

NOTICE

All drawings located at the end of the document.

IDENTIFICATION OF OPERABLE UNIT 3 AREA OF CONCERN

U. S. DEPARTMENT OF ENERGY
ROCKY FLATS PLANT
GOLDEN, COLORADO

ENVIRONMENTAL RESTORATION PROGRAM
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ADMIN RECORD

A-DU03-000105

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By *[Signature]*

Date 10/22/92 *[Signature]*

Identification of OU 3 Area of Concern

This report identifies concentrations of Pu⁻²³⁹ in surface soils that can serve as a basis for identifying the OU 3 offsite area of concern. This work expands upon the Generic Risk Assessment for Exposure to Plutonium Contaminated Soils previously reported in the Final Remedy Report (DOE, 1991). In the Remedy Report, DOE reported generic risks for hypothetical recreational and residential exposure scenarios that could arise from exposure to Pu⁻²³⁹ in surface soils. Both scenarios were reported as very conservative and the actual risk would not likely be higher (DOE, 1991). For a nominal 1 pCi/gram Pu⁻²³⁹ surface soil activity concentration the following lifetime excess cancer mortality risks (LECR-M) were estimated:

Exposure Scenario	LECR-M at 1 pCi/gram
Recreational	7E-8
Residential	2E-7

Though conservatively configured, these estimates did not take into account in-growth of Am⁻²⁴¹ as would be expected from equilibrium conditions. Reference levels reported herein do account for in-growth of Am⁻²⁴¹.

To calculate a PU⁻²³⁹ value for 1E-6, the methodology employed is an algebraic solution for one unknown given straight proportionality. As an example, using the recreational LECR-M of 7E-8 at 1 pCi/gram, a 1 E-6 reference level would be derived as:

$$7E-8 \text{ ===== } 1 \text{ pCi/gram as,}$$

$$1E-6 \text{ ===== } X.$$

Solving the proportional inequality gives: $X = 14.3 \text{ pCi/gr}^1$. This is essentially simple linear back-calculation.

All reference levels are based on an assumed residual LECR-M of 1E-6.

Americium can have a significant impact in the characterization of risk and attendant reference levels. Comparing cancer slope factors indicates that Am⁻²⁴¹ is 10-times more potent a carcinogen than Pu⁻²³⁹ by the ingestion route². Through inhalation, both

¹ Note that this is for plutonium only. As americium is factored-in, (assuming straight additivity from guidance (EPA, 1989)) the reference level will go down.

² Ingestion cancer potency factors for Am⁻²⁴¹ and Pu⁻²³⁹ are 3.1E-10 and 3.1E-11 respectively. Inhalation cancer potency factors for Am⁻²⁴¹ and Pu⁻²³⁹ are 4.0E-8 and 4.1E-8 respectively (EPA, 1991).

compounds are of comparable potency (see footnote 2). Am⁻²⁴¹ potency factors were also obtained from EPA (1991).

Americium's dose and risk component was factored-in by establishing the empirical relationship between Am⁻²⁴¹ and Pu⁻²³⁹ in OU3 surface soils using measured data from Jefferson County (JeffCo, 1991). Linear regression on samples analyzed for Am⁻²⁴¹ and Pu⁻²³⁹ estimated the following relationship:

$$\text{Am}^{-241} = 0.156 (\text{Pu}^{-239}) + 0.036, \quad R^2 = 0.89, \quad n = 48 \text{ pairs}$$

This relationship was also predicted by Krey et al. (1976). Based on serial transformation, the expected Am⁻²⁴¹ to Pu⁻²³⁹ ratio for an RFP plutonium isotopic concentration is following maximum ingrowth is about 0.15.

As reported in the Remedy Report, the Generic Risk Assessment for Exposure to Plutonium Contaminated Soils has limited use because it was intentionally biased through errs on the side of safety and consequently did not conform to Agency guidance³. DOE has taken the opportunity at this juncture to refocus the risk assessment through revision of certain input parameters so that reference levels will resemble a plausible Reasonable Maximum Exposure (RME).

Table 1 presents surface soil reference levels of Pu⁻²³⁹, including the Am⁻²⁴¹ component, for a recreational scenario. Table 2 presents surface soil reference levels of Pu⁻²³⁹, including the Am⁻²⁴¹ component, for a residential scenario. For illustration purposes, two cases are presented: (1) the Generic Remedy Report Case and, (2) the alternative Plausible-Reasonable Maximum Exposure Case (P-RME)⁴. Input parameters for the exposure variables and references are included in the Tables. Various alternative cases were developed to support selection of the P-RME. They are attached as Tables A and B.

³ In the Remedy Report, generic risk assessment was an upper-bound assessment and did not reflect EPA's intent in calculating risk based on the Reasonable Maximum Exposure (RME) concept. The RME should be comprised of a product of factors, such as concentration and exposure frequency and duration, that are an appropriate mix of values that reflect averages and 95th percentile distributions (EPA, 1990). EPA recognizes the need for professional judgement and offers guidance that the RME should estimate a conservative exposure scenario that is still within the range of possible exposures (EPA, 1989).

⁴ DOE is not presenting an official OU3 RME, nor are the subject reference levels intended as Preliminary Remediation Goals (PRG). Both the RME and PRG's will be addressed formally at their appropriate times in the RFI/RI, CMS/FS process.

Inspection of Table 1 shows a P-RME based surface soil reference level of 137 pCi/gram Pu⁻²³⁹ assuming a **recreational exposure scenario**. This is the soil activity concentration of Pu⁻²³⁹ that corresponds to 1E-6 LECR-M considering the concurrent dose and risk from plutonium and Am⁻²⁴¹ ⁵. In contrast, a reference level using Remedy Report assumptions for a recreational exposure scenario would be about 10.8 pCi/gram Pu⁻²³⁹. Currently, there are no known measured plutonium surface soil activity concentrations exceeding either of these values in OU3.

A review of Table 2 indicates a **residential scenario**, P-RME based surface soil reference level of 2.6 pCi/gram Pu⁻²³⁹. Similar to the recreational scenario, this is the soil activity concentration of Pu⁻²³⁹ that corresponds to 1E-6 LECR-M considering the concurrent dose and risk from plutonium and Am⁻²⁴¹ ⁶. In contrast, a reference level using Remedy Report assumptions (for a residential exposure scenario) would be about 0.5 pCi/gram. A map identifying the location of a 2.6 pCi/gram Pu⁻²³⁹ isocontour within OU 3 is attached.

The reference levels in Tables 1 and 2 (P-RME or Remedy Report) were computed using the most conservative portion of EPA's guidance for radiation risk assessment (EPA, 1989). Use of more traditional health-physic methods also presented in EPA guidance (1989), and used by EPA to estimate annual doses from chronic exposure to radionuclides in surface soils in the vicinity of RFP (Burley, 1990) would have produced higher (less conservative) reference levels.

The recreational scenario assumptions used to develop the P-RME based surface soil reference level of 137 pCi/gram Pu⁻²³⁹ involved developing values for a variety of exposure conditions. This was done to satisfy the requirement that the RME be a mixture of conservative and central tendency exposure parameters (see footnote 3). Review of Tables A and B indicate that reference level estimates ranged from 10.8 pCi/gram to 403 pCi/gram for the recreational scenario. In the residential scenario, reference levels range from 0.45 pCi/gram to 4.2 pCi/gram. Review of Tables 1 and 2 indicates that: (1) Remedy Report input assumptions, with one exception, are all conservative, upper-bound estimates and, (2) P-RME input assumptions reflect a mix of conservative and central tendency values. Notable in the P-RME case is exposure concentration, which as the master variable in these calculations, was fixed at the conservative Remedy Report value. Overall, the P-RME based reference level reflects EPA guidance while the Remedy Report-based estimates approximate a

⁵ This value assumes that LECR-M's are additive and is in accordance with EPA guidance. The premise of additivity has never been validated.

⁶ This value assumes that LECR-M's are additive and is in accordance with EPA guidance. The premise of additivity has never been validated.

worst-case setting⁷.

The likely potential future-land use is an important consideration when applying reference levels in a risk-management frame work. There are no current or planned development activities within the bounds outlined by the residential scenario of which DOE is aware, and no "Area of Concern" at all under the appropriate recreational scenario. It is on this basis that the recreational scenario-based surface soil reference level of 137 pCi/gram Pu⁻²³⁹ should be used for near-term, risk-management decisions.

A statistical comparison of the current and historical data used to krig the isocontour line for the residential scenario soil reference value of 2.6 pCi/gram Pu⁻²³⁹ is found in Appendix A. The kriging process used to develop the location of the isocontour line is found in Appendix B.

⁷ Previous guidance required developing an upper-bound estimate, however, that practice has been abandoned partly because the upper-bound estimates were implausible and could not be regarded as credible.

References

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TABLE 1

Reference Levels and Input Assumptions, OU3

Based on the Upper-Bound Recreational Exposure Scenario in the Remedy Report

(Reference Level for Pu-239 including Am-241)

Variable	Remedy Report (10.8 pCi/gr)	Category/ Ref.	P-RME (137 pCi/gr)	Category/ Ref.
Susp. Particulate	73 ug/m ³	Consrv/(1)	73 ug/m ³	Consrv/(1)
Inhalation Rate (2)	10 m ³ /day	Consrv/(2)	10 m ³ /day	Consrv/(2)
Annual Exposure Days/Year	56 day/yr	Consrv/(3a)	20 day/yr	Con Tend/(3c)
Exposure Period	40 yr	Consrv/(4a)	9 yr	Best. Est./(4c)
Incidental Soil Ingestion	115 mg/day	Consrv/(5a)	90 mg/day	Consrv/(5b)

Note Soil Fraction @ 1 (corrected) from Remedy Report causing a small increase in RR risk (7E-8 to 7.4E-8 @ 1 pCi/gr)

Conservative in the recreational setting where:

1. 73/57=double long-term RFP TSP actuals
2. Assumes 50% of daily volume occurs @ OU3
- 3a. 2 day/week, 4 week/mo., 7 mo./year (avg Temp> 40F. AMJJASO) (NOAA, 1987)
- 3c. 1 day/week, 4 week/mo., 5 mo./year (avg Temp> 60F. MJJAS) (NOAA, 1987)
- 4a. 40 year exceeds the upper 90th%-tile estimate (EFH, EPA, 1989) for sustained residence
- 4c. 9 year is the 50%-tile estimate (EFH, EPA, 1989) for sustained residence.
- 4d. 3 year is the best estimate for expected recreational use before the ROD.
- 5a. 115 mg/day is essentially 120 mg/day, upper-bound (OSWER 9285.6-03, EPA 1991)
- 5b. 90 mg/day, average-case is 1.5 X the 60 mg/day residential central tendency (LaGoy 1987)

TABLE 2

Reference Levels and Input Assumptions, OU3

Based on the Upper-Bound Residential Exposure Scenario in the Remedy Report

(Reference Level for Pu-239 including Am-241)

Variable	Remedy Report (0.45 pCi)	Category/ Ref.	P-RME (2.6 pCi)	Category/ Ref.
Surface Soil Activity/Conc.	1.0 pCi/gr	Constrv/(1)	1.0 pCi/gr	Constrv/(1)
Inhalation Rate (2)	20 m ³ /day	Constrv/(2)	20 m ³ /day	Constrv/(2)
Annual Exposure Days/Year	365 day/yr	Constrv/(3)	365 day/yr	Constrv/(3)
Exposure Period	30 yr	Constrv/(4a)	9 yr	Con Tend/(4b)
Incidental Soil Ingestion	120 mg/day	Constrv/(5a)	60 mg/day	Con Tend/(5b)
Intake of Leafy Vegetables	33 gr/day	Con Tend(6a)	50 gr/day	Con Tend(6b)
Intake of Tubor & Fruit	89 gr/day	V-Constrv/(6c)	42 gr/day	Constrv/(6d)
Dust Load-Scrub Fraction	0.01	Constrv/(7a)	0.005	Con Tend(7b)
Root Uptake-Scrub Fraction	0.001	Constrv/(7c)	0.000001	Con Tend(7d)
Fractional Time @ Home	1	Constrv/(8a)	1	Constrv/(8a)
Fraction of Households w/ gardens	1	Constrv/(9a)	1	Constrv/(9a)

Footnotes for Table 2

Conservative in the residential setting where:

1. Soil mixing from construction, tilling for a garden and general anthropogenic activity would reduce the soil concentration.
All Scenarios Are Overestimated By: 2 to 3 (Illsley, 1987)
2. 20 m³/day, reasonable upper-bound (OSMER 9285.6-03, EPA 1991)
3. 365 day/year is a worst-case estimate
- 4a. 30 year is the upper 90th%-tile estimate (EFH, EPA, 1989)
- 4b. 9 year is 50%-tile estimate (EFH, EPA, 1989)
- 5a. 120 mg/day, upper-bound (OSMER 9285.6-03, EPA 1991)
- 5b. 60 mg/day, average-case (Lagoy 1987)
- 6a. 33 gr/day is slightly less than typical (50 gr/day) (EFH, EPA, 1989)
- 6b. 50 gr/day is typical (EFH, EPA, 1989) correction made.
- 6c. 89 gr/day is double the reasonable worst-case (42 gr/day) (EFH, EPA, 1989)
- 6d. 42 gr/day reasonable worst-case (EFH, EPA, 1989)
- 7a. Fraction of soil concentration applied to leaves w/scrub-off, 0.01 conservative (Burley, EPA, 1990)
- 7b. Fraction of soil concentration applied to leaves w/scrub-off, 0.005 middle of range (Burley, EPA, 1990)
- 7c. Fraction taken-up w/ scrub-off. Top of range (Burley, EPA 1990)
- 7d. Fraction taken-up w/ scrub-off. Middle of range (Burley, EPA 1990)
- 8a. Maximum fractional time @ residence: 1, affects inhalation only, (EFH, EPA 1989)
- 9a. Maximal fraction of households w/ gardens: 1, affects food consumption only, (EFH, EPA, 1989)

TABLE A

Based on the Recreational Exposure Scenario in the Remedy Report
Major Risk-Exposure Assessment Input Variables

Variable	Remedy Report (10.8 pCi/gr)	Case A (14.4 pCi/gr)	Case B (80.6 pCi/gr)	Case C (134 pCi/gr)	Case D (137 pCi/gr)	Case E (403 pCi/gr)
Susp. Particulate	73 ug/m ³	73 ug/m ³	73 ug/m ³	73 ug/m ³	73 ug/m ³	73 ug/m ³
Inhalation Rate (2)	10 m ³ /day	10 m ³ /day	10 m ³ /day	10 m ³ /day	10 m ³ /day	10 m ³ /day
Annual Exposure Days/Year	56 day/yr	56	40 day/yr	20 day/yr	20 day/yr	20 day/yr
Exposure Period	40 yr	30	9 yr	9 yr	9 yr	3
Incidental Soil Ingestion	115 mg/day	115 mg/day	115 mg/day	115 mg/day	90 mg/day	90 mg/day
Note Soil Fraction @ 1 (corrected) from Remedy Report causing a small increase in RR risk (7E-8 to 7.4E-8 @ 1 pCi/gr)						

Conservative in the recreational setting where:

- 73/37=double long-term RFP TSP actuals
- Assumes 50% of daily volume occurs @ OUS (essentially)
 - 2 day/week, 4 week/mo., 7 mo./year (avg Temp> 40F. AMJJASO) (NOAA, 1987)
 - 2 day/week, 4 week/mo., 5 mo./year (avg Temp> 60F. MJJAS) (NOAA, 1987)
 - 1 day/week, 4 week/mo., 5 mo./year (avg Temp> 60F. MJJAS) (NOAA, 1987)
 - 40 Year exceeds the upper 90th-tile estimate (EFH, EPA, 1989) for sustained residence
 - 30 Year is 50X-tile estimate (EFH, EPA, 1989) for sustained residence
 - 9 Year is the 50X-tile estimate (EFH, EPA, 1989) for sustained residence.
 - 3 Year is the best estimate for expected recreational use before the ROD.
 - 115 mg/day is essentially 120 mg/day, upper-bound (OSWER 9285.6-03, EPA 1991)
 - 90 mg/day, average-case is 1.5 X the 60 mg/day residential central tendency (LaGoy 1987)

TABLE A

TABLE B

Based on the Residential Exposure Scenario in the Remedy Report

Major Risk-Exposure Assessment Input Variables

Variable	Remedy Report (0.45 pCi)	Category/ Ref.	Case A (1.3 pCi)	Category/ Ref.	Case B (2.6 pCi)	Category/ Ref.	Case C (4.2 pCi)	Category/ Ref.
Surface Soil Activity/Conc.	1.0 pCi/gr	Constrv/(1)	1.0 pCi/gr	Constrv/(1)	1.0 pCi/gr	Constrv/(1)	1.0 pCi/gr	Constrv/(1)
Inhalation Rate (2)	20 m ³ /day	Constrv/(2)	20 m ³ /day	Constrv/(2)	20 m ³ /day	Constrv/(2)	20 m ³ /day	Constrv/(2)
Annual Exposure Days/Year	365 day/yr	Constrv/(3)	365 day/yr	Constrv/(3)	365 day/yr	Constrv/(3)	365 day/yr	Constrv/(3)
Exposure Period	30 yr	Constrv/(4a)	9 yr	Con Tend/(4b)	9 yr	Con Tend/(4b)	9 yr	Con Tend/(4b)
Incidental Soil Ingestion	120 mg/day	Constrv/(5a)	120 mg/day	Constrv/(5a)	60 mg/day	Con Tend/(5b)	60 mg/day	Con Tend/(5b)
Intake of Leafy Vegetables	33 gr/day	Con Tend/(6a)	50 gr/day	Con Tend/(6b)	50 gr/day	Con Tend/(6b)	50 gr/day	Con Tend/(6b)
Intake of Tubor & Fruit	89 gr/day	V-Constrv/(6c)	42 gr/day	Constrv/(6d)	42 gr/day	Constrv/(6d)	42 gr/day	Constrv/(6d)
Dust Load-Scrub Fraction	0.01	Constrv/(7a)	0.01	Constrv/(7a)	0.005	Con Tend/(7b)	0.005	Con Tend/(7b)
Root Uptake-Scrub Fraction	0.001	Constrv/(7c)	0.001	Constrv/(7c)	0.000001	Con Tend/(7d)	0.000001	Con Tend/(7d)
Fractional Time @ Home	1	Constrv/(8a)	1	Constrv/(8a)	1	Constrv/(8a)	0.64	Con Tend (8b)
Fraction of Households w/ gardens	1	Constrv/(9a)	1	Constrv/(9a)	1	Constrv/(9a)	0.53	Con Tend (9b)

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Footnotes for Table B

Conservative in the residential setting where:

1. Soil mixing from construction, tilling for a garden and general anthropogenic activity would reduce the soil concentration. All Scenario's Are Overestimated By: 2 to 3 (Illistey, 1987)

2. 20 m³/day, reasonable upper-bound (OSMER 9285.6-03, EPA 1991)

3. 365 day/year is a worst-case estimate

4a. 30 year is the upper 90th%-tile estimate (EFH, EPA, 1989)

4b. 9 year is 50%-tile estimate (EFH, EPA, 1989)

5a. 120 mg/day, upper-bound (OSMER 9285.6-03, EPA 1991)

5b. 60 mg/day, average-case (LaGoy 1987)

6a. 33 gr/day is slightly less than typical (50 gr/day) (EFH, EPA, 1989)

- 6b. 50 gr/day is typical (EFH, EPA, 1989) correction made.
- 6c. 89 gr/day is double the reasonable worst-case (42 gr/day) (EFH, EPA, 1989)
- 6d. 42 gr/day reasonable worst-case (EFH, EPA, 1989)
- 7a. Fraction of soil concentration applied to leaves w/scrub-off , 0.01 conservative (Burley, EPA, 1990)
- 7b. Fraction of soil concentration applied to leaves w/scrub-off, 0.005 middle of range (Burley, EPA, 1990)
- 7c. Fraction taken-up w/ scrub-off. Top of range (Burley, EPA 1990)
- 7d. Fraction taken-up w/ scrub-off. Middle of range (Burley, EPA 1990)
- 8a. Maximum fractional time @ residence: 1 , affects inhalation only, (EFH, EPA 1989)
- 8b. Average fractional time @ residence: 0.64 , affects inhalation only, (EFH, EPA 1989)
- 9a. Maximal fraction of households w/ gardens: 1, affects food consumption only, (EFH, EPA, 1989)
- 9b. Maximal fraction of households w/ gardens: 0.53, affects food consumption only, (EFH, EPA, 1989)

APPENDIX A

STATISTICAL COMPARISON OF CURRENT AND HISTORICAL DATA

Three sources of data are used in this report to construct an isocontour map using the residential scenario surface soil reference level of 2.6 pCi/g Pu-239. Data from two "historical" data sources were first compared with 1991 data which meets current QA requirements. To compare the historical data with the current data the following methodology was used.

OBJECTIVE - Compare current (1991) and historical (1977, 1985) data in the north and south Settlement Agreement Lands.

Three comparisons of data are calculated using a two-tailed T test. Data sets and their sources are shown on accompanying pages. All T-test results are also shown.

Comparison #1 - Data set from untilled strips of the north area of Settlement Agreement lands sampled in 1991 vs. 1977 and 1985 data sets from same area. (labeled Set A)

Comparison #2 - Data set from untilled strips of the south area of Settlement Agreement lands sampled in 1991 vs. 1977 and 1985 data sets from same area. (labeled Set B)

Comparison #3 - Data set from untilled strips of the north area of Settlement Agreement sampled in 1991 vs. 1977 and 1985 data sets plus City of Broomfield property sampled in 1985. (labeled Set C)

RESULTS - The data for the plutonium soil samples were categorized into "Historical" (1977, 1985) and "Current" (1991) classifications. Composite values in pCi/g were entered as data in the two classifications and a T-test was performed on the mean values for each class.

The two-tailed T-test tests the null hypothesis that the mean values for each class are equal against the alternative hypothesis that one class mean is significantly larger than the other. Under the null hypothesis it is assumed that the data were all drawn from one distribution with a variance equal to the pooled sample variance from each class.

The procedure used for these comparisons was the SAS TTEST. This procedure tests for equal variance and calculates an f-ratio result and significance levels. This procedure also determines significance levels for the T-test when the equal variance assumption is being met and when it is not being met. If the F-test results do not show sufficient evidence to say that the variances are unequal (non-homogenous) then the P-value for un-equal variance should be used as the TTEST procedure makes compensating adjustments. The "equal variance" P-value is used when the data set distributions are similar as indicated by the f-ratio. In each comparison the equal and unequal p-values are similar and the F-test indicates similar distributions.

The level of significance for the T-test is the probability that one would see a difference in means of the magnitude indicated by the printout due to random chance if in fact all the data were drawn from the same population. In all cases the significance level of the test is much larger than 0.05 - the level ordinarily considered to be significant. For all data sets A, B and C the

results of the T-test indicates that there is insufficient evidence to conclude that a difference in mean plutonium levels exists between historical and current data.

MAP LEGEND

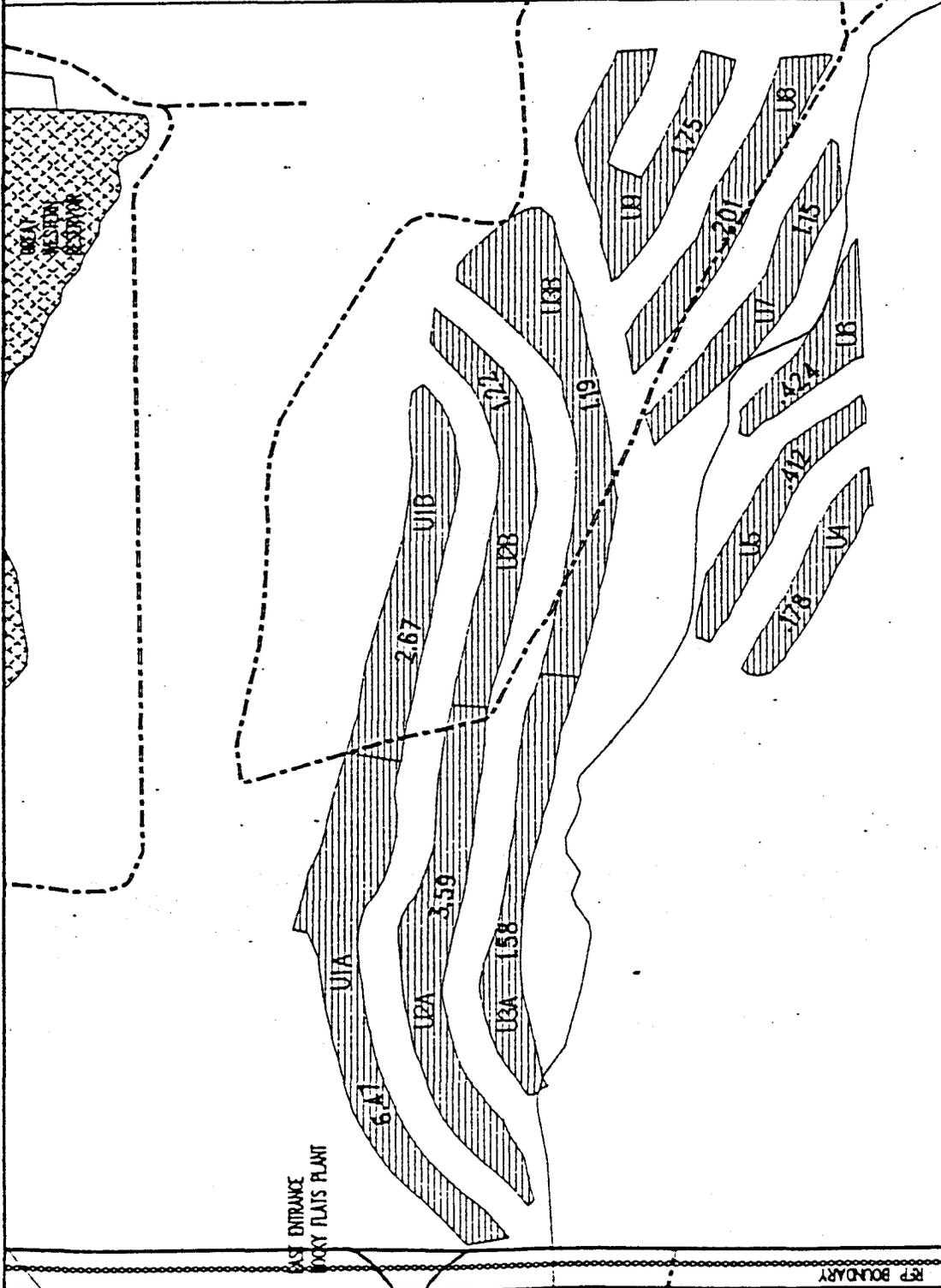
- RFP BOUNDARY
- STREAMS, DITCHES AND DRAINAGE FEATURES
- MEDIUM DUTY ROADS
- - - UNIMPROVED DIRT ROADS
- [Hatched Box] UNTILLED AREAS (VALUES IN pCi/G)
- [Cross-hatched Box] SURFACE WATER IMPOUNDMENTS

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of ENERGY
Rocky Flats Plant
Golden, Colorado



MAP OF NORTH AREA
UNTILLED STRIPS OF
REMEDY LAND SHOWING
SOIL SAMPLE LOCATION
SAMPLE NUMBER AND
RESULTS OF Pu 239,
240 ANALYSIS

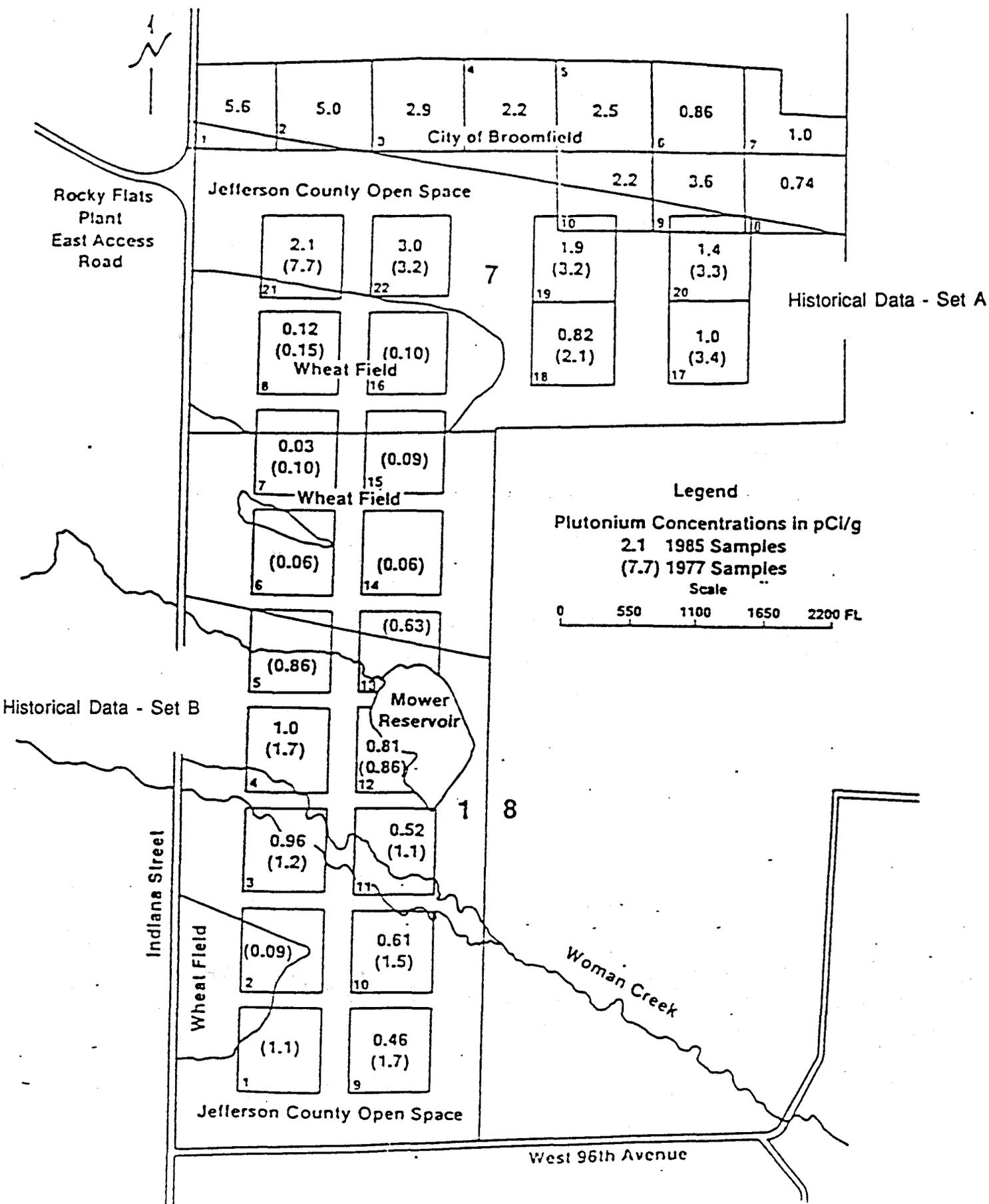
FIGURE 3



Current data - Set A
Source - Jefferson County Remedy lands, Semi-Annual Report, Summer 1991

NOVA STRIP

RFP BOUNDARY



Source - Rockwell International, Remedial Action Program on Jefferson County Open Space Land in Section 7, T2S, R69W, South of Great Western Reservoir, C.T. Illsley, EAC-420-87-1, 15 January 1987. (Remedy Report Document D-10)

MAP LEGEND

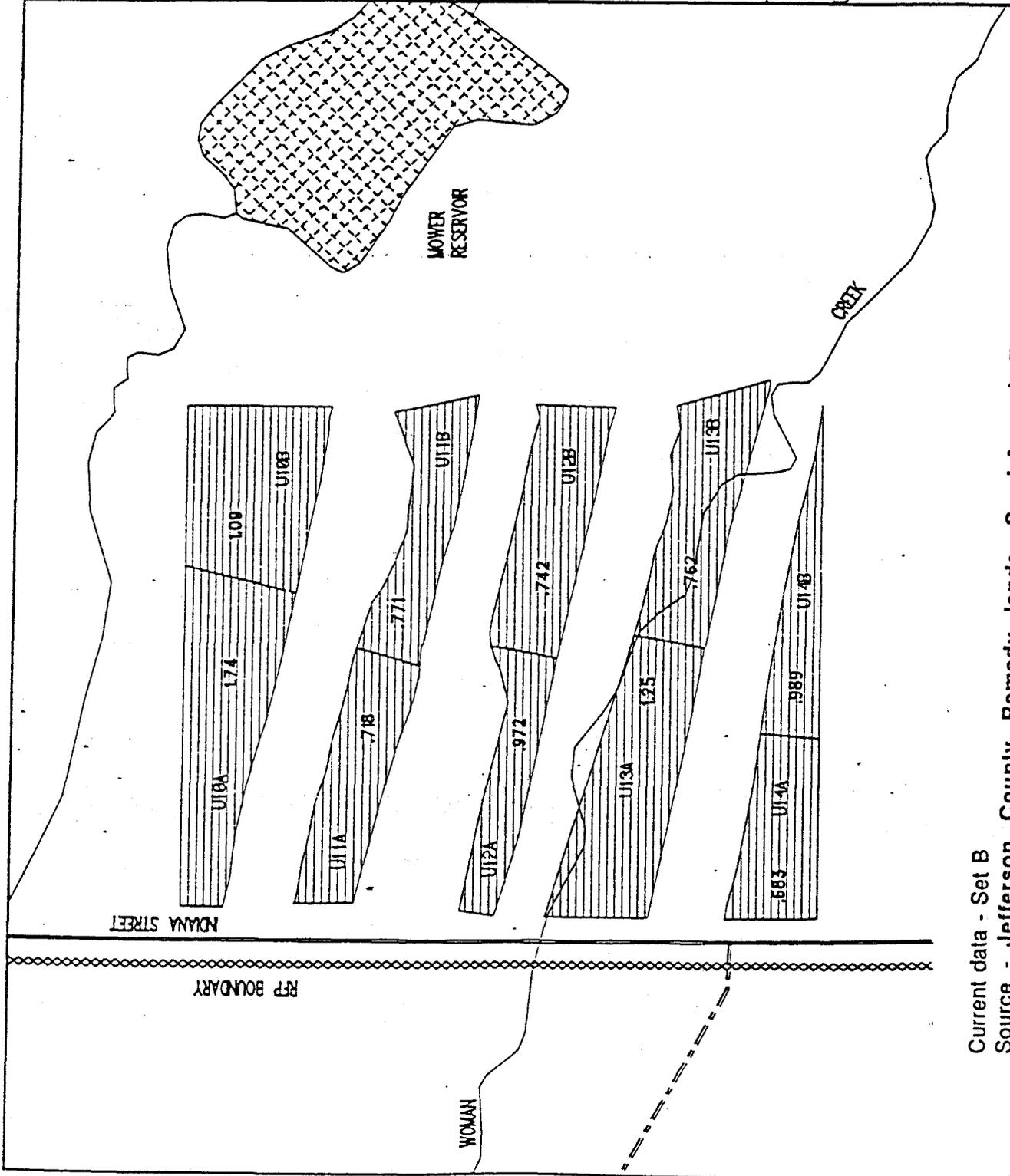
- RFP BOUNDARY
- STREAMS, DIICHES AND DRAINAGE FEATURES
- MEDIUM DUTY ROADS
- UNIMPROVED DIRT ROADS
- ▨ UNUTILLED AREAS (VALUES IN pCi/G)
- ▩ SURFACE WATER IMPOUNDMENTS

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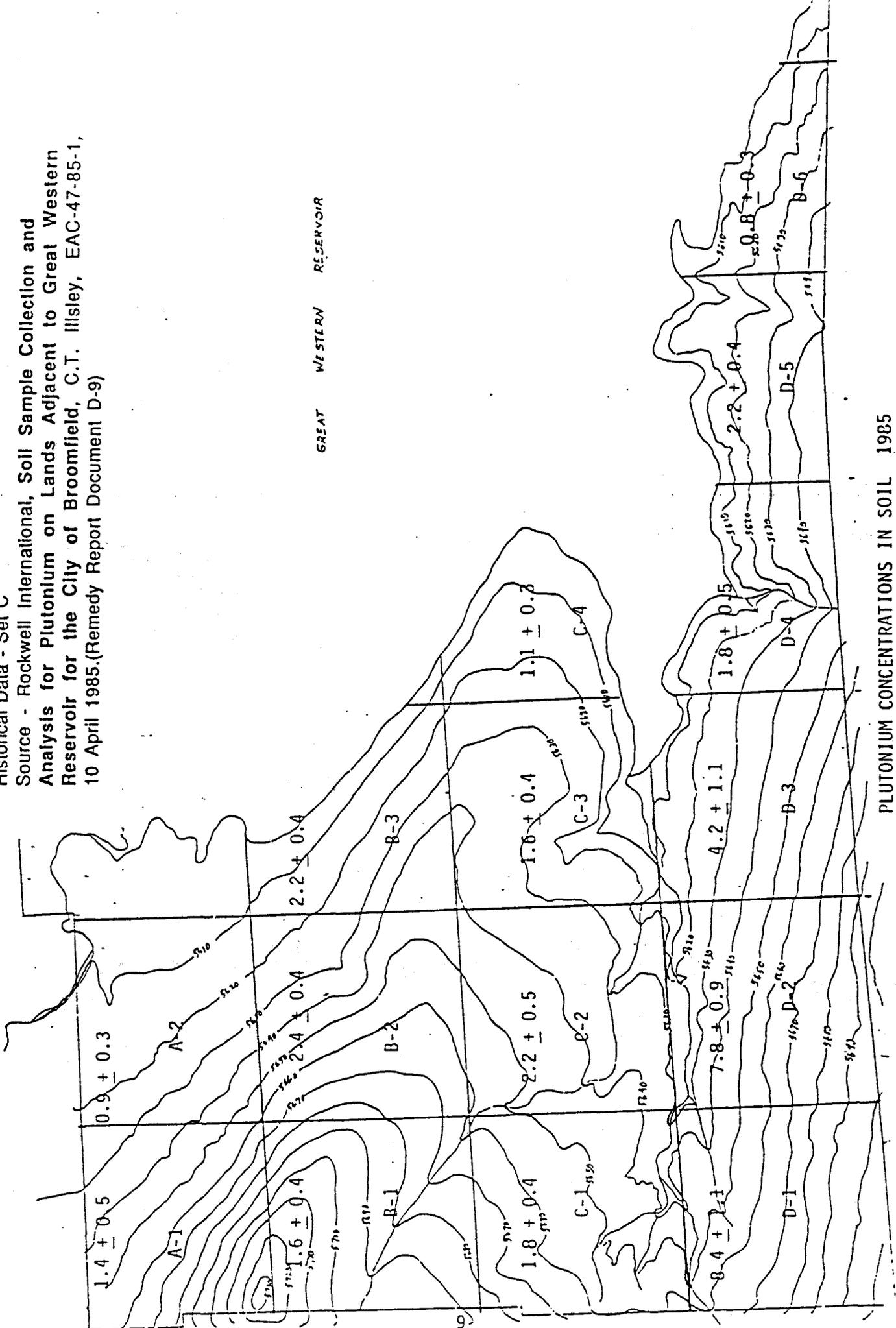
MAP OF SOUTH AREA
UNUTILLED STRIPS OF
REMEDY LAND
SHOWING SOIL
SAMPLE LOCATION,
SAMPLE NUMBER AND
RESULTS OF Pu 239,
240 ANALYSIS

FIGURE 4



Current data - Set B
Source - Jefferson County Remedy lands, Semi-Annual Report, Summer 1991

Historical Data - Set C
 Source - Rockwell International, Soil Sample Collection and
 Analysis for Plutonium on Lands Adjacent to Great Western
 Reservoir for the City of Broomfield, C.T. Illsley, EAC-47-85-1,
 10 April 1985.(Remedy Report Document D-9)



PLUTONIUM CONCENTRATIONS IN SOIL 1985
 (CDM METHOD-UNITS ARE D/M/G)

APPENDIX B

MAP CONSTRUCTION

KRIGING THEORY

Use of regionalized variable theory and the semivariogram as a means of describing spatial variation in soils is demonstrated by numerous authors (e.g., Burgess and Webster, 1980a, 1980b; McBratney et al. 1981; Burgess et al., 1981; Gilbert and Simpson, 1985; Webster and Oliver, 1990). The semivariogram describes the rate of change in a regionalized variable and measures the degree of spatial dependence between samples within geographical boundaries (i.e., 2-dimensional analysis) and/or with depth (i.e., 3-dimensional analysis). The spatial structure of the regionalized variable can be described by the semivariogram in the case of stationarity conditions (Bregt et al. 1991). The variogram splits the total variance of a data set into two parts. The first part represents the spatial variance between sample values relative to the distance between samples. The second part represents local or random variance. Because the semivariogram is a function of distance, the weights change according to the spatial arrangement of the samples (Isaaks and Srivastava, 1989).

By definition, the value of the theoretical variogram $\tau(h)$ for a given distance h , is the square of the expected difference (E) between the values of the samples separated by distance h :

$$\tau(h) = E\{Z(x) - Z(x + h)\}^2 \quad (1)$$

where $Z(x)$ and $Z(x + h)$ are the Pu activities at locations x and $x + h$ separated by the vector h , known as the lag. The

experimental semivariogram can be estimated from the data at hand by:

$$\tau(h) = \frac{1}{n(h)} \sum_{i=1}^{n(h)} [Z(x_i) - Z(x_i + h)]^2 \quad (2)$$

Modeling the experimental semivariogram provides the necessary parameters (i.e., nugget, sill, and range) for interpolation of soil-Pu activities. The calculated variance $\tau(h)$ between samples increases with increasing separation distances up to a distance (A) called the range, where it levels off to a constant value. Samples with a separation distance less than the range are spatially correlated, and those with separation distances greater than the range are statistically independent. The point that the semivariogram levels off is called the sill, and is equal to the overall variance of the sample population. The sill is composed of two components, C and C_0 . In most soil environs, $\tau(h)$ will remain nonzero as h approaches zero which is called the nugget effect ($\tau(h) = C_0, h > 0$). It reflects the inherent random variation of contaminant dispersion in the environment that cannot be predicted by any method, and may represent the variability between sampling points at distance less than that actually used or available, analytical error, or samples collected from different populations (i.e., depths, soil type, and other edaphic factors).

The kriging interpolation procedure uses the information from the semivariogram to find an optimal set of weights that are used in the estimation of soil-Pu at unsampled locations. The kriging procedure is optimal in the sense that it provides

estimates with minimum variance or uncertainty, and this variance can be estimated with a certain degree of confidence. The main sources of the uncertainty estimates are: 1) the number of nearby samples, 2) proximity of the samples, 3) spatial arrangement, and 4) the nature of the contaminant.

Kriging can be applied as a global or local estimator. Globally, the data would be used over the entire site with an estimation of the mean. Local estimation refers to an estimator of the average value of the regionalized variable over smaller soil areas from which a sample is collected. For example, the kriging estimator of the Pu level at a point $Z^*(x_0)$ in geographical space is:

$$Z^*(x_0) = \sum_{i=1}^n \lambda_i Z(x_i) \quad (3)$$

where $Z(x_i)$ is the observed datum at the point x_i within the local neighborhood about the point x_0 , and λ_i is the weight attached to that datum as obtained using a kriging estimator. If the assumptions underlying kriging are met, then the kriging estimator is a best linear unbiased estimator.

The assumptions for simple and ordinary kriging are strong stationarity and minimum kriging variance. These assumptions are expressed as follows:

$$E[Z^*(x_0) - Z(x_0)] = 0 \quad (4)$$

that implies zero drift and

$$\text{Var}[Z^*(x_0) - Z(x_0)] = \text{a minimum} \quad (5)$$

The variance in equation 5 provides a measure of the goodness of prediction. The variance depends on the sampling design and the model of the spatial structure of the data.

The assumption of strong stationarity is not always met. For example, Hamlett et al. (1986) showed that the assumption of strong stationarity should always be tested when analyzing the spatial variability of soil attributes. When the stationarity assumption is violated, it is necessary to model the drift function that underlies the semivariogram. In practice, this is achieved by using a universal kriging technique (i.e., non-stationary kriging) that estimates the order of the drift (k), models it, estimates the variogram, and solves the kriging equations (similar to Eq. 3). A complete formalization of the universal kriging is described by Karfritas and Bras (1981).

Geostatistical Approach

The first step to model spatially correlated data was to ascertain the data distribution and reduce the spread of the data using appropriate transformations. Next, a moving-window statistical algorithm was used (Murray and Baker, 1991) to assess the heteroscedasticity of the data. The experimental semivariogram calculations and the best-fit model were developed using GS+ software (Gamma Design Inc. 1991). Cross validation analysis and simple and ordinary kriging computations were performed using the GEO-EAS program (Englund and Sparks, 1988). The universal kriging for three orders of drift was computed using a modified UVKBLK algorithm originally described by Carr (1990). The modification included universal block kriging, five different types of semivariogram models, and numerous code modifications regarding input/output options.

The summary statistics that described the bias and the spread of the error distribution was the Mean Square Error (MSE). The MSE from the kriging estimates was defined as:

$$\text{MSE} = 1/n \sum_{i=1}^n [Z_i - Z^*_i]^2 \quad (6)$$

where Z_i was the observed value and Z^*_i was the estimated value. The kriging technique that gave the lowest MSE, the most evenly distributed error map, and the smallest scatter of the observed versus the estimated plot was used for Pu estimation. A computer code was written to compute the MSE, the Mean Kriging Variance (MKV), and the Gaussian confidence limits following the procedure outlined by Bregt et al. (1991). The kriging variances from each estimator were multiplied by the ratio MSE/MKV to compensate for the assumed underestimation of the kriging variance (see Bregt et al. 1991). These adjusted kriging variance estimates were used to determine confidence intervals for each point in the study area using the 90 percent Gaussian confidence limits:

$$Z^* \pm 1.645(\text{adjusted standard deviation}) \quad (7)$$

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Pu Values in pci/g

Data Sources

Phase 2 Operable Unit 2 W/RI Report (in production)

* Beckwell International, "Soil Sample Collection and Analysis for Plutonium on Lands Adjacent to Great Western Reservoir for the City of Provo, Utah," by C.T. Hilday, KAC-47-95-1, 10 April 1985. (Remedy Report D-5)

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