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ALL DRAWINGS ARE LOCATED AT THE END OF THE DOCUMENT

FINAL

TECHNICAL MEMORANDUM 3 PHASE II RFI/RI AQUIFER TEST WORK PLAN (ALLUVIAL)

ROCKY FLATS PLANT

903 PAD, MOUND, AND EAST TRENCHES AREAS (OPERABLE UNIT NO.2)

U S DEPARTMENT OF ENERGY

ROCKY FLATS PLANT

GOLDEN, COLORADO

ENVIRONMENTAL RESTORATION PROGRAM

June 12, 1992

REVIEWED FOR CLASSIFICATION/UCNI
By [illegible] (UNU)
Date 6/29/92

ADMIN RECORD

TECHNICAL MEMORANDUM 3

FINAL PHASE II RFI/RI AQUIFER TEST

WORK PLAN (ALLUVIAL)

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903 PAD, MOUND, AND EAST TRENCHES AREAS
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WORK PLAN FOR AQUIFER TESTING AND ANALYSIS PREPARED AS PART OF THE GEOLOGIC CHARACTERIZATION, PHASE II

1 0 INTRODUCTION

Aquifer testing is proposed to help understand the hydraulic characteristics of selected hydrostratigraphic units within Operable Unit 2 (OU2) at the Rocky Flats Plant (RFP) (Figure 1) OU2 consists of the 903 Pad, Mound and East Trenches areas This Work Plan incorporates part of the aquifer test work plan as outlined on pages 5-35 through 5-40 of the OU2 Phase II Work Plan (EG&G, 1991a), attached hereto as Appendix A and referred to here as the RFI/RI Work Plan

Three multi-well pumping tests will be performed to evaluate the hydraulic properties of the subsurface materials at OU2 The goals of this evaluation are to

- Develop parameters for rate of movement calculations (hydraulic conductivity, dispersivity, and effective porosity) for both the bedrock and alluvial materials
- Evaluate the degree of connection between the alluvium and the bedrock (both sandstone and claystone)

Alluvial materials in the study area are represented by unconsolidated surface materials ranging in texture from poorly graded sandy gravels to clayey sands For the most part the alluvial materials are coarse-grained and contain little to no clay The alluvium, absent locally, ranges to forty feet thick It is unconformably underlain by Arapahoe Formation claystones and sandstones Existing data, in the form of grain size analyses (EG&G, 1991b) and permeameter

tests (Personal Communication, Connie Dodge), suggest that both the alluvial material and the bedrock will have relatively low hydraulic conductivities The well diameters, pumping equipment and test design will reflect this concern

2 0 AQUIFER TEST SITES

Three distinct hydrogeologic situations are present at OU2 within the uppermost hydrostratigraphic unit (Figure 2) They are

- An unsaturated Rocky Flats Alluvium is underlain by a saturated uppermost Arapahoe Sandstone
- A saturated Rocky Flats Alluvium is underlain by a saturated uppermost Arapahoe Sandstone
- The Rocky Flats Alluvium is saturated and is underlain by claystone of the Arapahoe Formation

The test sites were selected to provide information about each of these three hydrogeologic situations, and additionally to

- Gain the maximum hydrologic information with a minimum test well network,
- Maximize the use of existing wells and minimize the construction of new wells as observation wells, and
- Be able to obtain the desired hydrologic information within a reasonable test period time

In order to satisfy these objectives, previous data and information related to aquifer testing at the RFP and geologic and hydrologic measurements made by EG&G and others (EG&G, 1991b) have been drawn upon These data and information have included stratigraphy based upon borehole core, water level measurements, laboratory hydraulic and physical tests on borehole cores, results of single-well packer and slug tests, and preliminary analysis of results of one multiple-well pumping test conducted at the RFP in 1989 The proposed locations of the alluvial and bedrock aquifer test sites are shown on Figure 3 In addition, 12 transducers have been installed in the OU2 area to monitor background water levels for use in implementation of the aquifer test work plan (Figure 3) A summary of the geologic and hydrogeologic characteristics

of each of the test sites is given in Table 1

Based upon the geologic model set forth in the Geologic Characterization Report (EG&G, 1991b), the uppermost Arapahoe Formation sandstone beneath the RFP site may consist of meandering paleochannels Therefore, aquifer test locations for Site Nos 1 and 2 were selected such that wells would penetrate the uppermost sandstone of the Arapahoe Formation (Figure 4) A separate location was selected for the alluvial aquifer test, Site No 3

The width of the paleochannel is expected to be in excess of 300 feet Although the channel consists of sandstones, siltstones and claystones which are discontinuous laterally and vertically, these discontinuities are expected to be on a small scale, allowing the sandstones an interconnectedness, and therefore allowing the unit to act as a single heterogeneous aquifer

Table 1

Geologic and Hydrologic Characteristics of Aquifer Test Sites at Rocky Flats Plant

Geologic or Hydrologic Characteristics*	Test No. 1	Test No 2	Test No. 3
Geologic Description	Alluvium, Sandstone, Silty Sandstone, Siltstone and Claystone	SW, GW, SC, Sandstone-clayey and silty	GC, SP, SC, GP, Clay-stone/Silty-Claystone
Ground Surface Elevation (Feet Above Mean Sea Level)	5980	5972	5949
Static Water Level Depth Below Ground Surface (feet)	34 1	26 9	13 0 (Assumed)
Depth to Top of Uppermost Arapahoe Sandstone Below Ground Surface (feet)	21 0	37 5	Not Present
Thickness of Uppermost Arapahoe Sandstone (feet)	21 0 - 63 5	37 5 - 66 0+	Not Present
Depth to top of Arapahoe Claystone (feet)	N/A	N/A	25 0
Saturated Thickness (feet)	30	40	12
Hydraulic Conductivity of Alluvial Aquifer (centimeters per second (cm/s))	N/A	1×10^{-3} to 1×10^{5}	1×10^{3} to 1×10^{-5}
Hydraulic Conductivity of Uppermost Arapahoe Sandstone (cm/s)	1×10^{-4} to 5×10^{-6}	1×10^{-4} to 5×10^{-6}	N/A
Hydraulic Conductivity of Alluvial Aquifer (gallons per day per square foot)	N/A	21 2 to 0 212	21 2 to 0 212
Hydraulic Conductivity of Uppermost Arapahoe Sandstone (gallons per day per square foot)	2 12 to 0 11	2 12 to 0 11	N/A
Transmissivity of Saturated Test Interval (gallons per day per foot)	3 2 to 63 6	5 2 to 271	2 5 to 254 4

NOTE Test Locations shown on Figure 3

* Data for this table were compiled from Well Logs 35-87 and 36-87 for Site No 1, 114-91 and 56-91 for Site No 2, and 17-87 and 18-87 for Site No 3, and from water level measurements for 1988-91 provided by EG&G

3 0 AQUIFER TEST DESIGN CONSIDERATIONS

Equations and calculations used to estimate certain design consideration parameters are attached to Appendix B Aquifer characteristics compiled in Table 1 are used

3 1 HYDRAULIC CONDUCTIVITY

If the hydraulic conductivity (K) of a specific test interval is believed to be 0 0212 gallons/day/ft^2 (gpd/ft^2) (1 x 10^{-6} cm/s) or less, based on the results of step-drawdown tests (Section 6 0), then it is recommended that an aquifer test not be conducted With hydraulic conductivity so low, an aquifer test would not achieve its goal, that is, measurement of hydraulic parameters representative of the aquifer for a considerable distance around the pumping well (small radius of investigation) Small radii of investigation would best be served by limiting the investigation to slug testing

3 2 RADIUS OF INFLUENCE

The possibility of low hydraulic conductivities in the uppermost Arapahoe sandstones implies a small radius of investigation Using an empirical equation from Bear (1979) to estimate the expected radius of influence (R) for a certain K (Table 1), and using a 20 percent drawdown in the pumping well (6 feet for a 30-foot saturated thickness of sandstone and 2 4 feet for a 12-foot saturated thickness of alluvium) the following values were obtained

Sandstone

for K = 0 11 gpd/ft^2 (5 x 10^{-6} cm/s),	R = 2 3 feet
for K = 0 212 gpd/ft^2 (1 x 10^{-5} cm/s),	R = 3 3 feet
for K = 2 12 gpd/ft^2 (1 x 10^{-4} cm/s),	R = 10 4 feet
for K = 21 2 gpd/ft^2 (1 x 10^{-3} cm/s),	R = 33 feet

Alluvium

for K = 0 212 gpd/ft^2 (1 x 10^5 cm/s), R = 0 83 feet

for K = 2 12 gpd/ft^2 (1 x 10^{-4} cm/s), R = 2 63 feet

for K = 21 2 gpd/ft^2 (1 x 10^3 cm/s), R = 8 33 feet

for K = 212 gpd/ft^2 (1 x 10^2 cm/s), R = 26 34 feet

(Appendix B, Part A)

It is obvious from these calculations that spacing of the observation wells is critical to the success of the testing If the spacing of the wells is greater than the radius of influence, then drawdown will not be observed The results of the step-drawdown tests performed after installation of pumping wells (Section 6 0) will provide enough information to evaluate the planned spacing and re-design, if necessary Additionally, continuous water level information collected through January, February and March of 1992 (Section 2 0) will indicate whether saturated thicknesses assumed for these calculations are representative of spring conditions and will provide data on water level trends during the pre-test period

3 3 PUMPING RATE

There is some uncertainty as to the pumping rate which would be used at each of the sites Because the hydraulic conductivity of the alluvial and bedrock systems may range from 0 11 gpd/ft^2 to 21 2 gpd/ft^2, with saturated thicknesses of between 12 ft and 40 ft (Table 1), a range of pumping rates must be anticipated Employing the radius of influence values calculated above (Subsection 3 2) in the Thiem Equation, estimated pumping rates are

Sandstone

for K = 0 11 gpd/ft^2 (5 x 10^6 cm/s), Q = 0 02 gallons per minute (gpm)

for K = 0 212 gpd/ft^2 (1 x 10^5 cm/s), Q = 0 04 gpm

for K = 2 12 gpd/ft^2 (5 x 10^{-4} cm/s), Q = 0 3 gpm

Alluvium

for K = 0 212 gpd/ft^2 (1 x 10^{5} cm/s), Q = 0 03 gpm

for K = 2 12 gpd/ft^2 (5 x 10^{-4} cm/s), Q = 0 2 gpm

for K = 21 2 gpd/ft^2 (5 x 10^{3} cm/s), Q = 1 4 gpm

(Appendix B, Part B)

Large pumping rates will cause the pumping well completed in a low hydraulic conductivity material to go dry in a very short time Therefore, a sustainable constant pumping rate is important to the success of the tests It is recommended that a Grundfos *Redi-Flo2* submersible pump (Appendix C), or equivalent, be used to deliver the low pumping rates estimated above The proposed submersible pump can fit into a 2-in diameter well, and its pumping rate ranges from 9 to 0 03 gpm, encompassing almost the full range of expected hydraulic conductivities

3 4 OTHER CONSIDERATIONS

Other considerations for test design include distance to boundaries, well bore storage and delayed yield Parameters for estimation of these considerations are taken from Table 1 Calculations supporting the values stated below are based on Walton, 1987 and are included in Appendix B

3 4 1 Well Bore Storage

Because the hydraulic conductivity (K) of the sandstone is expected to be relatively low, that is, on the order of 0 11 to 2 1 gpd/ft^2 (5 x 10^{6} cm/s to 1 x 10^{-4} cm/s), it is critical that well bore storage effects be kept to a minimum Using the low value of transmissivity for each of the sites, as set forth in Table 1, the time after which pumping begins beyond which well bore storage impacts are negligible are

Well diameter of two inches

for T = 5 2 gpd/ft, t_s = 618 minutes (10 hours)

for T = 3 2 gpd/ft, t_s = 1006 minutes (17 hours)

for T = 2 5 gpd/ft, t_s = 1287 minutes (22 hours)

(Appendix B, Part C)

Well diameter of four inches

for T = 5 2 gpd/ft, t_s = 2610 minutes (44 hours)

for T = 3 2 gpd/ft, t_s = 4248 minutes (71 hours)

for T = 2 5 gpd/ft, t_s = 5436 minutes (91 hours)

(Appendix B, Part C)

For low values of transmissivity, therefore, the well diameter is a critical factor in the duration of well bore storage effects and can be expected to last into 22 hours of pumping for a two-inch diameter well and 91 hours for a four-inch diameter well This is an important consideration for Site No 1 due to the possibility of very low hydraulic conductivity, and to Site No 3 because of a thin saturated interval which mandates a low pumping rate so as not to dry up the pumping well

3 4 2 Delayed Yield

All three test sites involve unconfined aquifers for which delayed yield is expected Using ranges of hydraulic conductivities and saturated thicknesses from Table 1, the following are estimates of the time after which pumping started beyond which delayed gravity yield impacts are negligible

Sandstone

for K = 2 1 gpd/ft^2 (1 x 10^{-4} cm/s), 30 feet saturated thickness, t_s = 53 days

for K = 0 2 gpd/ft^2 (1 x 10^{5} cm/s), 30 feet saturated thickness, t_s = 530 days

for K = 0 01 gpd/ft^2 (5 x 10^{6} cm/s), 30 feet saturated thickness, t_s = 1060 days

Alluvium

for K = 21 gpd/ft^2 (1 x 10^3 cm/s), 12 feet saturated thickness, t_s = 2 days

for K = 2 1 gpd/ft^2 (1 x 10^4 cm/s), 12 feet saturated thickness, t_s = 20 days

for K = 0 21 gpd/ft^2 (1 x 10^5 cm/s), 12 feet saturated thickness, t_s = 200 days

(Appendix B, Part D)

Except for the highest hydraulic conductivity anticipated in the alluvium at Site No 3, the duration of the effects of delayed yield are estimated to be too great to be accounted for in the pumping tests Therefore, values of storativity will be determined only for data which can be evaluated for the effects of delayed yield

3 4 3 Boundary Effects

It is assumed, that although geologic boundaries as a result of the geometry of the paleochannels may exist, the pumping rate and test duration at Site No 1 should be sufficiently low and short that the test results should not be influenced by these impermeable boundaries Based on the distance from the closest observation well to the edge of the channel sandstones (Figure 3) and using a range of hydraulic conductivities presented in Table 1, then the required durations of the test to realize the effects of boundaries are

for T = 63 6 gpd/ft, t_1 = 566 hours (24 days)

for T = 6 36 gpd/ft, t_1 = 5600 hours (240 days)

for T = 3 2 gpd/ft, t_1 = 11,000 hours (470 days)

(Appendix B, Part E)

However, Site No 2 may be located very close to the edge of the sandstone paleochannel and the observation well most distant from the pumping well could be placed a mere forty feet from the impermeable boundary Using a range of possible transmissivities from Table 1, the test durations which must be exceeded if boundary impacts are to be realized are

for T = 5 2 gpd/ft, t_1 = 270 hours (11 days)

for T = 27 gpd/ft, t_1 = 53 hours (2 days)

for T = 271 gpd/ft, t_1 = 5 3 hours

(Appendix B, Part F)

Only with transmissivity on the high end of the range will boundary effects be realized at Site No 2 In addition, depending on when and with what magnitude delayed drainage effects become appreciable and at what point in time and with what magnitude the effects of the impermeable boundaries influence the test results, the negative departure from the type curve caused by delayed drainage could be offset by the positive departure caused by the impermeable boundary effects

4 0 DETAILS OF THE WELLFIELD DESIGN

Figures 5 and 6 show the proposed wellfield layout for Sites Nos 1 and 3 The designs of Sites Nos 1 and 3 will remain as originally outlined on pages 5-35 through 5-40 of the OU2 Phase II RFI/RI Work Plan The design provided in the OU2 Phase II RFI/RI Work Plan will be implemented as stated with the exception of the omission of the most distant observation well at Site No 1 and the two most distant observation wells at Site No 3 However, it is noted that the OU2 RFI/RI Work Plan, as approved, includes a contingency for changing the well locations, pumping rates and duration of pumping to conform with the results of step-drawdown or other single hole tests performed in the pumping well

The test design of Site No 2 as set forth in the OU2 Phase II RFI/RI Work Plan includes two partially penetrating pumping wells, each completed in a different layer of a two-layer system (alluvium overlying sandstone) The solution proposed for this test does not include an analytical solution, relying instead on a numerical simulation which does not provide a unique solution The test design has been modified to include a single pumping well which fully penetrates the two-layer aquifer (Figure 7) This design will allow the use of an analytical solution As illustrated in Figure 8, two pairs of observation wells are spaced five and ten feet from the pumping well, with two existing wells serving as additional observation wells

To test the interconnectedness of the alluvium and the sandstone, the sandstone well of a pair of proposed observation wells, will be pumped while the other wells are monitored for changing water levels The results of this test will not be analyzed for aquifer hydraulic parameters, merely evaluated for an interconnectedness between the two layers

5.0 WELL INSTALLATION AND DEVELOPMENT

A minimum of two observation wells and one pumping well at each test site will be installed specifically for the aquifer tests The construction and installation will follow those guidelines set forth in Standard Operating Procedure (SOP), GW 08, Aquifer Pumping Test (EG&G, 1991c)

5 1 PUMPING WELLS

- Pumping wells will have an inside casing diameter of not more than two inches
- The annular space between the formation material and the casing will be filled with a filter pack designed specifically for that well by the site hydrogeologist
- The wells will have screened intervals which will fully penetrate the aquifer of interest and will be placed as specified by the site hydrogeologist
- The well installation for Site No 2, that is, where the alluvium and the uppermost sandstone are in hydraulic connection, will not include surface casing through the alluvium, but will consist of a single borehole diameter and casing diameter through both materials
- The pumping well will be thoroughly developed as specified by the site hydrogeologist

5 2 OBSERVATION WELLS

- Observation wells will be installed as specified by the SOP GT 06, Monitoring Well and Piezometer Installation (EG&G, 1991)
- Development of newly installed observation wells and the re-development of old wells will be performed according to SOP GW 2, Well Development (EG&G, 1991c) or as specified by the site hydrogeologist
- The annular space between the formation material and the casing will be filled with a filter pack as specified by the site hydrogeologist

- The wells will fully penetrate the aquifer of interest and screen will be placed as specified by the site hydrogeologist, and will fully screen the interval unless otherwise directed by the site hydrogeologist

- The screened interval of the Site No 3 observation well will be installed with the top of the screen two to three feet below the contact of the claystone with the sandstone

6 0 WELLFIELD DEVELOPMENT AND HYDROLOGIC TESTING

The well-drilling contractor will supply the drill rig and well materials EG&G will supply the pump, flow control equipment, power supply, and monitoring equipment Well drilling and pumping tests will be monitored by the subcontractor

After drilling and completion of the pumping wells and before the installation of the observation wells, step-drawdown tests will be performed as set forth in the aquifer test SOP, GW 08 for the purpose of refining the design of each test, including pumping rate, and observation well spacing The performance of slug tests will be subject to the presence of favorable conditions at each of the pumping wells After drilling and completion of the well clusters by EG&G, one constant-rate pumping test will be performed at each of the three areas During the constant rate pumping test, time-drawdown data in the pumping and observation wells will be collected using data loggers and pressure transducers provided by EG&G In this way, a logarithmic time step for drawdown measurements can be used to obtain early-time data during the test Manual drawdown measurements will be made periodically during the test to check the performance of the data loggers and pressure transducers

Water pumped during the step-drawdown and constant-rate pumping tests will be collected in containers at the test sites The water will not be re-injected as proposed in the RFI/RI Work Plan, but will be held for treatment on plant site Periodic field water-quality indicator measurements of the water being discharged to storage during the constant rate pumping tests will be made These field water-quality indicator measurements will include water temperature, pH, and specific conductance as set forth in SOP GW 5, Field Measurement of Groundwater Field Parameters (EG&G, 1991c) EG&G will provide the field water-quality measurement instruments

7 0 ANALYSIS METHODS

Analytical methods for Sites Nos 1 and 3 will follow the OU2 Phase II RFI/RI Work Plan as closely as possible The interpretation of time-drawdown data from a constant rate pumping test is a special pattern-recognition problem The time-drawdown data will be analyzed using type-curve matching techniques for the aquifers tested Least-squares curve fitting methods will be used to supplement and enhance the analysis of time-drawdown data to obtain estimates of transmissivity and storativity If a hydrostratigraphic unit is found to be sufficiently homogeneous, the method of Papadopulos (1965) will be used to analyze for directional hydraulic conductivity

Site No 2 requires the development of an analytical solution specifically derived for application to the hydrogeologic conditions present at the test site, specifically, a two-layer aquifer, consisting of a thinner, but more permeable alluvial layer overlying a thicker, but less permeable bedrock layer, which are assumed to be in hydraulic connection The development of this method, a sensitivity analysis of the method, and a reference from the literature supporting the analytical solution are included as Appendix D

Results of the analyses for the constant-rate pumping tests at the three areas will include estimates of the hydraulic characteristics (transmissivity and storativity) for the aquifers tested Tabular results, as well as graphical results for the directional hydraulic conductivity if possible, will be provided as part of the draft and final reports All raw data and calculations will be included as appendices

8.0 REFERENCES

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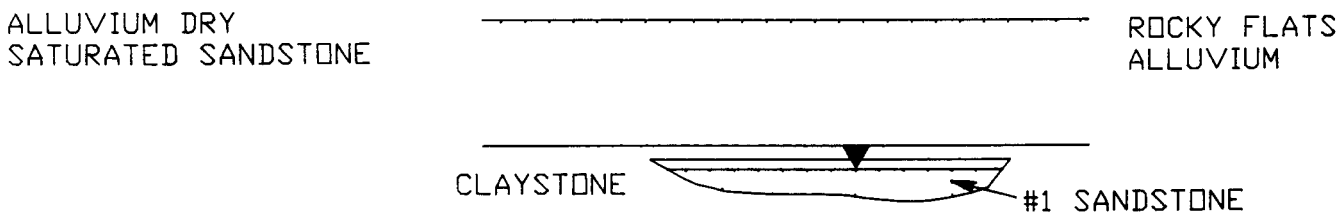
SITE No 1



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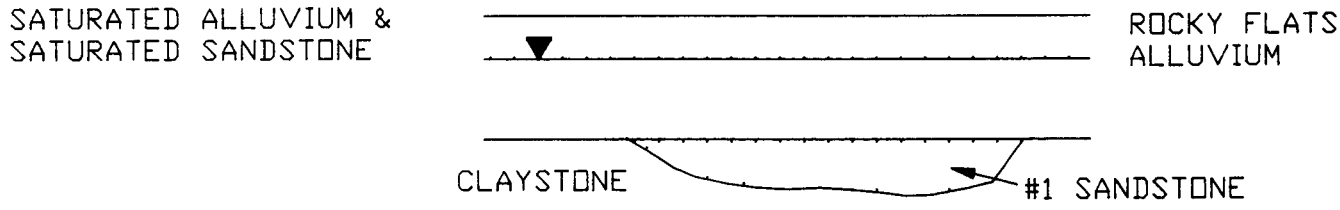

SITE No 3

NOTE NOT TO SCALE

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WORK PLAN (ALLUVIAL)

HYDROLOGIC CONDITIONS
UPPERMOST HYDROSTRATIGRAPHIC UNIT

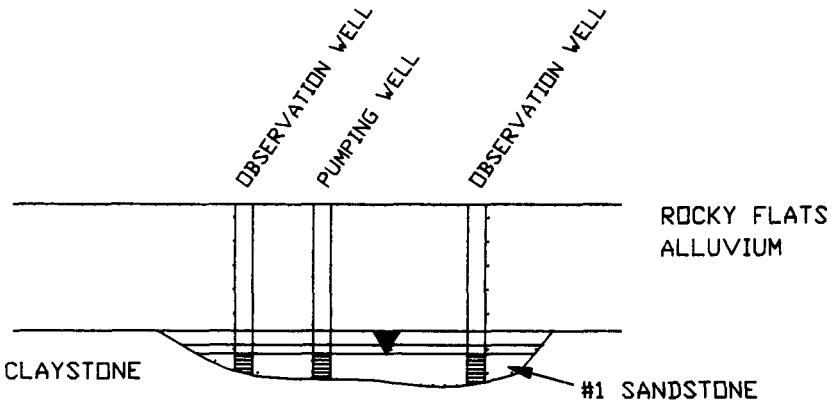
FIGURE 2

JUNE, 1992

SITE No 1

ALLUVIUM DRY
SATURATED SANDSTONE

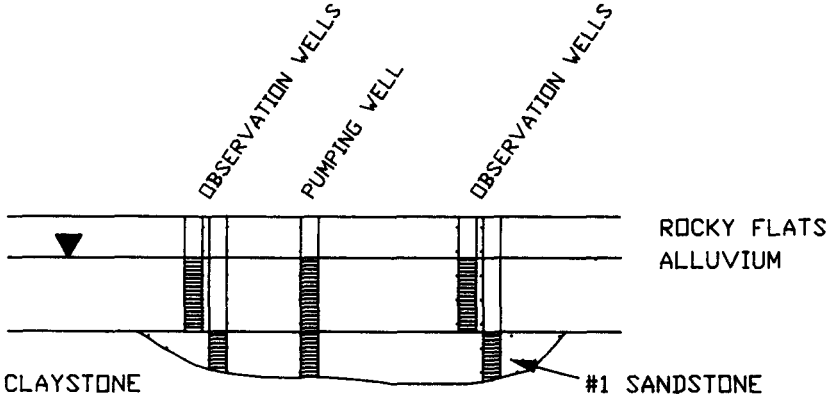
MULTI-WELL PUMPING TEST



SITE No 2

SATURATED ALLUVIUM &
SATURATED SANDSTONE

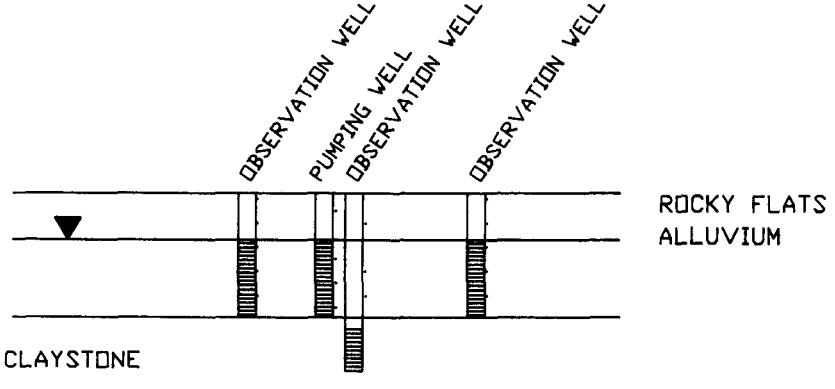
PUMPING TEST OF ALLUVIUM AND
SANDSTONE WITH PAIRED OBSERVATION
WELLS IN ALUVIUM AND SANDSTONE



SITE No 3

SATURATED ALLUVIUM
UNDERLAIN BY CLAYSTONE

PUMPING TEST OF ALLUVIUM WITH
OBSERVATION WELL IN CLAYSTONE



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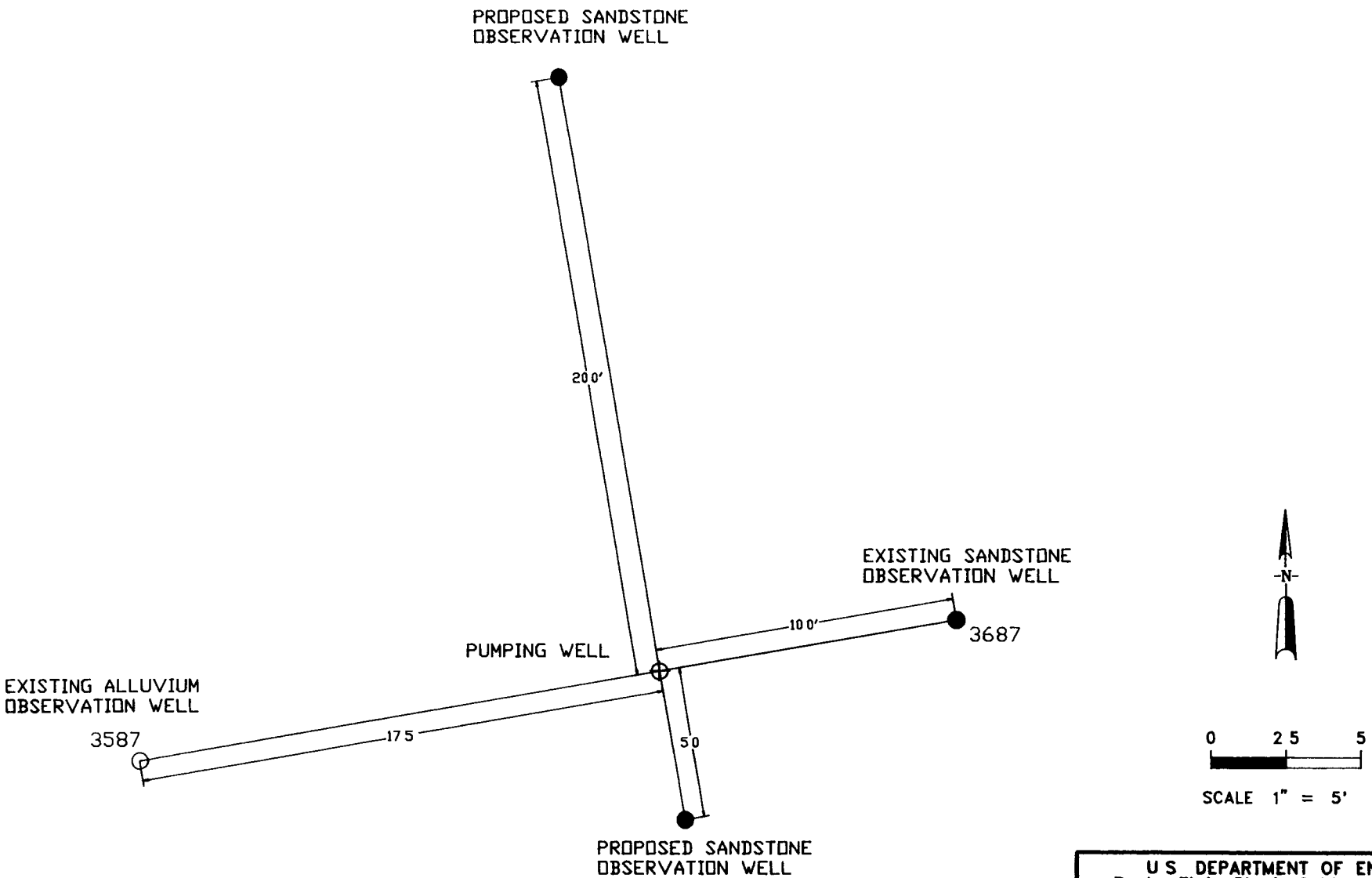
AQUIFER TEST DIAGRAMS
UPPERMOST HYDROSTRATIGRAPHIC UNIT

FIGURE 4

JUNE, 1992



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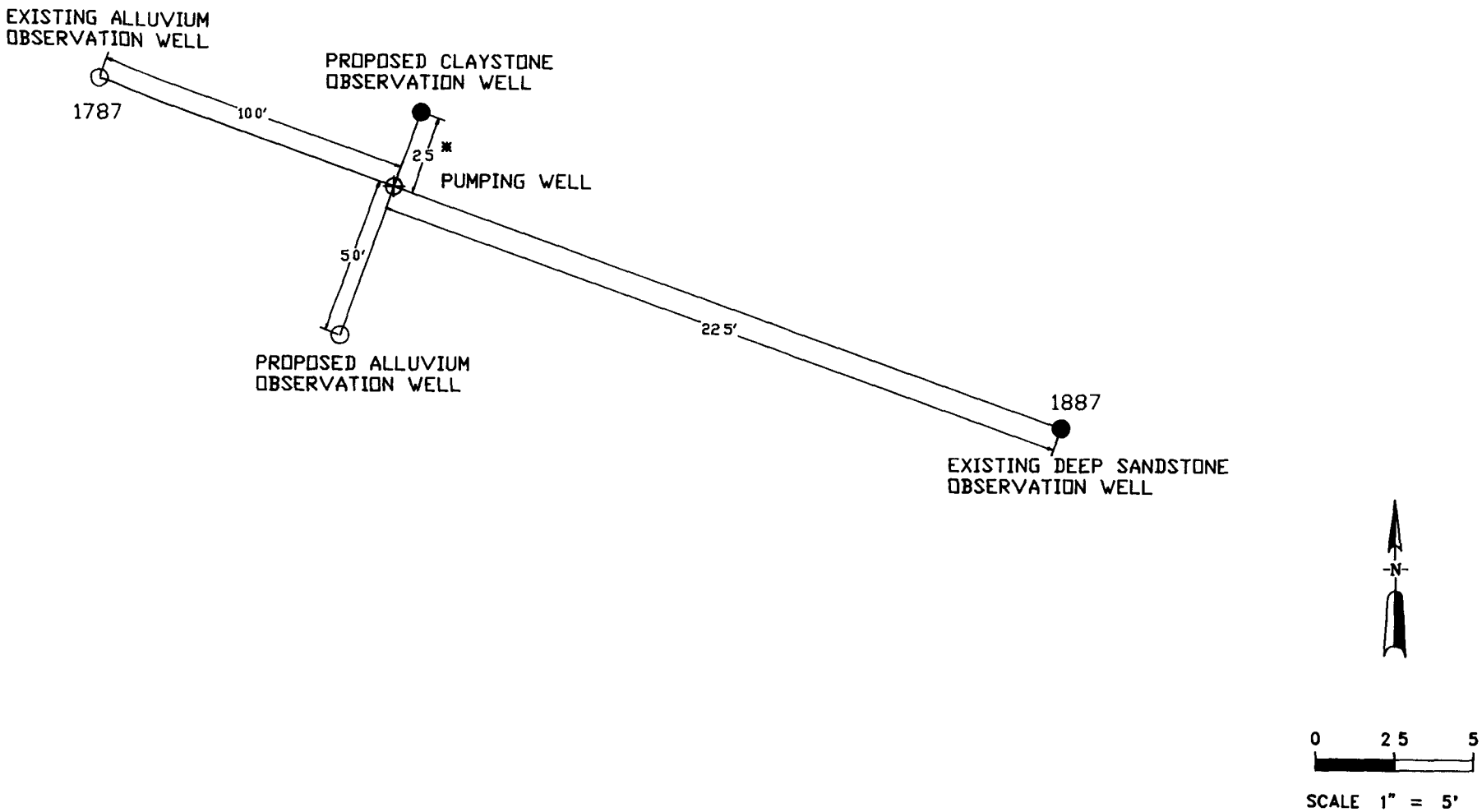
SITE No 1 – WELL SPACING

FIGURE 5

JUNE, 1992



* OR AS CLOSE AS PRACTICABLE

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SITE No 3 – WELL SPACING

FIGURE 6

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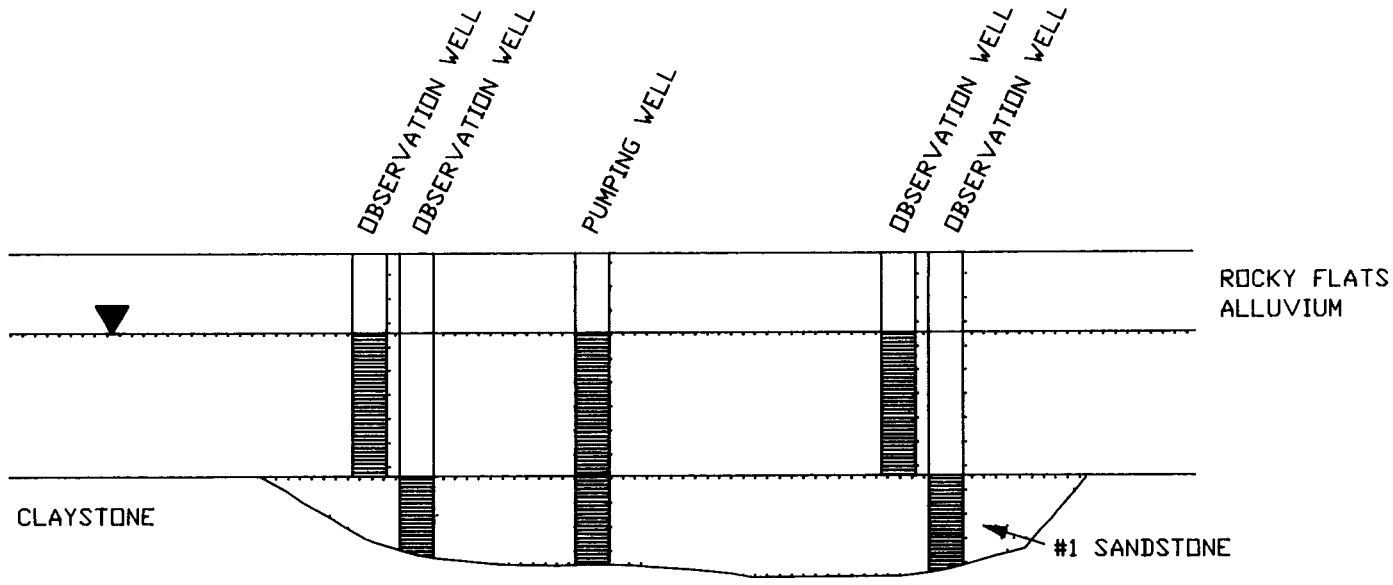
SATURATED ALLUVIUM &
SATURATED SANDSTONE

PUMPING TEST OF ALLUVIUM
AND SANDSTONE WITH PAIRED
OBSERVATION WELLS IN
ALLUVIUM AND SANDSTONE



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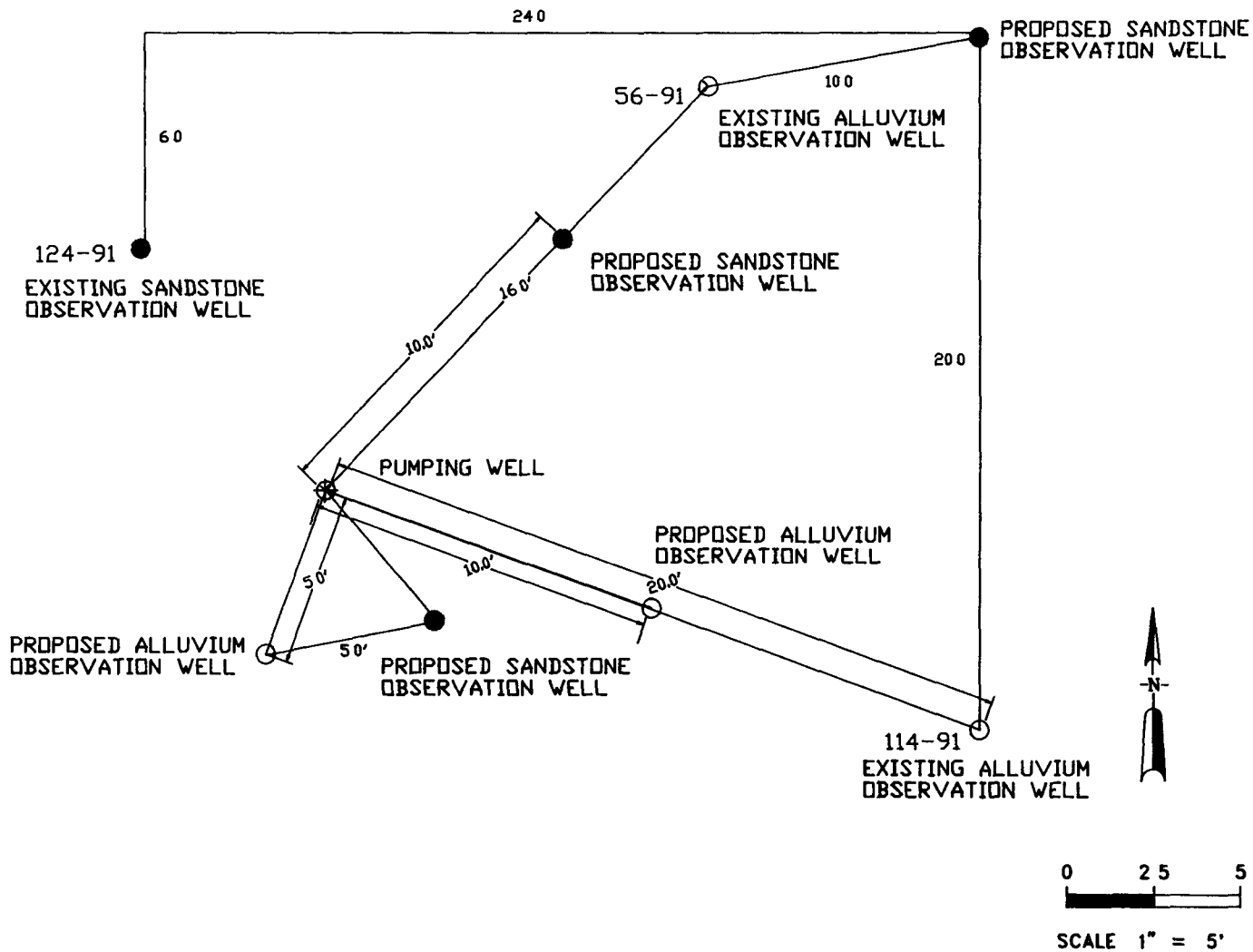
SITE No 2 DIAGRAM

FIGURE 7

JUNE, 1992



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Rocky Flats Plant, Golden, Colorado

OPERABLE UNIT NO 2
PHASE II RFI/RI AQUIFER TEST
WORK PLAN (ALLUVIAL)

SITE No 2 - WELL SPACING

FIGURE 8

JUNE, 1992

APPENDIX A

AQUIFER AND TRACER WORK PLAN
PHASE II RFI/RI WORK PLAN
903 PAD, MOUND, AND EAST TRENCHES
AUGUST 19, 1991

5 5 1 Hydraulic Testing Program

Three multi-well pumping and tracer tests will be performed to evaluate the hydraulic properties of the subsurface materials at the 903 Pad, Mound, and East Trenches Areas The goals of the program are to

- Develop parameters for rate of movement calculations (hydraulic conductivity and effective porosity) for both the bedrock and alluvial materials
- Evaluate the degree of connection between the alluvium and the bedrock (both sandstone and claystone)
- Develop parameters for estimation of production rates from remedial ground-water collection systems

The testing program has been designed based on the hydrogeologic model of the subsurface described in earlier sections of this plan Three distinct hydrogeologic situations are present in the upper HSU at the 903 Pad, Mound, and East Trenches Areas

1) The Rocky Flats Alluvium is unsaturated and is directly underlain by the of the Arapahoe Number One Sandstone Formation (saturated)
2) The Rocky Flats Alluvium is directly underlain by the Number One Sandstone and both are saturated
3) The Rocky Flats Alluvium is saturated and is underlain by claystone of the Arapahoe Formation

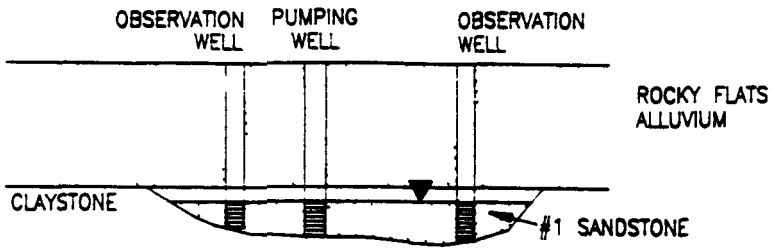
Hydrologic pumping tests have been designed to evaluate hydraulic conductivity, storage properties, and the effective porosity for each of these situations Schematics of the subsurface conditions and test well layouts are shown on Figure 5-9

Detailed designs for each of the hydrologic pumping tests are presented below, however, before the tests are actually performed, the production wells will be installed and tested (step-drawdown or other single hole technique) to establish better estimates of the hydraulic properties at the test locations The hydrologic tests will then be re-evaluated and possibly re-designed (observation well locations, pumping rates and duration of pumping) After re-evaluation of the test designs, the observation wells will be installed and the hydrologic tests will be performed All water produced during the hydrologic pumping testing of the production wells will be stored in tanker trucks and reinjected into the production well from which the water was produced

TEST T-1

ALLUVIUM DRY
SATURATED SANDSTONE

MULTI-WELL PUMPING TEST
CONVERGING RADIAL TRACER TEST

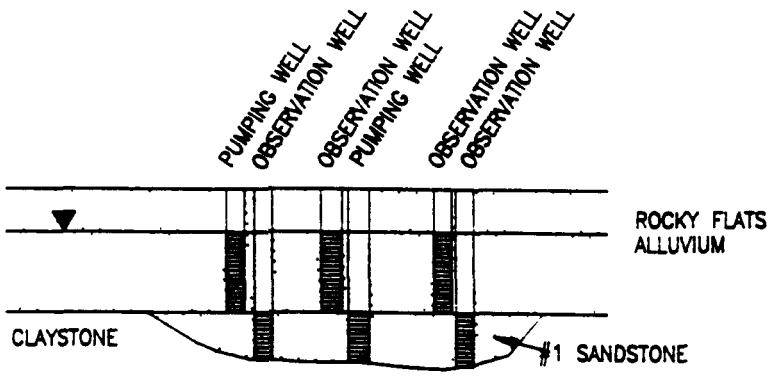


TEST T-2

SATURATED ALLUVIUM &
SATURATED SANDSTONE

PUMPING TEST OF ALLUVIUM WITH
OBSERVATION WELLS IN SANDSTONE

PUMPING TEST OF SANDSTONE WITH
OBSERVATION WELLS IN ALLUVIUM

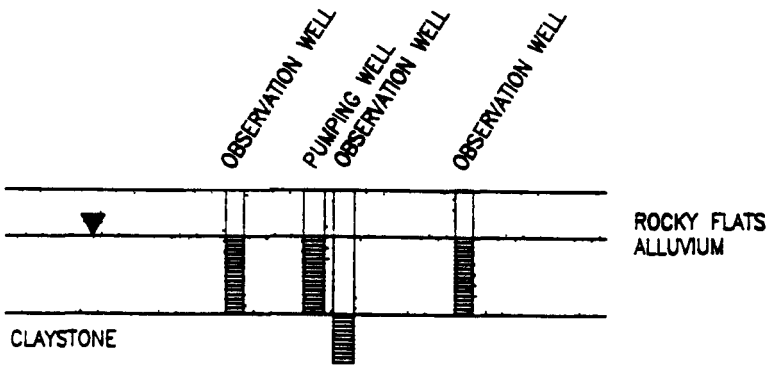


TEST T-3

SATURATED ALLUVIUM
UNDERLAIN BY CLAYSTONE

PUMPING TEST OF ALLUVIUM WITH
OBSERVATION WELL IN CLAYSTONE

CONVERGING RADIAL TRACER TEST



U S DEPARTMENT OF ENERGY
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OPERABLE UNIT NO 2
PHASE II RFI/RI WORK PLAN (ALLUVIAL)

HYDRAULIC TEST DIAGRAMS

FIGURE 5-9

August, 1991

R33149 PJcwpj 080691

5 5 1 1 Case 1. Unsaturated Alluvium over Saturated Sandstone

A multi-well pumping test followed by a converging radial tracer test will be performed at the T-1 location shown on Plate 1 An array of 1 production well and four observation wells will be completed in the Number One Sandstone The observation wells will be located at distances of 5, 10, 20 and 40 feet from the production well (Figure 5-10)

Initial pump rates will be determined by using Theis (1935) and hydraulic properties developed in the Phase I RI (hydraulic conductivity of $4x10^{-4}$ centimeter/s, storage coefficient of 0 1 and saturated thickness of 15 feet) A steady pumping rate of 1 gpm is estimated for wells at the T-1 location If the test array is located approximately 40 feet from the edge of the sandstone channel, significant interference from the boundary (additive drawdown of 0 5 feet) should be observable in the most distant observation well after 5 days of pumping All produced water (7,200 gallons) will be stored in tanker trucks and then reinjected into the production well at the end of the recovery period (see below)

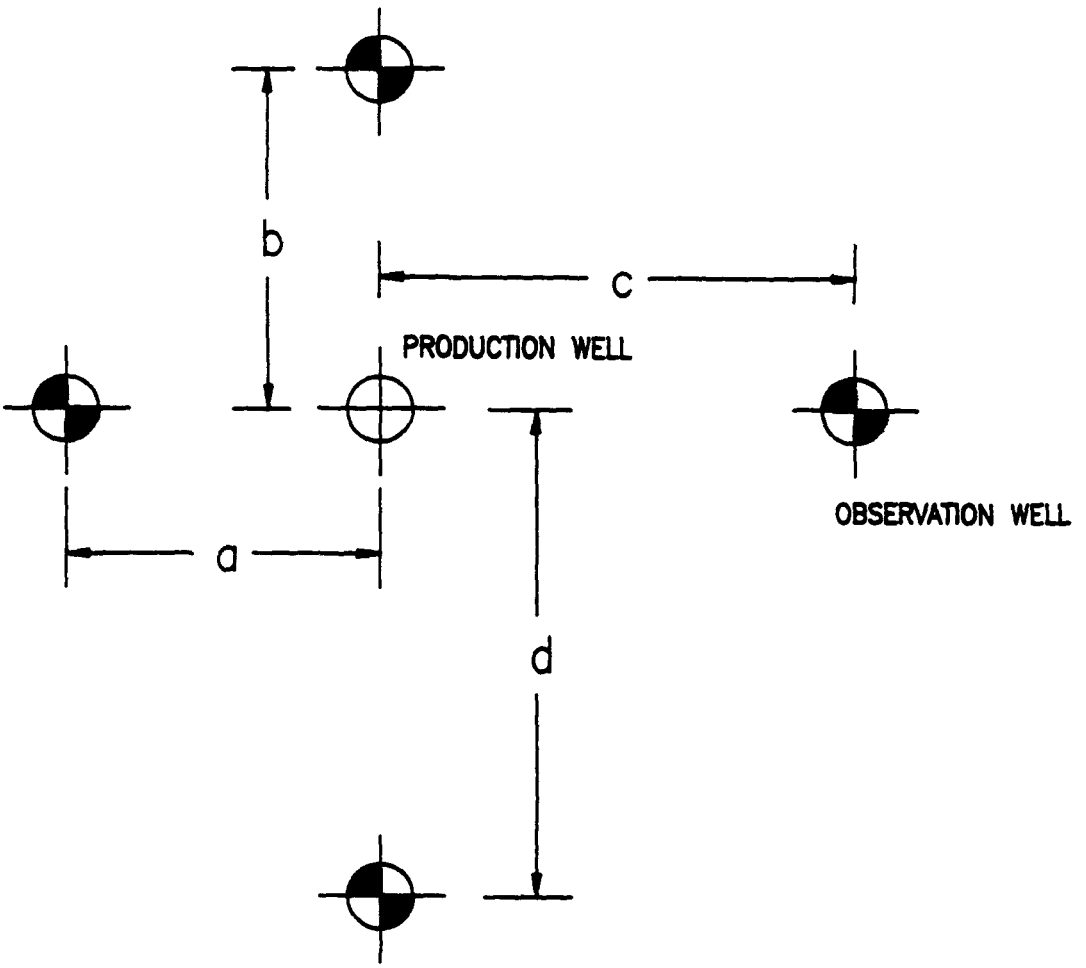
Immediately following the 5 days of steady pumping, a converging radial tracer test will be performed by injecting rhodamine-WT dye into the observation well located 5 feet from the production well (steady pumping will continue throughout the tracer test) It is anticipated that the 50 percent concentration (C_{50}) will arrive at the production well approximately ten hours after introduction of the fluorescent dye The entire pump test will require approximately 24 hours to complete The tracer test results will be analyzed using methods described by Sauty (1980)

After completion of the tracer test recovery of the system will be monitored for an additional 6 days Drawdowns in the observation and production wells will be evaluated using methods described in Bedinger and Reed (1988), such as Neuman (1972 and 1973)

5 5 1 2 Case 2 Saturated Alluvium over Saturated Sandstone

Two multi-well pumping tests will be performed at the T-2 location shown on Plate 1 An array of one production well and four observation wells will be completed in the Rocky Flats Alluvium, and a second array of one production well and four observation wells will be completed in the Number One Sandstone The observation wells in the Rocky Flats Alluvium will be located at distances of 5, 10, 30 and 75 feet from the production well The observation wells in the Number One Sandstone will be located at distances of 5, 10, 20 and 40 feet from the production well (Figure 5-10)

A 5-day production test of the Rocky Flats Alluvium will be performed with an additional 5 days of recovery Water level responses will be measured in wells that monitor in both the alluvium and the sandstone A second



EXPLANATION OF WELL SPACINGS (FEET)

	a	b	c	d
Sandstone	5	10	20	40
Alluvium	5	10	30	75

U.S. DEPARTMENT OF ENERGY
Rocky Flats Plant, Golden, Colorado

OPERABLE UNIT NO. 2
PHASE II RFI/RI WORK PLAN (ALLUVIAL)

OBSERVATION WELL LAYOUT

FIGURE 5-10

August, 1991

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5-day production test of the sandstone will be performed with monitoring of observation wells in both the alluvium and the sandstone The test period will be designed based on previous pump test data A tracer test will not be performed as part of this test because of expected interference (dilution effects) from the overlying or underlying units

The pumping test of the sandstone will be conducted at 1 gpm (see discussion of Case 1 above for expected production volume and aquifer responses) An estimated steady pumping rate of 3 gpm flow from the alluvium has been calculated using the Theis Method (1935), and alluvial hydraulic properties developed in the Phase I RI (hydraulic conductivity of $1x10^{2}$ cm/s, storage coefficient of 0 1 and saturated thickness of 5 feet) At the end of the recovery period for the second test, all produced water (22,000 gallons from the alluvium and 7,200 gallons from the sandstone stored in separate tanker trucks) will be reinjected into the production well from which the water came

Drawdowns in the observation and production wells will be evaluated using numerical modeling techniques, such as Lappala, et al (1987), as well as the more standard methods described in Bedinger and Reed (1988) However, because the hydrogeologic conditions do not meet the assumptions of the standard leaky-aquifer analyses, it is anticipated that numerical modeling will be the effective method to evaluate the interconnection between the alluvium and the sandstone

5 5 1 3 Case 3 Saturated Alluvium over Claystone

A multi-well pumping test followed by a converging radial tracer test will be performed at the T-3 location shown on Plate 1 An array of one production well and four observation wells will be completed in alluvium The observation wells will be located at distances of 5, 10, 30 and 75 feet from the production well (Figure 5-10) In addition, a single observation well will be installed adjacent to the production well to monitor head response at a depth of approximately 5 feet into the claystone

An estimated steady pumping rate of three gpm flow from the alluvium has been calculated using the Theis Method (1935), and alluvial properties developed in the Phase I RI (hydraulic conductivity of $1x10^{2}$ cm/s, storage coefficient of 0 1 and saturated thickness of 5 feet) All produced water (22,000 gallons) will be stored in tanker trucks and reinjected into the production well at the end of the recovery period Using a simple finite-difference evaluation, it is estimated that a water level response will be measurable in the claystone (0 1 feet of drawdown for a vertical conductivity of $1x10^{-6}$ cm/s) after 5 days of pumping

Immediately following the 5 days of steady pumping, a converging radial tracer test will be performed by injecting rhodamine-WT dye into the observation well located 5 feet from the production well It is anticipated that the 50 percent concentration will arrive at the production well approximately 1 hour after the introduction

of the fluorescent dye, and that the entire test will require approximately 24 hours to complete The tracer test will be analyzed using methods described by Sauty (1980)

After completion of the tracer test, recovery of the system will be monitored for an additional 6 days Drawdowns in the observation and production wells in the alluvium will be evaluated using methods described in Bedinger and Reed (1988) The response of the observation well in the claystone will be evaluated using methods described in Bedinger and Reed (1988), such as Lappala, et al (1987)

5 5.2 Ground-water Sampling Program

Ground-water samples will be collected on a quarterly basis from all new and existing monitoring wells at the 903 Pad, Mound, and East Trenches Areas upon completion of well development Samples will be analyzed for the parameters listed in Table 5-3 during the first round of sampling after completion of new wells. This parameter list may be reduced in subsequent quarterly sampling events if certain parameter groups are not detected, or are not significantly above background levels and if approved by EPA and CDH Ground-water samples will be analyzed in the field for pH, conductivity, temperature, and dissolved oxygen Sample aliquots designated for metals and radionuclide analyses will be filtered with the exception of tritium All sample filtration and preservation will be performed in the field

5 5 3 Borehole Sampling Program

Borehole samples will be collected from boreholes within and adjacent to IHSSs to characterize both plumes and sources Selected borehole samples will be analyzed for the chemical parameters listed in Table 5-3 following CLP methods or the methods provided in the GRRASP (EG&G, 1990k) plan These parameters are essentially the same as those analyzed in the Phase I RI except that oil and grease and RCRA characteristics are eliminated Oil and grease have not proven useful in determining extent of soil contamination, and RCRA hazardous waste characteristics have been within acceptable limits The TCL list for organics and the TAL list for inorganics are nearly the same as the previously used HSL list for organics and inorganics

The physical properties of on-site geologic materials will also be characterized to support the evaluation of remedial action alternatives Bulk samples will be collected from continuous core of alluvial wells to characterize each of the materials found within the 903 Pad, Mound and East Trenches Areas (Rocky Flats Alluvium, colluvium, valley fill alluvium, and weathered bedrock) Specifically, 10 samples of each geologic material type will be submitted for grain size analyses (sieve and hydrometer analyses), Atterberg limits testing, and recompacted permeability testing to evaluate the variability of these parameters across the site

PART A

Using Bear (1979), R = 575 s(hK)^.5
R = Radius of Influence
K = Hydraulic Conductivity
h = Initial Head = 12' = 3.66m
For 12' saturated thickness, allowing 20% drawdown
s = Drawdown = 2.4' = 0.73m

K (cm/s)	R (m)	R (ft)
1 0E-05	0.25	0.83
1 0E-04	0.80	2.63
1.0E-03	2.54	8.33
1 0E-02	8.03	26.34

h = 30' = 9.14m
For 30' saturated thickness, allowing 10% drawdown
s = 6.0' = 1 83 m

K (cm/s)	R (m)	R (ft)
5.0E-06	0.71	2.33
1 0E-05	1.01	3.30
1 0E-04	3.18	10.43
1 0E-03	10.06	32.99

PART B

Using Thiem, Q = [3.14K(h^2-hw^2)]/ln (R/rw)
Q = pumping rate
rw = radius of well = 0.08'
hw = head in the well

K (cm/s)	K (gpd/ft^2)	K (ft/min.)	Q (ft^3/m)	Q (gpm)
1 0E-05	0.212	0.0000197	0.004	0.03
1 0E-04	2.12	0 000197	0.024	0.19
1 0E-03	21.2	0.00197	0.184	1 40
1 0E-02	212	0 0197	1 475	11.21

Using Thiem, Q = [3.14K(h^2-hw^2)]/ln (R/rw)
rw = radius of well = 0.08'

K (cm/s)	K (ft/sec.)	Q (ft^3/s)	Q (gpm)
5.0E-06	1.6E-07	4.95E-05	0.02
1 0E-05	3.3E-07	8.97E-05	0.04
1 0E-04	3.3E-06	6.85E-04	0.31
1 0E-03	3.3E-05	5.54E-03	2.53

PART C

Well Bore Storage Calculations - 2" Well Diameter

ts = 5.4*10^5 (rw^2-rc^2)/T (Walton, 1987)
(ts = time (min) beyond which effects of storage are negligible)
rw = radius of the pumping well = 2" diam well = 1" rad = 0 08'
rc = radius of pump column, = 0.25" = 0 021
T = Transmissivity = Km = K*30'

K (gpd/ ft^2)	m (ft)	T Km (gpd/ft)	ts (hr)
0 212	12	2 5	21 5
0.11	30	3 2	16 8
0 11 0.212	40	5 2	10.3

Well Bore Storage Calculations - 4" Well Diameter

ts = 5 4 10^5 (rw^2-rc^2)/T (Walton, 1987)
(ts = time (min) beyond which effects of storage are negligible)
rw = radius of the pumping well = 4" diam well = 2" rad = 0 16'
rc = radius of pump column, = 0.25" = 0 021
T = Transmissivity = Km = K*30'

K (gpd/ ft^2)	m (ft)	T Km (gpd/ft)	ts (hr)
0 212	12	2 5	90 6
0 11	30	3 2	70 8
0 11 0.212	40	5 2	43 5

PART D

DELAYED YIELD

td = 5 4 10^4 m Sy/K (Walton, 1962)
td = time (min)beyond which delayed yield impacts are negligible
m = aquifer thickness = 12.0'(Test No 3) 30 0'(Test No 1)
Sy = Specific Yield = 0 1
K = Hydraulic Conductivity

K (gpd/ft^2)	m (ft)	td (min)	td (days)
0 1060	30	1528301.9	1061 3
0 2120	30	764150.9	530 7
2.1200	30	76415.1	53 1
0.2120	12	305660.4	212.3
2.1200	12	30566.0	21 2
21.2000	12	3056.6	2.1
0 212	40	1018867 9	707 5
2.12	40	101886.8	70 8
21 2	40	10188 7	7 1

Valid only for 0 7'<r<20' (Boulton 1954)

PART E

Boundary Effects - Test Site No. 5

ti = 5.4*10^2(ri^2)Sy/T (Walton, 1967)
ti = time (min) after pumping begins during which boundary impacts are negligible
T1 = 30'(0.11 gpd/ft) = 3.2
T2 = 30'(212 gpd/ft) = 6.4
T3 = 30'(2.12 gpd/ft) = 64

Sy = 0.1

Yi = Max distance from boundary to observation well = 200 ft.

T (gpd/ft^2)	ti (min)	ti (hr)
3 2	675000.0	11250.0
6.4	339622.6	5660.4
63 6	33962.3	566.0

PART F

Boundary Effects - Test Site No. 6

ti = 5.4*10^2 (ri^2)Sy/T (Walton, 1967)
10' saturated alluvium + 26' saturated Sandstone
K = 5*10^-6 (SS) and K = 1 10^-5 (Alluv)
K = 5*10^-5 (SS) and K = 1 10^-4 (Alluv)
K = 5 10^-4 (SS) and K = 1 10^-3 (Alluv)

T1 = 10'(0.212 gpd/ft) + 26'(0.11 gpd/ft) = 5 2
T2 = 10'(2 12 gpd/ft) + 26'(0.21 gpd/ft) = 27 1
T3 = 10'(21.2 gpd/ft) + 26'(2.12 gpd/ft) = 271 4

Sy = 0.1

Max. distance from boundary to observation well = 40 ft

T (Kama+ Kasmas)	ti (min)	ti(hr)
5 2	16615.4	276 9
27 1	3184 0	53.1
271 4	318.4	5 3

PART G

Boundary Effects - Test Site No. 4

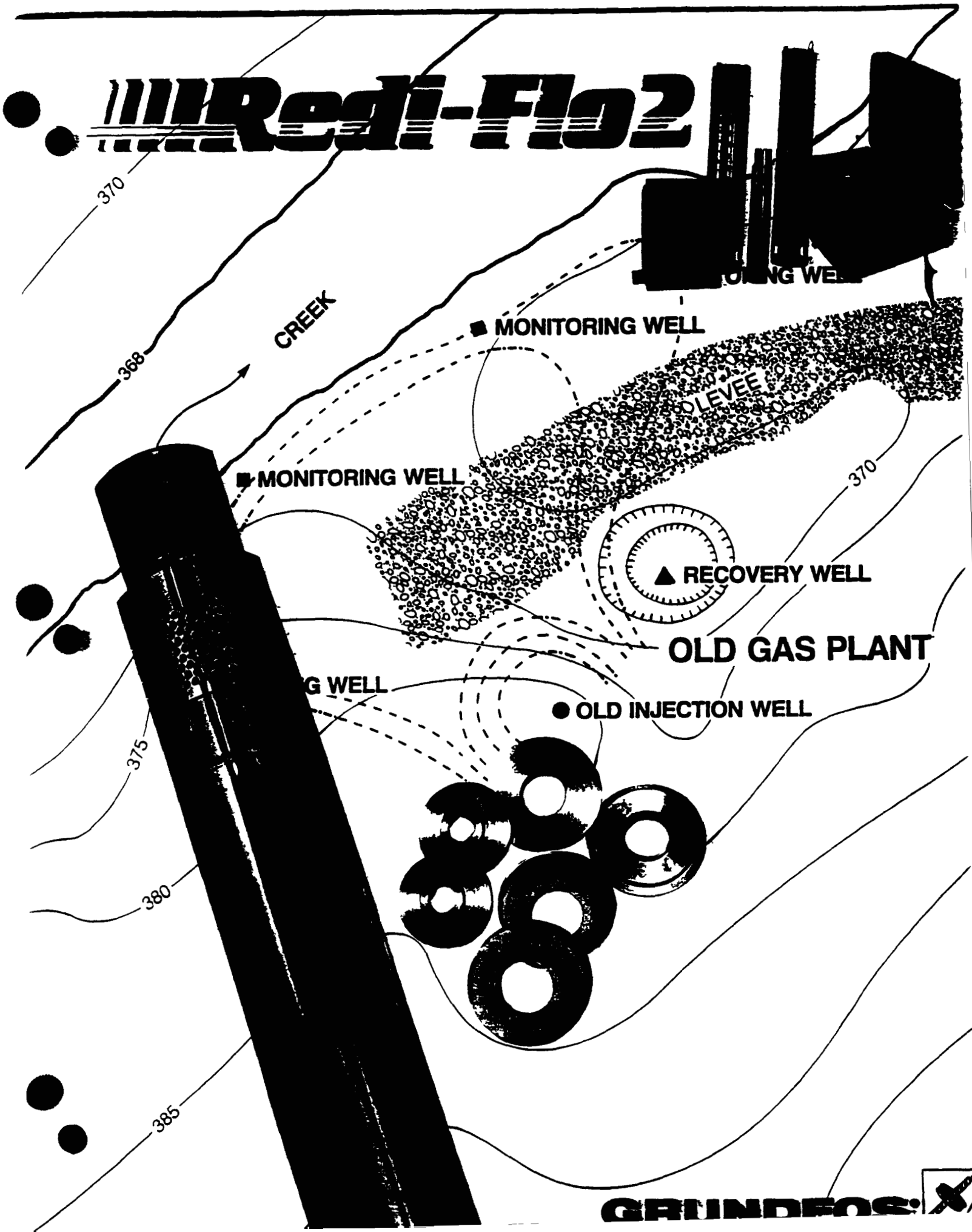
ti = 5.4*10^2 (ri^2)Sy/T (Walton, 1967)
12' Saturated Alluvium
K = 0 212
K = 2.12
K = 21 2

T1 = 12'(212 gpd/ft) = 2 5
T2 = 12'(2.12 gpd/ft) = 25 44
T3 = 12'(21 2 gpd/ft) = 254 4

Sy = 0 1

Max distance from boundary to observation well = 150 ft

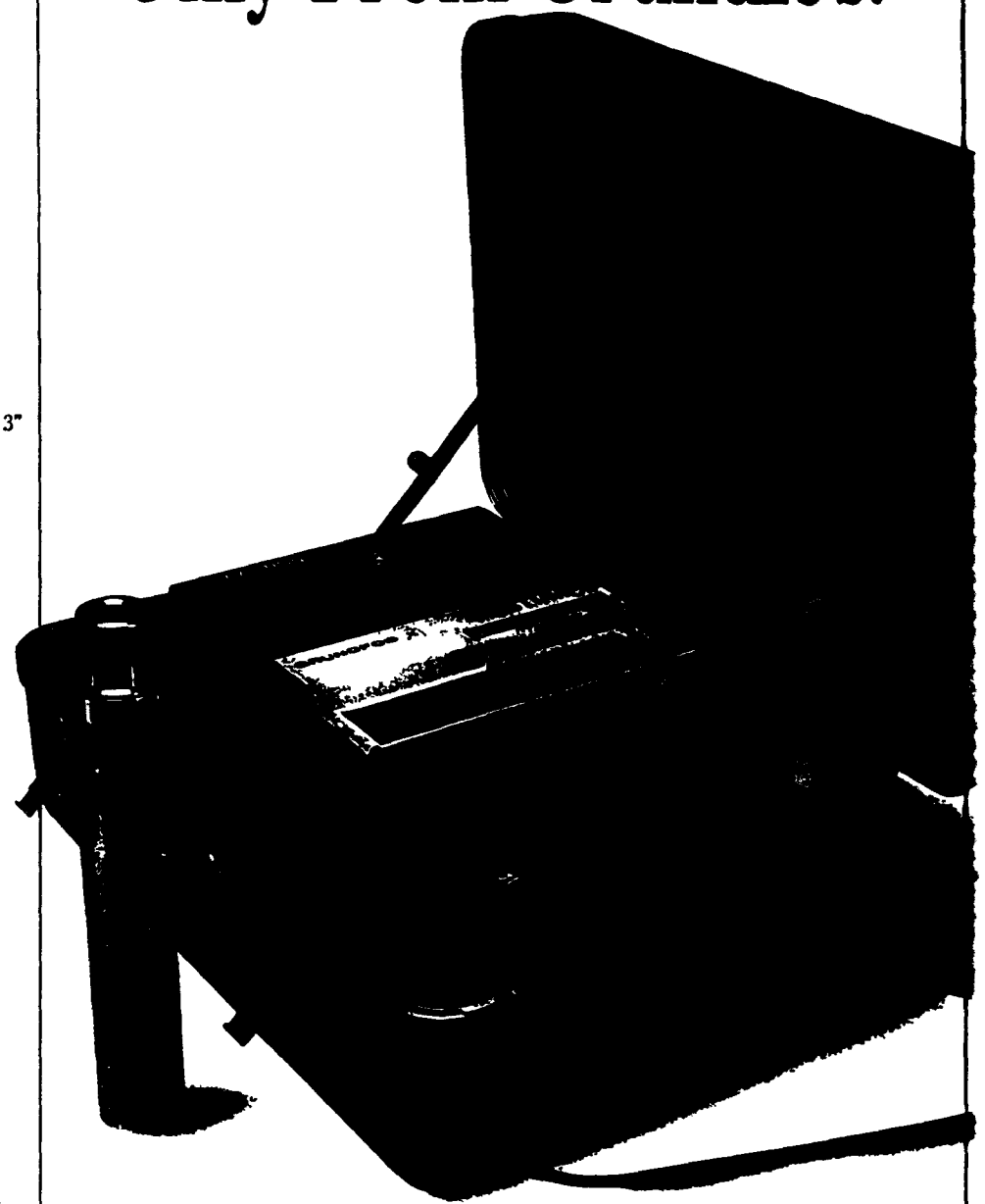
T	ti (min)	ti(hr)
2 5	33962.3	566.0
25 4	3396.2	56 6
254 4	339 6	5 7


Redi-Flo2
370
368
CREEK
MONITORING WELL
LEVEE
MONITORING WELL
370
RECOVERY WELL
OLD GAS PLANT
OLD INJECTION WELL
375
380
385
GRUNDFOS

Redi-Flo2 Compact Design

No other pump on the market combines compact design and power like Redi-Flo2. Measuring just over 11" tall, 1 8" in diameter and weighing 5 5 pounds, this pump

The Complete Purge & Sample System Only From Grundfos.



Redi-Flo2 is designed for dedicated or non-dedicated sampling installations By attaching the pump to a reel of tubing, it becomes fully portable

Put the power of Redi-Flo2 into your daily operation Once this pump is part of your sampling protocol, you'll wonder how you ever got along without Redi-Flo2.

Redi-Flo2

Materials & Components

1 **INLET SCREEN** (316 Stainless Steel) — non-corrosive inlet screen prevents impellers from clogging

2 **PUMP HOUSING** (316 Stainless Steel) — corrosion resistant with 1/2 inch NPT discharge connection

3 **GUIDE VANE** (316 Stainless Steel) — increases pump efficiency and resists clogging

4 **WEAR RING** (Teflon) — placed at each stage, reduces upthrust and vibration

5. **IMPELLER** (316 Stainless Steel) — long-wearing, abrasion and corrosion resistant with high strength-to-mass ratio The fabricated design allows for optimum hydraulic performance

6 **SPACER RING** (316 Stainless Steel) — heavy-duty, corrosion resistant.

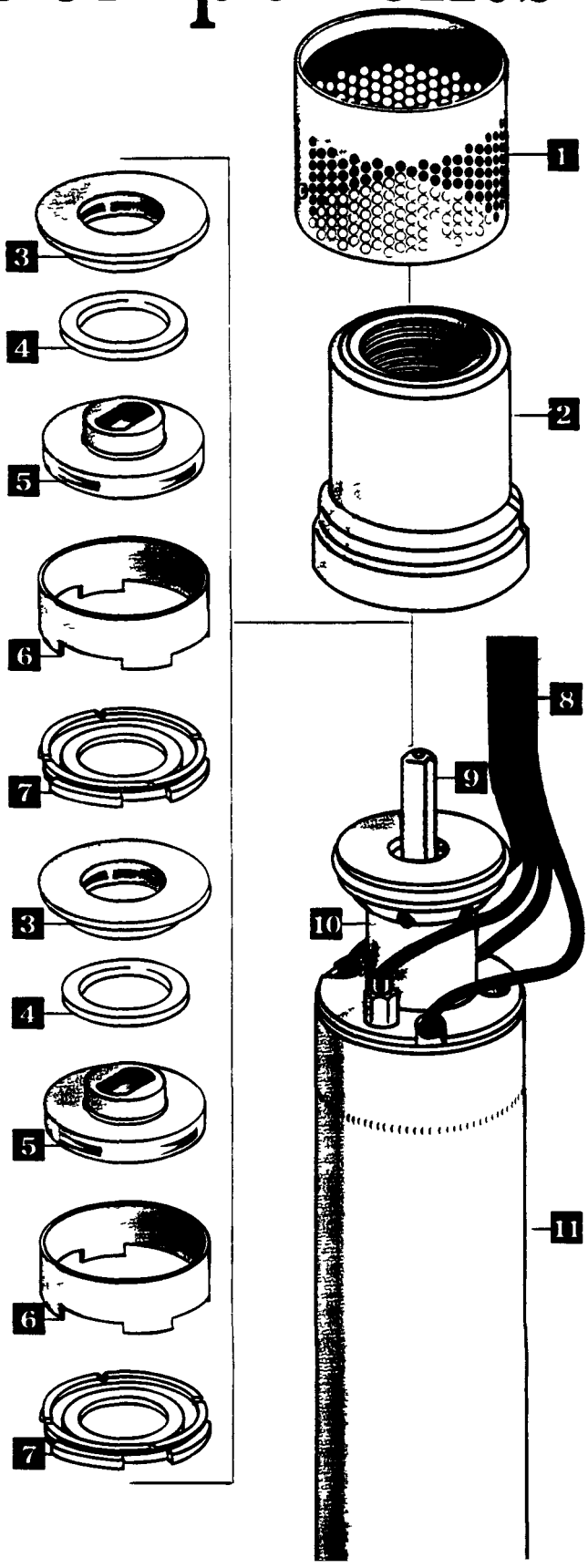
7 **WEAR PLATE** (Teflon) — placed at each stage, eliminates vibration and maintains pump efficiency

8 **MOTOR LEAD** (Teflon insulated wire) — corrosion resistant, reduces the risk of sample bias

9 **SHAFT** (329 Stainless Steel) — splined shaft prevents slippage of the impellers while allowing for easy disassembly and re-assembly of the pump for cleaning or service

10. **SUCTION INTERCONNECTOR** (316 Stainless Steel) — rugged design with large flow openings Provides positive pump and motor alignment.

11. **MOTOR HOUSING** (316 Stainless Steel) — meets the specifications required for environmental applications



Redi-Flo2 Delivers Sample Integrity You Need The Purging Power You Want!

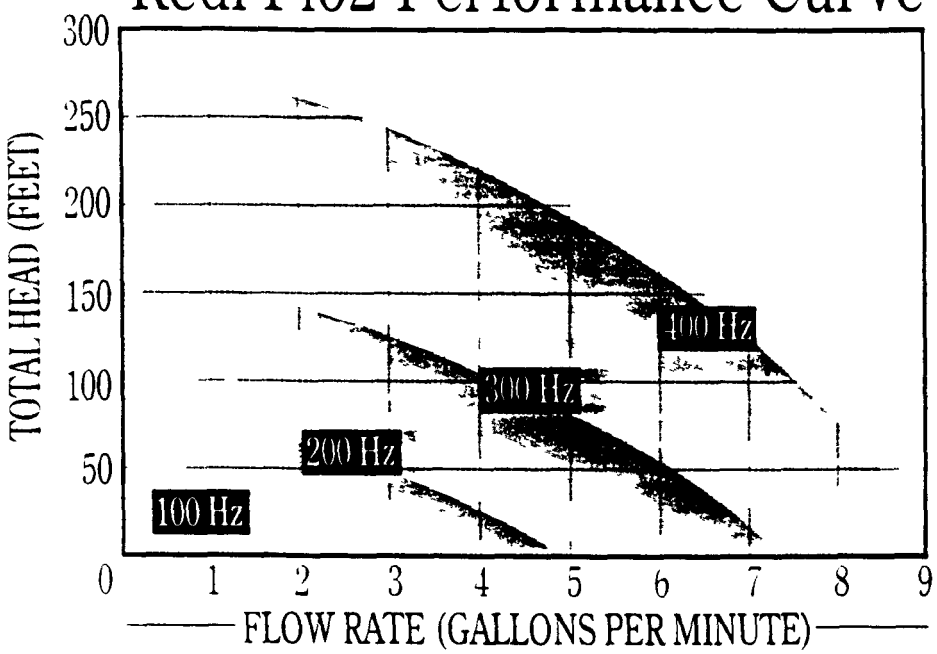
IMUM SAMPLE INTEGRITY INANTS. WITH REDI-FLO2, AT THEIR BEST.

100 ML/MIN FLOW RATE allows for maximum control when sampling In addition, the 100 ml/min flow rate recommended for volatile compound sampling is easily achieved in seconds, simply by turning a dial

OPTIMUM SAMPLE INTEGRITY is critical! With dedicated installations of Redi-Flo2 there is no risk of cross-contamination between wells In addition the risk of contaminants from the surface or well casing entering into samples is reduced

FAST DECONTAMINATION is achieved each and every time The unique design and superior materials of construction make decon' a snap Redi-Flo2 is designed for easy disassembly and re-assembly in minutes That means less down time and higher productivity

Redi-Flo2 Performance Curve



CONTINUOUS FLOW is available from 100 ml/min to 9 gpm

MINIMAL TRAINING is required to effectively operate the converter Its construction and dial design make the Redi-Flo2 system easy to operate without extensive training Operator error is virtually zero

SAMPLE EXPOSURE IS MINIMIZED since the pump is submerged and water flows directly into your sample container Less contact with the atmosphere produces better samples

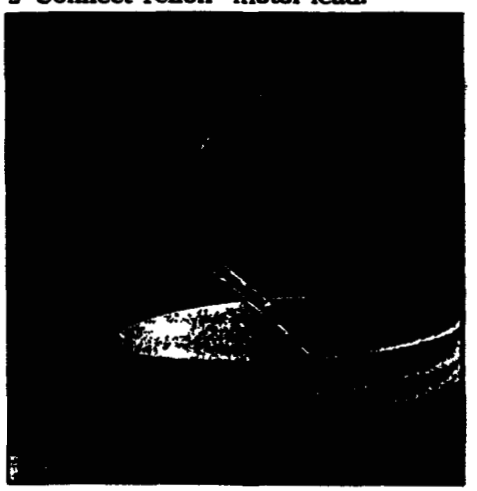
Redi-Flo2

Purge & Sample With Redi-Flo2

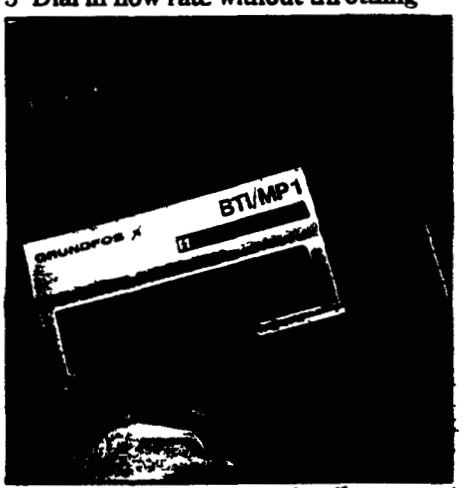
1 Lower Redi-Flo2 into the well.

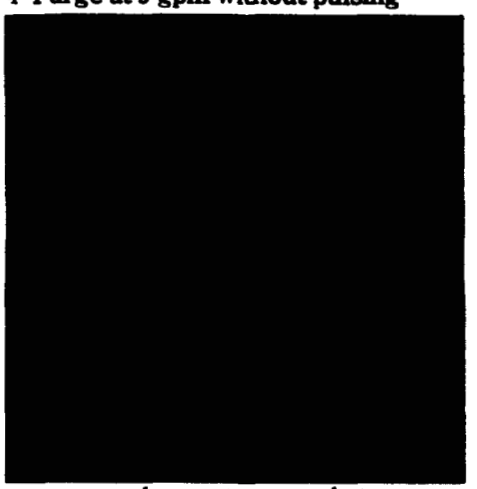
2 Connect Teflon® motor lead.

3 Dial in flow rate without throttling



4 Purge at 9 gpm without pulsing





5 Adjust the flow rate and collect samples from a smooth, uninterrupted stream.

Th
With

REDI-FLO2 ALLOWS FOR
FOR GROUNDWATER CO
YOUR SAMPLE

PURGING & SAMPLING

with the same pump is extremely efficient. With Redi-Flo2, there is no delay between purging the well and collecting your sample

FASTER PURGING is

achieved with the powerful 9 gpm capacity Using a bailer for purging can be costly and tiresome Field tests demonstrate operators prefer the Redi-Flo2 system because of its purging power

CONTINUOUS FLOW

allows for a cleaner, simpler sample catch Partially filled sample containers are a thing of the past. Redi-Flo2 allows you to fill your containers completely, without having to wait for additional water to be extracted from the well. Uninterrupted sample collection improves sample integrity

APPENDIX D

Solving for Transmissivities in a Two-Layer Pumping Test

Using the Jacob approximation of the Theis equation See Molz, F J et al (1989) The Impeller Meter for Measuring Permeability Variations, Water Res Research, Vol 25, No 7, pp 1677-1683 for precedent.

$$Q_1 = \frac{4\pi T_1 \overline{s_1}}{2\,3\log_{10}\dfrac{2\,25 T_1 t}{S_1 r_1^2}}$$

$$Q_2 = \frac{4\pi T_2 \overline{s_2}}{2\,3\log_{10}\dfrac{2.25 T_2 t}{S_2 r_2^2}}$$

$$Q_1 + Q_2 = Q$$

$$\frac{4\pi T_1 \overline{s_1}}{2\,3\log_{10}\dfrac{2.25 T_1 t}{S_1 r_1^2}} + \frac{4\pi T_2 \overline{s_2}}{2\,3\log_{10}\dfrac{2\,25 T_2 t}{S_2 r_2^2}} = Q$$

$$T = T_1 + T_2, \quad T_2 = T - T_1$$

$$\frac{T_1 \overline{s_1}}{\log_{10}\dfrac{2\,25 T_1 t}{S_1 r_1^2}} + \frac{(T - T_1)\overline{s_2}}{\log_{10}\dfrac{2\,25 T_2 t}{S_2 r_2^2}} = \frac{2\,3Q}{4\pi} = C$$

Rearrange for Newton-Raphson Method

$$T_1 = \left[C - \frac{(T-T_1)\overline{s_2}}{\log_{10} \dfrac{2\,25t(T-T_1)}{S_2 r_2^2}} \right] \frac{\log_{10} \dfrac{2\,25T_1 t}{S_1 r_1^2}}{\overline{s_1}}$$

Find T_1 by successive approximation using Newton-Raphson method

$$T_{1(n+1)} = \frac{f(T_{1(n)}) - T_{1(n)} f'(T_{1(n)})}{1 - f'(T_{1(n)})}$$

Find the derivative $f'(T_1)$

d(uv) = udv + vdu is differential formula

$$\left[C - \frac{(T-T_1)\overline{s_2}}{\log_{10} \dfrac{2\,25t\,(T-T_1)}{S_2 r_2^2}} \right] \frac{1}{\overline{s_1}}\; 0\,43 \frac{S_1 r_1^2}{2\,25T_1 t} \frac{2\,25t}{S_1 r_1^2} + \frac{\log_{10} \dfrac{2\,25\,T_1 t}{S_2 r_1^2}}{\overline{s_1}} \left[-d \frac{(T-T_1)\overline{s_2}}{\log_{10} \dfrac{2\,25\,(T-T_1)t}{S_2 r_2^2}} \right]$$

$$d\left(\frac{u}{v}\right) = \frac{vdu - udv}{v^2} \quad \textit{is differential formula}$$

$$d\,\frac{(T-T_1)\overline{s_2}}{\log_{10}\dfrac{2\,25t(T-T_1)}{S_2r_2^2}} = \frac{\left(\dfrac{\log_{10}2\,25t(T-T_1)}{S_2r_2^2}\right)\left(-\overline{s_2}\right) - \left[(T-T_1)\overline{s_2}\right]\dfrac{43Sr_2^2}{2\,25t(T-T_1)} * \dfrac{2\,25t}{S_2r_2^2}\,(-1)}{\left[\log_{10}\dfrac{2.25t(T-T_1)}{S_2r_2^2}\right]^2}$$

$$= -\frac{\overline{s^2}\left[\log_{10}\dfrac{2.25t(T-T_1)}{S_2r_2^2} - 0\,43\right]}{\left(\log_{10}\dfrac{2\,25t(T-T_1)}{S_2r_2^2}\right)}$$

The derivative is

$$\acute{f}(T_1) = \left[C - \frac{(T-T_1)\overline{s_2}}{\dfrac{\log_{10}2\,25t(T-T_1)}{S_2r_2^2}}\right]\frac{43}{S_1T_1} + s_2\,\frac{\left[\log_{10}\dfrac{2\,25t(T-T_1)}{S_2r_2^2} - 0\,43\right]}{\left(\log_{10}\dfrac{2.25t(T-T_1)}{S_1r_2^2}\right)^2}\;\frac{\log_{10}\dfrac{2\,25T_1t}{S_1r_1^2}}{\overline{s_1}}$$

Reference for Newton-Raphson Method

McCracken, Daniel D and William S Darn (1964) Numberical Methods and Fortran Programming
John Wiley & Sons, pp 135-145

```
      PROGRAM TRANS2
C     Transmissivity In Layered Aquifer System
C     This program uses Newton-Raphson iteration to solve for transmissivity
C     of individual Layers in a two Layered system when pumping test data is
C     available   Drawdown must have been monitored in each layer   A gross
C     transmissivity must have been obtained from an normal Theis analysis

C     Select a time when conditions for application of the Jacob method are
C     satisfied
C     Use consistent units, such as feet-day
      DOUBLE PRECISION TIME,Q T,R1 S1,R2 S2 C1 C2 C3,CLOG TT1,T1 A,B
      DOUBLE PRECISION F,TEMP,FXN,TEST,NUMER,DENOM,NUMER1,NUMER2,SS1,SS2
      REAL COUNT, LIMIT
      INTEGER T1GET
      CHARACTER YN*1

      WRITE(*, (A\)')'OTime since start of pumping - ->
      READ(* *)TIME
      WRITE(* '(A\)')'OPumping rate - -> '
      READ(*,*)Q
      WRITE(*, (A\)') OCombined transmissivity - -> '
      READ(*,*)T
      WRITE(*,'(A\)')'OStorativity in layer 1 - -> '
      READ(*,*)SS1
      WRITE(* '(A\)')'OStorativity in layer 2 - -> '
      READ(* *)SS2
      WRITE(*,'(A\)')'Distance to monitoring well in layer 1 - -> '
      READ(*,*)R1
      WRITE(*,'(A\)')'ODrawdown at monitoring well in layer 1 - -> '
      READ(* *)S1
      WRITE(*, (A\)') ODistance to monitoring well in layer 2 - ->
      READ(* *)R2
      WRITE(* '(A\)')'ODrawdown at monitoring well in layer 2 - -> '
      READ(* *)S2
500 WRITE(*,'(A\) )'OInitial estimate of Transmissivity in layer 1 - -
      1>  '
      READ(* *)T1
      C1=2 25*TIME/(SS1*R1**2)
      C2=2 25*TIME/(SS2*R2**2)
      C3=2 3*Q/(4 *3 1415027)
      CLOG=0 43429448190325182765
      TEST=T1/1 E8
      LIMIT=100000
      T1GET=0
100 IF(T1 GE T)THEN
        T1=T-1 E-13
        T1GET=1
      ENDIF
      TT1=T-T1
      A=(C3-(TT1*S2/DLOG10(C2*TT1)))*CLOG/(S1*T1)
      NUMER1=(DLOG10(C2*TT1)-CLOG)
      IF(T1 LE O )THEN
        WRITE(*  (A)') OESTIMATE TOO FAR FROM SOLUTION
        WRITE(*  (A)')  WILL NOT CONVERGE
        GOTO 400
      ENDIF
      NUMER2=DLOG10(C1*T1)
```

```
      NUMER=S2*NUMER1*NUMER2
      DENOM=(S1*(DLOG10(C2*TT1))**2 )
      B=NUMER/DENOM
C     F is the derivative for the Newton-Raphson formula
      F=A+B
      FXN=(C3-TT1*S2/DLOG10(CZ*TT1))*DLOG10(C1*T1)/S1
      TEMP=(FXN-T1*F)/(1 -F)
      IF(DABS(TEMP-T1) LT TEST)GOTO 200
      COUNT=COUNT+1
      IF(COUNT GT LIMIT)THEN
        WRITE(*,'(A)I)'OITERATION LIMIT EXCEEDED '
        IF(T1GET EQ 1)WRITE(*,'(A)')' Generated transmissivity in layer
      11 greater than combined transmissivity
        GOTO 400
      ENDIF
      T1=TEMP
      GOTO 100
200   WRITE(*, (A,G12 4)')'OTransmissivity of layer 1 = ' T1
      WRITE(*  (A,G12 4)')'OTransmissivity of layer 2 = ',T-T1
600   WRITE(*,*)
400   WRITE(*, (A\) ) ODo you want to try another estimate? ( Y'/'N'
      1) - ->  '
      READ(*,*,ERR=600)YN
      IF(YN EQ  Y')THEN
        COUNT=0
        GO TO 500
      ENDIF
300   CONTINUE
      END
```

TEST OF TRANS2

Scenerio #1

Thickness of layer 1 = 11 ft. (Saturated thickness)
Hydraulic Conductivity of layer 1 = $1 * 10^{3}$ cm/sec - K_1

Thickness of layer 2 = 28 ft
Hydraulic Conductivity of layer 2 = $5 * 10^{5}$ cm/sec

r_w = 2 inches = 0 17 ft

t = 5 days

S_y = 0 1 (from OU2 Work Plan)
$S_2 = 28 * 10^{-6}$

Let drawdown be 25% of saturated thickness of layer 2

$$0\,25 * 11 = 2\,75 \; feet$$

$$K_1 = 1 * 10^{-3} \frac{cm}{sec} * 2834\,794 \frac{ft/day}{cm/sec} = 2\,8348 \frac{ft}{day}$$

$$K_2 = 5 * 10^{-5}\; 2834\,784 = 0\,1417392 \frac{ft}{day}$$

$$T_1 = 11 * 2\,8348 = 31\,1828 \frac{ft^2}{day}$$

$$T_2 = 28 * 0\,1417392 = 3\,968698 \frac{ft^2}{day}$$

$$T = 31\,1828 + 3\,968698 = 35\,1515$$

$$Q_1 = \frac{4\pi T_1 \overline{s_1}}{\ln \frac{2.25 T_1 t}{S_y r_w^2}} = \frac{4\pi * 31.1828 * 2.75}{\ln \frac{2.25 * 31.1828 * 5}{0.1 * 0.17^2}} = 92.0496 \frac{ft^3}{day}$$

$$Q_2 = \frac{4\pi * 3.968698 * 2.75}{\ln \frac{2.25 * 3.968698 * 5}{28E-6 * 0.17^2}} = 7.69371 \frac{ft^3}{day}$$

$$Q + Q_1 + Q_2 = 99.7433$$

Calculate drawdown in each layer at r = 5 ft at 5 days

$$S_1 = \frac{Q_1}{4\pi T_1} \ln \frac{2.25 T_1 t}{S_y r_1^2} = \frac{92.0496}{4\pi * 31.1828} \ln \frac{2.25 * 31.1828 * 5}{0.1 * 5^2} = 1.16136$$

$$S_2 = \frac{14.2192}{4\pi * 3.968698} \ln \frac{2.25 * 3.968698 * 5}{28E-6 * 5^2} = 1.70671$$

```
Pumping rate - -> 99 7433
Combined transmissivity - -> 35 1515
Storativity in layer 1 - ->  1
Storativity in layer 2 - -> 28E-6
Distance to monitoring well in layer 1 - -> 5
Drawdown at monitoring well in layer 1 - -> 1 16136
Distance to monitoring well in layer 2 - -> 5
Drawdown at monitoring well in layer 2 - -> 1 70671
Initial estimate of Transmissivity in layer 1 - -> 31
Transmissivity of layer 1 = 31 00 (vs  31 18)
Transmissivity of layer 2 = 4 151 (vs  3 97)

Do you want to try another estimate? ('Y'/'N') - ->
```

```
Do you want to try another estimate? ('Y'/ N') - -> 'Y'

Initial estimate of Transmissivity in Layer 1 - - > 2

ESTIMATE TOO FAR FROM SOLUTION
WILL NOT CONVERGE

Do you want to try another estimate? ( Y /'N') - -> 'Y'

Initial estimate of Transmissivity in layer 1 - -> 1

ESTIMATE TOO FAR FROM SOLUTION
WILL NOT CONVERGE

Do you want to try another estimate? ('Y'/'N') - -> 'Y'

Initial estimate of Transmissivity in layer 1 - ->  5

Transmissivity of layer 1 =  2411  |  Alternate mathematical solution
Transmissivity of layer 2 = 34 91  |  Not consistent with physical conditions


Do you want to try another estimate? ('Y / N ) - ->
```

Sensitivity to Error in Drawdown Measurement

s_1	s_2	T_1	T_2	Remarks All other parameters unchanged
1 16136	1 70671	31 00	4 151	Actual Case T_1 = 31 1828, T_2 = 3 968698
1 2	1 7	27 04	8 114	
1 1	1 7			Generated $T_1 > T$
1 3	1 71	20 63	14 52	
1 5	1 71	14 24	20 91	
1 16	1 8	30 36	4 79	
1 16	1 9	29 18	5 98	If s_2 too high, T_1, will be too low (Remember that T is held constant)
1 16	1 6	31 89	3 26	
1 16	1 16	33 41	1 74	
1 16	0 9	33 83	1 32	
1 16	0 0	34 43	0 72	Remember this is an erroneous drawdown measurement

Sensitivity to Error in Combined Tranmissivity

T	T_1	T_2	Remarks All other parameters unchanged
35 1515	31 00	4 151	Actual case
36	28 78	7 22	
38 6667	23 31	15 31	10% increase in T in T produces 25% decrease in T_1
31 6364			10% decrease in T generated $T_1 > T$

Sensitivity to Error in Storativity

S_1	S_2	T_1	T_2	Remarks All other parameters unchanged from original values
0 1	28E-6	31 00	4 151	Actual Case T_1 = 31 1828, T_2 = 3 968698
0 15	28E-6	22 00	13 16	
0 25	28E-6	14 45	20 70	
0 1	28E-5	24 86	10 29	
1 5	28E-7	32 63	2 52	

5

Roots of Equations

5 1 Introduction

Finding the roots of equations is one of the oldest problems in mathematics and one that is encountered frequently in modern computing, since it is required in a great variety of applications

Consider the simple quadratic equation

$$ax^2 + bx + c = 0$$

We say that

$$x = \frac{-b \pm \sqrt{b^2 - 4ac}}{2a}$$

are the *roots* of this equation because, for these values of x, the quadratic equation is satisfied More generally, we are given a function of x, $F(x)$, and we wish to find a value of x for which

(5 1) $$F(x) = 0$$

The function F may be algebraic or transcendental, we generally assume it to be differentiable

In practice, the functions with which we deal have no simple closed formula for their roots, as the quadratic equation has We turn instead to methods of approximating the roots, which involves two steps

1 Finding an approximate root
2 Refining the approximation to some prescribed degree of accuracy

We will not concern ourselves now with step 1, which is taken up in Section 5 11 Often a first approximation is known from physical

considerations Graphical methods can sometimes be used if this is not the case * Special methods exist for the important case in which $F(x)$ is a polynomial † $a_0 x^n + a_1 x^{n-1} + a_2 x^{n-2} + \cdots + a_{n-1} x + a_n$

We turn our attention to the second step—refining an initial approximation of or "guess" at the solution A numerical method in which a succession of approximations is made is called an *iterative* technique Each step, or approximation, is called an *iteration* If the iterations produce approximations that approach the solution more and more closely, we say that the iteration method *converges*

We will now discuss several iterative techniques for the solution of equations and investigate their convergence properties

5 2 Method of successive approximations

Suppose that (5 1) is rewritten in the form

(5 2) $$x = f(x)$$

This can usually be done in many different ways For instance, if

$$F(x) = x^2 - c = 0$$

where $c \geq 0$, we may add x to both sides to get

(5 3) $$x = x^2 + x - c$$

or we may divide by x to get

(5 4) $$x = \frac{c}{x}$$

As a last example, we may rearrange the equation to get

(5 5) $$x = x - \frac{x^2 - c}{2x} = \frac{1}{2}\left(x + \frac{c}{x}\right)$$

It should be obvious that the values of x which are solutions to these equations are $\pm\sqrt{c}$

Let x_0 be an initial approximation to the solution of (5 2) Then, as the next approximation, take

$$x_1 = f(x_0)$$

As the next approximation take

$$x_2 = f(x_1)$$

* See, for instance, Kaiser S Kunz, *Numerical Analysis*, McGraw-Hill, 1957
† See, for instance, Anthony Ralston and Herbert S Wilf, editors, *Mathematical Methods for Digital Computers*, Wiley, 1960, pp 233–241

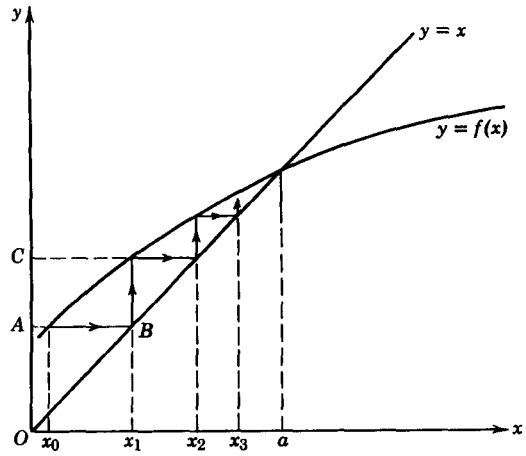


FIGURE 5 1 Diagrammatic representation of the method of successive approximations for $0 < f'(x) < 1$

Proceeding in this way, the nth approximation, or, as it is often called, the nth *iterate*, is

$$x_n = f(x_{n-1}) \tag{5 6}$$

The fundamental question is do the x_n converge to a solution of (5 2) as n increases?

We will now develop *sufficient* conditions of $f(x)$ for this desired convergence That is to say, we will develop conditions that will guarantee that x_n will get closer and closer to a solution of (5 2) These conditions are not *necessary*, however, that is, there may be functions $f(x)$ that do not satisfy these conditions but for which the iteration method (5 6) nevertheless produces a solution

Let us first consider a geometrical representation of the process When we wish to solve (5 2), we look for the intersection of the curve $y = f(x)$ (the right-hand side of the equation) and the line $y = x$ (the left-hand side) See Figure 5 1, in which the curve $y = f(x)$ is unspecified, except that it has the characteristic $0 < f'(x) < 1$ * Let $x = a$ be the value of x at the point of intersection, then a is a root of (5 2), which we naturally do not know at the outset

* A prime denotes a derivative with respect to x

Now consider a guess x_0 The value of x_1 is $f(x_0)$ Since OA in Figure 5 1 is $f(x_0)$, we can find x_1 by tracing a horizontal line until we meet the 45° line $y = x$ as shown (point B) The value of $f(x_1) = x_2$ is then obtained by drawing a vertical line through x_1 (point B) to the curve $y = f(x)$ Thus x_2 is OC We proceed in this manner, as indicated by the arrows in the figure

We seem, in this case, to be converging toward the solution $x = a$, since each successive approximation is closer to a It is important to remember that we took a curve $y = f(x)$ for which $0 < f'(x) < 1$

Consider now another shape for the curve $y = f(x)$, one in which the derivative is negative but less than 1 in absolute value (See Figure 5 2) Again the arrows indicate the pattern of the iterations, and again the approximations seem to converge to $x = a$ Now, however, each successive approximation is on the opposite side of $x = a$ from its predecessor, whereas in the first example of Figure 5 1 all the approximations were on the same side of $x = a$

Finally, we consider approximation formulas for which the derivatives are greater than 1 (Figure 5 3) and less than -1 (Figure 5 4) In both cases the iterations do not converge Each succeeding guess is farther from $x = a$ than its predecessor It seems, therefore, that

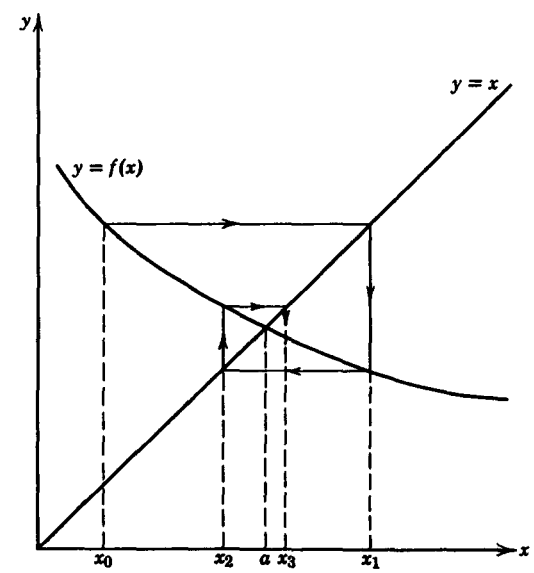


FIGURE 5 2 Diagrammatic representation of the method of successive approximations for $-1 < f'(x) < 0$

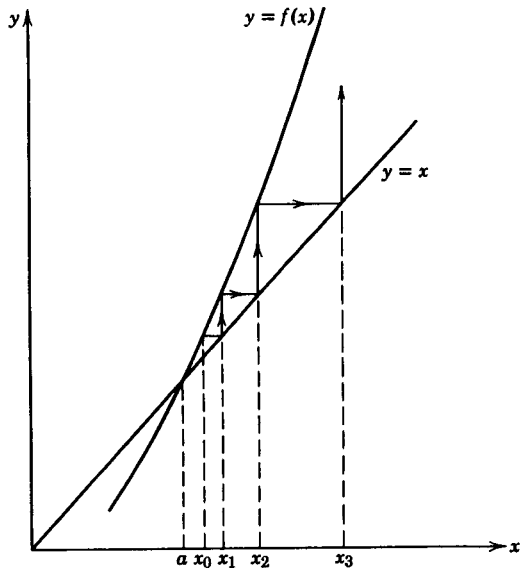


FIGURE 5 3 Diagrammatic representation of the method of successive approximations for $f'(x) > 1$

if $f'(x)$ is less than 1 in absolute value, the iteration method described by (5 6) will converge

This, in fact, is the case, as we can readily prove by an elementary argument Note that

$$a = f(a)$$

$$x_n = f(x_{n-1})$$

so that

$$x_n - a = f(x_{n-1}) - f(a)$$

Multiplying on the right by $(x_{n-1} - a)/(x_{n-1} - a)$ and using the mean value theorem,* we have

$$x_n - a = f'(\xi)(x_{n-1} - a)$$

where ξ lies between x_{n-1} and a

* The mean value theorem states that given two points, a and b, on a curve $y = f(x)$, where $f(x)$ has a continuous derivative, the slope of the chord between a and b

$$\frac{f(b) - f(a)}{b - a}$$

is equal to the slope of the tangent to the curve at some intermediate point

Now let m be the maximum absolute value of $f'(x)$ over the entire interval in question (the interval including $x_0, x_1, \ldots, x_n, a$) Then

$$|x_n - a| \leq m|x_{n-1} - a|$$

Similarly,

$$|x_{n-1} - a| \leq m|x_{n-2} - a|$$

so

$$|x_n - a| \leq m^2|x_{n-2} - a|$$

Continuing in this way,

$$|x_n - a| \leq m^n|x_0 - a| \tag{5 7}$$

Now, if $m < 1$ over the entire interval, then, no matter what the choice of x_0, as n increases the right-hand member becomes small, and x_n comes closer to a

On the other hand, for $|f'(x)| > 1$, $|x_n - a|$ becomes indefinitely large as n increases The proof is left to the reader as an exercise *Thus if $|f'(x)| < 1$, the process (5 6) converges If $|f'(x)| > 1$, the process (5 6) diverges* Observe that the inequalities are assumed to hold at *all* the approximations $(x_0, x_1, \ldots, x_n)$

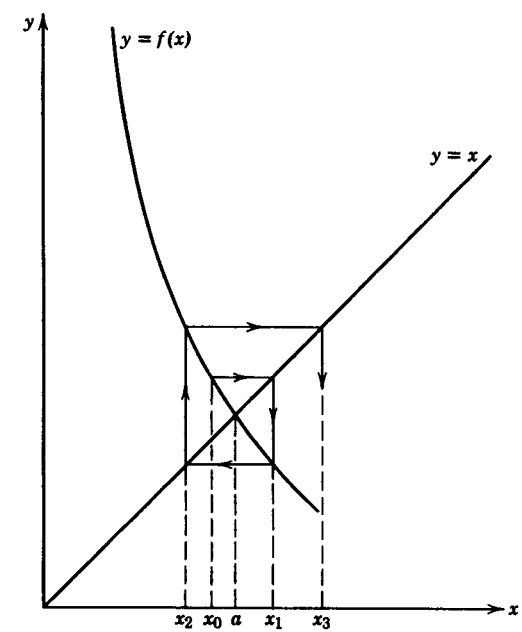


FIGURE 5 4 Diagrammatic representation of the method of successive approximations for $f'(x) < -1$

What happens if at some points x_i the derivative $f'(x_i)$ is less than 1 in absolute value and at some other points x_j the derivative $f'(x_j)$ is greater than 1 in absolute value? The answer to this question is unresolved. The process sometimes converges and sometimes does not.

Let us return for a moment to our example of finding the square root of c. In (5.3)

$$f(x) = x^2 + x - c$$

so that

$$|f'(x)| < 1 \quad \text{if} \quad -1 < x < 0$$

If we are searching for the square root of a number c which is less than 1, the process converges to the negative square root of c.

In (5.4), however,

$$f'(x) = \frac{-c}{x^2}$$

and, if x is close to $\sqrt{c}$ (as it must eventually be in order to converge to the square root of c), $f'(x) \simeq 1$, and indeed the process diverges.

Finally, using (5.5),

$$f'(x) = \frac{1}{2}\left(1 - \frac{c}{x^2}\right)$$

and again, if $x \simeq \sqrt{c}$, $f'(x) \simeq 0$, and the process converges (rapidly, as a matter of fact). Formula 5.6 is a special case that we shall encounter again in a later section on the Newton-Raphson method.

It should be clear that, although for any equation there is in general a wide choice of functions $f(x)$ for use in the method of successive approximations, a judicious choice is necessary if convergence is to be obtained.

5.3 A modified method of successive approximations

Consider Figure 5.1 again. Notice that although each iterate is closer to the solution than its predecessor each falls short of the correct answer. It might be advantageous, therefore, to make a larger correction in each iteration. That is to say, instead of letting

$$x_{n+1} = x_n + \Delta x$$

where

$$\Delta x = f(x_n) - x_n$$

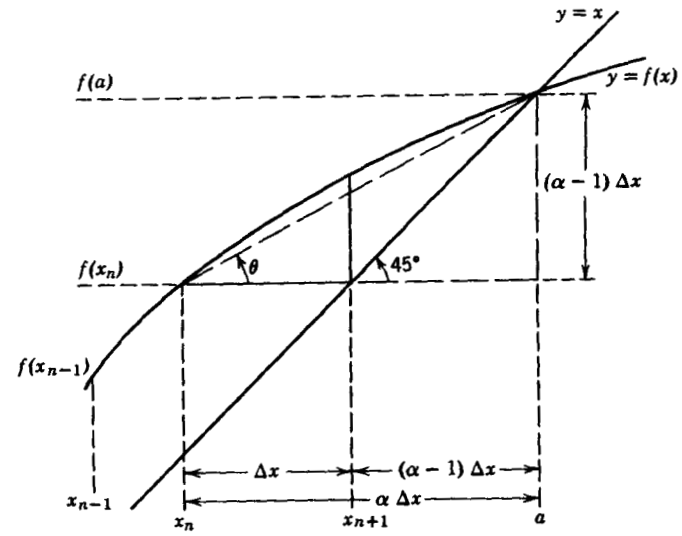


FIGURE 5.5 Diagrammatic representation of the modified method of successive approximations for $0 < f'(x) < 1$

we might choose the next iterate after x_n to be

$$x_{n+1} = x_n + \alpha\,\Delta x$$

where $\alpha > 1$.

The situation is displayed in Figure 5.5, which is an enlargement of a small section of Figure 5.1. The best choice of α is the one shown, which would produce $x_{n+1} = a$. Let us try to determine the best value for α.

Notice that the distance between x_{n+1} and a is $(\alpha - 1)\,\Delta x$, and, since $y = x$ is a 45° line, the distance between $f(a)$ and $f(x_n)$ is also $(\alpha - 1)\,\Delta x$. Therefore, the tangent of the angle θ is

$$\tan\theta = \frac{(\alpha - 1)\,\Delta x}{\alpha\,\Delta x} = \frac{\alpha - 1}{\alpha} \tag{5.8}$$

On the other hand,

$$\tan\theta = \frac{f(a) - f(x_n)}{a - x_n}$$

and, using the mean value theorem,

$$\tan\theta = f'(\xi) \tag{5.9}$$

where $x_n \le \xi \le a$

From (5 8) and (5 9), then,

$$\alpha = \frac{1}{1 - f'(\xi)} \tag{5 10}$$

The value of ξ is unknown, of course, but we can approximate the value of $f'(\xi)$ by

$$f'(\xi) \simeq \frac{f(x_n) - f(x_{n-1})}{x_n - x_{n-1}} = \frac{f(x_n) - x_n}{x_n - x_{n-1}} \tag{5 11}$$

Geometrically, this amounts to drawing the chord between the points $(x_n, f(x_n))$ and $(x_{n-1}, f(x_{n-1}))$ and finding its intersection with the line $y = x$

The process is now

$$x_{n+1} = x_n + \alpha(f(x_n) - x_n) \tag{5 12}$$

where α is determined as in (5 10) and (5 11)

The question arises how convergence is affected by the modified method Notice from (5 10) that if $0 < f'(x) < 1$ then $1 < \alpha < \infty$ This is the case illustrated in Figure 5 1, in which the steps were too small, since $\alpha > 1$, the modified method will make them larger and therefore speed up convergence

For $-1 < f'(x) < 0$, $\frac{1}{2} < \alpha < 1$ from (5 10), which is the situation in Figure 5 2 There, each step was too large, the modified method decreases each step by a factor between $\frac{1}{2}$ and 1

More important, perhaps, are the divergent cases If $f'(x) > 1$, then $\alpha < 0$ As shown in Figure 5 3, each step is in the wrong direction, that is, the iterates are moving away from the solution Since α for this case is negative, the modification reverses the direction as needed

Finally, for $f'(x) < -1$, $0 < \alpha < \frac{1}{2}$ Here, as seen in Figure 5 4, the steps were too large, the modification reduces them by a factor between zero and $\frac{1}{2}$ It is appropriate that the reduction should be greater in this case then in Figure 5 2, since it is divergent, whereas the other was convergent

This modification is due to Wegstein * The processes of extrapolation (overshooting) or interpolation (undershooting) is common in iterative methods We shall encounter them again in Chapter 8 in connection with the iterative solution of simultaneous linear equations

* Comm ACM, 1, 9–13 (1958)

A further slight modification of the method of successive approximations leads to one of the best-known numerical techniques, the Newton-Raphson method, for finding the roots of equations Those already described, however have a practical advantage over the Newton-Raphson in certain cases We shall return to this question after considering the Newton-Raphson method

5 4 The Newton-Raphson method

Recall that in (5 11) we approximated the derivative $f'(\xi)$ by a difference Recall also that the optimum choice of ξ lay in the range $x_n \leq \xi \leq a$

Suppose that for computational simplicity we chose $\xi = x_n$ Then we have

$$\alpha = \frac{1}{1 - f'(x_n)} \tag{5 13}$$

and

$$x_{n+1} = \frac{f(x_n) - x_n f'(x_n)}{1 - f'(x_n)} \tag{5 14}$$

We now note that (5 14) is equivalent to a method of successive approximations given by

$$x_{n+1} = g(x_n)$$

where

$$g(x) = \frac{f(x) - x f'(x)}{1 - f'(x)}$$

Recall also that if $|g'(x)| < 1$ then the method converges Now

$$g'(x) = \frac{f''(x)[f(x) - x]}{(1 - f'(x))^2}$$

From (5 2), however, if x is sufficiently near a root, the term in brackets is small Therefore, the iteration method described in (5 14) converges, provided

1 x_0 is sufficiently close to a root of $x = f(x)$
2 $f''(x)$ does not become excessively large
3 $f'(x)$ is not too close to 1

This is the celebrated Newton-Raphson method It is usually written in the more familiar form

$$x_{n+1} = x_n - \frac{F(x_n)}{F'(x_n)} \tag{5 15}$$

$$x_{n+1} = x_n - \frac{f(x_n) - x_n}{f'(x_n) - 1} = \frac{x_n f'(x_n) - x_n - f(x_n) + x_n}{f'(x_n) - 1}$$

where

$$F(x) = f(x) - x = 0$$

That is to say, we have returned to the form given in (5 1)

The conditions for convergence now become

1 x_0 is sufficiently close to a root of $F(x) = 0$
2 $F''(x)$ does not become excessively large
3 $F'(x)$ is not too close to zero

The last condition means that no two roots are too close together We shall return to a discussion of this problem in the following section

Let us find a geometrical interpretation of the Newton-Raphson method In (5 13) we chose the point to be at x_n In Figure 5 5 this means that the angle θ is chosen to be the slope of the tangent to $y = f(x)$ at x_n The process then is to draw the tangent to the curve $y = f(x)$ at $x = x_n$ and find the intersection of the tangent with the line $y = x$ Doing so produces the new value x_{n+1} A vertical line is drawn through x_{n+1} to the curve $y = f(x)$ and a new tangent drawn The path traced in Figure 5 6 is for the case in which $0 < f'(x) < 1$

Notice that the convergence is much more rapid than that in Figure

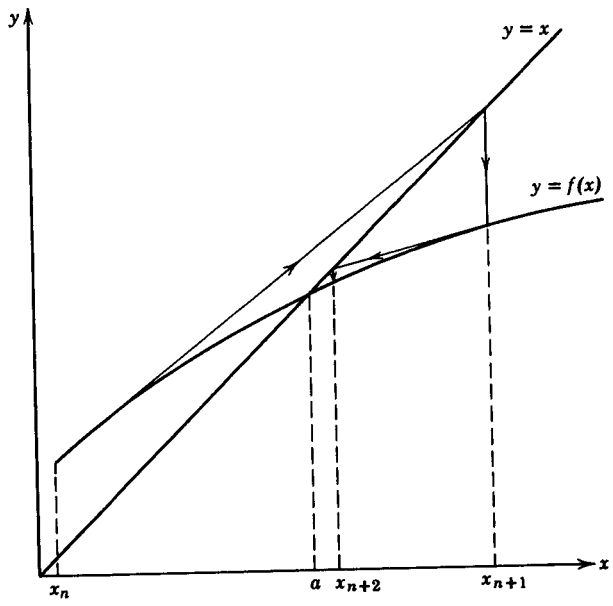


FIGURE 5 6 Diagrammatic representation of the Newton Raphson method for $f(x) = x$

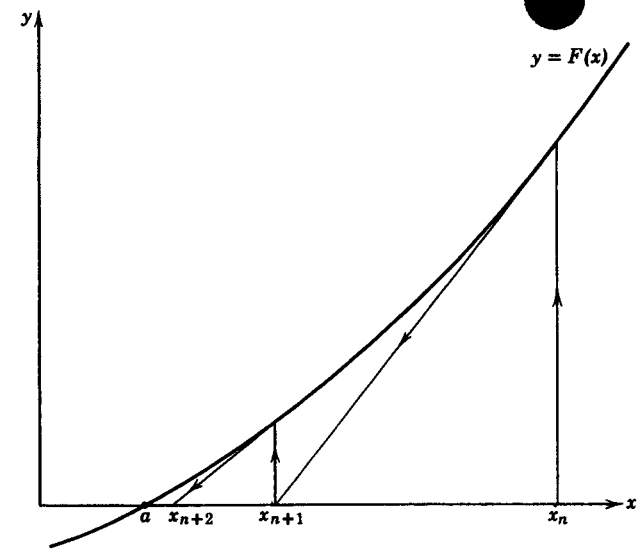


FIGURE 5 7 Diagrammatic representation of the Newton Raphson method for $F(x) = 0$

5 1, which is typical of the Newton-Raphson method, since $g'(x)$ is very small

If the equation is put in the form of (5 1) and the iterative formula (5 15) is used, the geometric picture is that of Figure 5 7 We are now looking for the intersection of $y = F(x)$ and $y = 0$ Given a guess x_n, the tangent to $y = F(x)$ is drawn, and its intersection with the x-axis produces the new value of $x = x_{n+1}$ It is easily determined that this is the x_{n+1} in (5 15) find the equation of the line through the point x_n, $F(x_n)$ with slope $F'(x_n)$ and then find the intersection of this line with the x-axis

5 5 Nearly equal roots

We have already pointed out that difficulties may arise in the Newton-Raphson method if (5 1) or (5 2) has nearly equal roots In that case, condition 3 for convergence is violated close to the nearly equal roots The phenomenon is illustrated in Figure 5 8 (The scale is greatly enlarged) Notice that the derivative of $f(x)$ is near 1 at the two roots, a_1 and a_2 Moreover, from the mean value theorem the derivative is equal to 1 somewhere between a_1 and a_2

Let us now examine what happens if we choose x_0 as an initial guess

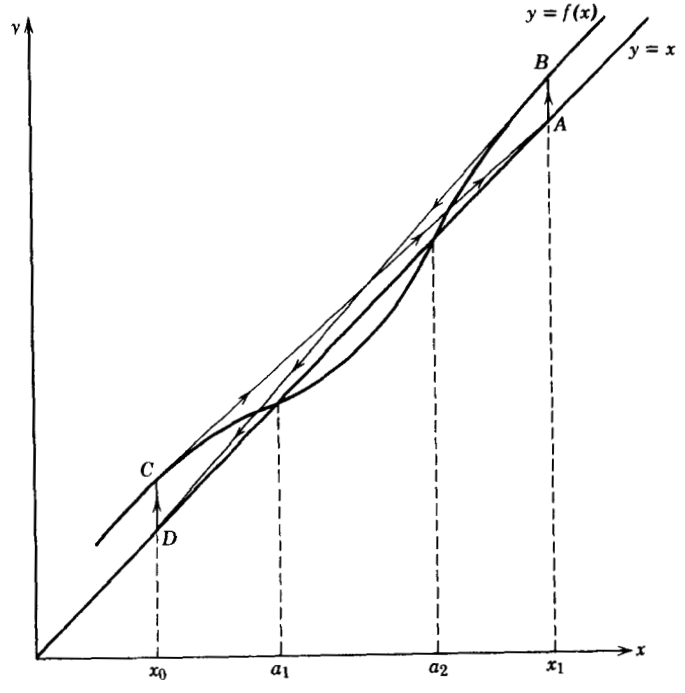


FIGURE 5 8 Diagrammatic representation of the non convergence of the Newton Raphson method for $|f'(x)|$ near 1

to the root a_1 The tangent constructed at C intersects $y = x$ at 1 and the new iterate is x_1 The tangent at B intersects $y = x$ at D, yielding x_0 again The iteration, therefore, alternates between x_0 and x_1 indefinitely The process cannot *resolve* the two roots because they are too close together Of course, we might say that it is condition 1 that is being violated and that x_0 was not sufficiently close to a_1

Indeed, this is true We should therefore explore a method by which a close first approximation may be found Numerically, difficulties arise because the evaluation of the denominator in (5 14) requires the subtraction of two nearly equal numbers, which, as we have seen repeatedly, gives rise to inaccuracies

Following Macon,* we will first find the value of x where $f'(x) = 1$, that is, we solve the equation

$$x = x + f'(x) - 1$$

* Nathaniel Macon, *Numerical Analysis*, Wiley, New York, 1963, pp 34–36

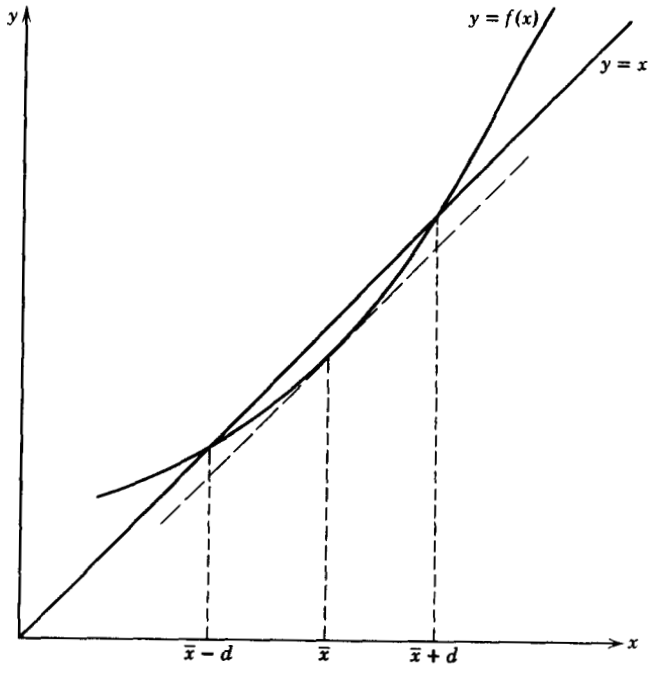


FIGURE 5 9 Diagrammatic representation of the modified Newton Raphson method for $|f'(x)|$ near 1

Let the solution be $x = \bar{x}$ This point lies between the two roots, a_1 and a_2 In order to obtain a first approximation, we may assume that $\bar{x}$ lies midway between a_1 and a_2 (See Figure 5 9) That is to say, we let $\bar{x} + d$ and $\bar{x} - d$ be the two roots Expanding $f(x)$ in a Taylor series about $\bar{x}$ and noting that $f'(\bar{x}) = 1$, we have

$$f(x) = f(\bar{x}) + (x - \bar{x}) + \tfrac{1}{2}f''(\bar{x})(x - \bar{x})^2 +$$

We now terminate the series after three terms as shown and let $x = \bar{x} + d$, so that

$$f(\bar{x} + d) = f(\bar{x}) + d + \tfrac{1}{2}f''(\bar{x})d^2$$

But

$$f(\bar{x} + d) = \bar{x} + d$$

so, solving for d,

$$d = \sqrt{\frac{2(\bar{x} - f(\bar{x}))}{f''(\bar{x})}}$$

For the case in which we are solving the equation in the form

$$F(x) = 0$$

we get

$$d = \sqrt{\frac{-2F(\bar{x})}{F''(\bar{x})}}$$

noting that $F'(\bar{x}) = 0$. The reader should satisfy himself that the quantity under the square root sign is positive by referring to Figure 5.8.

A recapitulation is in order. Given an equation with two nearly equal roots and knowing at least approximately where they are, we solve the equation

$$x = x + f'(x) - 1$$

for a value $\bar{x}$, using any convenient method, such as Newton-Raphson. Using this value of $\bar{x}$, solve for d with the expressions shown above. Finally, the values $\bar{x} - d$ and $\bar{x} + d$ are used as starting approximations for a Newton-Raphson solution for a_1 and a_2, respectively.

Of course, we may run into trouble if $f''(x)$ is near zero. This means that $f'(x) = 1$ has more than one root near x. In this event we would first find a solution for $f''(x) = 0$. The details are not discussed here, the interested reader is referred to Macon's text.

5.6 Comparison of the methods and their roundoff errors

Since the Newton-Raphson method converges much more rapidly than the method of successive approximations, we might ask why the latter is ever used. The answer lies in the requirement, in Newton-Raphson, of the evaluation of both the function and its derivative at each iteration. These evaluations may be difficult, time-consuming, or impossible. For example, the function $f(x)$ may not be given by a formula at all but by a table of values. The derivative may not even exist at all points. The method of successive approximations or its modification is often applied in such cases.

The choice of methods depends, in other words, on the particular function $f(x)$ or $F(x)$.

It is interesting and important to notice that the roundoff error does *not* build up as the iterations proceed. The total roundoff error is just the error committed in the final iteration and does not depend on the arithmetic operations in previous iterations. This property is characteristic of iterative processes and is one of their major advantages over nonitrative techniques. The reason for the nonaccumulation of roundoff errors is clear: each iterate, including the next-to-last x_n, may be considered to be the *initial* approximation. The roundoff error in the last iterate therefore depends only on the operations that produce it from the next-to last.

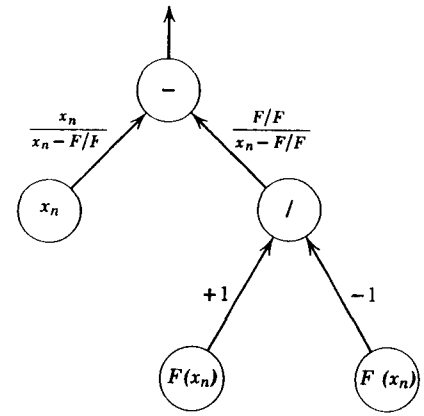


FIGURE 5.10 The process graph for the Newton-Raphson method

The process graph for the Newton-Raphson method of (5.15) is shown in Figure 5.10. There is no inherent error in x_n, since it may be considered to be an infinite decimal with zeros for any missing digits at the end. There are relative roundoff errors in computing $F(x_n)$ and $F'(x_n)$, call them r and r', respectively. Call the relative roundoff error in the division d and that in the subtraction, s. Then the absolute roundoff error in x_{n+1} is

$$e = \frac{F(x_n)}{F'(x_n)}\left(r - r' - d + \frac{s}{x_{n+1}}\right)$$

In most cases the error is dominated by the errors r and r' in evaluating F and F'.

5.7 Roots of polynomials

We now consider the very important special case in which $F(x)$ is a polynomial of degree m

$$F(x) = a_0 + a_1x + a_2x^2 + \qquad + a_mx^m \tag{5.16}$$

We use the Newton-Raphson method in the form given by (5.15)

The evaluation of $F(x_n)$ by Horner's rule has already been discussed in Section 3 5 We recursively find

$$(5\ 17)\qquad \begin{cases} b_m = a_m \\ b_j = a_j + x_n b_{j+1} \qquad j = m-1, \qquad , 0 \end{cases}$$

and

$$F(x_n) = b_0$$

Now recall from Section 3 4 (3 11) that

$$F(x) = (x - x_n)\,G(x) + b_0$$

where

$$G(x) = b_1 + b_2 x + \qquad + b_m x^{m-1}$$

Now

$$F'(x) = (x - x_n)\,G'(x) + G(x)$$

so

$$F'(x_n) = G(x_n)$$

But $G(x)$ is a polynomial of degree $m - 1$, so we can use Horner's rule to evaluate $G(x_n)$ and thereby find $F'(x_n)$ Letting

$$(5\ 18)\qquad \begin{cases} c_m = b_m \\ c_j = b_j + x_n c_{j+1} \qquad j = m-1, \qquad , 1 \end{cases}$$

It follows that

$$F'(x_n) = G(x_n) = c_1$$

From (5 15), then, the Newton-Raphson method for a polynomial reduces to

$$x_{n+1} = x_n - \left(\frac{b_0}{c_1}\right)$$

where b_0 and c_1 are calculated from (5 17) and (5 18) This procedure is often referred to as the Birge-Vieta method

Example

Let

$$F(x) = x^3 - x - 1$$

We wish to find the root near $x_0 = 1\ 3$ The sequence of calculations is shown in Table 5 1

We see that x_2 and x_3 agree through seven digits, x_3 therefore has at least seven reliable digits and almost certainly more

A further discussion of finding the roots of polynomials appears in Case Study 7

Table 5 1

i	a_i	b_i	c_i
3	1	1	1
2	0	1 3	2 6
1	−1	0 69	4 07
0	−1	−0 103	

$$x_1 = x_0 - \frac{b_0}{c_1} = 1\ 3 - \frac{-0\ 103}{4\ 07} = 1\ 325$$

i	a_i	b_i	c_i
3	1	1	1
2	0	1 325	2 65
1	−1	0 755625	4 267
0	−1	0 001203	

$$x_2 = x_1 - \frac{b_0}{c_1} = 1\ 325 - \frac{0\ 001203}{4\ 267} = 1\ 3247181$$

i	a_i	b_i	c_i
3	1	1	1
2	0	1 324718	2 649436
1	−1	0 154878	4 264634
0	−1	0 0000004	

$$x_3 = x_2 - \frac{b_0}{c_1} = 1\ 324718 - \frac{0\ 0000004}{4\ 264634} = 1\ 3247179$$

5 8 Effect of uncertainty in the coefficients

Often the coefficients a_i in a polynomial (5 16) are obtained from experimental equipment or as a result of prior calculations In either case there is some uncertainty in the values of the coefficients, that is, the a_i contain inherent errors It is important to determine how errors in the coefficients affect the error in a computed root

This error is independent of the method of computation used We shall assume that there is no roundoff error in the computed root or, more precisely, that the roundoff error is negligible compared with the error due to inaccuracies in the coefficients This is in fact often a valid assumption For example, it is not uncommon to work with coefficients that are known to only a few percent in a computer that carries 10 digits in each number Except in unlikely circumstances, roundoff error will not matter

Let the error in a_i be δ_i, that is, the *true* polynomial is

$$F^*(x) = (a_0 + \delta_0) + (a_1 + \delta_1)x + (a_2 + \delta_2)x^2 + \quad + (a_m + \delta_m)x^m \tag{5 19}$$

where the $|\delta_i|$ are small compared with the $|a_i|$ We will let $\bar{x}$ be a root of the original polynomial

$$F(x) = a_0 + a_1x + a_2x^2 + \quad + a_mx^m \tag{5 20}$$

Finally we let

$$x^* = \bar{x} + \epsilon \tag{5 21}$$

be a root of (5 19), and we proceed to estimate ϵ under the assumption that $|\epsilon|$ is much less than $|\bar{x}|$ If the estimate of ϵ does not satisfy this assumption, the analysis will not be valid In many cases, however, the assumption is justified, and in any case its validity can easily be checked after the estimate has been obtained

Substituting (5 21) in (5 19) and noting that

$$F^*(x^*) = 0$$

we have

$$(a_0 + \delta_0) + (a_1 + \delta_1)(\bar{x} + \epsilon) + \quad + (a_{m-1} + \delta_{m-1})(\bar{x} + \epsilon)^{m-1} + (a_m + \delta_m)(\bar{x} + \epsilon)^m = 0$$

Expanding $(x + \epsilon)^j$ and neglecting terms of second or higher powers in ϵ, we get

$$(a_0 + \delta_0) + (a_1 + \delta_1)(\bar{x} + \epsilon) + + (a_{m-1} + \delta_{m-1})(\bar{x}^{m-1} + (m - 1)\bar{x}^{m-2}\epsilon) + (a_m + \delta_m)(\bar{x}^m + m\bar{x}^{m-1}\epsilon) = 0$$

Again neglecting terms in $\delta_i\epsilon$ and noting that $F(\bar{x}) = 0$,

$$\delta_0 + \delta_1\bar{x} + \quad + \delta_{m-1}\bar{x}^{m-1} + \delta_m\bar{x}^m + \epsilon(a_1 + 2a_2\bar{x} + + (m - 1)a_{m-1}\bar{x}^{m-2} + ma_m\bar{x}^{m-1}) = 0$$

so that

$$\sum_{i=0}^{m} \delta_i\bar{x}^i + \epsilon F'(\bar{x}) = 0$$

A bound on ϵ then is

$$|\epsilon| \le \frac{\left|\sum_{i=0}^{m} \delta_i\bar{x}^i\right|}{|F'(\bar{x})|} \tag{5 22}$$

We now consider two special cases

1 The coefficients are experimental data given to a fixed number of decimal places p

2 The coefficients are the results of previous floating point calculations and have a given number of significant figures

The difference is that between absolute and relative accuracy in the coefficients

CASE 1 If the a_i are each given to p decimal places,

$$|\delta_i| \le \tfrac{1}{2}\ 10^{-p}$$

and from (5 22)

$$|\epsilon| \le \frac{\frac{1}{2}\ 10^{-p}}{|F'(\bar{x})|}\left|\sum_{i=0}^{m} \bar{x}^i\right|$$

Now

$$\left|\sum_{i=0}^{m} \bar{x}^i\right| \le \sum_{i=0}^{m} |\bar{x}|^i$$

by the triangle inequality The right-hand member of this last inequality is a geometric series and equal to

$$\frac{1 - |\bar{x}|^{m+1}}{1 - |\bar{x}|}$$

so that

$$\epsilon \le \frac{10^{-p}(1 - |\bar{x}|^{m+1})}{2|c_1|(1 - |\bar{x}|)} \tag{5 23}$$

where c_1 has replaced $F'(\bar{x})$ and was calculated by (5 17) and (5 18)

Example

$F(x) = x^3 - x - 1$ Suppose the coefficients are accurate to four decimals ($p = 4$) One root of this equation, as shown before, is $x = 1\ 324718$ The bound (5 23) becomes

$$0\ 75\ \ 10^{-4}$$

which indicates that

$$x = 1\ 324718 \pm 0\ 000075$$

It is not profitable, therefore, to iterate further to find the root to any greater accuracy

CASE 2 If the a_i are each given to t significant figures,

$$|\delta_i| \le 5\ \ 10^{-t}|a_i|$$

and from (5 22)

$$|\epsilon| \leq 5 \quad 10^{-t} \frac{\sum_{i=0}^{m} |a_i \bar{x}^i|}{|c_1|}$$

Example

$F(x) = x^3 - x - 1$ Suppose the coefficients are computed numbers accurate to four significant digits ($t = 4$) Then for $x = 1\ 324718$

$$|\epsilon| \leq 0\ 00055$$

so that

$$x = 1\ 324718 \pm 0\ 00055$$

The root should therefore be stated as 1 325, with a possible error of one unit in the last place

5 9 Simultaneous equations

Often we are faced with problems involving several unknowns and an equal number of equations For example, we may wish to find x and y such that

$$x^2 + y = 3$$

and

$$y^2 + x = 5$$

In this case we may solve the first for y and substitute in the second to get

$$x^4 - 6x^2 + x + 4 = 0$$

Now we have a polynomial in x that can be solved by methods we know One root is $x = 1$ and therefore $y = 2$

Many times, however, it is difficult or impractical to reduce the problem in this way to the solution of one equation in one unknown The most common situation occurs when the equations are linear, this special case is considered in detail in Chapter 8, since there are special methods for its solution Here, we state results for the solution of two nonlinear equations in two unknowns, using a generalization of the Newton-Raphson method The derivation is left to the student (see Exercise 32)

Let the equations be

$$F(x, y) = 0$$

$$G(x, y) = 0$$

and let x_n, y_n be some approximate root

Define

$$J(x_n, y_n) = \frac{\partial F}{\partial x}(x_n, y_n) \frac{\partial G}{\partial y}(x_n, y_n) - \frac{\partial F}{\partial y}(x_n, y_n) \frac{\partial G}{\partial x}(x_n, y_n)$$

This is called the Jacobian of the system and is assumed to be nonzero The assumption is analogous to assuming that $F'(x_n) \neq 0$ in the single variable case

The next approximation is then given by

$$x_{n+1} = x_n - \frac{F(x_n, y_n) \dfrac{\partial G}{\partial y}(x_n, y_n) - G(x_n, y_n) \dfrac{\partial F}{\partial y}(x_n, y_n)}{J(x_n, y_n)}$$

$$y_{n+1} = y_n + \frac{F(x_n, y_n) \dfrac{\partial G}{\partial x}(x_n, y_n) - G(x_n, y_n) \dfrac{\partial F}{\partial x}(x_n, y_n)}{J(x_n, y_n)}$$

The iterations are continued until two successive approximations are found to be sufficiently close to each other Numerical examples appear in Exercises 33 and 34

A generalization of the method of successive approximations to two simultaneous equations is given in Exercise 35

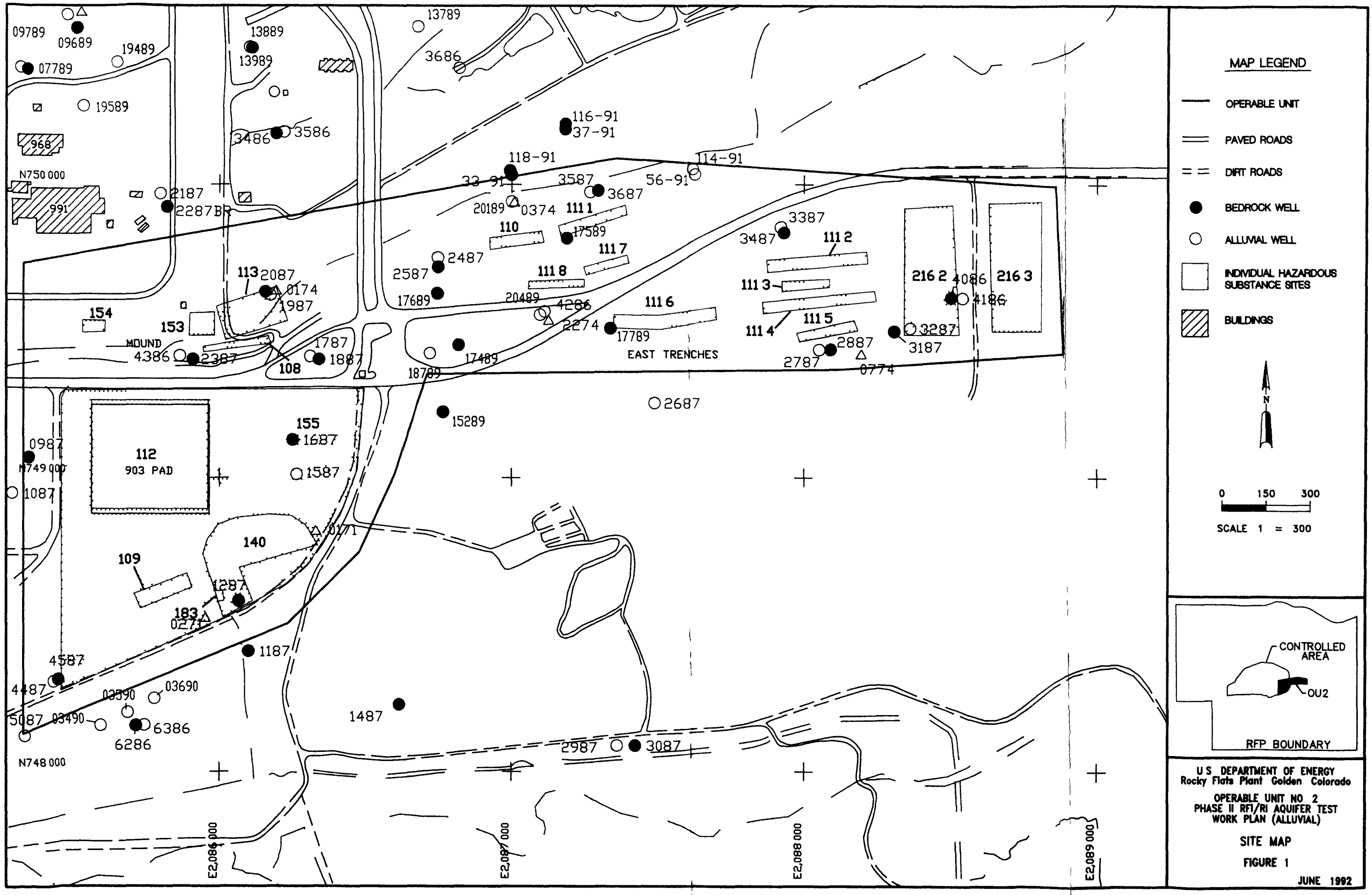
5 10 Complex roots

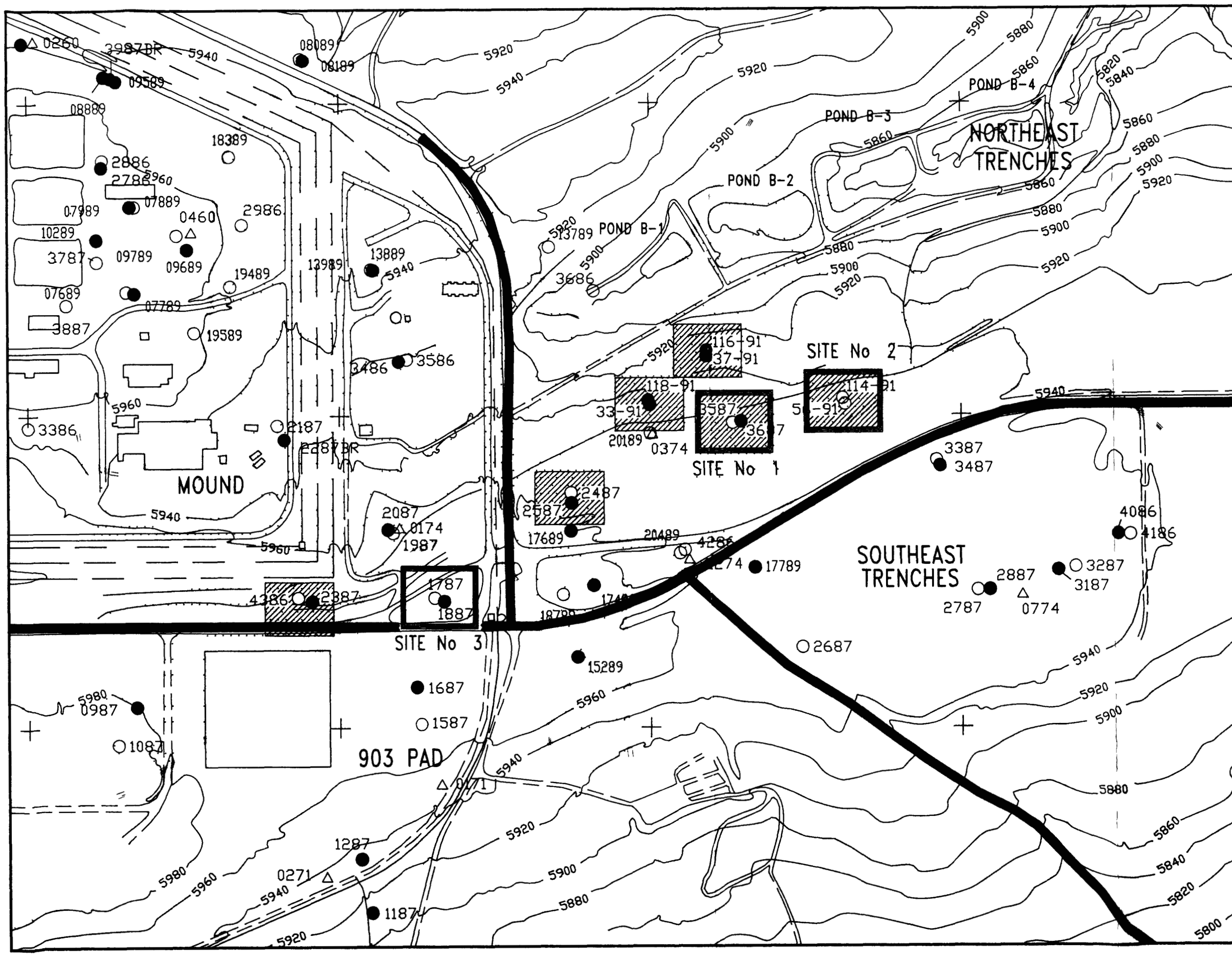
All the techniques described so far find the real roots of an equation or pair of equations We will now discuss very briefly the solution of equations whose roots are complex numbers

It should be clear that if the function is real-valued and if the initial guess x_0 is real, only real numbers will be produced However, if x_0 is a complex number, then succeeding x_i may also be complex Indeed, the methods described previously work equally well for complex numbers Many FORTRAN systems have provisions for complex arithmetic, in these systems it is a minor problem to modify the program to make it find complex roots

Finally, for polynomials with real coefficients we note that if $a + bi$ (where $i = \sqrt{-1}$) is a root $a - bi$ is also a root Thus, if $p_n(x)$ is the polynomial of degree n, it can be factored into the form

$$p_n(x) = (x^2 - 2ax + (a^2 + b^2))\, p_{n-2}(x)$$


MAP LEGEND
OPERABLE UNIT
PAVED ROADS
DIRT ROADS
BEDROCK WELL
ALLUVIAL WELL
INDIVIDUAL HAZARDOUS SUBSTANCE SITES
BUILDINGS
N
0 150 300
SCALE 1 = 300
CONTROLLED AREA
OU2
RFP BOUNDARY
U S DEPARTMENT OF ENERGY
Rocky Flats Plant Golden Colorado
OPERABLE UNIT NO 2
PHASE II RFI/RI AQUIFER TEST
WORK PLAN (ALLUVIAL)
SITE MAP
FIGURE 1
JUNE 1992
EAST TRENCHES
MOUND
903 PAD
N750 000
N749 000
N748 000
E2,086 000
E2,087 000
E2,088 000
E2,089 000



U S DEPARTMENT OF ENERGY
Rocky Flats Plant Golden Colorado

OPERABLE UNIT NO 2
PHASE II RFI/RI AQUIFER TEST
WORK PLAN (ALLUVIAL)

TEST SITE LOCATION MAP

FIGURE 3

JUNE 1992