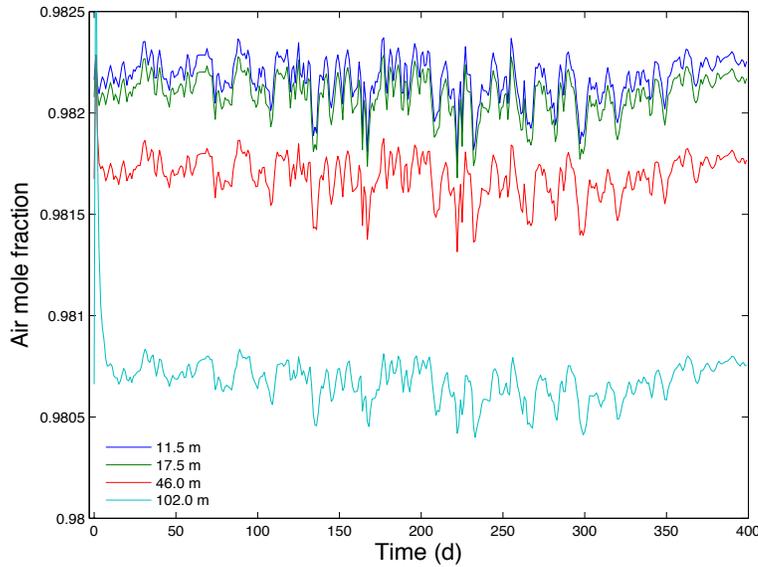


330 **Figure 14.** Concentration histories of argon-37 at depth of 11.5, 17.5, 46, and 102 m.

331 Figures 15 and 16 show the concentration histories of water and air at four locations.
 332 These concentration profiles are mainly controlled by barometric pressure boundary and
 333 steam production by test residual heat. The water mole fraction keeps the highest in the
 334 chimney and lowest away from the working point.

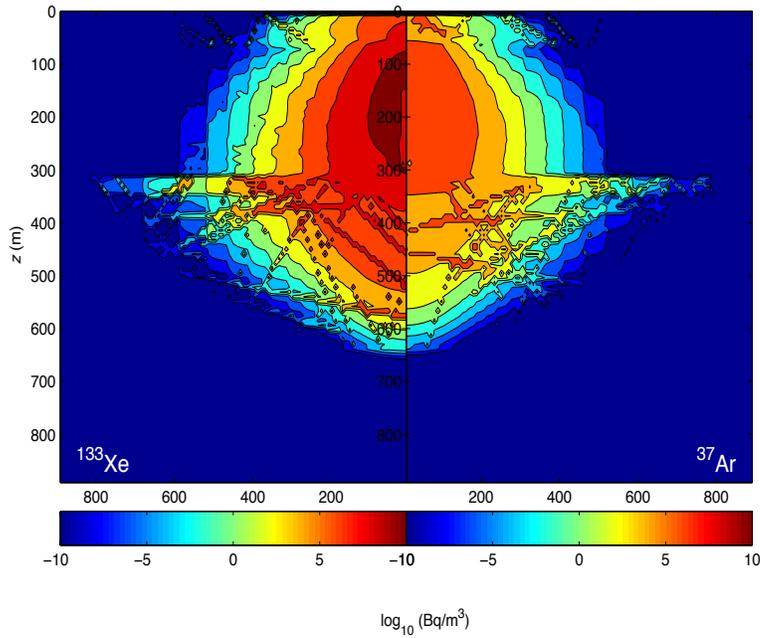


335 **Figure 15.** Concentration histories of water at depth of 11.5, 17.5, 46, and 102 m.

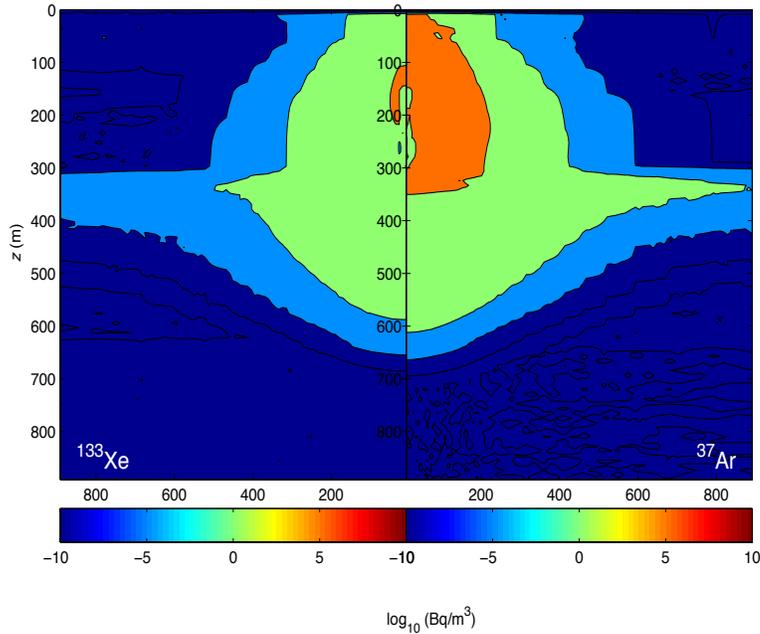


336 **Figure 16.** Concentration histories of air above chimney at depth of 11.5, 17.5, 46, and 102 m.

337 **4.2.3. Spatial Distributions of Noble Gas Components.** Test-related ^{133}Xe and
 338 ^{37}Ar concentrations (Bq/m^3) at various times reflect the transport processes in the fractured
 339 rock. Figures 17 and 18 show the ^{133}Xe and ^{37}Ar plumes at 1 day and 100 days. The ^{37}Ar
 340 plume is widely spread because of its higher diffusivity.

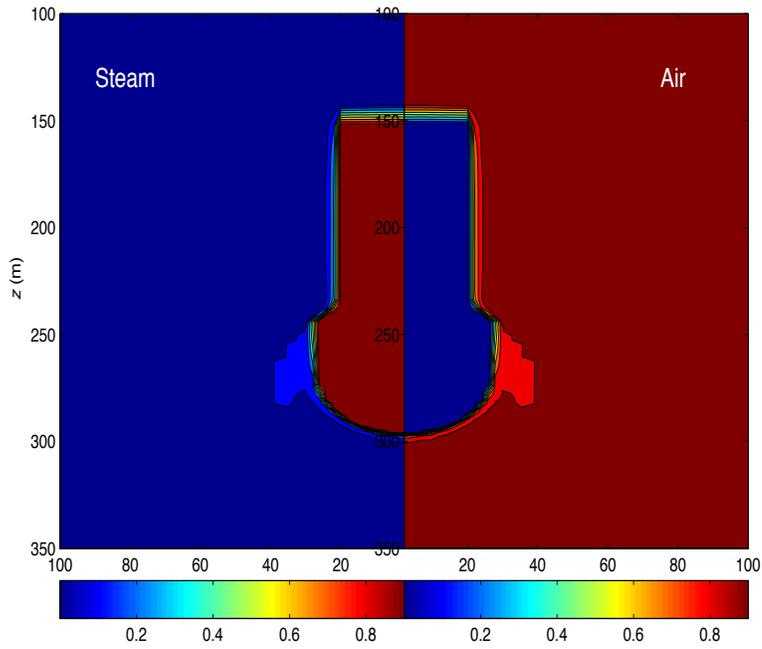


341 **Figure 17.** Contour plots of ^{133}Xe and ^{37}Ar activities (Bq/m^3) at 1 day. Note that the half-symmetry domain of ^{133}Xe plume is flipped to the left for the comparison purpose.

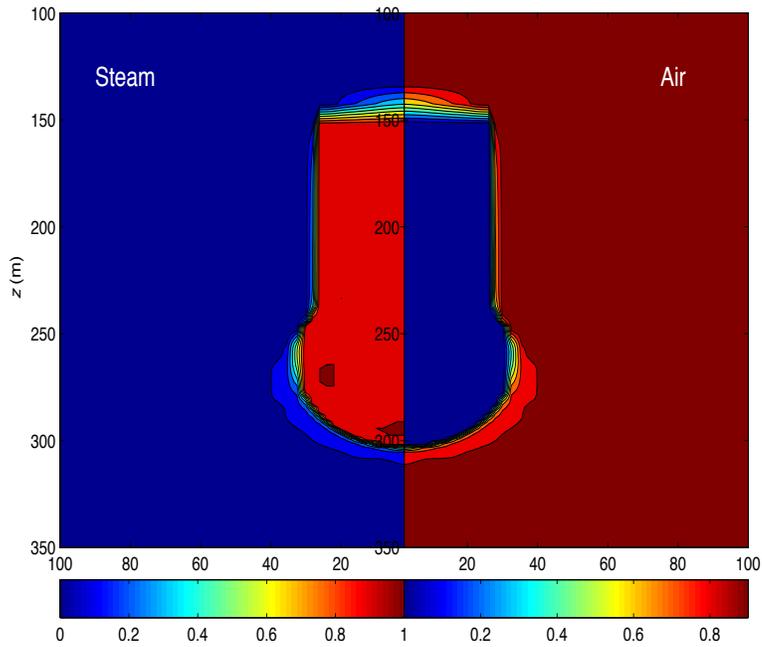


342 **Figure 18.** Contour plots of ^{133}Xe and ^{37}Ar activities (Bq/m^3) at 100 days.

343 Figures 19 and 20 show the distribution of the mole fraction of steam and air at 1 day
 344 and 100 days. The steam bubble is expanded from the working point in the chimney and
 345 mainly contained within the boiling front. Both boiling and condensation fronts expand and
 346 drive the test-related noble gas away from the chimney.



347 **Figure 19.** Contour plots of steam and air at 1 day.



348 **Figure 20.** Contour plots of steam and air at 100 days.

349 5. Conclusions

350 The detectability of noble gas ^{133}Xe and ^{37}Ar is quantitatively characterized using (1)
 351 arrival time, (2) detection window width, and (3) detection window height. The transport of
 352 ^{133}Xe and ^{37}Ar is described by a single-gas-phase model and a two-phase multi-component

353 model. In this study, we demonstrated the processes of ^{133}Xe and ^{37}Ar transport in fractured
354 rock.

355 When the temperature is below the boiling point and the subsurface system is sufficiently
356 dry, the system can be modeled as a single-gas-phase transport. Then, the barometric
357 pumping becomes the major driving force to deliver ^{133}Xe and ^{37}Ar to ground surface.
358 If the fractured rock is not covered by alluvia, the diffusivity in rock matrix and fracture
359 aperture size are sensitive parameters contributing the detectability of noble gases at ground
360 surface. When the ground surface is covered by alluvia, the permeability in the overburden
361 layer replaces the fracture aperture size to become a sensitive parameter. The detection
362 zone is provided in possible ranges of sensitive parameters.

363 The above-boiling test is modeled as a two-phase and multi-component transport. Steam
364 production and bubble expansion are the major process to drive noble gas components to
365 ground surface. Geologic heat pipe keeps constant (at boiling point) from its boiling front
366 to the condensation front. Capillary-pressure in the rock matrix drives liquid water to
367 move toward the boiling front and the pressure gradient elevated by phase change (steam
368 production) drives steam away from the chimney through fractures. The steam bubble
369 becomes a major driver for noble gas transport. The arrival time is usually shorter compared
370 to that in the single-gas model. After the temperature in the chimney drops below boiling
371 point, the barometric pumping takes over the role as the major driving force.

372 Both models show that the detection window width for ^{133}Xe is smaller than that for ^{37}Ar
373 because of the shorter half life. To take advantage of ^{133}Xe detection sensitivity, the mon-
374 itoring is suggested at the early stage. This study is limited to two specific tests. Further
375 study is necessary for a wide range of yields and geological conditions.

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