TA 40

Data Analysis

and

Vapor Plume Modelling

New Mexico Environmental Improvement Division Visit

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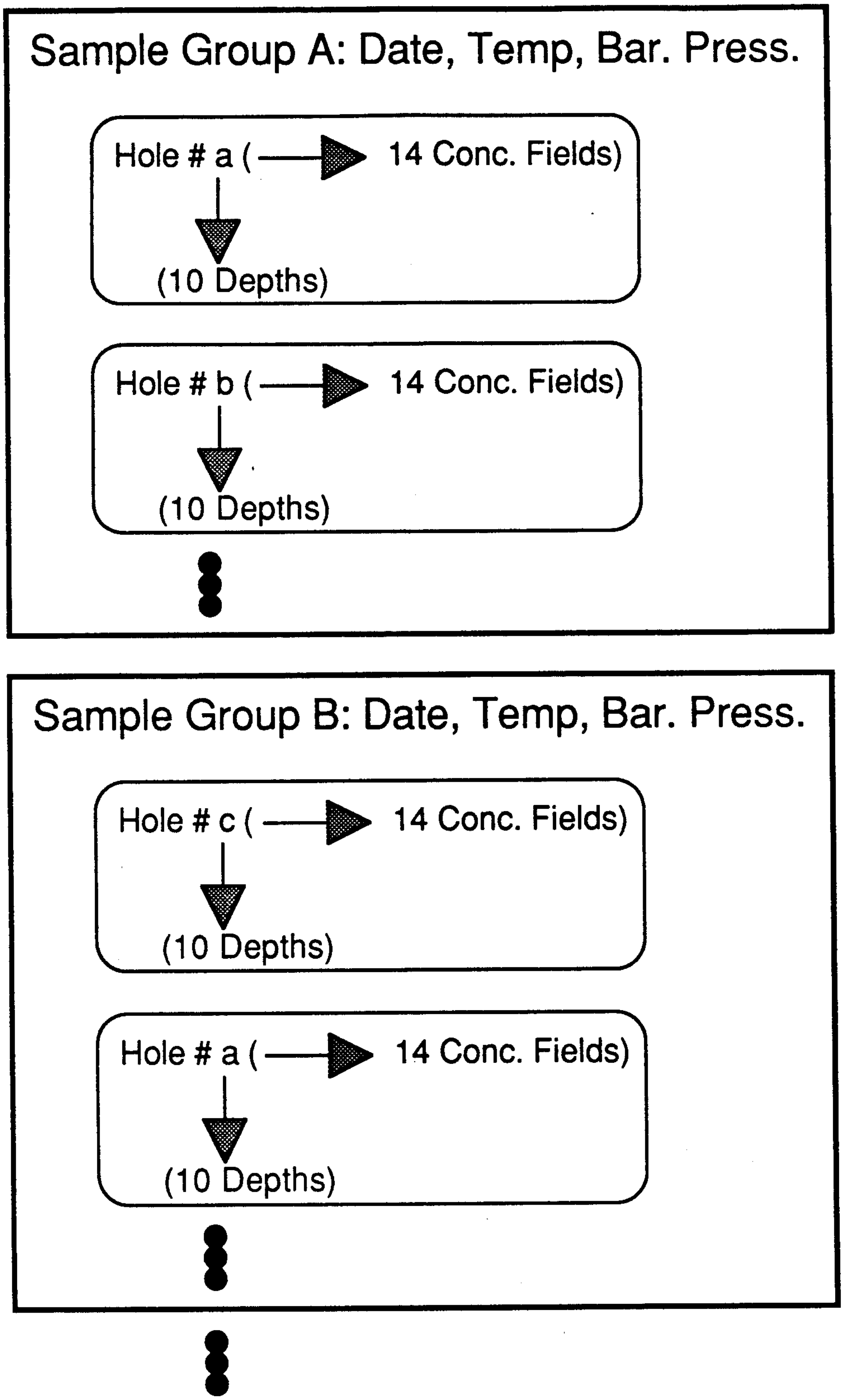
Presentation Outline

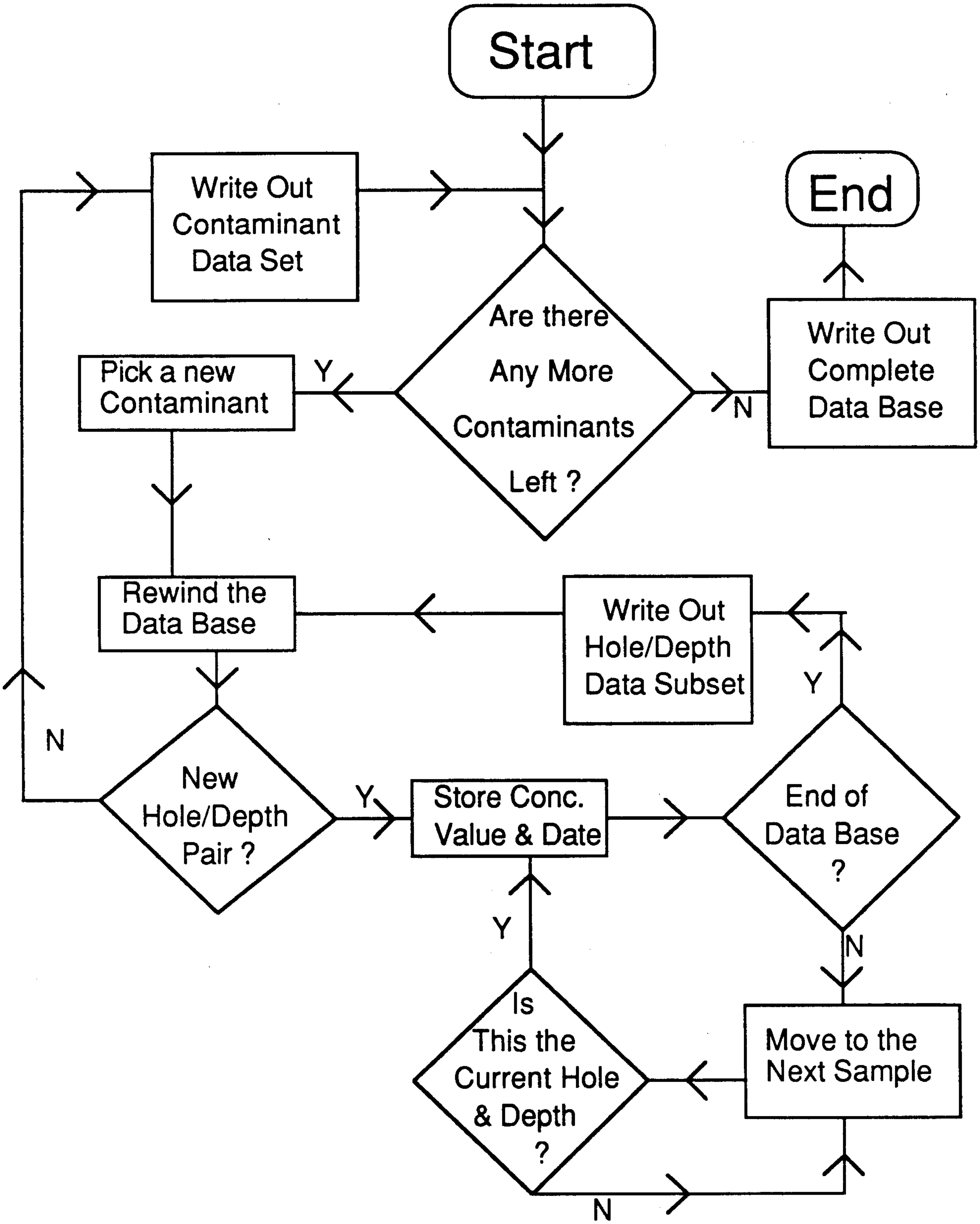
- **Data Analysis**
- **Computational Tools**
- **Vapor Extraction Simulation**

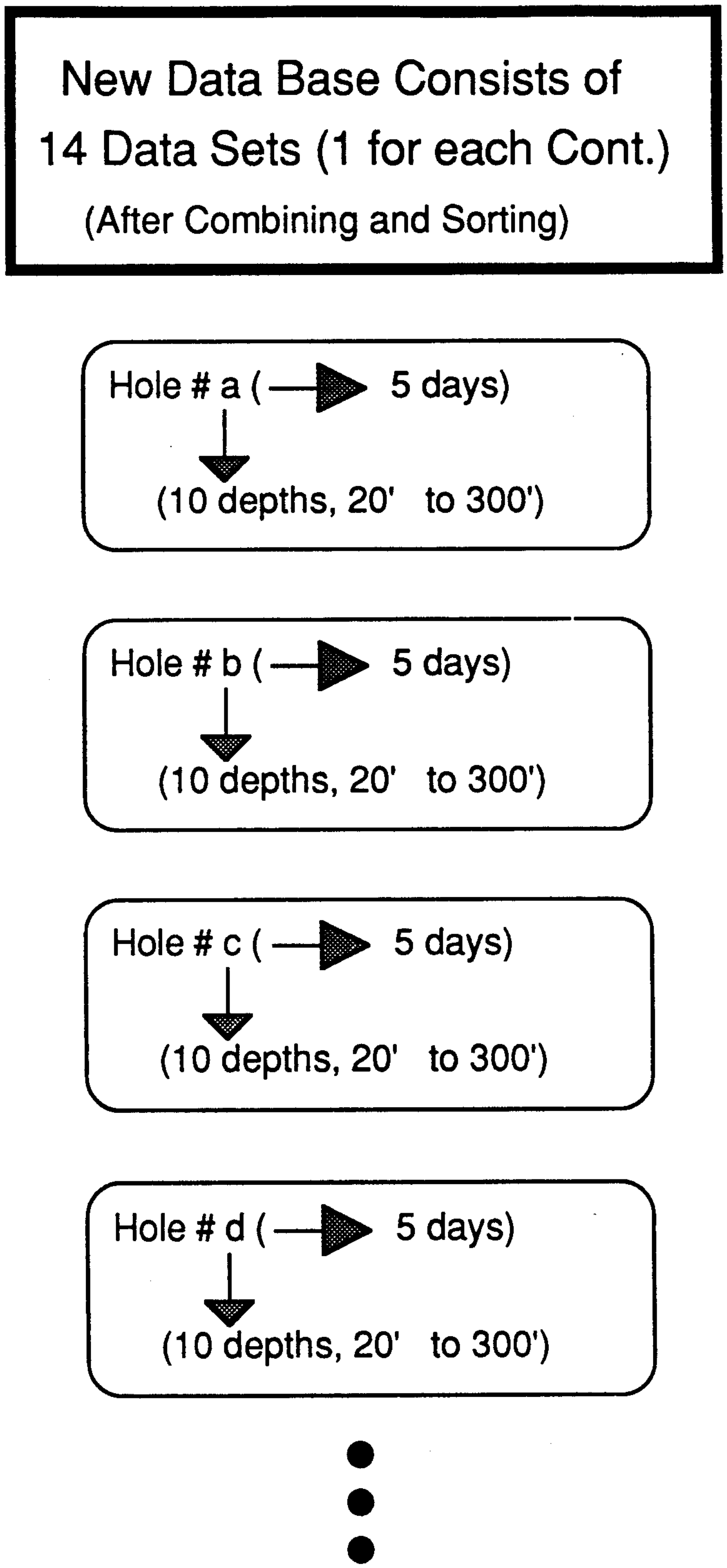
Raw Data from Pore Gas Measurements



26 holes
10 depths
*14 contaminants/depth

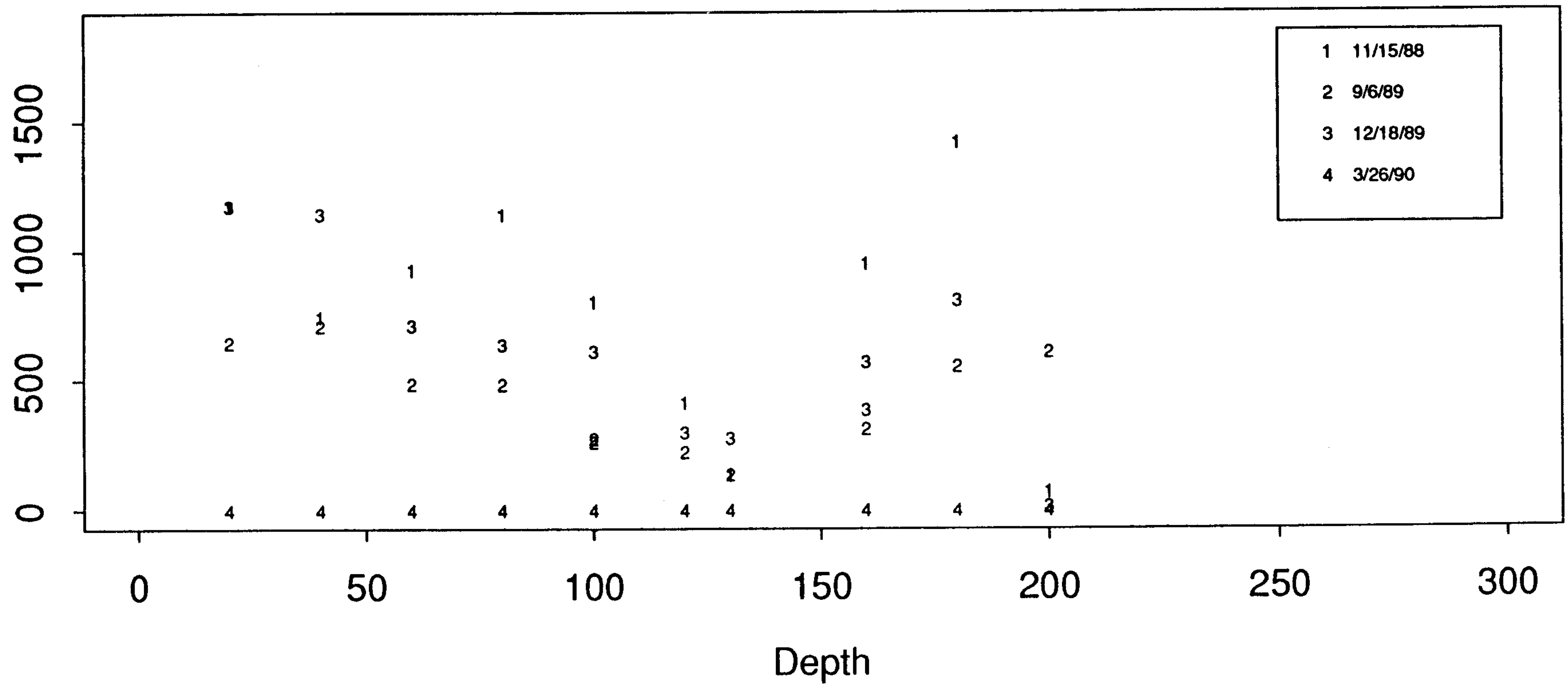
Organizing the Data

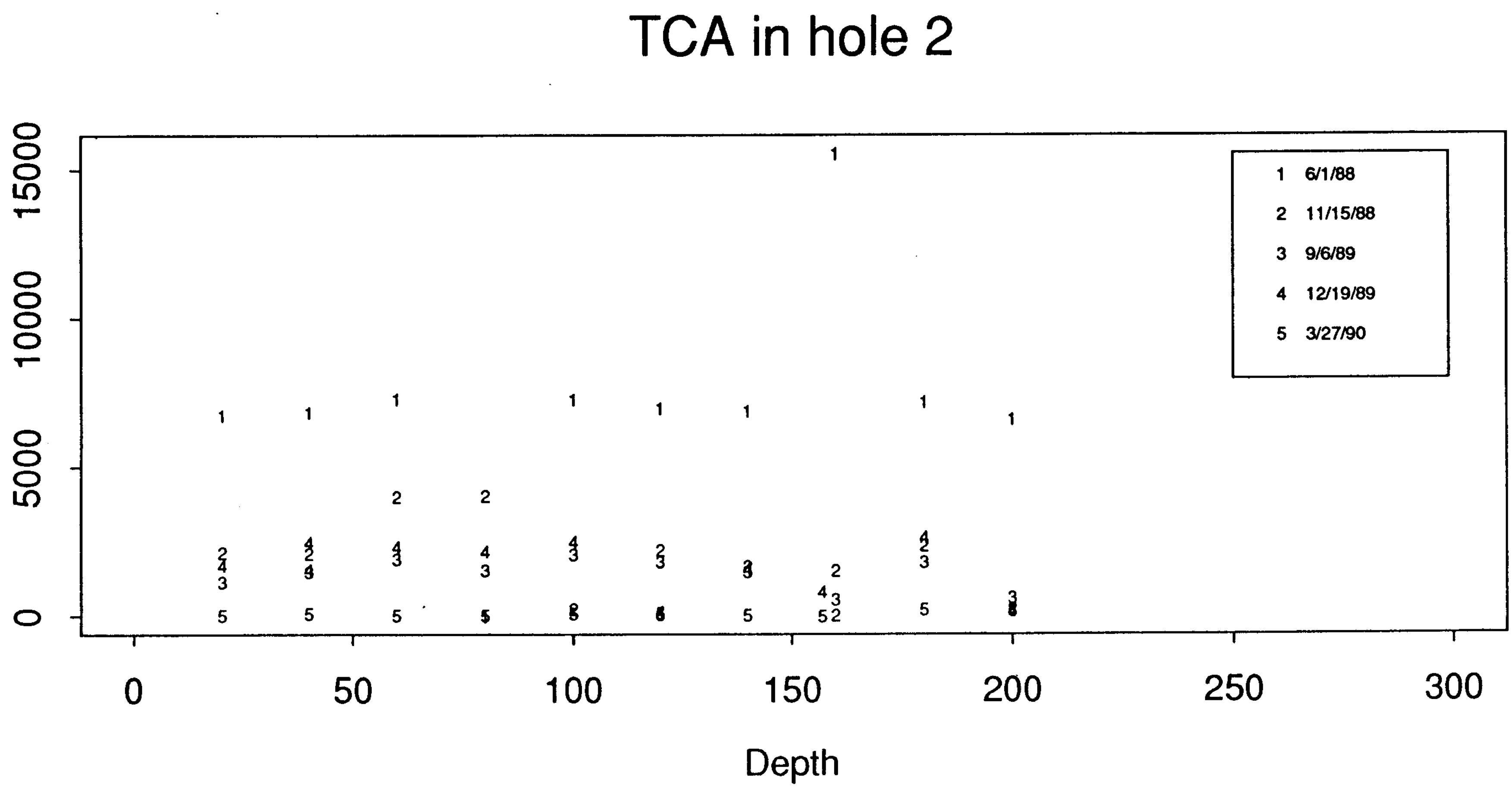



New Data Base Consists of
14 Data Sets (1 for each Cont.)
(After Combining and Sorting)
Hole # a (5 days)
(10 depths, 20' to 300')
Hole # b (5 days)
(10 depths, 20' to 300')
Hole # c (5 days)
(10 depths, 20' to 300')
Hole # d (5 days)
(10 depths, 20' to 300')

TCA in hole 1

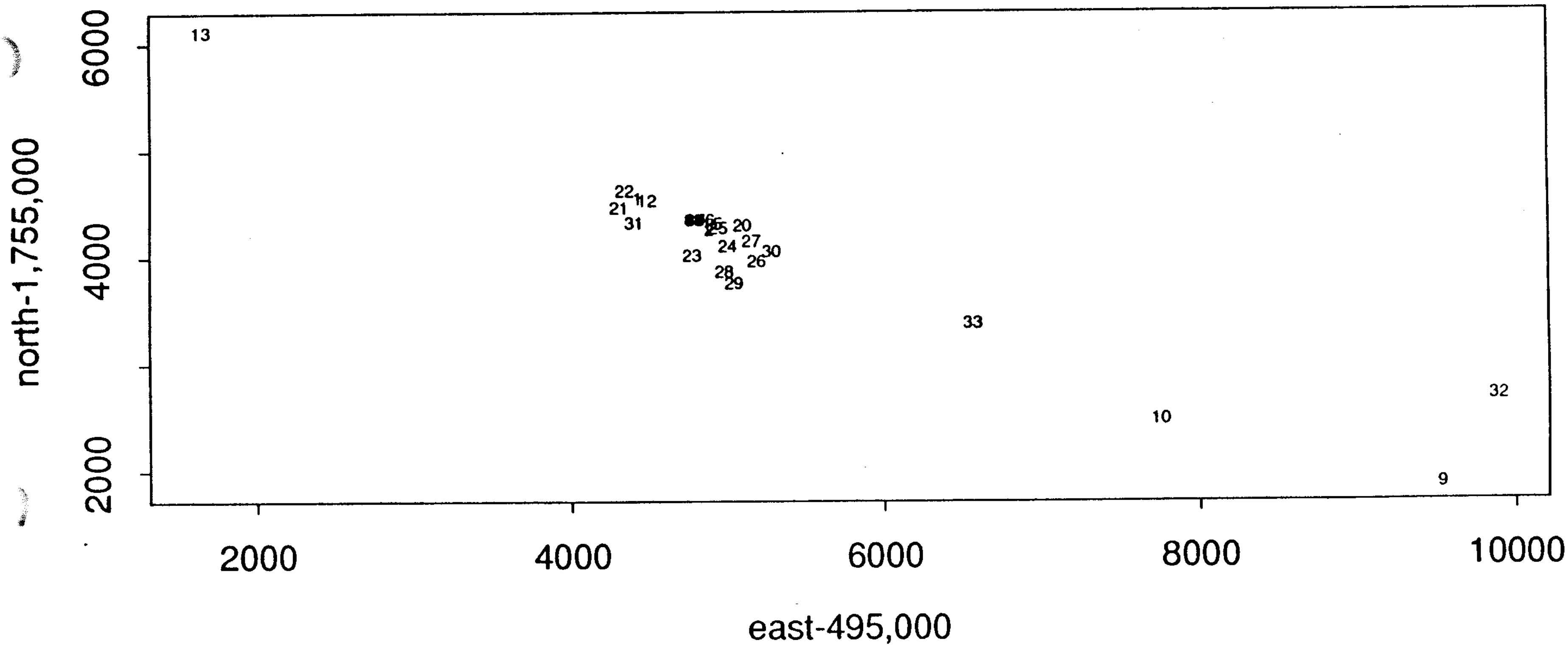
outside fence area ✓



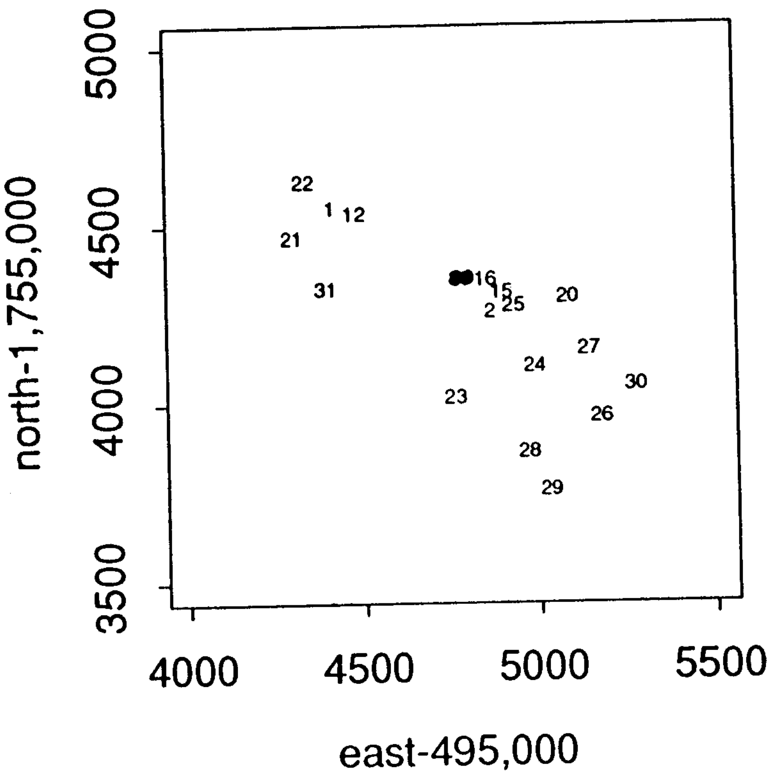


TCA in hole 2
0
5000
10000
15000
0
50
100
150
200
250
300
Depth
1 6/1/88
2 11/15/88
3 9/6/89
4 12/19/89
5 3/27/90

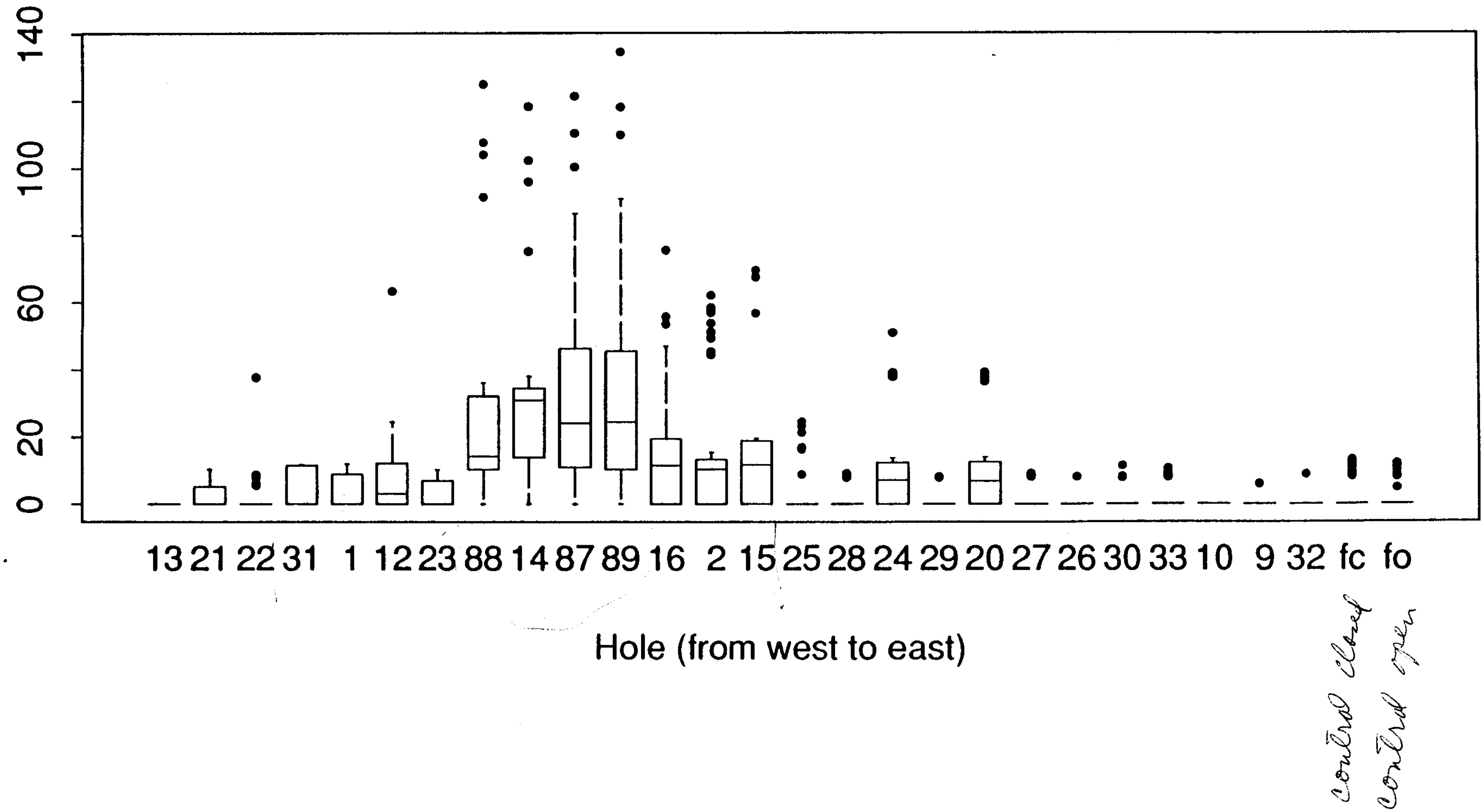
All holes at area L



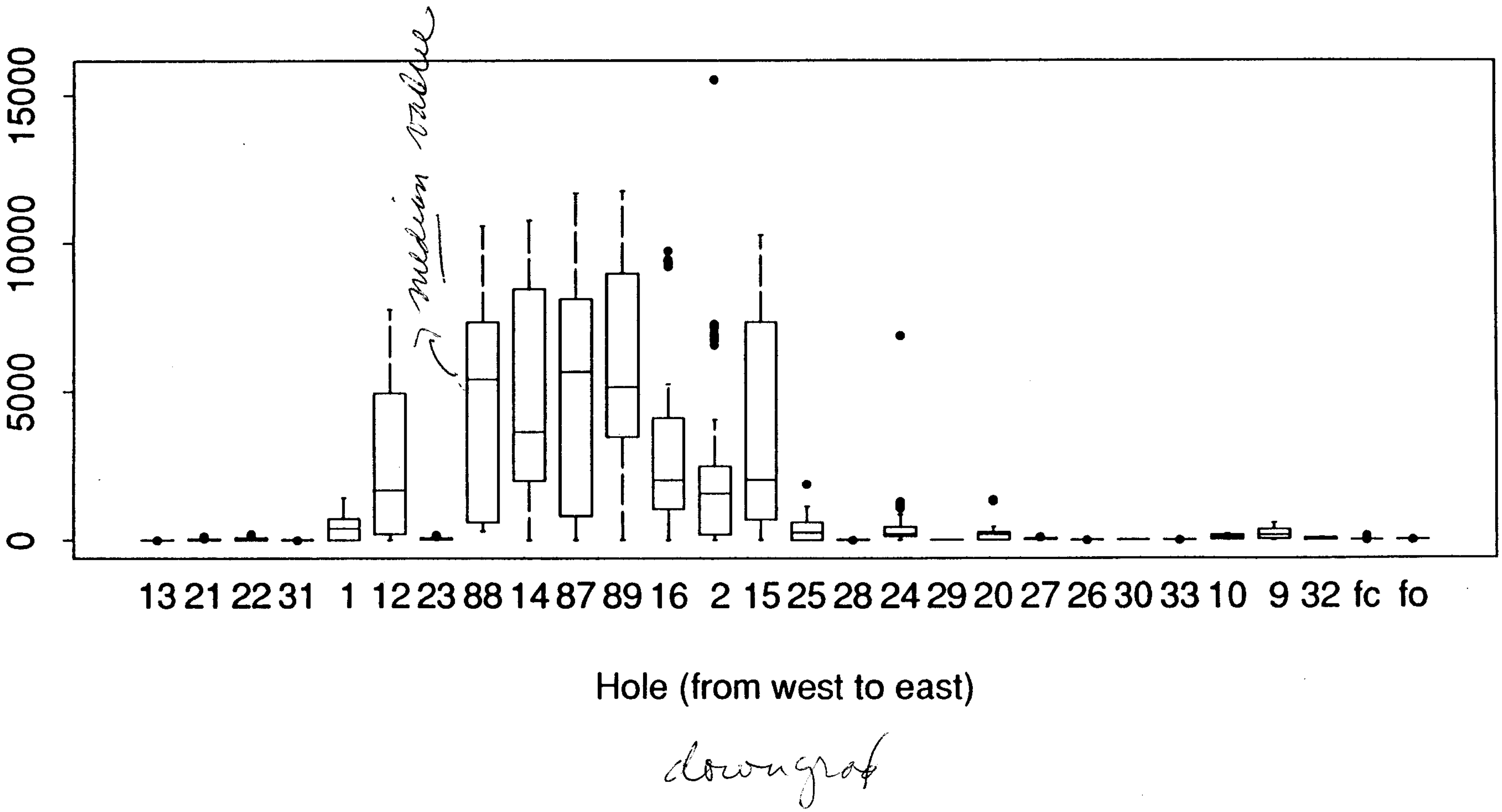
Central holes at area L



12 : CTC


0
20
60
100
140
13 21 22 31 1 12 23 88 14 87 89 16 2 15 25 28 24 29 20 27 26 30 33 10 9 32 fc fo
Hole (from west to east)
control closed
control open

15 : TCA


15000
10000
5000
0
13 21 22 31 1 12 23 88 14 87 89 16 2 15 25 28 24 29 20 27 26 30 33 10 9 32 fc fo
Hole (from west to east)
median value
downgrad

SUBSURFACE ENVIRONMENTAL MODELING CAPABILITIES AT LOS ALAMOS NATIONAL LABORATORY
Geoanalysis Group EES-5

The Geoanalysis Group at Los Alamos National Laboratory has developed modeling capabilities for a wide range of subsurface environmental problems over a wide range of scales. The capabilities use finite difference, finite element, distinct element, and lattice gas approaches for solving comprehensive sets of governing equations for flow and transport in porous and fractured media, and for rock mechanics problems. In addition to these numerical tools advanced visualization techniques have been developed to maximize the knowledge gained from the calculations.

TRACR3D

TRACR3D is a family of codes that solve problems in general purpose flow and transport through porous/fractured media under isothermal conditions. It can simulate transient, saturated and unsaturated flow with couple two-phase (gas and liquid) flow, in isotropic or anisotropic nonhomogeneous media, and in 1-3 dimensions. The code is implemented on a variety of computer systems, including SUN4, VAX, and CRAY machines.

TRACR3D can also simulate movement of reactive or passive solutes. A variety of transport mechanisms are included: advection, diffusion, sorption (equilibrium and reversible to irreversible, saturable, and non-equilibrium), radioactive decay and decay chains. In addition, the transport of dilute, volatile organics is treated through the use of Henry's law for the partitioning of organics between liquid and air-vapor phases. A biodegredation package is available which simulates biological (microbial) action on one or two mobile substrates under aerobic and anearobic conditions. This package solves five equations for the two substrates, oxygen, nutrient, and bacteria.

The code uses an integrated finite-difference solution method with very fast matrix solution techniques. It has been tested against analytic solutions and some experimental data. A user's manual is available.

FEHMS

FEHMS (*F*inite *E*lement *H*eat, *M*ass, and *S*tress code) calculates nonisothermal transient multiphase flow of noncondensible plus condensible fluids in porous media. It is finite element based, thereby allowing mixtures of elements and irregular mesh geometry. It allows for reactive multicomponent tracers in both gas and liquid phases. Several models of deformable media coupled with Darcy flow are available. Solution geometries include two- and three-dimensions. A dual porosity module is available, in addition to several effective continuum models. Several sorption and reaction models are available for transport calculations, in addition to radioactive decay. The code uses an adaptive solution strategy and has been implemented on SUN4, VAX, and CRAY computers. A user's manual is available.

CTCN

This code calculates the migration of toxic colloids through porous and fractured aquifers, mitigated by negative charges on both colloids and the aquifer. Solutions are obtained for population and species balances for up to four spatial dimensions. The nonlinear dynamic second-order partial differential equations are solved by utilizing the Method of Lines, which converts the partial differential equations into a system of ordinary differential equations which are solved by a robust solver. The code is being used to help assess the environmental impact and role of particulate transport at specific toxic waste sites.

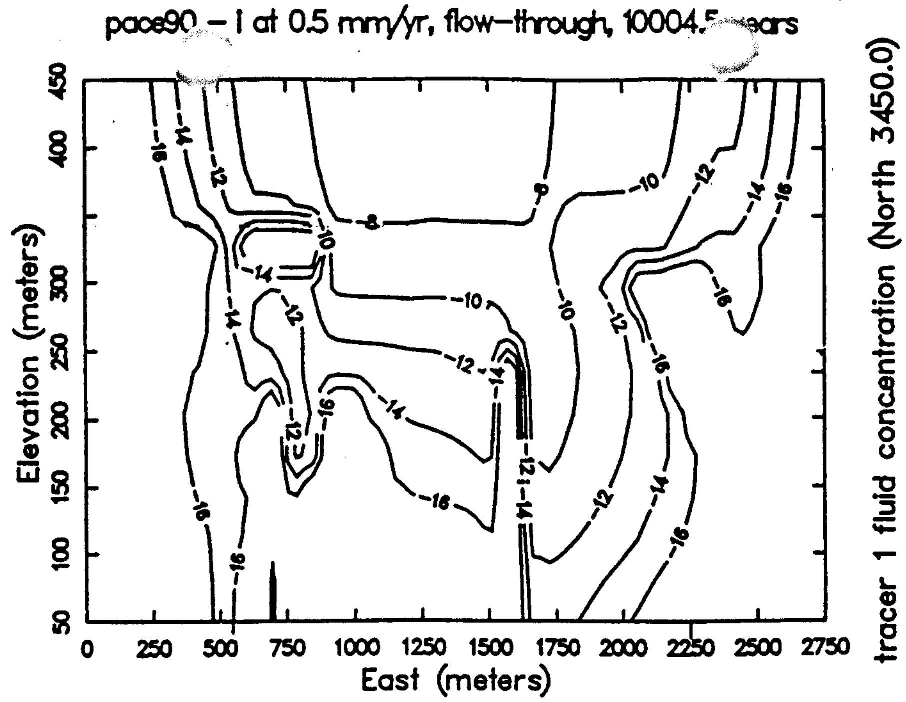


Figure 1. A 2-D slice from a 3-D unsaturated radionuclide transport calculation, 10,000 years after beginning of contaminant release. Contours show the logarithm of mass concentration of ^{129}I in water. The contaminant source resides on the top of the plot on the middle of the east axis. The irregular nature of the contours (as opposed to a simple plume) are the result of 3-D inhomogeneities in the rock types and displacement of layers along faults. Calculation performed with TRACR3D.

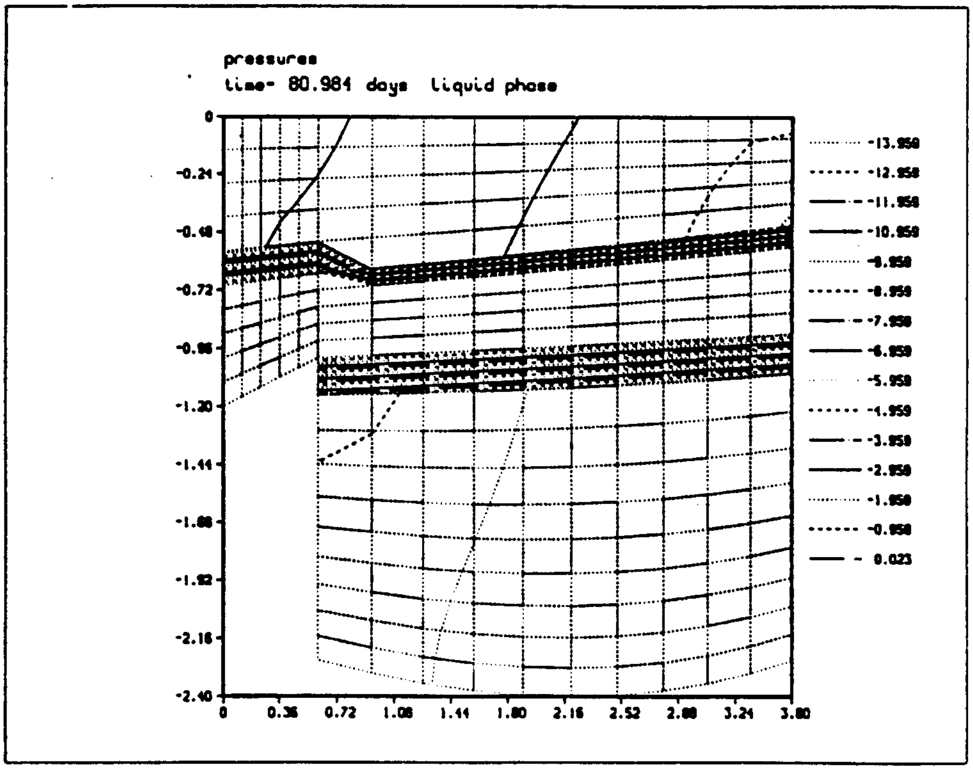


Figure 2. Water capillary pressure contours, overlayed on the computational mesh, from a detailed waste trench-cap simulation. Using a finite element code, all geometric details of such an engineered feature can be simulated. By simultaneously carrying out field experiments and numerical calculations such as this engineered barrier design can be optimized. Calculation performed with FEHMS.