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***Impacts of Source Term Heterogeneities on Water
Pathway Dose***

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IMPACTS OF SOURCE TERM HETEROGENEITIES ON WATER PATHWAY DOSE

Sub-Group 2 water pathway analysis

T. Sullivan, A. Guskov, P. Poskas, N. Ruperti, V. Hanusik, and V. Stefula

Report

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1.0 INTRODUCTION

Radioactive sealed sources are used extensively throughout the world in different field and various activities such as medicine, agriculture, industry, research, education military applications, as well as nuclear facilities. The International Basic Safety Standards for Protection against Ionizing Radiation and for the Safety of Radiation sources [1] defines a sealed source as “radioactive material that is (a) permanently sealed in capsule or (b) closely bounded and in a solid form. The capsule or material of sealed source shall be strong enough to maintain remain leak free under the conditions of use and wear for which the source was designed, also under foreseeable mishaps”.

When a radioactive sealed source is no longer needed, or becomes unfit for the intended application it is considered spent. A spent sealed source is not necessarily a waste because it can be used in other applications. If for any technical or economic reason (decay, obsolete equipment and technique, worn out equipment) no further use is foreseen, the spent sealed source is considered spent and becomes radioactive waste [2] [3]. In addition, a source may be taken out of service temporarily or indefinitely. In this case the source is out of used (“disused”) but not considered spent [4]. Sources that are not in active use and have not being declared as spent are considered as disused sealed sources [4].

Considering the potential radiation hazards associated with such waste it has to be managed and disposed of in a way that will ensure that the potential radiation hazards are adequately managed and controlled in compliance with the appropriate safety principles and criteria. It is recognised that there exists today experience and means for all steps in the management of disused sealed sources, except disposal of [2].

In many countries, disused sealed sources represent a part of the radioactive waste inventory being characterised generally with high specific activities and small physical sizes and for which a solution has to be found in term of long-term disposal. Together with their casing and packaging, they are one form of heterogeneous waste; many other forms of waste with heterogeneous properties exist. They may arise in very small quantities and with very specific characteristics in the case of small producers, or in larger streams with standard characteristics in others.

This wide variety of waste induces three main different levels of waste heterogeneity: (i) hot spot (e.g. disused sealed sources); (ii) large item inside a package (e.g. metal components); and (iii) very large items to be disposed of directly in the disposal unit (e.g. irradiated pipes, vessels). Safety assessments generally assume a certain level of waste homogeneity in most of the existing or proposed disposal facilities. There is a need to evaluate the appropriateness of such an assumption and the influence on the results of safety assessment.

This need is especially acute in the case of sealed sources. There are many cases where are storage conditions are poor, or there is improper management leading to a radiological accident, some with significant or detrimental impacts. Disposal in a near surface disposal facility has been used in the past for some disused sealed sources. This option is currently in use for others sealed sources, or is being studied for the rest of them. The regulatory framework differs greatly between countries. In some countries, large quantities of disused sealed sources have been disposed of without any restriction, in others their disposal is forbidden by law. In any case,

evaluation of the acceptability of disposal of disused sealed sources in near surface disposal facility is of utmost importance.

1.1. Background

The International Atomic Energy Agency's (IAEA) coordinated research project (CRP) "Improving Long Term Safety Assessment Methodologies for Near Surface Radioactive Waste Disposal Facilities" (ISAM) was launched in 1997 and completed in the year 2000. The main outcome of the project was the development of a harmonised methodology for carrying out post-closure safety assessment of near surface disposal facilities that can be applied iteratively to provide for the various purposes required of such safety assessment. The methodology has since found widespread acceptance and is being published in a series of reports dealing with scenario development, modelling and confidence building, together with three documented test cases for vault, borehole and Radon-type disposal facilities. Upon completion of the ISAM project, it was recognised that a need existed to investigate further application of the ISAM methodology to a range of practical issues.

Therefore, the IAEA launched a new and complementary CRP "Application of Safety Assessment Methodologies for Near-Surface Radioactive Waste Disposal Facilities" (ASAM). It builds on the experience gained with the ISAM programme, with special emphasis on application of the ISAM methodology to practical problems of topical interest with the prime objective to:

- Explore practical application of the ISAM methodology to a range of near surface disposal facilities for a number of purposes, such as development of design concepts, safety reassessment and upgrading of existing facilities; and
- Develop practical approaches to assist regulators, operators and other specialists reviewing safety assessments.

The emphasis of the ASAM project is on evaluating the post-closure safety of radioactive waste disposal facilities, although, where considered appropriate, operational safety might also be assessed.

Initially the ASAM project focuses on the analysis of issues related to the safety of near surface disposal facilities, namely:

- Assessing the safety of existing disposal facilities and facilities built to safety standards different from current standards;
- The disposal of disused sealed sources and other heterogeneous waste in near surface disposal facilities; and
- The disposal of mining and minerals processing waste and other waste with an enhanced content of naturally occurring radionuclides.

The project is also addressing :

- review of safety assessments and associated regulatory aspects; and

- important common issues in the application of safety assessment methodologies to different facility types such as the assessment of disruptive events (e.g. human intrusion) and the performance of engineered barriers.

Withing this programme, the role of the Disused Sealed Sources and Heterogeneous Wastes (DSSHW) Working Group is to investigate application of the ISAM methodology with a view to studying the importance of considering the heterogeneity of waste in the safety assessment of near surface disposal facilities.

During the first RCM held in Vienna from 11 to 15 November 2002 it was decided by the DSSHW Working Group to split the WG in four Sub-groups. The Sub-Group named “Water Pathway Analysis” has the mission to analyse the influence of heterogeneity on the long-term safety of a near surface disposal facility in the water pathway. Currently, safety assessment work relies on the assumption of uniform distribution of waste within a disposal facility. Sealed sources due to their small volume and high activity do not match the average radionuclide concentrations in the facility. This sub-group will analyze the impact of non-uniform inventory distributions on concentrations in the groundwater pathway.

Specifically this sub-group has performed a series of assessments to address the impacts of heterogeneities in the waste caused by spent sealed sources and other non-routine wastes on projected concentration in the water pathway. The assessment is structured around the data from the Saratov site and data collected on the inventory characteristics of sealed sources.

1.2 Objectives

The main objective of the sub-group is to study the applicability of the ISAM methodology in evaluating the safety implications and acceptability for the water pathway of disposing heterogeneous waste in near surface facilities.

The specific objectives are:

- Evaluate the impacts of heterogeneities on radionuclide concentrations in the aquifer below the disposal facility.
- Determine guidelines for assessing whether heterogeneities in waste inventory are important for the groundwater pathway
- Demonstrate the methodology using site-specific data for the Saratov site.

1.3 Scope

This study addresses the impact of heterogeneities on the concentration/dose from the groundwater pathway on two scales: site-wide and within a single disposal facility. At many sites, a series of disposal facilities including trenches, vaults, and boreholes may be present. In some cases, for safety assessment, the entire inventory is combined into a single ‘representative’ disposal facility. In contrast, analyzing each disposal facility individually adds spatial heterogeneity due to the separation of facilities and due to the different inventories that will exist in each facility. The next level of heterogeneity is within a single disposal facility where the wastes themselves are heterogeneous and may contain (i) hot spots such as sealed sources; (ii)

large items inside a package such as a metal component; and (iii) very large items to be disposed directly in the disposal unit. The impacts of combining the entire inventory into a single facility will be compared with analysis of multiple facilities at the same site and spatial variability within a single disposal facility will also be investigated.

The scope of these studies include the following constraints:

- Disposal facilities such as vaults, trenches, and boreholes, with the existing associated practices are considered in the study.
- Operational safety is not considered in this study. It is recognized that heterogeneity may have significant influence on safety during the handling and disposal of the wastes, this will most likely not impact groundwater concentrations.
- Health impacts associated with non-radiological components of the wastes are not considered in this study.
- As a basis of comparison, a reference case using the same inventory, release rates, and transport properties with a homogeneous distribution of wastes will be used.

The intent of the first phase of these investigations is to provide guidelines on when treatment of the inventory on an average basis (homogeneous distribution) within a single disposal facility and across the entire disposal site is acceptable from the perspective of safety assessment of the groundwater pathway. The guidelines will be derived following the safety assessment methodology recommended by IAEA. It is important to provide these guidelines as the issue of heterogeneities has not been previously addressed in the literature. By inspection, it can be guaranteed that there will be some heterogeneous distribution of waste within a single facility that will lead to a higher peak concentration/dose than a homogeneous distribution. The question is how much higher will the dose be and does this impact on safety assessment. For example, Cs at Saratov has a site-specific K_d of 10,000. If a safety assessment for the groundwater pathway is performed, the results will show the dose at a receptor well is exceedingly small (for example, assume it is $1E-8$ mSv/y). If we have a heterogeneous distribution with a peak heterogeneity of 10:1, the dose will increase by less than a factor of 10 (dispersion will smooth this peak). Therefore, the peak dose will be less than $1E-7$ mSv/y. Thus, it can be stated with confidence that modelling Cs using a heterogeneous model will not alter the conclusion about the safety of the disposal site. In contrast, if the predicted dose was close to the standard, for example, within a factor of 2, heterogeneities may be important in determining if disposal is acceptable.

The impacts of heterogeneities will be site- and problem-specific. Therefore, general guidelines will be developed for four classes of radionuclides :

- Mobile, short half-life,
- Immobile, short half-life
- Mobile, long-half-life
- Immobile, long half-life

The exact definition of these classes is arbitrary, but for this study, the mobile radionuclides are defined as those having a saturated zone retardation coefficient of less than 50 and short-half-life radionuclides are those with a half-life of less than 50 years. Ideally, the distinctions would be based on travel time to the receptor and radionuclide half-life, but this leads to site-specific definitions of the four classes. A half-life of 50 years is reasonable in that it includes radionuclides that often have a very high inventory Cs-137, Sr-90, and Co-60 and based on their inventory warrant analysis of the groundwater pathway. Other radionuclides of importance in the assessment of the groundwater pathway have half-lives of greater than 1000 years.

The intent of the second phase of these investigations is to apply the IAEA methodology to the Saratov site incorporating heterogeneities in waste distribution throughout the site and within individual disposal facilities.

Ideally, the For this reason, it is not necessary to focus on the same radiounuclides as for analyzing inadvertent intruders. For the inadvertent intruder scenarios, radionuclides that undergo gamma decay and have large inventories (e.g. Cs-137, Co-60) are often of great concern. For the groundwater pathway, radionuclides that are mobile in groundwater and have a long-half-life are often of great concern. For example, Tc-99, a beta-emitter, due to its relatively low concentration compared to Cs and Co is often not a concern for inadvertent intruders, while, due to its much longer half-life and mobility it may be of concern in the groundwater pathway.

1.4 Expected Outcomes

For this sub-group the outcomes are:

- the production of an assessment of the impacts of heterogeneities in inventory both within the site and within a single near-surface disposal facility on the concentration in the water pathway.
- the derivation of qualitative guidance on the impact to the water pathway of sealed sources and other heterogeneities in a near-surface disposal facility,
- the application of this generic assessment in the case of the Saratov site,
- the quantitative application on the Saratov site in order to allow the verification of the acceptability of the disposed and forecast DSS.

1.5. Structure

Section 2 outlines the approach that is used to evaluate the influence of heterogeneity in near-surface disposal facility. The different steps of the approach described in this document:

- assessment context (Section 3)
- disposal system description (sections 4),
- data requirements for modelling (Section 5),
- analysis framework and basis for evaluation of the impact of heterogeneities (Section 6),

- model formulation, implementation, and analysis of results (Section 7), and
- summary and conclusions (Section 8).

In addition to the main sections of the report there are five Appendices. The first provides the details of the test problem for the Saratov Site including the major assumptions and data. The next four are the detailed reports of the assessment of the impact of heterogeneities performed by the four groups.

2.0 APPROACH TO BE USED TO EVALUATE THE INFLUENCE OF HETEOGENEITY IN NEAR SURFACE DISPOSAL FACILITY SAFETY

As part of the ISAM project, a consistent safety assessment methodology was developed (the ISAM safety assessment methodology) which is presented in figure 1. This approach has been used in order to evaluate the influence of the presence of heterogeneous waste for the safety of near-surface disposal facility.

The purpose of this study is to derive guidelines for the impact of heterogeneities in waste distribution caused by sealed sources or other waste streams to be disposed in near-surface disposal facility. Currently, the standard practice is to homogenize the inventory within a single disposal facility and base the safety assessment on a uniform distribution of contamination within a facility. Many analyses go one step further and combine the inventory of all disposal facilities at a site into a single 'effective' disposal facility. The guidelines will be a function of radionuclide half-life and transport parameters. For example, short-lived mobile radionuclides may exhibit one type of response in the groundwater pathway to heterogeneities while short-lived immobile radionuclides may exhibit another. The use of the safety assessment approach allows for the derivation of guidelines in a relevant, adequate, understandable and credible manner. Therefore it is proposed to apply the safety assessment approach to assessing the impacts of heterogeneities in wastes on water pathway dose.

The key components of the ISAM safety assessment approach, adapted to the purpose of derivation of activity limits for disused sealed sources, are presented in figure 1. They consist on:

- the specification of the assessment context (Step 1, Section 3);
- the description of the disposal system (Step 2, Section 4);
- the development and justification of scenarios (Step 3, Section 5 and 6);
- the formulation and implementation of models (Step 4, Section 7); and
- the calculation and derivation of illustrative groundwater concentrations (Step 5, Section 7)
- the interpretation of the impact of heterogeneities on groundwter concentrations (Step 6, Section 7 and 8).

For an actual disposal system iterations of the assessment process will be performed when comparing the derived groundwater concentration with regulatory limits. In most cases, regulatory limits are set on dose, not groundwater concentration. However, dose is linearly proportional to groundwater concentration. Therefore, in the first phase of these studies, where the objective is to derive guidelines for when heterogeneities are important in the groundwater pathway, the groundwater concentration is used as a basis of comparison. In a complete safety assessment, the groundwater concentrations would be used to estimate dose based on a suite of exposure scenarios (e.g. drinking water, food grown with irrigation of contaminated waters, etc.). This will be done when applying the methodology to the Saratov site.

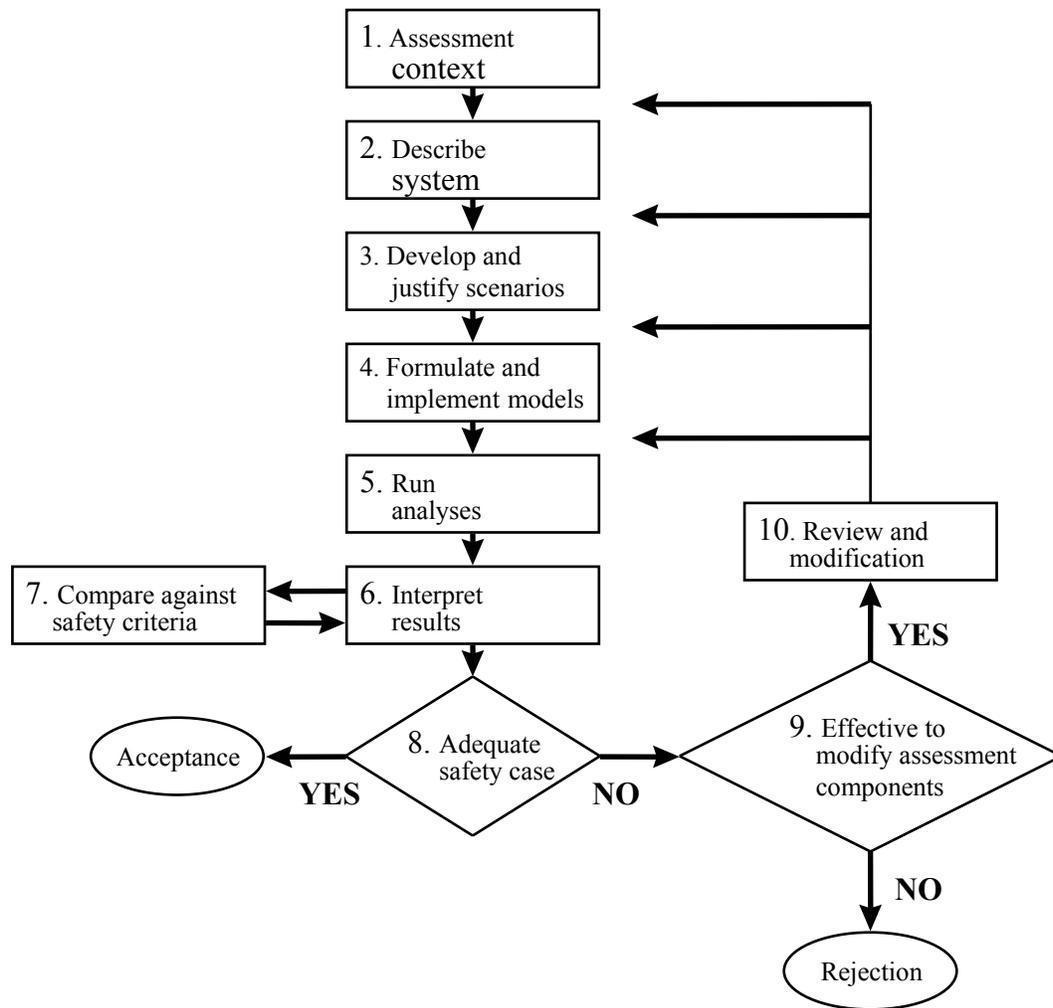


Figure 1 The safety assessment process.

3.0 ASSESSMENT CONTEXT

3.1 Purpose

Perform generic and site-specific analysis to assess the impacts of heterogeneities on peak concentration and flux at selected receptor locations in the water pathway.

3.2 Calculational end points

The dose is directly proportional to the water concentration for the water pathway. The proportionality constant depends on site-specific plant and animal uptake factors and human consumption factors. To focus on the impacts of heterogeneities, the peak water concentration and peak flux at selected receptor locations are the calculational endpoints.

The receptor locations are:

- the bottom of the facility,
- the bottom of the vadose zone,
- wells at approximately 100, 1000, and 2000 meters.

The first two locations are used to assess the changes in concentration due to release from the wastes (bottom of the facility) and transport in the vadose zone (bottom of the vadose zone). Coupled with the receptors in the aquifer, assessment of the role of each of these regions in mitigating impacts of heterogeneities can be assessed.

3.3 ASSESSMENT PHILOSOPHY

The assessment philosophy is to develop a set of test problems that strikes a balance between a generic and site-specific analysis. The balance is needed to generalize the findings of these studies to other disposal sites. The site-specific analysis is needed to provide a framework and foundation in an actual problem. For this reason, analyses are based on the Saratov site and its associated disposal facilities and environmental conditions (e.g. precipitation, geology, hydrology, etc.). A detailed site-description for Saratov was prepared as part of the ISAM project and this forms the basis of the water pathway analysis. To increase generality, deviation will be made from the Saratov conditions as needed. For example, the Saratov inventory is not representative of the range of inventories found in sealed sources. Therefore, some calculations will be performed using an inventory that is more representative of sealed sources.

3.4 TIME FRAMES

The time frames to be considered are radionuclide specific and will be the time to peak dose at the relevant locations used in the analysis.

4.0 DISPOSAL SYSTEM DESCRIPTION

A summary of key site parameters is provided below. More details can be found in Appendix A which is the test problem description. These parameters are to be used in all assessments and are meant to be representative of the information found in the Saratov site description.

4.1 Disposal Options

The exercise will include simulations of vaults, trenches, and boreholes. The analyst may choose to examine any or all of these facilities. Figure 2 provides a site map with surface dimensions for all of the disposal facilities (vaults A, B, C, and D, trenches (facility F), and boreholes (facility E). These are the outer dimensions of the facilities. The waste-bearing zone is often smaller due to walls and service areas that are not used for wastes. For the purposes of this assessment, the facility boundary can be assumed to be 200 m from the lower right corner of trench F1 in Figure 1. The direction of water flow is marked on the figure. This information may be used when placing receptor wells. The following section discusses the dimensions that should be used in the analysis. These dimensions are summarized in Table 1.

4.1.1 Trenches

There are five trenches with a total volume of 150 m^3 . In each trench, the waste region is 1.8 m deep from -3.5 m to -1.7 m in elevation. For multi-dimensional analysis, assume the width in the direction of groundwater flow is 6 m and the length perpendicular to flow is 2.7 m. If more than one trench is simulated, use the same dimensions for each trench.

Assume the trench cap does not provide a barrier to infiltration.

4.2.2 Vaults

Saratov contains four vaults, A, B, C, and D. All contain solidified radioactive wastes.

Vaults A, B, and D.

Disposal volume – 200 m^3 in each vault. Wastes are placed in a 2.7-meter zone from -0.30 to -3.0 m deep.

Vault C

Disposal Volume – 960 m^3 . Depth 3.0 meters with wastes in 2.7 meter zone.

4.2.3 Sealed Source Borehole

The borehole has a 4 meter cover followed by a 1.5 meter source region. The borehole diameter is 0.4 m. The container lifetime for materials in the borehole is 45 years. After this time, assume the natural infiltration rate for water flow. If more than one borehole is simulated, use the same dimensions for each borehole.

5.0 Data required for simulations

To assess the impacts of heterogeneities data are required for water flow, engineered barrier performance, transport, source term release rates, and source term distribution. This information is needed in step 4 of the safety assessment process, develop and implement models. In the first set of analyses, the source term distribution will define the heterogeneities. Later analyses may examine the impacts of waste container and waste form performance on heterogeneities. The data that are the basis for analysis are presented in full in Appendix A and summarized next.

5.1 Water flow parameters

5.1.1 Engineered Barrier

Assume that the engineered barrier has a lifetime of 100 years. After which, it no longer prevents infiltration. Prior to failure assume that the barrier reduces infiltration to 1% of the natural infiltration.

5.1.2 Infiltration

After failure of the caps and covers, assume that the average infiltration into the wastes includes all of the snowmelt and precipitation, 350 mm/yr. This value should be used for the source zone Darcy velocity after engineered barrier failure. Prior to barrier failure, the flow rate is 3.5 mm/yr, 1% of natural infiltration.

5.1.3 Vadose Zone Thickness

The actual vadose zone has a complicated layered geology. The purpose of this assessment does not include detailed characterization of the flow that occurs. Instead the conceptual model will involve a homogeneous vadose zone underneath the repository. Two cases may be considered. The first will use the actual vadose zone thickness. The second will assume no vadose zone. This test is meant to stress the impacts of heterogeneities.

Case a) Vadose zone thickness is 70 m. In this case, analysts should also track the concentration and mass flux out of the bottom of the facility.

Case b) Vadose zone thickness is 0 m.

5.1.4 Vadose Zone Darcy Velocity and Moisture Content

The vadose zone Darcy velocity is 350 mm/yr (same as infiltration rate into waste zone after failure of engineered barriers). Due to the small width of the disposal vaults, the regional flow is deemed the appropriate value. The model has a different velocity in the waste zone and the vadose zone until the engineered barriers fail. If it is a problem to have a different velocity in the source zone and vadose zone, the analyst should provide a rationale for choosing one over the other.

The vadose zone moisture content is 0.05 and it has a porosity of 0.53, representative of a dry sandy soil.

5.1.5 Saturated Zone Water Flow Parameters

The saturated zone thickness at Saratov is 10 m. The saturated zone Darcy velocity is 2.92 m/yr and the porosity is 0.4.

5.2 Inventory

The Saratov inventory for each of the boreholes, vaults, and trenches is found in the tables in the Appendix A. For the purposes of evaluating the impacts of heterogeneities we will emphasize several classes of radionuclides:

- a) Short-lived, low mobility, high inventory (e.g. Cs-137, Co-60, etc.)
- b) Short-lived, high mobility, high inventory (e.g. H-3)
- c) Long-lived, high mobility (C-14, I-129, Tc-99, Cl-36)
- d) Long-lived, low mobility (Am-241, Pu-239, U-235, etc).

Not all radionuclides will be present in each disposal option. For example, long-lived beta emitters such as C-14, Tc-99 and I-129 are typically not used as sources and therefore, are not in the sealed source boreholes. The trenches at Saratov contain radium-contaminated soils that are essentially homogeneous and therefore the only heterogeneity is in the spatial locations of the trenches. To better represent sealed sources and other heterogeneities, additional inventory was added to some of the disposal facilities. This additional inventory focused on mobile radionuclides such as H-3, Tc-99, and I-129 and those with long-half lives and found in sealed sources, such as Pu.

5.2.1 Inventory estimates for boreholes and vaults at Saratov

The inventory estimates found in tables 2 – 7 of Appendix A are based on data from the Saratov site and modified to include additional radionuclides to represent sealed sources and other heterogeneities. Modifications to the Saratov data are marked in the accompanying tables.

5.2.2 Inventory of the trenches

In 5 trenches the total volume of contaminated ground is 150m³ with the average specific activity 24000 Bq/kg on Ra-226 (there are also small amount of other radionuclides: 6.2 Bq/kg of U-238; 7.7 Bq/kg U-234, 45 Bq/kg Th-232 and 56 Bq/kg Th-228). The total activity in all trenches is estimated, assuming a density of 1.9 g/cm³ as follows:

Ra-226	6840.0 MBq
U-238	1.767 MBq
U-234	2.1945 MBq
Th-232	12.825MBq
Th-228	15.96MBq

5.3 Transport Parameters

5.3.1 Distribution Coefficients, Kd's

An extensive review of Kd's for four different soil types has been made by Thibault et al. 1990 and median values are presented for sand, loam, clay, and organic soils. Sand is the most representative soil type for Saratov and Kd values for sand are recommended for use in the problem. In general, C, I, Np, H, and Tc had Kd values less than 5 and will be mobile at the Saratov sitem. Sr, U, Co, Pd, and Zr had Kd values between 15 and 100. All other radionuclides had a Kd value greater than 100. Site-specific measurement of the Kd for Cs was determined to be 10,000 cm³/g and should be used in place of the literature value in Appendix A.

5.3.2 Diffusion/Dispersion Coefficients

For dispersion coefficients, use a dispersion that is 1/10 of the distance to the receptor in the longitudinal direction and 1/100 in the transverse direction. This will allow little spreading of the plume and maximize the impacts of heterogeneities. Table 2 presents the dispersion values suggested for the test problem. In the unsaturated zone, dispersivity is highest in the z-direction, which is the presumed direction of flow. For the saturated zone, the x-direction is the assumed flow direction and consequently, dispersivity is highest along this axis. Dispersivity values are assumed to be independent of the radionuclide.

Table 2 Dispersivity values (m) for the unsaturated and saturated zone.

Case	Dispersivity (a _x) (m)	Dispersivity (a _y) (m)	Vertical dispersivity (a _z) (m)
Saturated zone	10	1	0.1
70 meter unsaturated zone	0.7	0.7	7
3 meter unsaturated zone	0.03	0.03	0.3

For diffusion coefficients use 10⁻⁶ cm²/s for all radionuclides, as diffusion is typically only a small component of transport.

5.4 Source Term Release Rates

At Saratov there are three main types of wastes: cement solidified, sealed sources, and activated metals. Each may have unique release characteristics. In addition, other facilities may have other waste streams including bitumen, compacted lab trash, de-watered resins, etc. Unfortunately, the values for the release rates from various waste forms are not well known. Therefore, in the first stage of these analyses, the inventory will be released subject to geochemical constraints (sorption and solubility). In other words, no credit will be taken for the waste form or container

with the exception of sealed sources that are assumed to isolate the inventory for 45 years. In the absence of site-specific estimates of solubility, it will be assumed that releases are not solubility limited. Further refinements could consider container lifetime, diffusive releases from cement and bitumen, and dissolution of metals.

5.5 Source Term Distribution

5.5.1 Heterogeneity Within a single Disposal Cell

A base case will be performed where the source term is homogeneous throughout the disposal cell. Supplemental cases will place high concentration zones throughout the repository while maintaining the total inventory constant.

Suggested source term distributions:

- a) Homogeneous (base case)
- b) High concentrations at the bottom. Place 10% of the inventory in the bottom 1% of the facility. This example provides a difference of approximately 10 in strength between the two regions.
- c) As in b except the wastes are in the top 1% of the repository.

5.3.2 Heterogeneity Across Multiple Disposal Cells

Frequently when modeling multiple facilities at a single site, the wastes are all placed in one hypothetical disposal facility. One important question to analyze is the impact of combining all of the wastes into one facility as opposed to modeling the spatial distribution of wastes in the various facilities more accurately.

The test case to simulate is a comparison of placing all of the wastes in the largest disposal cell at the site, Vault C, versus maintaining the spatial and inventory distribution of each of the individual disposal cells at the Saratov site. For this test case, the analyst is requested to place the entire site inventory into an “extended vault C”. To accommodate the additional volume, the width perpendicular to flow for “extended Vault C” should be increased to 28.1 m.

For the simulation using the actual geometry and inventory, it is assumed that there is a well 88.5 m downgradient of Vault C. This well is assumed to have the ability to collect all of the water leaving all of the trenches. Therefore, when simulating the actual distribution of wastes, the effective distance to the well for all of the facilities becomes the distance from the edge of the facility to the hypothetical well. This is a conservative assumption because the spatial layout at Saratov would prevent a single well from capturing the plumes from all vaults without substantial dilution.

To isolate the impacts of spatial heterogeneity, when modeling multiple facilities in this test case, the analyst should use all assumptions pertaining to vault C. For example, boreholes and trenches should be modeled with the water infiltration appropriate for Vault C. Similarly other modeling

assumptions should be consistent between the “extended Vault C” and the spatially distributed sources.

6.0 Analysis Framework

Section 5 contained the site geometry, inventory, and other data required for the analysis. This section provides the context for the analysis including the locations for comparison of results (called receptor locations) and the basis for comparison between the base case (homogeneous distribution of wastes) and the non-homogeneous distributions of waste. In addition,

6.1 Receptor Locations

Three receptor well locations are to be used if possible. The objective of having multiple receptor wells is to examine the effects of heterogeneity in the source term as a function of distance. The general approach is to place receptor locations in the aquifer at distances of approximately 100 m, 1000 m, and 2000 m (nearest distance to the river) from the edge of the disposal facility. With multiple facilities it is cumbersome to model slightly different distances but it can be done. Table 3 presents the distance from each facility to the site boundary in the direction of flow. If the analyst is simulating the effects of heterogeneities in a single facility, the distances can be simplified to 100, 1000, and 2000 m if desired. If the analyst is simulating more than one disposal facility to examine the impacts of spatial distribution on receptor concentrations, the values in Table 3 should be used. The final column in Table 3 provides the distances to be used when comparing releases from multiple facilities to releases from a single ‘representative’ facility.

Table 3 Distance to receptor locations for each disposal facility

Facility	Distance to first receptor	Distance to second receptor	Distance to third receptor (m)	Distance to the first receptor Spatial Heterogeneities Case*
Vault A	122	1022	2022	127.6
Vault B	116.5	1016.5	2016.5	122.6
Vault C	88.5	988.5	1988.5	88.5
Vault D	101	1001	2001	108
Borehole E	51	951	1951	63.7
Trench F1	149.5	1049.5	2049.5	173.4
Trench F2	126.5	1031.5	2031.5	153.3
Trench F3	149.5	1049.5	2049.5	169.3
Trench F4	126.5	1031.5	2031.5	148.5
Trench F5	149.5	1049.5	2049.5	166.5

- Special test case that looks at the impacts of multiple facilities on release described in the next section.

6.3 Basis for Comparison

For each radionuclide simulated in each test case, the following summary results should be reported for each receptor location.

- Peak concentration
- Time to peak concentration
- Ratio of Peak Concentration to Base Case (homogeneous) peak concentration
- Ratio of Time of Peak Concentration to Time of Base Case Peak concentration.
- Peak Flux out of the bottom of the facility (note in 2 or 3-dimensions this will require integration over the area of the facility).
- Time to Peak Flux at the bottom of the facility
- Ratio of Peak Flux to Base case Peak flux
- Ratio of Time to Peak Flux to Time of Base Case Peak Flux.

Other parameters, such as the time evolution of concentration at a receptor location or the total mass passing through a receptor location should be reported as necessary to support scientific observations on the impacts of heterogeneities. For example, if the heterogeneous source has a high peak concentration but short duration, this could be plotted against the homogeneous case to illustrate the differences. Another important case that will arise with long-lived radionuclides is that the heterogeneities may impact the timing and peak flux at a receptor location, but the total mass (mass flow rate integrated over time) may not change much. This would have important implications for flux based regulatory limits.

For multi-dimensional analysis, peak and average flux and concentration leaving the disposal facility should be calculated through integration over the distance (2-D) or area (3-D) perpendicular to flow at the receptor location.

7.0 Analysis Results

Step 5 of the performance assessment process involves running the models and obtaining the results for interpretation. Four groups (Lithuania, two from Slovakia, and Brazil) have taken the data presented in Sections 5 and 6 and performed the initial analysis of the impacts of heterogeneities on water pathway concentrations. These four studies examined the following issues:

- Spatial heterogeneities within a single disposal facility (deterministic distribution of wastes)
- Spatial heterogeneities within a single disposal vault (probabilistic distribution of wastes).
- Spatial heterogeneities caused by having multiple disposal cells at a single site. Three-dimensional analytical solutions were used to assess the impacts of a spatially distributed source term. Results for the heterogeneous (spatially) distributed wastes were compared to the homogeneous case where all wastes are placed into a single 'effective' vault.
- Spatial heterogeneities caused by having multiple disposal cells at a single site. This study used the AMBER computer model to represent the 3-dimensional distribution of wastes at the site. In addition the impacts of modelling spatial heterogeneities in inventory in the vault and modelling transport in 1 or 2-dimensions was investigated.

Additional areas of study could include examining heterogeneities introduced by having different waste streams (e.g., large metallic equipment components from decommissioning of nuclear facilities), different waste forms (e.g., many facilities have a mixture of cement and bitumen waste forms), or different waste containers (e.g. carbon steel, stainless steel, cement, etc.). In most cases, processes that spread the release over time (e.g. different release rates from cement and bitumen waste forms) will lead to lower peak release rates from a disposal cell. However, with multiple disposal cells with the opportunity for overlapping plumes this may not always be the case.

The remainder of this section presents the major results and findings of the four studies discussed above. The complete reports on these studies are in Appendices B – E.

7.1 Impact of spatial heterogeneities in source distribution within a single disposal cell using a deterministic approach.

The release from a single disposal cell at the Saratov facility and predicted concentrations at receptor wells was assessed for the case of homogeneous source term and for the case of waste heterogeneity at the bottom of the Vault and at the top as well. The heterogeneity placed 90% of the inventory in 10% of the volume of the disposal cell. Leading to an approximately 10 :1 ratio in concentration between the two zones. Concentrations were uniform outside of the high concentration zone. The system description, material properties, inventory, water flow parameter, calculation scheme, calculation results and analysis of impacts of source term heterogeneities on releases followed the test problem description in Section 5 and are presented in detail in Appendix B.

7.1.1 Computational Approach

DUST-MS v.3 and **GWSCREEN v.2.03** codes were employed for the performance of the calculations. The assessment of the transport in the Waste Zone and Vadose Zone has been performed using DUST-MS code. The assessment of the transport in the Saturated Zone has been performed using GWSCREEN code.

The *base case* of homogeneous source term and two options of the *test case* for heterogeneous source term of high concentration 1) at the bottom and 2) at the top of the repository have been assessed. The 1-D transport of the nuclides has been assessed in flow direction for the Vault and Vadose Zone. The 2-D transport of the nuclides has been assessed in flow and in transverse directions for the Saturated zone. The calculations has been split in to the three consecutive steps (runs):

- 1) Assessment of the vault and generation of the boundary conditions data file of fluxes for the vadose zone run (DUST-MS);
- 2) Assessment of the vadose zone and generation of the boundary conditions data file of fluxes for the saturated zone run (DUST-MS);
- 3) Assessment of the saturated zone (GWSCREEN).

The same calculation scheme has been used for both homogeneous and heterogeneous calculation cases.

From the over 30 radionuclides found in the inventory, the following were selected for assessment :

- H-3 (short-lived, high mobility)
- I-129, C-14 (long-lived, high mobility)
- Pu-239, Ra-226 (long-lived, low mobility).

Short-lived low mobility radionuclides such as Cs-137, were not analyzed in detail. Screening calculations suggested that these would not reach the aquifer in measurable concentrations. The inventory, half-life, and Kd value for the selected radionuclides is in Table 4. Figure 3 presents the geometry used in the analysis.

7.1.2 Results

The values for peak concentration and peak flux was monitored as well as the time of the peaks for each radionuclide at the following locaitons :

- The bottom of the cement vault
- The bottom of the vadose zone
- Receptor well 70, 100, 1000, and 2000 m from the edge of the facility.

Figures showing the time evolution of concentration and flux at each of these points was generated for each test case and radionuclide. The complete set of figures is in Appendix B. Figure 4 shows a representative example for H-3 concentrations at the different locations for the homogeneous test case. Figure 5 shows the same information for I-129.

Table 4 : Inventory, half-life, and Kd of modeled radionuclides.

Class	Nuclide	Half Life, yrs	*) K _d , cm ³ /g	Activity, MBq
SLW, <i>high mobility</i>	H-3	12.33	0	916 023
LLW, <i>high mobility</i>	I-129	1.590*10 ⁷	1	3 726
	C-14	5.730*10 ³	5	74
LLW, <i>low mobility</i>	Pu-239	2.411*10 ⁴	550	209 3707
	Ra-226	1.600*10 ³	500	56 120

Both figures 4 and 5 use a log scale for concentration on the Y-Axis. The X-axis is the time in years. For H-3, figure 4, concentrations are quite high at the bottom of the vault and decrease with distance. The concentrations at the bottom of the vadose zone follow very closely with those at the bottom of the vault. This is due to the relatively fast travel time through the 70 m vadose zone for H-3. At 100 years, there is a marked increase in concentration at the bottom of the vault caused by the increased flow at this time due the simulation of the failure of the engineered barrier. Peak aquifer concentrations of H-3 are 3-4 orders of magnitude lower than at the bottom of the vault. This is due to dilution from the higher flow rate in the aquifer as well as radioactive decay and dispersion.

For I-129, figure 5, the behavior is different. Even with a K_d of 1, the travel time through the unsaturated zone becomes on the order of a few hundred years as evidenced by the time t_{peak} concentration. Note, the time scales in figures 4 and 5 are different. Again, peak aquifer concentrations are much lower than in the vadose zone due to dilution. In this case, the peak concentration at 100 meters is approximately a factor of 5 greater than at 2000 m. The cause for the decrease is dispersion, as decay does not come into play due to the long half-life of I-129.

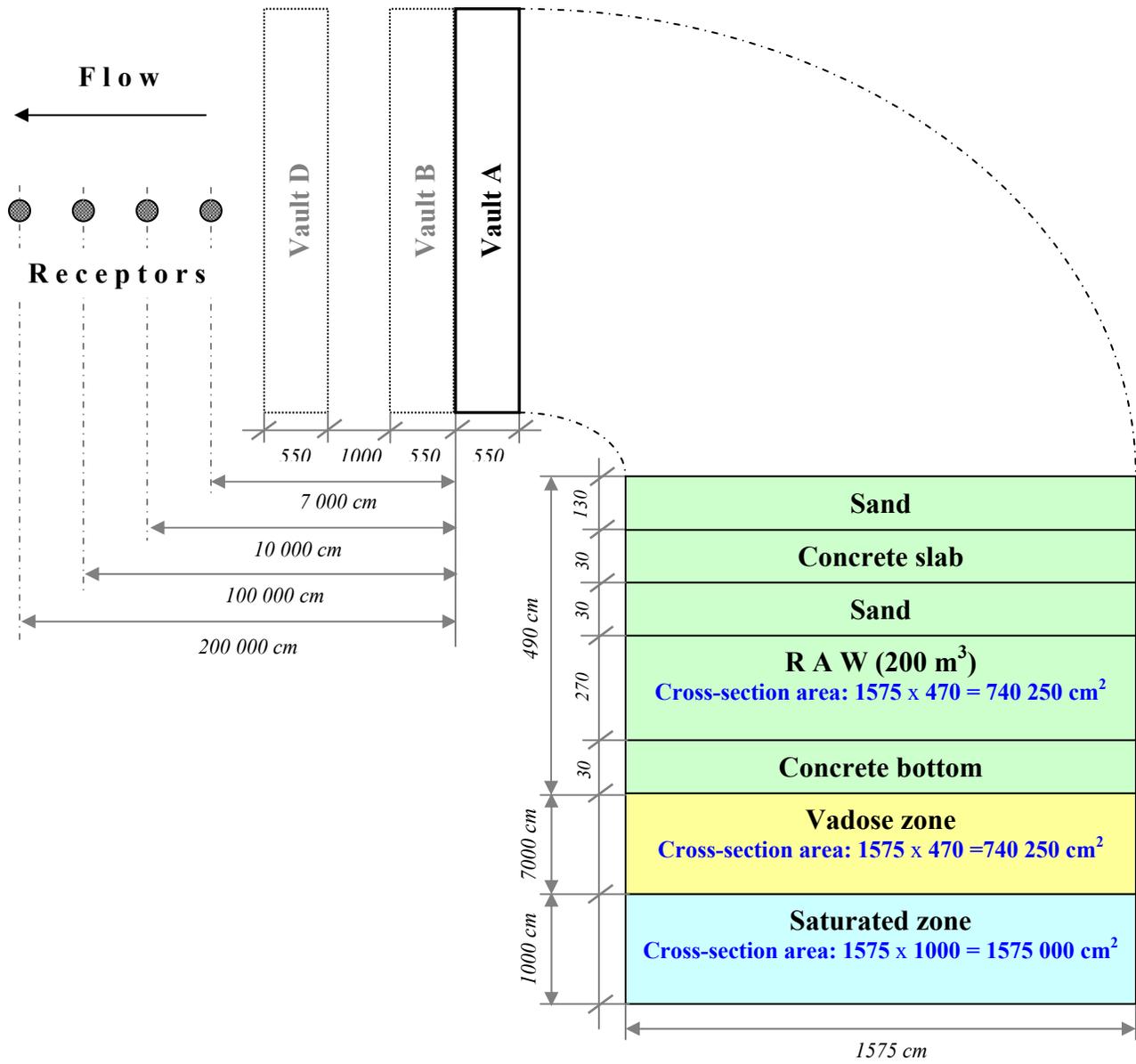


Figure 3. Geometry used to analyze the impact of heterogeneities from a single Vault.

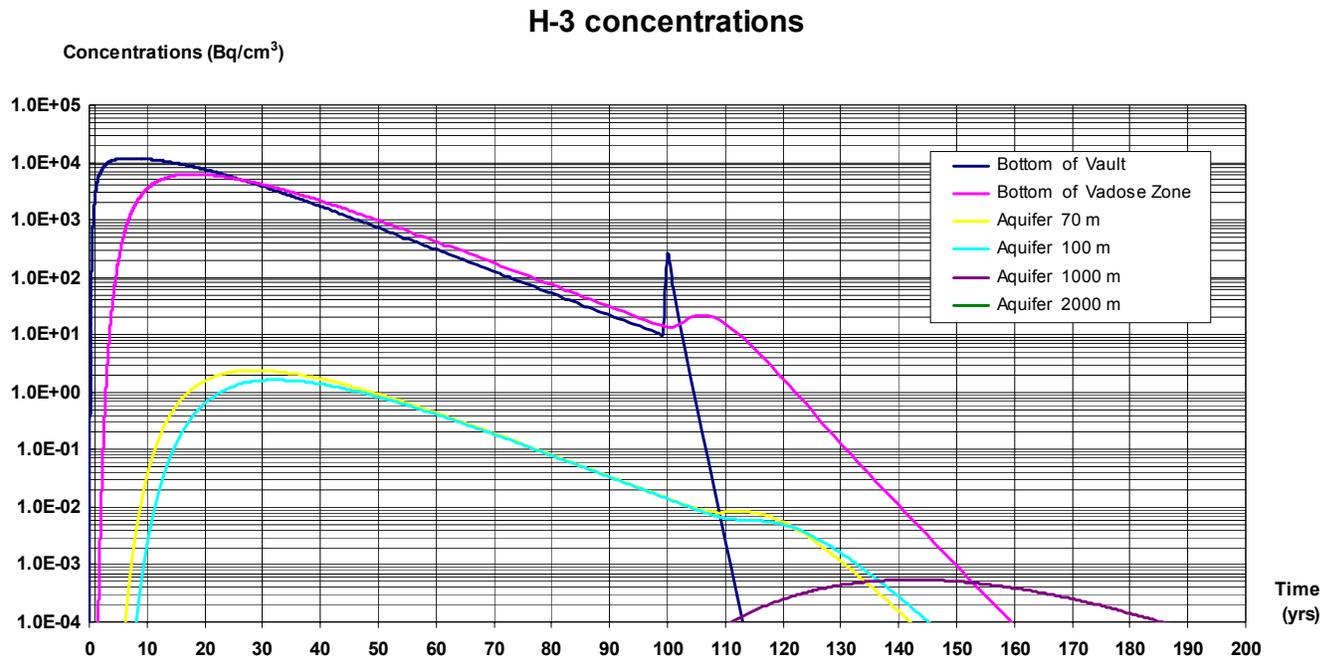


Figure 4. H-3 concentrations at the receptor locations for the homogeneous distribution of wastes within the vault.

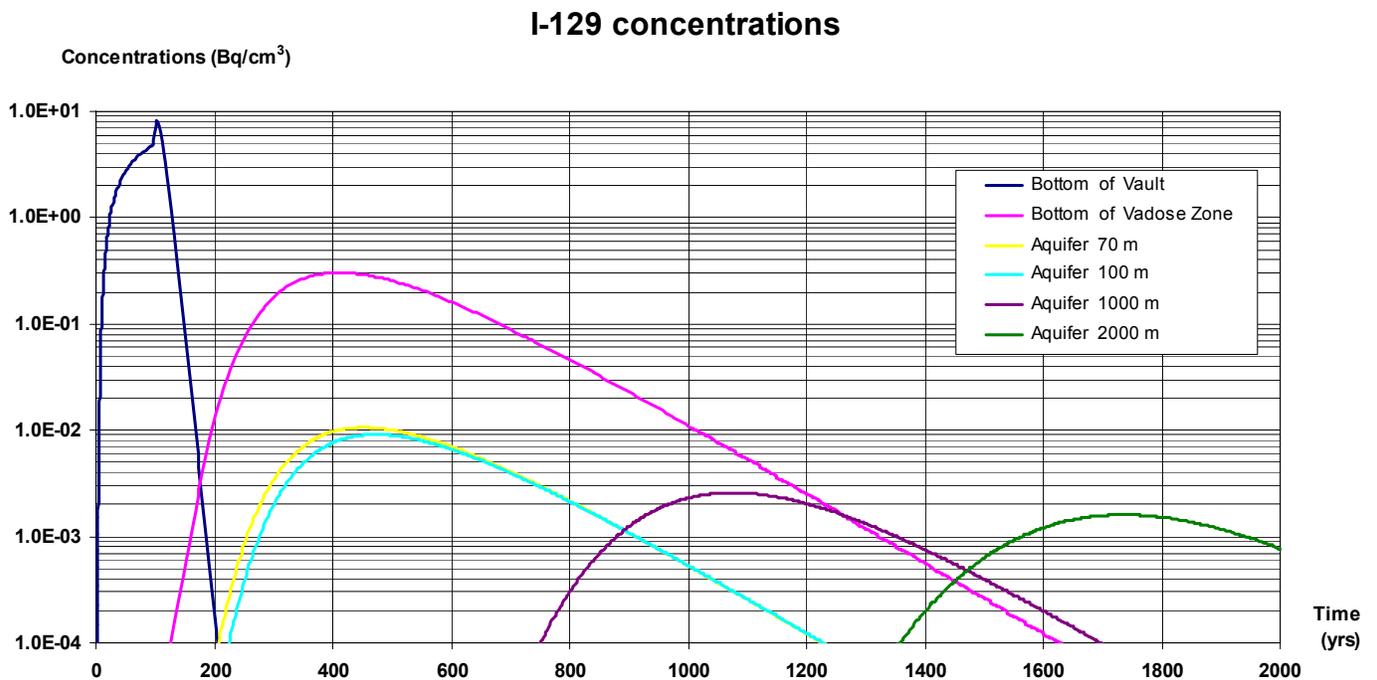


Figure 5 I-129 concentrations at the receptor locations for the homogeneous distribution of wastes within the vault.

Figure 6 and 7 show a graphical comparison of the concentrations at the bottom of the vault for H-3 and I-129 for the three cases : a) homogeneous distribution, b) high concentrations of waste at the bottom of the vault, and c) high concentrations at the top of the vault. For H-3, having the high concentrations near the bottom of the vault lead to 60% increase in peak concentration over the base case. Considering this location is less than 1 meter from the waste zone and that a concentration difference of approximately a factor of 10 exists between the high concentration region in the heterogeneous case and the homogeneous case, it is clear that diffusion/dispersion quickly reduce the concentration differences. The peak time for concentration is very early (10 – 15 years) due to the radioactive decay of H-3. The homogeneous case actually had a slightly higher peak concentration than the heterogeneous case with the high concentration at the top of the facility. This is due primarily to radioactive decay effects.

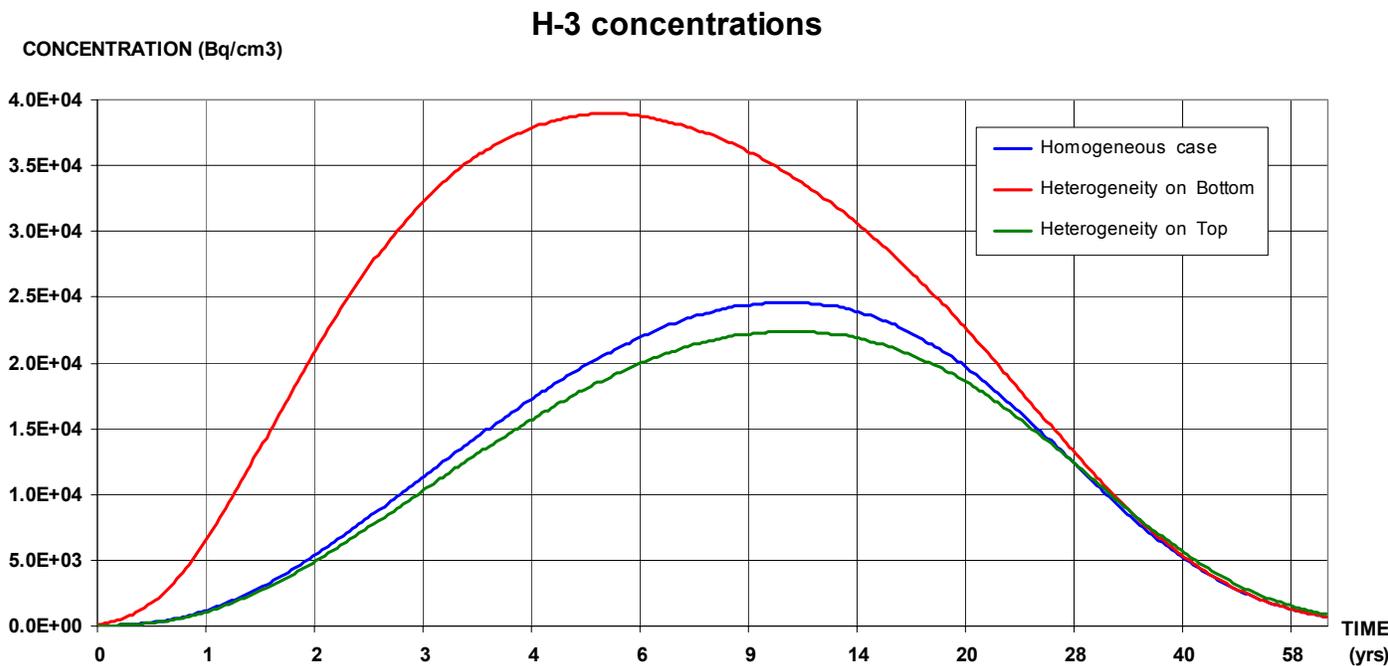


Figure 6 H-3 concentrations at the bottom of the vault for the three distributions of wastes in the vault.

Figure 7 shows the same information for I-129 at the bottom of the vault. In this case, the peak concentration (and flux) occur shortly after the engineered barrier fails at 100 years. Once again, the high concentration waste zone at the bottom of the facility leads to highest predicted concentrations. However, this time the difference is less than 20%. The homogeneous case and the high concentration at the top of the facility showed similar results. This indicates that over a distance of approximately 3 m, dispersion and diffusion have worked to smooth out the order of magnitude difference in initial concentrations in the heterogeneous case.

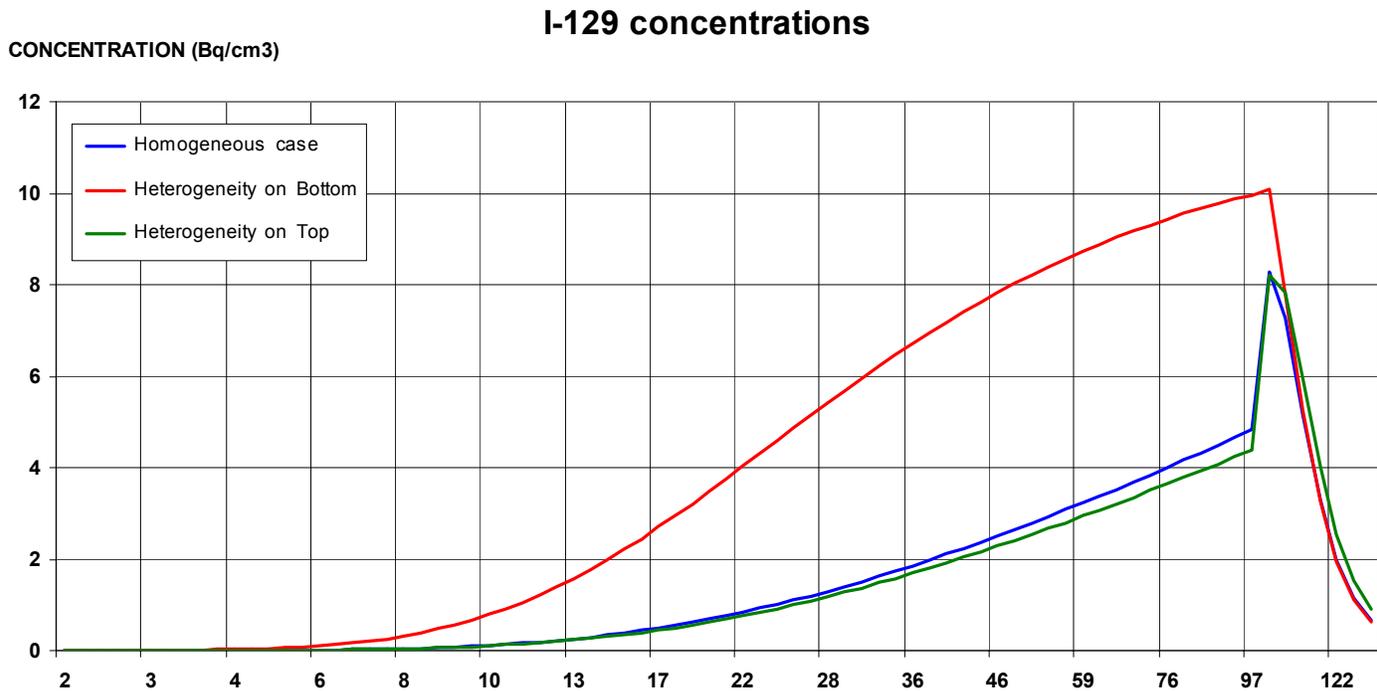


Figure 7 I-129 concentrations at the bottom of the vault for the three test cases.

Plots similar to figures 6 and 7 for the bottom of the vadose zone, and 70, 100, 1000, and 2000 m distances in the aquifer for all of the radiounuclides are in Appendix B. Appendix B also contains tables comparing the peak concentrations for the heterogeneous cases to the homogeneous case.

7.1.3 Analysis of results

1. The calculation results presented for **homogeneous case** demonstrate nuclide dependent behavior of the concentration and flux at various selected locations of receptors. In general the degradation of engineered barriers after 100 years has no impact to the release of *nonsorbing* nuclide (H-3) because it leaves the Vault Zone before degradation of the barriers nuclides due to high mobility. The same is with *strong sorbing* nuclides (Pu-239, Ra-226), but these nuclides leave the Vault far after Vault failure due to low mobility. The peak concentration/flux of *poor sorbing* nuclides (I-129, C-14) at the bottom of the Vault is reached approximately just after 100 years due to increased water flow after Vault failure. The peak concentration is approximately of the same order at various distances in Aquifer Zone for long-lived nuclides of high mobility (I-129, C-14) due to slow decay.

2. From the calculation results presented for **heterogeneous case at the Bottom of the Vault** the ratio of peak concentration value in the heterogeneous case to the homogeneous case is less than twice at the bottom exterior of the vault. This occurs even though there is a 10 :1 difference in initial concentrations in the vault due to the heterogeneity. The ratio of time to peak concentration asymptotically increases from 0.5 for H-3 (earlier for heterogeneous waste) to 1.0 with the increase of distance from the waste zone to the point of comparison.

3. From the calculation results presented for **heterogeneous case at the Top of the Vault** it is observed that the ratio of peak concentration values for the heterogeneous and homogeneous case varies within range of $\pm 10\%$ for all nuclides. In this case with the 10 :1 difference in initial concentrations at the top of the vault, the discrepancy becomes smoothed out over the 3 m transport distance to the bottom of the vault. The ratio reaches definite value for LLW nuclides (I-129, C-14, Pu-239, Ra-226) but asymptotically moves to 1 for SLW nuclide (H-3) with the increase of distance from the Vault to the receptors. The ratio of peak times is close to 1.0 for all nuclides at various distances of the receptors.

4. It is concluded that the impact of heterogeneity on releases of nuclides has stronger effect in case of heterogeneous RAW at the Bottom of the Vault than in case of heterogeneity at the Top of the Vault when it is close to homogeneous case for the option of heterogeneity at the Top of the Vault.

7.2 Impact of spatial heterogeneities in source distribution within a single disposal cell using a probabilistic approach.

The impacts of a random distribution of wastes within the a disposal vault with a region of high concentration has been analyzed for a single disposal cell at the Saratov facility and predicted concentrations at receptor wells was assessed for the case of homogeneous source term and for the case of waste heterogeneity throughout the facility with high concentrations at either the top or the bottom of the facility. To accomplish this, a probabilistic wrapper was prepared to use in conjunction with the DUST-MS computer code and the inventory was allowed to vary randomly. Details of the mathematical model, conceptual approach and the results are presented in Appendix C.

7.2.1 Computational Approach

DUST-MS is deterministic code developed for low-level waste source term analysis. DUST-MS simulates one-dimensional release of radionuclides from a wasteform and transport. To perform a probabilistic calculation an adapted version MCDU of the LISA code (developed by A. Saltelli at the CEC JRC at Ispra) has been applied. The DUST-MS code is used as a subroutine in the MCDU code. MCDU uses Latin Hypercube Sampling to sample parameter values for stochastic calculations. In conjunction with MCDU, DUST-MS calculates the distribution of flux and concentration at the specified locations. In addition MCDU performs sensitivity analysis for 20 parameters of DUST-MS. After development of the combined code, a verification run was performed using the combined MCDU/DUST-MS code and comparing the results to the deterministic DUST-MS code.

For the probabilistic test problem, 10 containers were simulated, Figure 8. For the base case, each container starts with an initial ^{129}I inventory of $5.55 \cdot 10^8$ Becquerels. From there, a series of ten cases were simulated with 90% of the inventory in one container with the remaining 10% distributed randomly through the other containers. Parameters for water flow were Darcy velocity 35 mm/yr prior to failure of the engineered barriers 0-100yr ; 350 mm/yr after failure engineered barriers. Release from the waste form was simulated using rinse release with a zero partition coefficient. Simulations were also performed for a homogeneous distribution of wastes outside of the hot-spot region as a basis for comparison.

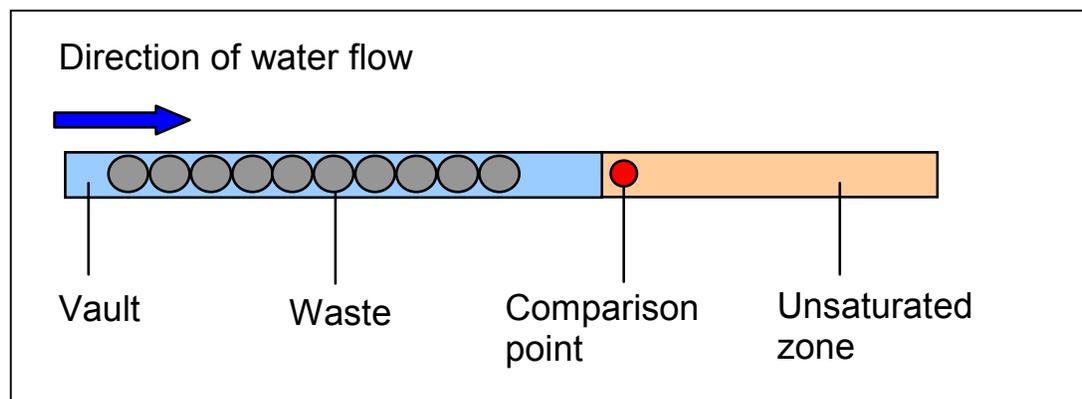


Figure 8 Location of waste containers and comparison point for probabilistic analysis.

7.2.2 Results and Discussion

Table 5 provides the maximal flux for deterministic and probabilistic simulations with

- a) Uniform (homogeneous) inventory distribution
- b) 90% of inventory in the designated location and the remaining 10% being randomly distributed in the other containers. For the non hot-spot containers, the inventory was allowed to vary between $\pm 20\%$ of the mean value with the sum of the inventories the same as for homogeneous deterministic case.

For I-129, which is relatively mobile, there were two local and distinct maximums in flux. The first came after approximately 50 years, while the second came immediately after the engineered barrier was assumed to fail at 100 years. In Table 5, subscript 1 refers to the first local maximum, while subscript 2 refers to the second local maximum. The flux was much greater immediately after the engineered barrier failure due to the 100-fold increase in flow rate. These effects are shown in Figure 8. The concentration only showed one maximum and this occurred at approximately 50 years for all cases. After failure of the engineered barrier, the concentration quickly decreased as the majority of the ^{129}I moves out of the waste zone.

Table 5 Comparison of maximal flux and time of the maximal flux for the different inventory distribution in the deterministic and probabilistic cases.

Simulation	Time of maximum [y]		Maximal flux [Bq/cm ² /y]	
	T _{1max}	T _{2max}	F _{1max}	F _{2max}
Deterministic				
uniform waste distribution	52	101	17.1	75.5
90% of inventory in the top	65	101	15.9	92.9
90% of inventory in the middle	54	101	17.3	78.5
90% of inventory in the bottom	38	101	20.4	55.4
Probabilistic				
uniform waste distribution	52	101	16.9* 17.1**	74.5* 76.5**
90% of inventory in the top	65	101	15.9* 15.9**	92.4* 93.3**
90% of inventory in the middle	54	101	17.3* 17.3**	78.4* 78.7**
90% of inventory in the bottom	38	101	20.2* 20.5**	55.0* 55.9**

* 5th percentile

** 95th percentile

Table 5 provides the following information.

- The time of the first local maximum T_1 depends on the location of the hot-spot and is independent of whether a probabilistic or deterministic analysis is performed.
- The differences introduced by having small variations ($\pm 20\%$) in the inventory in the non-hot spot locations lead to small changes ($< 1\%$) in predicted maximum flux.
- The range of predicted maximum flux (F_2) was between 55 and 93.3 Bq/cm²/yr depending on the location of the hot-spot. While the predicted maximum for a uniform distribution was 75.5 Bq/cm²/yr, which is in the middle of the range.
- For 90% of the inventory in 10% of the volume, the difference in waste form concentrations between the hot-spot and other waste forms is approximately 99:1. However, the maximal flux difference for a hot-spot as compared to a uniform waste distribution is only 24%.
- The highest flux occurs when the hot-spot is located at the bottom of the facility. At this location, there is only 0.5 meters distance between the hot-spot and the comparison point.

The last two bullets suggest that dispersion/diffusion quickly smooth out large changes in concentration that could arise due to non-uniform distribution of wastes.

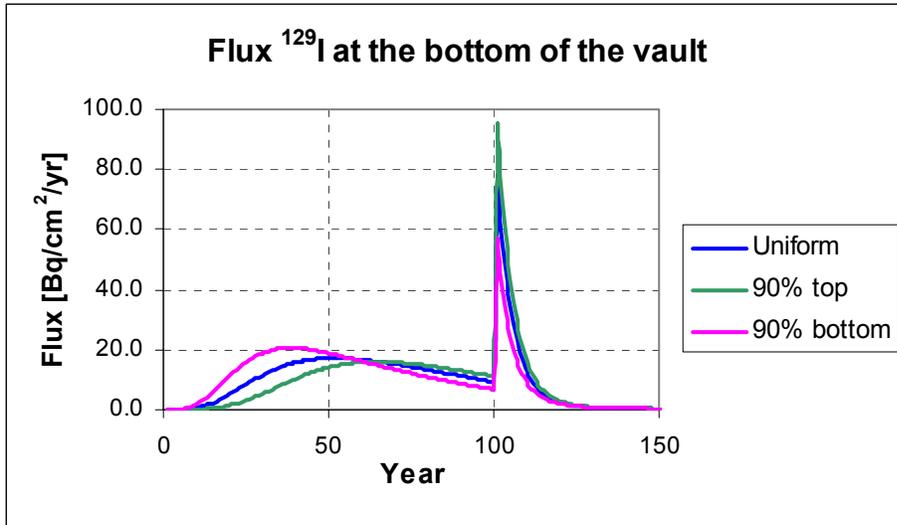


Figure 9 ¹²⁹I flux at the bottom of the vault for three distributions of wastes in the facility.

7.3 Impacts of Spatial Heterogeneity in Disposal Cells using 3 dimensional groundwater transport modeling

The objective of this analysis was to investigate the influence of the spatial heterogeneity of wastes on the site scale on peak concentrations and fluxes at selected locations. The disposal units and geometry at the Saratov site were used as the basis for these calculations. Each disposal unit has its own waste inventory and characteristics. For this test problem, the wastes were distributed homogeneously within each disposal unit. 3-D analytical solutions were developed specifically for the ASAM project to evaluate the influence of the facility heterogeneities on the performance of the whole disposal system.

A test case, Appendix A, was developed to analyze the impact of lumping all of the wastes into one extended facility as opposed to considering the same spatial and inventory distribution of the Saratov site. Details of the approach and the results are presented in Appendix D.

7.3.1 Computational Approach

The 3-D conceptual model considers the projection of the Saratov disposal facilities (vaults, trenches and borehole) on a horizontal plane, at the top of the groundwater pathway, as shown in Figure 10. The five trenches are in the lower-left, the four vaults are in the center section and the borehole is in the upper right of this figure.

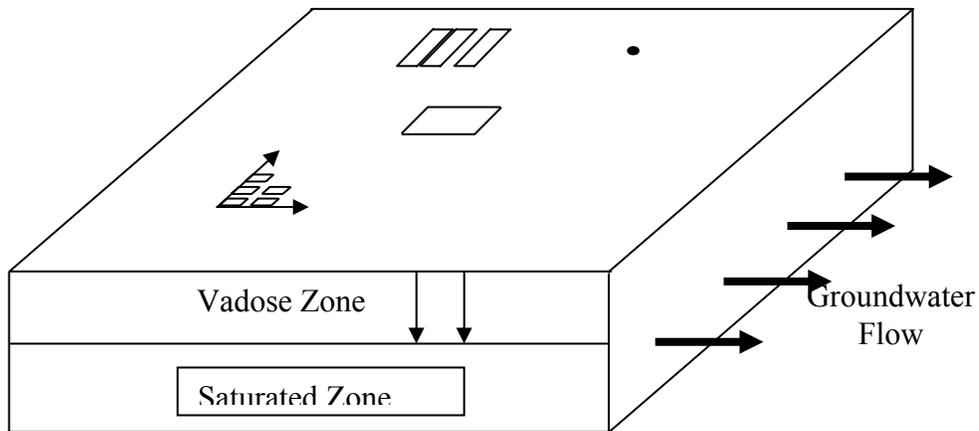


Figure 10 3-dimensional model of the site.

In order to represent spatial heterogeneities of the Saratov site, a coordinate system was defined in the horizontal x - y plane (Figure 11), where the position of each facility can be identified by its (x_{min}, x_{max}) and (y_{min}, y_{max}) boundary coordinates (see Appendix D Table 1). The receptor wells, used for the concentration calculations, were intentionally located along the centerline of each group of facilities, represented by the 3 lines on Figure 11, with the corresponding coordinates given by Appendix D, Table 2.

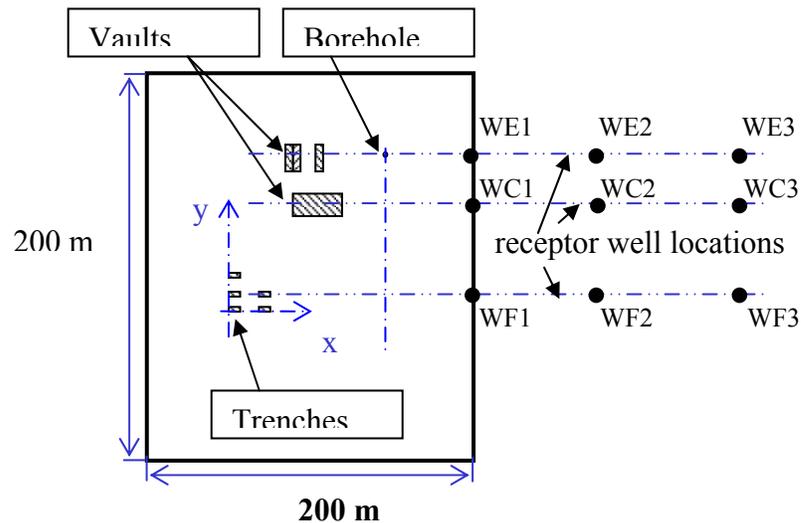


Figure 11 x - y co-ordinate system for disposal facilities and wells.

The model assumes one-dimensional vertical transport in the vadose zone using the flow rates consistent with the prescribed engineered barrier performance (3.5 mm/yr for time < 100 years and 350 mm/yr after that). Three-dimensional transport is considered in the saturated zone with flow along the X-axis and diffusion/dispersion leading to transport along the other axes. Release from the waste forms is assumed to occur instantaneously. Transport parameters defined in Appendix A were used for the simulations. For H-3, a special case was simulated in which the dispersion parameters were reduced by a factor of 10. This set of analysis led to improved understanding on the effects of dispersion on peak concentrations and fluxes.

Instead of analyzing for all radionuclides, two radionuclides from the Saratov inventory were analyzed from each of the four classes defined in the test problem as follows.

- a) Short-lived, low mobility, high inventory (Cs-137 and Ni-63);
- b) Short-lived, high mobility, high inventory (H-3 and Sr-90);
- c) Long-lived, high mobility (I-129 and Tc-99);
- d) Long-lived, low mobility (Am-241 and Pu-239).

The impact of lumping all of the wastes into one facility as opposed to modeling the spatial distribution of facilities was investigated. A comparison was made for each radionuclide between a test case that considers the same spatial and inventory distribution of the Saratov site and a homogeneous base case that lumps all of the wastes in an “extended vault C”, with the same properties of Vault C, however with different dimensions to accommodate the increased volume of waste from the other disposal cells.

For each radionuclide simulated in each test case, the following summary results are reported in Appendix D for each receptor location:

- Peak concentration, C_{max} (MBq/m³);
- Time to peak concentration t_c (yr);
- Ratio of Peak Concentration to Base Case (homogeneous) peak concentration, C_{max}/C_r ;
- Ratio of Time of Peak Concentration to Time of Base Case Peak concentration, t_c/t_{cr} ;
- Ratio of Peak Flux to Base case Peak flux, ϕ_{max}/ϕ_r ;
- Ratio of Time to Peak Flux to Time of Base Case Peak Flux, t_{pf}/t_{fr} ;
- Peak Concentration at the bottom of the facility, C_b (MBq/m³);
- Time to Peak Flux at the bottom of the facility, t_{bc} (yr);
- Peak Flux out of the bottom of the facility, ϕ_b (MBq/yr);
- Time to Peak Flux at the bottom of the facility, t_{bf} (yr).

7.3.2 Results and Discussion

The main objective of this study was to compare concentrations and fluxes from two cases: wastes modeled in their actual spatial distribution at the site, and a hypothetical situation in which all of the waste is placed in one hypothetical vault at the center of the site. For these simulations, this hypothetical vault was chosen to be an extension of the largest vault at Saratov, Vault C.

The flux and concentrations at the bottom of the facility are reported in Appendix D, Table 14 and 15 for the distributed facilities case and Table 20 for the homogeneous facility in an extended Vault C. The distributed facilities case had at least one facility that had fluxes and concentrations 50 – 100% higher than the homogeneous case. The cause for this is the non-uniform distribution of inventory in the different facilities. Smaller vaults often contain a higher percentage of the inventory than the ratio of the vault volume to the total volume of all vaults. Therefore, depending on the vault size and inventory, the flux and concentration out of the bottom can be higher than for the homogeneous case.

In this simulation, there are three lines of receptor wells. One line is located in front of the Vaults A, B, and D and the spent source borehole. The second is located in front of Vault C, and the third is located in the center of the soil disposal trenches. The radionuclides in these simulations were not found in the trenches and therefore, the fluxes and concentrations in front of the trenches were several orders of magnitude lower than at the other locations. Comparison of fluxes and concentration between the two cases was not straightforward. For the distributed facilities simulation, in some cases, the well in front of Vaults A, B, and D had the highest values, in other cases the wells in front of Vault C had the highest values. For the extended vault C case, the highest values are always in front of the source. The extended vault C values along the line in front of vault C are used as the homogeneous case basis for comparison. Due to the higher values being in different locations, comparisons were made between the concentration and flux for three cases: a) values in front of Vaults A, B, and D to the extended vault C, b) front of Vault C (distributed source) to the extended Vault C, and c) sum of values in front of Vaults A, B, and D and Vault C to the extended vault C case. Comparison C is conservative as it does not count for dilution that would occur by mixing the concentrations from the two regions.

The peak flux and concentration at the receptor wells at 155 m, 1055 m, and 2055 m from the Saratov site centerline are presented in Appendix D, Tables 16 – 19 for the distributed facility case and in Tables 21 and 22 for the homogeneous extended vault C. The ratios of peak concentration and flux for the distributed case to the homogeneous case are presented in Tables 23 – 26. A ratio of greater than 1 indicates that the distributed case had a higher peak flux or concentration. The fluxes and concentrations for the comparison of Case a) or b) from above, Tables 23 and 24, were greater than the homogeneous case at the nearest receptor well for Sr-90, Tc-99, and I-129. The distributed vaults led to 17 to 78% higher concentrations and 53 to 78% higher flux than the homogeneous case. For H-3, the homogeneous case gave slightly higher concentrations in Case a and b. The conservative case c) above which adds the concentrations at the two different wells to get a concentration always had higher peak concentrations than the homogeneous case, Table 25. Peak concentrations were 43 to 78% higher for the distributed case as compared to the homogeneous case.

The ratio of the peak concentrations and fluxes from the distributed case to the homogeneous case increased with distance from the source (i.e. homogeneous case becomes less conservative with distance). This is believed to be due to mixing of the plumes with the distributed source leading to lower dilution from dispersion. With a distributed source, the plumes from Vault C and Vaults A, B, and D have more and more overlap as the distance from the source increases. This overlap causes gradients in concentration to decrease and therefore, dispersion decreases leading to higher concentrations.

The saturated zone travel times from each facility for each radionuclide to a well at the facility boundary ($X = 155.5$ m) is presented in Appendix D, Table 13. The travel times indicate that the peak arrival time can vary by as much as 25% from different facilities due to the different travel distances. This suggests that accounting for different facilities will lead to longer duration of contamination at the well, but at lower peak concentrations due to the different travel times. This suggests that using a single 'lumped' facility will generally lead to higher predicted doses and fluxes as compared to distributing the facilities consistent with their spatial arrangement based on travel time alone. Since the results suggest higher fluxes and concentrations from the individual facilities, it is clear that the impacts of travel time have only a secondary effect under the test conditions. The table also shows that due to low-mobility caused by sorption, radionuclides such as Cs-137, Ni-63, Am-241, and Sr-90 will not reach the wells in high concentrations as the travel time exceeds 10 half-lives.

H-3 was chosen to study the effects of dispersion ($\alpha_x = 10$ m, $\alpha_y = 1$ m and $\alpha_z = 0.1$ m) on the merging of contaminant plumes. Appendix D Figures 3 to 8 show the concentration isolines (values ranging from $1.E-07$ to 50 MBq/m³) and isosurfaces ($C = 0.5$, $1.E-02$ and $1.E-04$ MBq/m³) obtained at $t = 5, 25, 50, 75, 100$ and 150 yr. One can see that the vertical distribution of concentrations is nearly uniform due to vertical dispersion.

The use of dispersion coefficients more representative for smaller distances was adopted as an additional test case for the migration of H-3, considering a characteristic length of 100 m to calculate the dispersion coefficients ($\alpha_x = 1$ m, $\alpha_y = 0.1$ m and $\alpha_z = 0.01$ m). The results are shown in Tables 14 to 26 and in Figs. 9 to 14 in Appendix D, where one can observe a small spreading of the contaminant plumes and higher values of concentration than in the previous case. The values of concentration calculated at the bottom of each facility are almost one order of magnitude higher than in the previous case, indicating a strong influence of dispersion on the mass transport of high mobile nuclides.

7.3.3 Conclusions

Many sites would like to use a single effective facility to represent all of the individual disposal facilities at the site. The question arises as to whether this is conservative or not. For the inventory distribution and conditions at the Saratov site use of a single homogeneous vault to simulate the entire waste contained at the facility underpredicted the release obtained using the actual spatial distribution of facilities. Using the complete spatial distribution led to as much as 78% higher fluxes and concentrations. The major cause for this lack of conservatism is that the non-uniform distribution of wastes in different facilities leading to higher than site-wide average inventory concentrations in some of the facilities. To overcome the lack of conservatism, the highest concentration for any individual disposal facility could be used to represent the site in an homogeneous simulation.

7.4 Impacts of Spatial Heterogeneity on the Site and in the Source Using One and Two-Dimensional Groundwater Transport Modeling

The objective of this analysis was to investigate the influence of the spatial heterogeneity of wastes on the site scale on peak concentrations and fluxes at selected locations. The disposal units and geometry at the Saratov site were used as the basis for these calculations. Each disposal unit has its own waste inventory and characteristics. The AMBER computer code was used to provide a 3-D representation of the site with 2-dimensional transport simulations in the vadose and saturated zones.

A test case, Appendix A, was developed to analyze the impact of lumping all of the wastes into one extended facility as opposed to considering the same spatial and inventory distribution of the Saratov site. In addition, simulations were performed for the site examining the impacts on groundwater concentration caused by differences in the spatial distribution of wastes inside the individual disposal vaults. Details of the approach and the results are presented in Appendix E.

7.4.1 Computational Approach

The AMBER computer model was used to simulate the releases from the different facilities at the Saratov site. AMBER uses a compartmental approach that can be generalized to provide a 3-dimensional representation of the site using multiple sources and changes in flow between compartments. Coupling between adjacent compartments is allowed through simulation of advection and dispersion processes. Figure 12 provides a plan view of the site and the stream channels used in the simulation. Figure 13 shows the 3-dimensional representation of the site. Coupling between adjacent compartments is designated by the green arrows in the vadose zone and the blue arrows in the saturated zone. Both figures label the disposal vaults (A – D), trenches (F1- F5) and spent-sealed source borehole (labelled as E).

Three major categories of simulation were conducted as part of the ASAM program :

a) Fully heterogeneous two-dimensional transport approach

The contaminants are released from individual disposal facilities into the compartments of top layer of the vadose zone. The vaults A, B and D and the borehole E contribute into the stream B, the vault C contributed into the stream D while trench F5 contributes to stream G and trenches F1 through F4 contribute to stream H. These transfers are visualised in Figure 13 by means of red arrows.

Advection, longitudinal and transversal dispersion are modelled between groundwater compartments (see blue arrows), advection and transversal dispersion are modelled between vadose zone compartments (green arrows). The longitudinal dispersion in vadose zone is omitted.

b) Homogenous two-dimensional transport approach

Under this approach, the geographic distribution of the sources is disregarded and all the sources are deemed to contribute into single stream (D). Figure 14 shows the modelled plan view of the all of the vaults contributing to stream D. However, once the contaminants are released from the facility into the vadose zone, they are allowed to spread through the streams to enable transverse dispersion as under the heterogeneous approach.

c) . Homogeneous One-dimensional transport

This approach is rather typical for the water pathway analysis. All the sources are deemed to contribute into single stream as above, but in addition there is no communication whatsoever with neighbouring streams and the contaminants transport takes place in “closed tube”. This prevents the dilution that will occur due to spreading of the contamination between “tubes” and will lead to the highest predicted concentrations. For this case, additional studies were conducted that examined the variation of radionuclide inventory in the vault. In these studies, 99% of the inventory was placed in one compartment and 1% was placed in a second compartment.

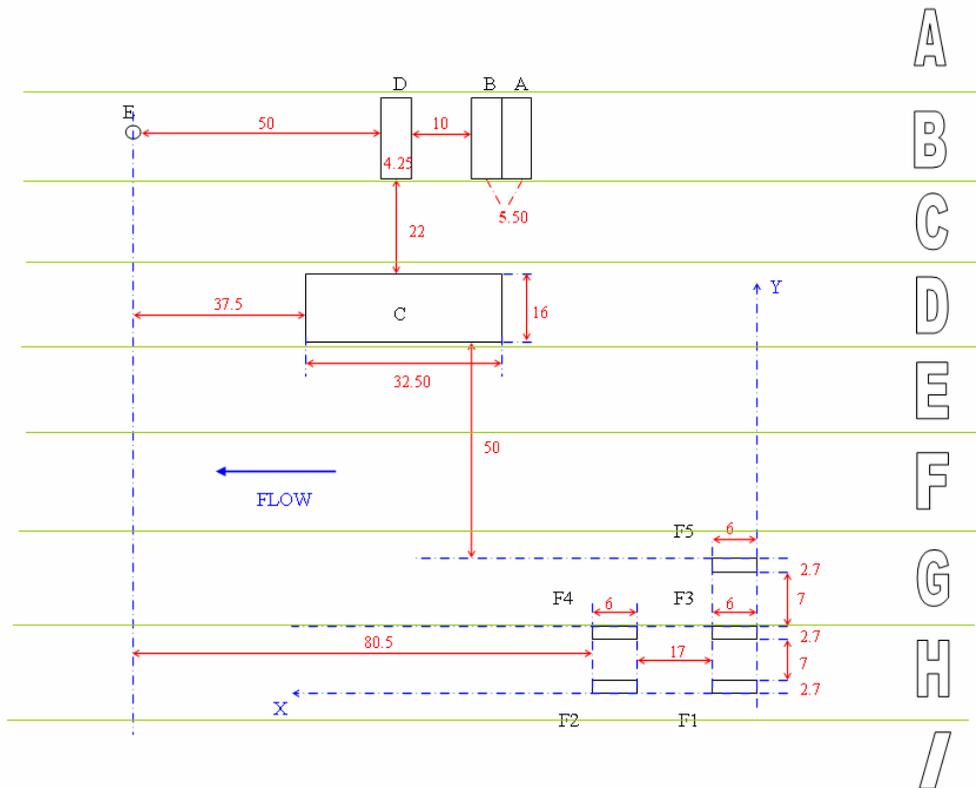


Figure 12 Plan view of the Saratov site showing the stream channels (A – I) used in the simulation.

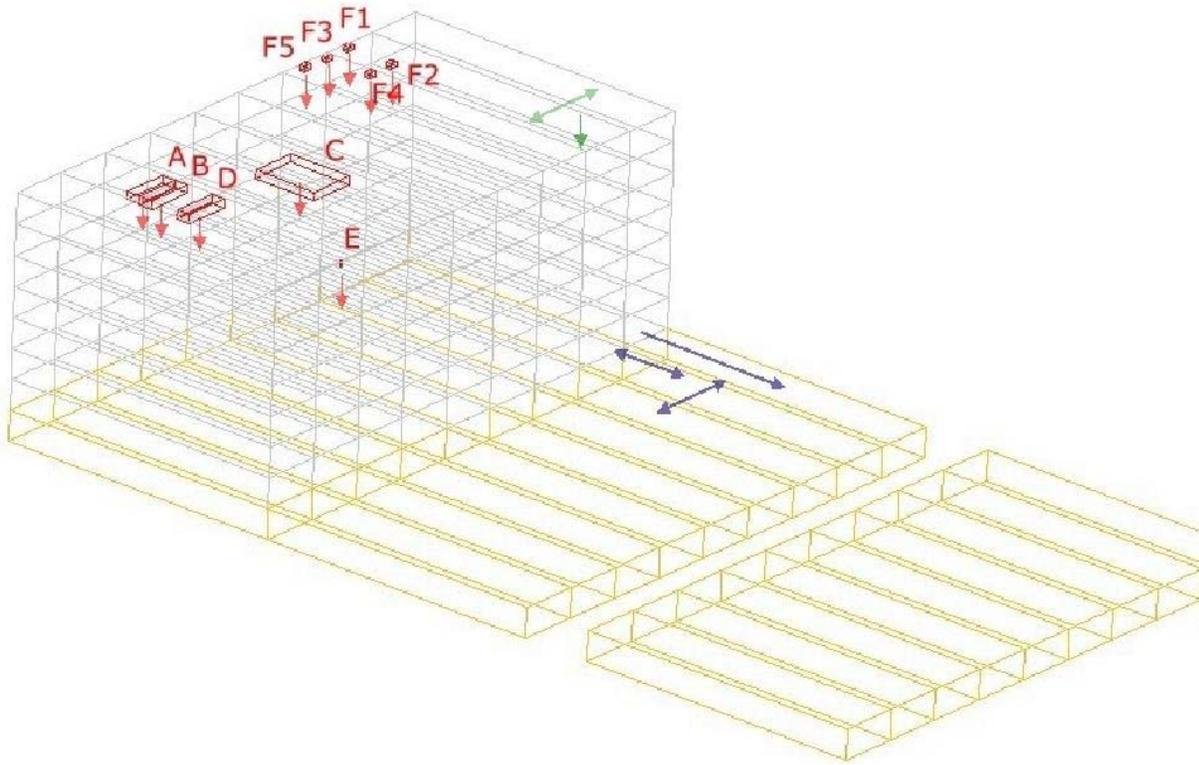


Figure 13 Three-dimensional representation of the Saratov site.

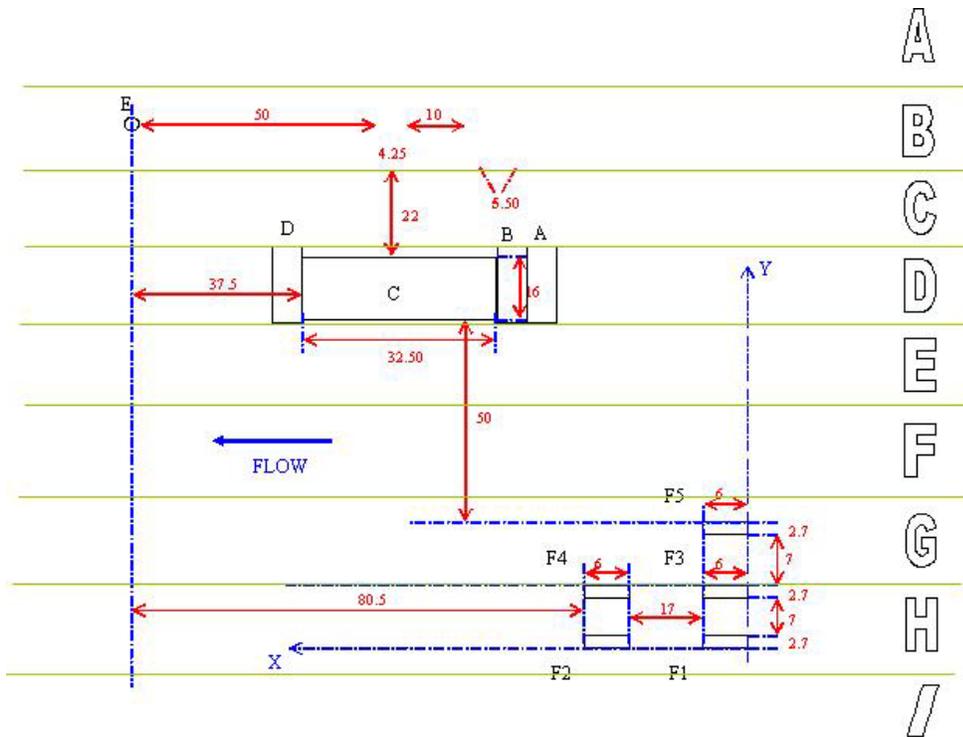


Figure 14 Plan view of the vault layout for the homogeneous test case. All vaults lie above stream tube D.

7.4.2 Results and Discussion

The following radionuclides were modelled in all three cases:

- H-3
- C-14
- Co-60
- Ni-63
- Sr-90
- Tc-99
- I-129
- Cs-137
- Po-210a
- Ra-226 with long-lived chain daughters Pb-210, Po-210
- Th-232 with long-lived chain daughters Ra-228, Th-228c
- U-238 with long-lived chain daughters U-234, Th-230, Ra-226, Pb-210, Po-210
- Pu-238 with long-lived chain daughters U-234, Th-230, Ra-226, Pb-210, Po-210
- Pu-239 with long-lived chain daughters U-235, Pa-231, Ac-227
- Am-241 with long-lived chain daughters Np-237, U-233, Th-229

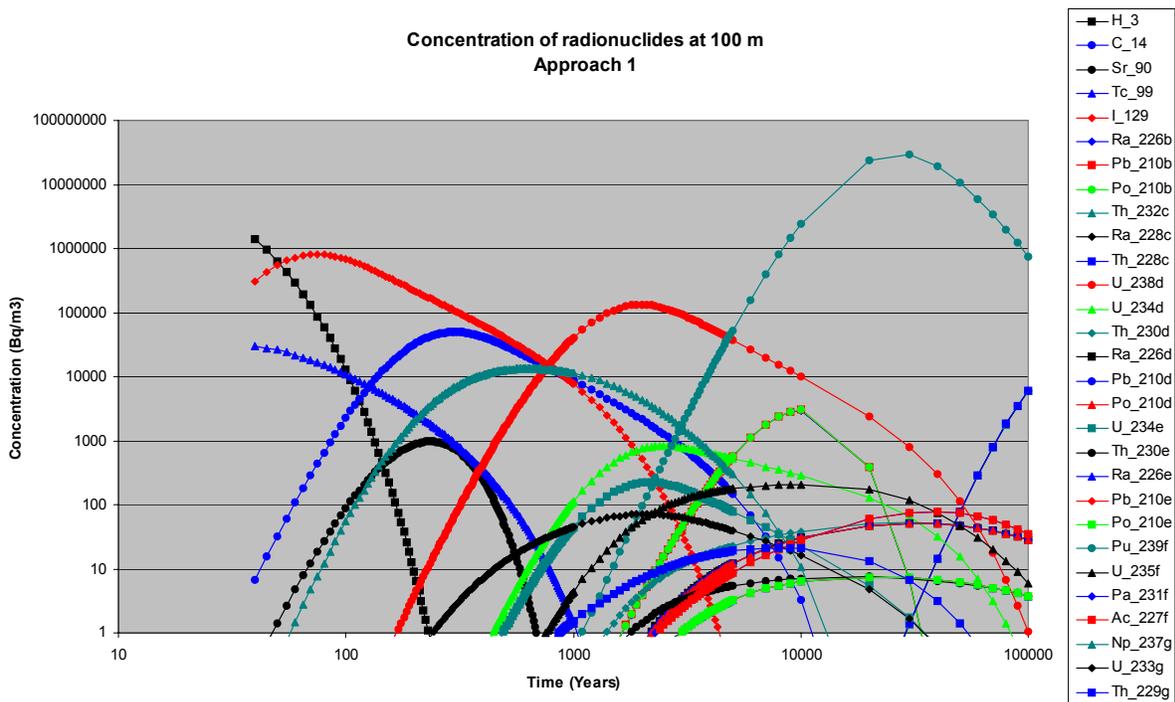


Figure 15 Simulation results for groundwater concentrations at 100 m for the fully heterogeneous case (Case 1).

Concentrations in the groundwater were monitored at 100, 1000, and 2000 m downstream from the facility. Figure 15 provides the results for the peak concentrations at the 100 m distance for the fully heterogeneous case, Case a). Similar figures are supplied in Appendix E for all three cases at distances of 100, 1000, and 2000 m.

Table 6 presents the peak concentrations at 100 m for each test case and each radionuclide. Similar tables are presented in Appendix E for the 1000 and 2000 m distances. Several important findings can be developed from the data in Table 6. First, short-lived immobile radionuclides (e.g. Cs-137, Co-60, Ni-63) do not reach the well. This occurs even though the Cs-137 and Co-60 inventories are the first and second highest in the facility, respectively. Short-lived mobile radionuclides such as H-3 are able to reach the well at 100 m with an appreciable concentration. They also reach the well before the engineered barrier fails completely at 100 years. The engineered barrier was modeled to limit flow to 1/100 of the flow after failure (site annual precipitation rate of 35 cm/yr). This indicates the importance of a barrier at early times for short-lived radionuclides. Release rates would be modeled to be 100 times higher for H-3 if the barrier was not initially present.

Table 6 shows that in general, the predicted concentrations are lowest for the fully heterogeneous case, Case A and highest for the homogeneous case with 1-dimensional transport of the radionuclides in the aquifer. In general, the fully heterogeneous simulation, Case A, has concentrations that are 1 – 1.7 times lower than combining all of the vaults into a region above a single stream tube, Case B. The highest concentrations were predicted by the lumped vault approach without transverse dispersion in the aquifer. Concentrations in Case C were 2 – 5 times higher than in Case B. This supports the importance of dispersion in reducing peak concentrations and fluxes.

Table 6 Peak concentrations at 100 m for each test case.

Concentration of radionuclides in groundwater at a distance of 100 m from source [Bq/m ³]			
Radionuclide	Case a	Case b	Case c
H_3	1 414 933	2 125 595	9 704 302
C_14	49 777	60 973	159 611
Co_60	0	0	0
Ni_63	0	0	0
Sr_90	970	1 206	1 586
Tc_99	30 158	58 519	226 917
I_129	815 968	975 863	2 597 971
Cs_137	0	0	0
Po_210	0	0	0
Ra_226b	2 976	3 382	4 821
Pb_210b	3 018	3 430	4 889
Po_210b	3 018	3 430	4 889
Th_232c	6 090	125 059	214 262
Ra_228c	6 104	125 221	214 588
Th_228c	6 104	125 221	214 588
U_238d	132 968	133 061	352 056
U_234d	831	831	2 797
Th_230d	53	53	333
Ra_226d	51	51	327
Pb_210d	51	51	327
Po_210d	51	51	327
Pu_238e	0	0	0
U_234e	224	302	802
Th_230e	7	9	37
Ra_226e	7	9	37
Pb_210e	7	9	37
Po_210e	7	9	37
Pu_239f	28 807 239	32 830 928	79 318 225
U_235f	206	225	869
Pa_231f	78	84	376
Ac_227f	78	84	376
Am_241g	0	0	0
Np_237g	13 380	13 806	45 799
U_233g	71	73	319
Th_229g	21	22	124

*The letters in the end of radionuclide names indicate membership in the same decay chain

8.0 Conclusions and Future Directions

The issue of the impacts of heterogeneities in source distribution has not been addressed previously in the literature. There is a concern that hot spots originating from sealed sources and other non-routine wastes could cause localized groundwater concentrations that are much greater than would be predicted based upon a homogeneous distribution of wastes. Within the context of the ISAM methodology, the impacts of spatial heterogeneities in waste distribution on groundwater concentrations and fluxes have been examined on two scales: within a single disposal cell and throughout the disposal facility. Four studies have been performed. The first two examined the impacts of spatial heterogeneities within a single disposal cell. One study used a deterministic approach and examined releases for three classes of radionuclides (short-lived high mobility, long-lived high mobility, and long-lived low-mobility). In this study, the hot spot contained 90% of the inventory in 10% of the facility volume. The second study on the disposal cell scale used a probabilistic approach for a long-lived mobile radionuclide that had 99% of the inventory in 10% of the volume. Two studies were also conducted that examined the impacts of heterogeneities on the site scale. Both examined one case using the actual spatial distribution and wastes at the Saratov site; and a second case that combined all of the vaults into a geometry that caused all of the inventory to enter the aquifer in essentially the same location. The major finding of these studies were:

- Heterogeneities within a single disposal vault do not have a major impact on groundwater concentrations. For simulations with 90% of the inventory in 10% of the volume, peak concentrations and fluxes differed by less than a factor of 2 for all radionuclides. This suggests that if predicted dose is more than a factor of two below regulatory concerns, addressing heterogeneities for the water pathway is not important. Care should be taken when applying this finding to sites and conditions other than that which was simulated. However, the studies showed that differences in concentration will be quickly damped by diffusion/dispersion processes.
- For the Saratov conditions, simulating the actual disposal geometry and inventory in the disposal cells had only a marginal effect on groundwater concentrations compared to combining the entire inventory into a single effective facility. In one study, differences between the two cases were less than 5% with the single effective facility giving slightly higher results. In the second simulation, using the actual geometry and inventory had slightly higher peak concentrations (up to 78%) for some radionuclides. The differences in the two simulations are related to modeling assumptions. The important point is that for the Saratov site, there is not a large difference in end results between combining all of the inventory into a single effective vault and considering the detailed spatial distribution in inventory.

Specific findings of the studies that examined heterogeneities within a single disposal vault include:

- Results are radionuclide dependent. For the inventory used in the analysis and conditions at the Saratov site short-lived low mobility radionuclides do not reach the aquifer in any appreciable quantity. This is due in part to the thickness of the unsaturated zone which is 70 m. Long-lived low mobility radionuclides reach the aquifer after a long period of time. The high mobility short and long-lived radionuclides can reach nearby receptor wells at appreciable concentrations
- Introducing heterogeneity with 90% of the inventory in 10% of the volume led to less than a factor of 2 difference in peak concentration and flux immediately under the vault as compared to a homogeneous distribution of wastes for any radionuclide. This indicates that dispersion and diffusion are effective mechanisms for reducing high concentration gradients. The difference between the heterogeneous case and the homogeneous case decreased with distance from the source. Since low-mobility radionuclides reach the aquifer at low-levels, minor changes in peak concentration and flux due to heterogeneities will not be important in demonstrating safety. For the high-mobility contaminants, the impacts of heterogeneities may be important in the groundwater pathway if the homogeneous case is within a factor of 2 of regulatory guidelines. Although, the vadose zone was 70 m in this simulation, the factor of 2 applies just outside the bottom of the vault and therefore, these results should generalize to situations with a thin vadose zone.
- The high concentration heterogeneity at the bottom of the vault led to the largest deviation from the homogeneous inventory distribution base case.
- In the probabilistic simulations, 99% of the inventory was placed in a single container. The results show that use of a homogeneous distribution outside of the high concentration region, gave results essentially the same as the median of the probabilistic simulations. The 95th percent confidence level of the probabilistic simulations was less than 5% greater than the median value. This tight distribution suggests that the peak fluxes and concentrations in the groundwater pathway are more controlled by the total inventory than the distribution of inventory. The highest predicted flux and concentration occurred when the heterogeneity was at the bottom of the facility. In this case, the peak flux was approximately 40% greater than for the homogeneous distribution.

Part of the reason that large heterogeneities in source term distribution do not have a major impact on groundwater concentrations is that the waste zone is only 3 m thick and the first receptor well is approximately 100 m away. Thus, there is ample distance for dispersion and diffusion to smooth out the heterogeneity.

Many sites would like to use a single effective facility to represent all of the individual disposal facilities at the site. The question arises as to whether this is conservative or not. Specific findings of the studies that examined the impact of heterogeneities in spatial distribution of disposal facilities at a site include:

- For the inventory distribution and conditions at the Saratov site use of a single homogeneous vault to simulate the entire waste contained at the facility underpredicted the release obtained using the actual spatial distribution of facilities in one study. Using the complete spatial distribution led to as much as 78% higher fluxes and concentrations. The major cause for this lack of conservatism is that the non-uniform distribution of wastes in different facilities leading to higher than site-wide average inventory concentrations in some of the facilities. To overcome the lack of conservatism, the

highest concentration for any individual disposal facility could be used to represent the site in a homogeneous simulation.

- In the second study, use of a geometry that placed all of the vault releases into a single stream tube was shown to provide essentially the same results as the distributed source case.
- The difference in results between the two studies arises from assumptions on how to model the geometry of the extended vault.
- Both studies found that dispersion was more important than source geometry in estimating peak concentrations and fluxes.

Future Directions

Depending on the participant's interest, three additional areas of study are being contemplated:

- Additional studies to examine the impacts of non-uniform waste release rates (e.g. part cement wastes, part bitumen, large metallic components, etc.) could be performed. This may be useful in addressing the degree of conservatism found in baseline assumptions.
- A complete Safety Assessment of the Saratov site could be performed using a heterogeneous source term. However, if the only changes are in the treatment of source term heterogeneities, the studies reported in this document suggest that the impact on predicted dose will be minimal (< a factor of 2).
- Multi-dimensional analysis of the impact of heterogeneities on release from a vault. All of the studies conducted for this report consider one-dimensional source terms. The impacts of heterogeneities may be greater when modeling in 2 or 3 dimensions where there is the possibility of less communication between the high and low concentration regions due to greater spatial separation. This is not anticipated to be a major issue unless the vaults are approximately the same size as the distance to the nearest well. Preliminary guidance on this issue obtained from the two studies of distributed sources conducted as part of this program suggests that differences will be less than a factor of 2.

9.0 References

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