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GLACIAL OVERBURDEN/UPPER GREAT MIAMI AQUIFER MODELING IMPROVEMENT TECHNICAL APPROACH/WORK PLAN

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REPORT

Glacial Overburden/Upper Great Miami Aquifer Modeling Improvement Technical Approach/Work Plan

Operable Unit 5
Project Order 61

September 1993
Revision 3

Environmental Remedial Action Project
Fernald Environmental Management Project
Fernald, Ohio
FERMCO Subcontract No. 2-21487

PARSONS

Fairfield Executive Center
6120 South Gilmore Road
Fairfield, Ohio 45014

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CONTENTS

SECTION

1.0 Introduction 1-1
- 1.1 Scope of Work 1-1
- 1.2 Objectives 1-1
- 1.3 Technical Approach 1-2

2.0 Conceptual Model Development 2-1
- 2.1 Model Construction Steps 2-1
- 2.2 Geologic Setting 2-3
- 2.3 Hydrogeologic Setting 2-10
- 2.4 Contamination and Geochemical Conditions 2-14
- 2.5 Conclusions from the April 15-16, 1993, Industrial Workshop 2-15
- 2.6 Expected Data from the Glacial Till/Vadose Zone Hydraulic Studies 2-15
- 2.7 Definition of the Conceptual Model 2-17
- 2.8 Preliminary Boundary Conditions 2-21

3.0 Code Selection 3-1
- 3.1 Selection Criteria 3-1
- 3.2 Selection of Codes 3-3
- 3.3 Verification of SWIFT and MSTS 3-4

4.0 Technical Plan 4-1
- 4.1 Introduction 4-1
- 4.2 Model Implementation 4-1
- 4.3 Test Simulations 4-5
- 4.4 Final Report 4-6

4776

CONTENTS (Continued)

5.0 Management Plan 5-1

5.1 Hardware and Software Requirements 5-1

5.2 Quality Assurance 5-1

5.3 Project Team Organization 5-2

5.4 Deliverables 5-2

5.5 Schedule 5-2

6.0 References 6-1

APPENDICES

A Auxiliary Code Selection

B Applicable PARSONS Procedures

LIST OF ILLUSTRATIONS

FIGURES

1-1 Improvement of the Till Zone Model Logic Diagram

2-1 Surface Geology of the Study Area
2-2 Isopach of In Situ/Undisturbed Glacial Overburden
2-3 B-B'(South - North) Cross Section
2-4 E-E' (West - East) Cross Section
2-5 Water Table Elevation Map for Glacial Overburden (Averaged, 1/88 - 7/92)
2-6 Major Features of the Conceptual Model
2-7 Conceptual Model
2-8 Preliminary Boundary Conditions

5-1 Organization Chart

LIST OF ACRONYMS

ASI	Advanced Sciences, Inc.
CERCLA	Comprehensive Environmental Response, Compensation, and Liability Act
CRU	CERCLA/RCRA Unit
ERA	Environmental Remedial Action
FD	finite difference
FEMP	Fernald Environmental Management Project
FERMCO	Fernald Environmental Restoration Management Corporation
GMA	Great Miami Aquifer
GO/UGMAS	Glacial Overburden and Upper Great Miami Aquifer System
HSU	Hydrostratigraphic Unit
IGWMC	International Groundwater Modeling Center
IT	International Technology Corporation
MSTS	Multiphase Subsurface Transport Simulator
ODAST	One Dimensional Analytical Solute Transport
QA	Quality Assurance
RCRA	Resource Conservation and Recovery Act
SWIFT	Sandia Waste Isolation Flow and Transport
US EPA	United States Environmental Protection Agency

SECTION 1

INTRODUCTION

The purpose of this effort is to improve the present computer model that predicts groundwater flow and contaminant transport through the Glacial Overburden and the Upper Great Miami Aquifer System (GO/UGMAS) at the Fernald Environmental Management Project (FEMP). Currently, the GO/UGMAS is modeled with the One-Dimensional Analytical Solute Transport (ODAST) code. Under certain conditions, a one-dimensional code is not an effective tool for simulating flow and transport conditions in the GO/UGMAS due to the presence of multiple sources of contamination and possible lateral migration along sand lenses.

1.1 Scope of Work

This work plan defines the GO/UGMAS modeling effort and consists of three parts. First, existing site and literature data are reviewed to develop a conceptual model of the GO/UGMAS. Second, code selection criteria are defined based on this conceptual model, different computer codes are evaluated against these criteria, and a code(s) is selected for this modeling. Third, the plan for completing the construction and calibration of the GO/UGMAS model using the selected code.

The conceptual model will be refined during the project with the results from the FEMP glacial overburden hydraulic studies (slug tests, packer tests, lysimeter sampling, and pumping tests), the results of hydrologic analysis of existing data, and the results of an independent study on the distribution of K_d (FERMCO 1993). The FEMP glacial overburden hydraulic studies are presently being performed under a separate task (PARSONS 1993a).

1.2 Objectives

Presently, the ODAST model is used for fate and transport in the GO/UGMAS. The ODAST model is a one dimensional analytical code for solute transport in homogeneous, semi-infinite media. ODAST represents a simplified but very conservative method of modeling fate and transport of constituents. ODAST assumes constant pore velocity, dispersion, and retardation. The surface oxidized (brown) clay is also ignored in ODAST modeling since it may be highly fractured and may not represent a barrier to contaminant transport. Material properties are assumed to be homogeneous and conservative values of these properties are selected. Straight vertical transport is also assumed, when in fact lateral migration may occur in sand lenses (see more detailed discussion below).

A similar conservative approach will be followed in developing an improved model of the GO/UGMAS. The primary objectives associated with the improvement of the GO/UGMAS model are:

1) The model needs to be available to support current studies and remedial design efforts.

2) The model should account for the relevant hydrogeologic pathways for the CERCLA/RCRA Unit 5 (CRU5) Risk Assessment. The improved model needs to include lateral movement/migration capability and multiple source loadings in the glacial overburden.

3) The model should provide a level of conservatism that is appropriate for a Comprehensive Environmental Response, Compensation, and Liability Act (CERCLA) Risk Assessment.

4) The model should be defensible with respect to the United States Environmental Protection Agency (US EPA) and Ohio Environmental Protection Agency and should help satisfy current regulatory compliance needs including the Resource Conservation and Recovery Act (RCRA) program.

5) The model needs to address the influence of Paddy's Run on the hydrogeologic regime.

1.3 Technical Approach

The approach to the improvement of the GO/UGMAS model is provided as a logic diagram in Figure 1-1. The center set of boxes in Figure 1-1 represents the steps in the development of the GO/UGMAS model, consisting of the definition of the conceptual model, the process of code selection, the construction of model mesh, the establishment of boundary and initial conditions, the calibration, and sensitivity analysis. As shown in the blocks to the left on Figure 1-1, the collection of additional hydraulic data will be conducted by Fernald Environmental Restoration Management Corporation (FERMCO) in parallel to model construction and calibration (see PARSONS 1993a). These hydraulic studies are currently being planned to determine which migration pathways are applicable to the GO/UGMAS model and to calculate specific parameter values. Since these results will not be available in time for use in model selection and model mesh construction, a code will be selected based on defined conservative conditions and the model mesh will be constructed based on available cross section data. Also in parallel (see right side of Figure 1-1), existing hydrologic data will be reviewed and additional analysis will be performed to help define model boundary conditions and input parameters. The final boundary conditions and input parameters will be incorporated in the model when the final field tests and an in depth review of existing data are completed.

In performing this task, two models will be developed with two different codes. A three-dimensional depiction of the conceptual model will be constructed with the main code. A second auxiliary code will be used to study the impacts of the assumptions/simplifications in the main model and to support verification of the main model.

Improvement of the GO/UGMAS Model Logic Diagram

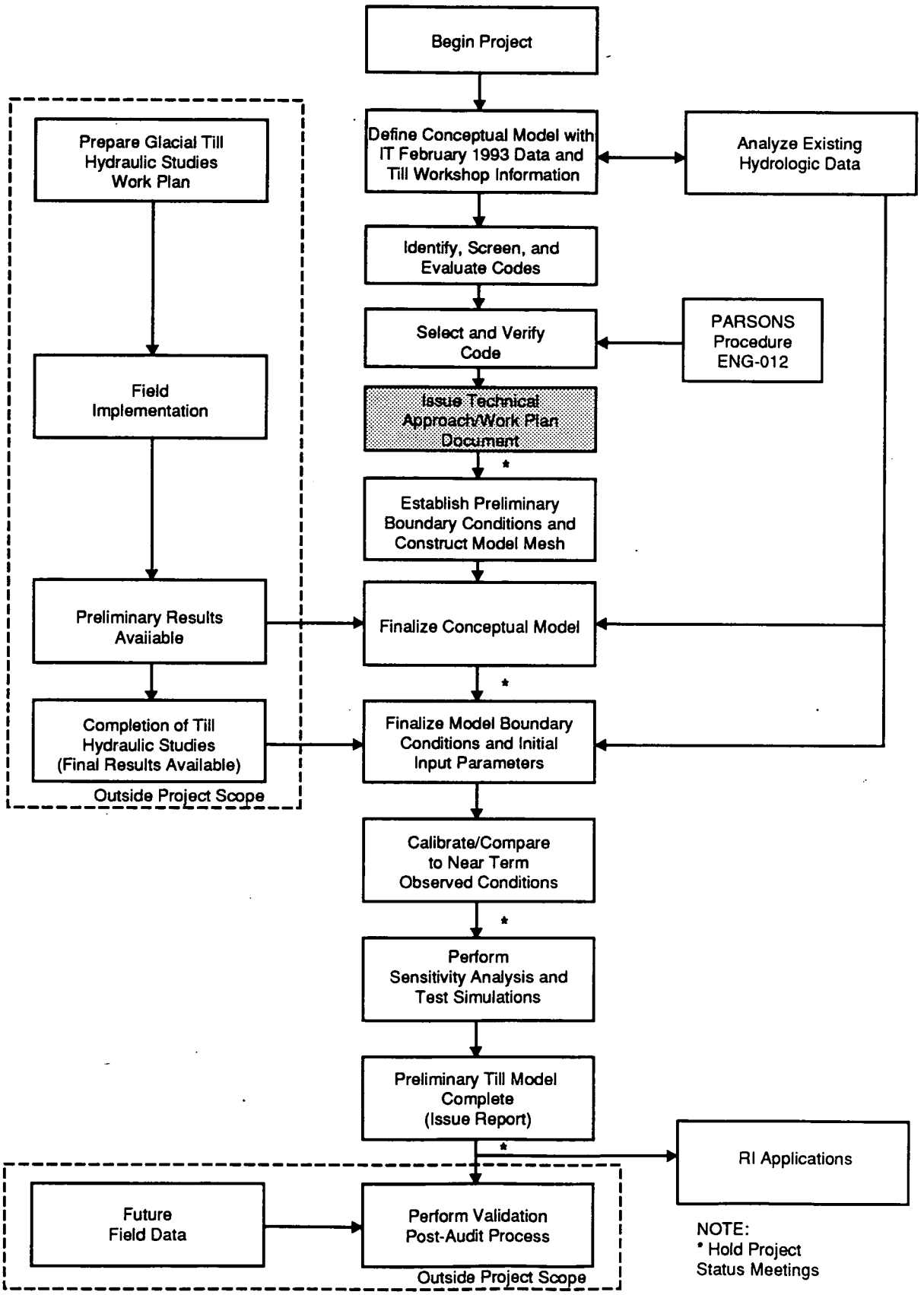

Figure 1-1 - Improvement of the Till Zone Model Logic Diagram

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SECTION 2

CONCEPTUAL MODEL DEVELOPMENT

A conceptual model provides the basis for accurately constructing a numerical model for the GO/UGMAS. The conceptual model represents surface and subsurface geologic and hydrogeologic features contained within the area to be numerically modeled. The conceptual model for the GO/UGMAS numerical model has been developed through the CERCLA remedial investigation of the FMPC. Figure 2-1 illustrates the extent of the area used to develop the conceptual model and the surficial geology of that area. Figure 2-1 also shows the boundaries of the numerical model and the boundary of the FEMP property.

2.1 Model Construction Steps

A representative model requires a conceptual understanding of the geologic and hydrogeologic conditions and the physical features of the site such as topography and the drainage system. The conceptual model presented here is based upon these data and the results of the FEMP Industrial Workshop: "Characterization of the Vadose Zone," conducted on April 15-16, 1993 (DOE 1993a). The conceptual model provides the basis for the code selection and the development of the numerical model which will be presented in Sections 3 and 4. As shown on Figure 1-1, the initial conceptual model will be revised during the project as dictated by the results of investigative activities (see Subsection 1.3).

A review of various site-specific data is conducted as a part of this task. These data were collected in the past and applied to the development of a conceptual model of the GO/UGMAS. The majority of these data were collected during the Remedial Investigation process. Data used to build the conceptual model include: United States Geological Survey quadrangle maps and site-specific topographic plots, lithologic logs from project soil borings, slug test results, hydrography, barometric pressure data, geotechnical data, and contaminant distribution data. Two key reports were used to derive the conceptual model: the Site-Wide Characterization Report (DOE 1993b) and the Preliminary Presentation of Geology and Hydrogeology of the Glacial Overburden (International Technology Corporation [IT] Corporation 1993). Figures in this section are based on IT's work which are presently undergoing minor revisions as a result of the QA/QC process. Because some figures are still under revision, several which are presented in this report are incomplete and should be considered "preliminary." Finalized figures will be included in the final GO/UGMAS modeling report.

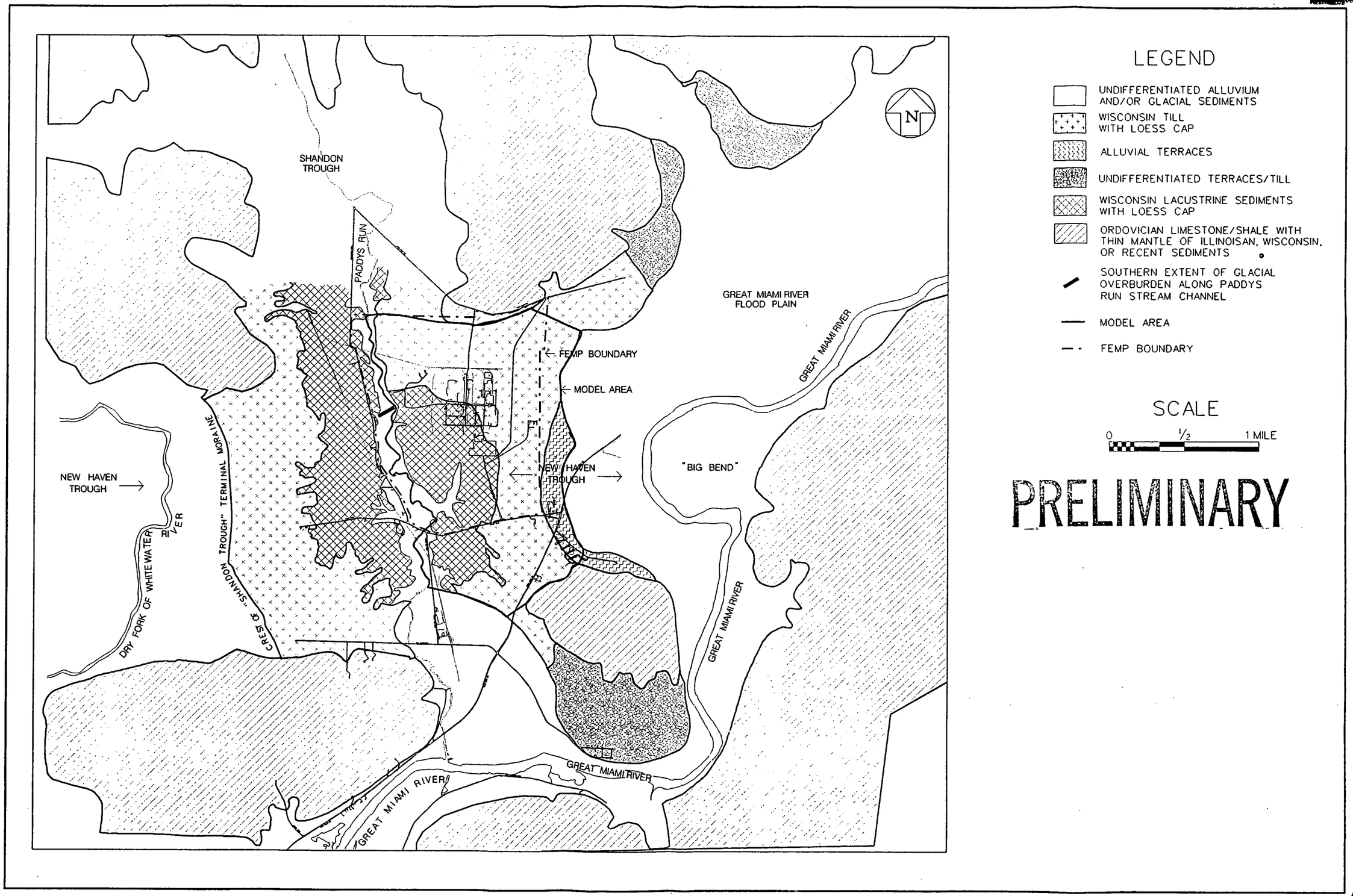


Figure 2-1 - Surface Geology of the Study Area

The geology of the glacial overburden is being characterized concurrently with the development of the improved glacial overburden model via the hydraulic studies in the glacial till/vadose zone program (PARSONS 1993a). Results of the characterization program will be incorporated into the glacial overburden model as they become available. The description of the glacial overburden geology in the final glacial overburden modeling report will be consistent with the most recent field data and the RI reports.

2.2 Geologic Setting

The geologic setting includes surficial geology, the geologic history of the area, surface topography and drainage features, and the local stratigraphy and hydrostratigraphy. Existing information on these issues is summarized below.

2.2.1 Physiographic Province

The main physiographic features in the portion of southwestern Ohio that contains the FEMP and the area to be modeled are gently rolling uplands and steep hillsides along the major stream valleys. The dominating features in the area of the FEMP are the New Haven Trough carved by the Ancestral Ohio River and the current Great Miami River Valley. The New Haven Trough, a relatively broad flat-bottomed valley, is flanked on either side by bluffs that rise to as much as of 200 feet above the level of the valley floor. The Great Miami River flows across the east end of the New Heaven Trough and then south within its own smaller outwash filled valley. Paddys Run flows south within the western boundary of the FEMP property and joins the Great Miami River about two miles south of the FEMP.

2.2.2 Geologic History

The modeling effort focuses on the glacial overburden. Therefore, the aspects of geologic history related to the deposition of the glacial overburden materials and their horizontal and vertical spatial distribution are of critical importance to the model.

As described in the Sitewide Characterization Report (DOE 1993b), the FEMP is located within a 2- to 3-mile-wide, east-west oriented, buried valley known as the New Haven Trough (see Figure 2-1). This valley was eroded in the mid-Pleistocene and then partially filled with glacial outwash sands and gravels which now comprise the Great Miami Aquifer (GMA). The valley was carved by the Ancestral Ohio River which formed during the ice advance and flowed within this trough in a westward direction across the study area. Outwash deposits filled the valley as the continental glaciers retreated.

Later during the Wisconsin glaciation a thin veneer of glacial overburden consisting of till covered with heterogeneous clays, silts, and sands was deposited. The lobe of the Wisconsin glacial advance came

from the north and was aligned along the Shandon Trough (see Figure 2-1). The veneer, from its base to its top, consists of a widely-distributed basal till, locally deposited lacustrine and outwash sediments that are aligned along the present day Paddys Run, and a thin mantle of ubiquitously-distributed loess. These features are illustrated in Figure 2-1 which shows the surface geology of the study area as it would appear without the loess mantle.

The southern most advance of the Wisconsin ice lobe is delineated by a moraine that arcs around the site to the south and west depicting the extent of glacial advancement and till deposition in those directions. The till consists predominantly of fine clay and silt, but also contains unsorted fractions of sand, gravel, and larger erratics. Within the till are sand and silt channel deposits that appear to be less laterally extensive than coarser-grained portions of the lacustrine deposits. These sand and silt deposits within the till may transmit groundwater in the present-day system. Overall, the till appears to act as a low-permeability barrier inhibiting the downward flow of groundwater across the portions of the study area in which it is present as is shown in Figure 2-1. Since till underlies the lacustrine deposits on the site, downward groundwater flow is inhibited by both the fine grained lacustrine sediments as well as till.

As the ice melted, a lake formed in the central portion of the area defined by the moraine. Coarser-grained lacustrine sediments appear to be more laterally extensive than sand lenses within the underlying glacial till.

The coarser-grained, lacustrine sediments appear most significant for the modeling effort because they are thought to contain the most likely pathways for lateral contaminant transport. The lacustrine sediments were deposited in and around a meltwater lake as the Wisconsin-aged glacier retreated. Because these sediments were deposited by flowing water they differ in character from the underlying till. Waterlain sediments will selectively settle according to mass, or grain size, and stream velocity as well as other factors, or become sorted after deposition, due to the reworking action of waves or currents.

2.2.3 Surface Topography and Surface Water

The Pleistocene valley-fill materials occupying the New Haven Trough (see Figure 2-1) are topographically low compared to the much older bedrock which underlies the highlands that flank the area to the north, south, and east. Elevations in valley fill materials across the central portions of the FEMP range from 570 to 580 feet above sea level. The slopes in the western portion of the FEMP increase as they approach Paddys Run where elevations drop from 580 feet to about 530 feet above sea level. Elevations on the northern portion of the FEMP property rise to about 700 feet against the steep bedrock supported valley wall. In the northeast corner of the FEMP property, the land gradually slopes downward into a small, unnamed stream that discharges to the east directly into the Great Miami River. The majority of runoff and drainage across the FEMP is from east to west, into Paddys Run.

Immediately south of the former production area of the FEMP is the Storm Sewer Outfall Ditch which discharges to Paddys Run. As shown on Figure 2-1, both the outfall ditch and Paddys Run have eroded through the entire section of glacial overburden exposing the underlying GMA outwash sediments. Because of this exposure, these channels become losing streams south of the point where they have eroded through the glacial overburden and flow directly on the GMA.

2.2.4 Surficial Geology

The surficial geology of the immediate area of the FEMP has been carefully studied. The extent of glacial overburden has been mapped according to its grain-size, color, and texture. Mapping and sample analyses under the CERCLA Remedial Investigation have led to the current understanding of the geologic history and depositional environments that created the glacial overburden, as discussed in the preceding sections. The distribution of the material within the glacial overburden has been plotted on numerous cross sections and maps to delineate the extent of each of these materials. A preliminary presentation of the geology and hydrogeology has been produced by IT (1993). This interpretation is undergoing some refinement as part of the development of the Operable Unit 5 RI Report and as the results of the analysis of new data from ongoing investigations.

The areas on Figure 2-1 that have been delineated as Ordovician bedrock north of the FEMP are covered with a thin mantle of till and loess.

The model will contain a thin layer of these glacially related materials in the upland bedrock areas. The bedrock which forms the sides and bottom of the valleys is considered impermeable and will not be considered in the model. However, it will be assumed that till and loess are present in all areas of the Paddys Run watershed north of the portion of the New Haven Trough that has been actively studied during the Remedial Investigation.

2.2.5 Stratigraphy

The stratigraphic units contained in the GO/UGMAS conceptual model have been discussed in the preceding section dealing with surface geology. Further information is presented in this section. The units are presented from oldest to youngest, and vertically from the bottom to the top.

1) Bedrock: The deepest and oldest unit of interest is the Ordovician bedrock, which consists of the shales and limestones. In the areas outside of the buried valleys, bedrock will serve as an impermeable boundary for the model. The depth to bedrock in the FEMP area can be as great as 250 feet. In the buried valleys or glacial troughs, the depth to bedrock is well below the water table, and will not be a part of the model.

2) Outwash: The coarse-grained glacial outwash was deposited in areas where bedrock had been deeply eroded. These areas have been buried primarily with this outwash. Only the upper, unsaturated portion of these outwash materials will be included in this modeling exercise. The underlying saturated interval is the Great Miami River Aquifer which is included in a separate modeling effort.

3) Glacial Overburden: This model focuses on the materials that have been defined as the glacial overburden. The glacial overburden consists of glacially derived sediments stratagraphically above the Great Miami Aquifer outwash sands. These sediments include till, lacustrine, outwash, and loess units. As illustrated in Figure 2-2, the glacial overburden in the FEMP area, which is primarily till, ranges from 20 to 50 feet in thickness. The till is likely to be thicker in the northern portions of the Paddys Run watershed within the Shandon Trough. IT(1993) describes the till as silty, sandy, gravelly clay. Borings drilled in the FEMP area have encountered coarse-grained, permeable, saturated sand bodies. The existing understanding of these sands is that they are thin and discontinuous, although additional boring log correlations and other studies are underway to better determine their extent. North-south and east-west cross sections, which depict typical stratigraphic relationships between the various units, are presented in Figures 2-3 and 2-4, respectively (see Figure 2-2 for locations of cross sections).

4) There are important color contrasts in the glacial overburden. The upper part is generally brown, whereas the lower part is grey. The brown color is caused by oxidation of sediments due to exposure to oxygenated groundwater. The gray clays have not been oxidized because they are thought to be saturated by stagnant groundwater. Other groundwater-related mechanisms, including rate of groundwater flow, may contribute to these distinct soil colorings.

5) Lacustrine Sediments: The delineation of lacustrine-related sediments in the FEMP area began in 1988 when the Soil Conservation Service mapped these deposits. The lacustrine deposits consist primarily of clay and silt. This type of clay can be distinguished from till clays because it lacks any component that is sand-sized or greater. This clay also generally is more homogeneous.

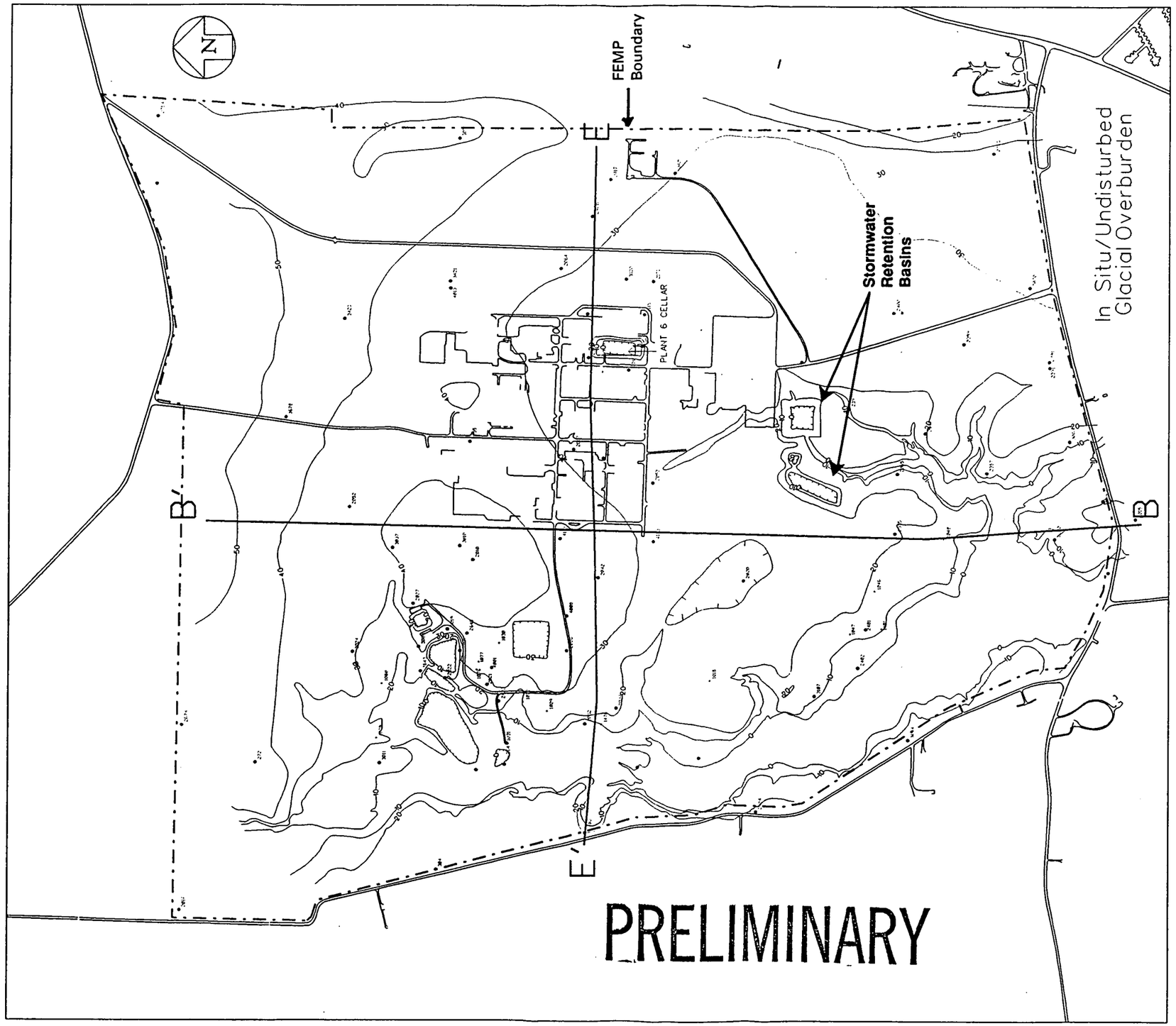
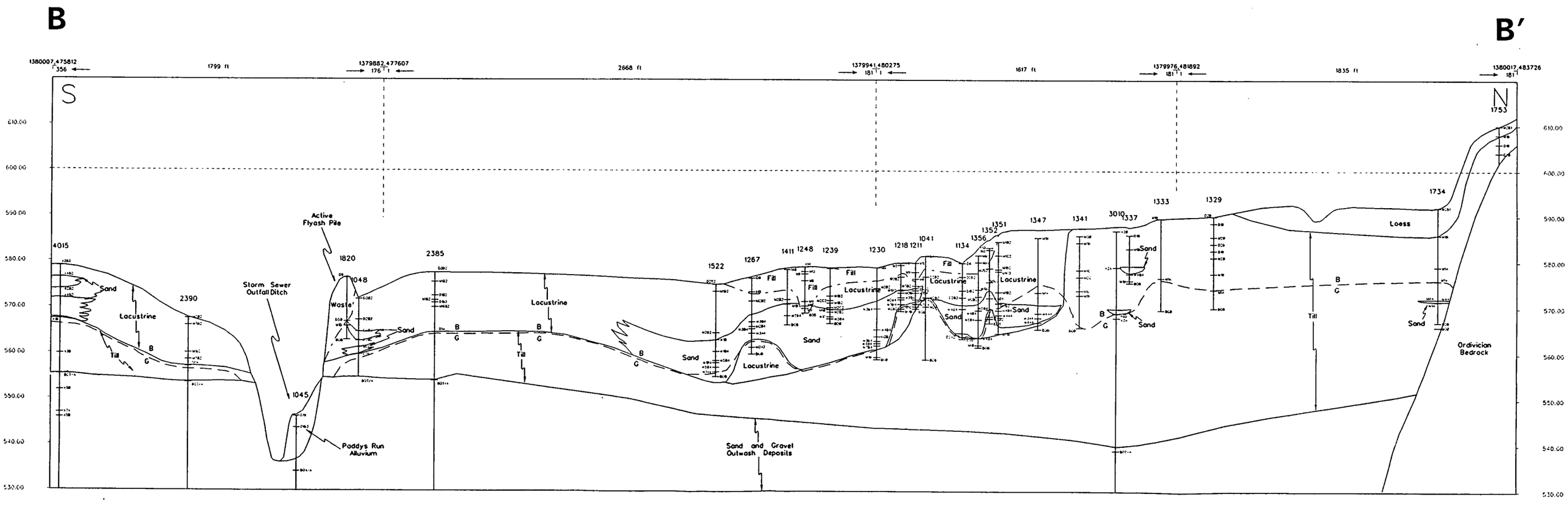
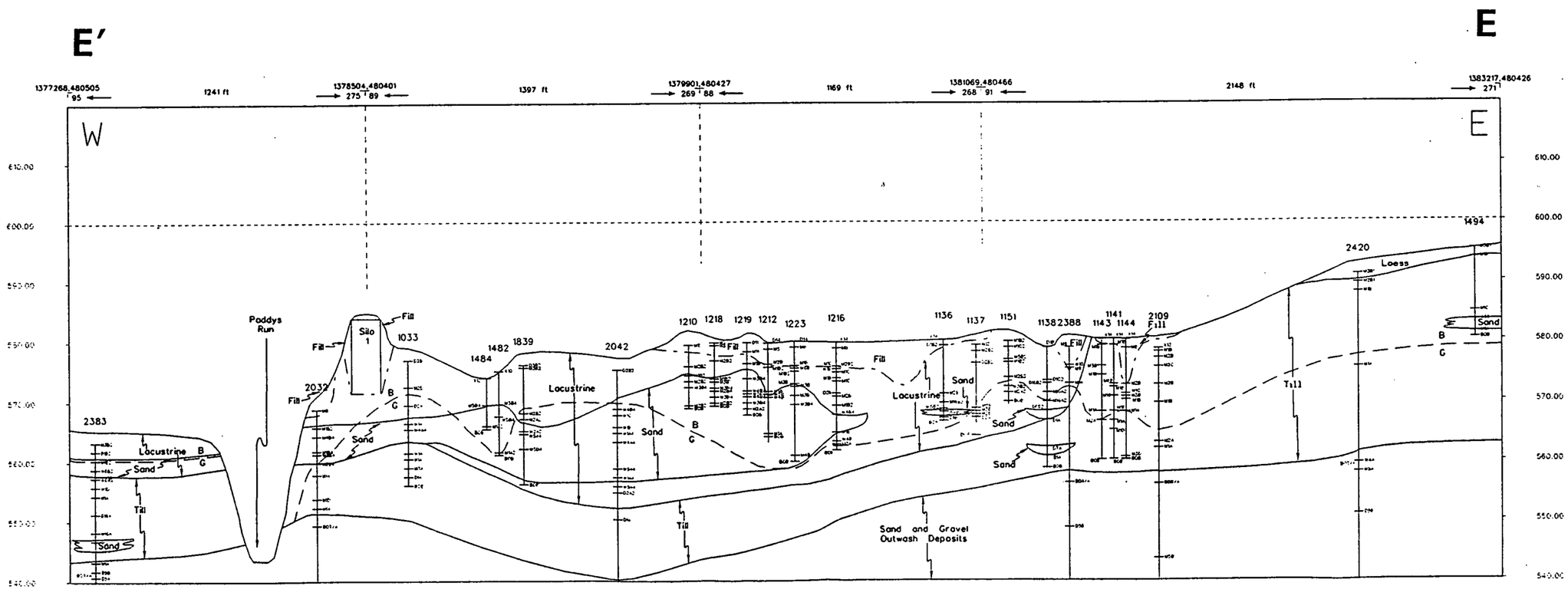


Figure 2-2 - Isopach of In Situ/Undisturbed Glacial Overburden



PRELIMINARY

Figure 2-3 - B-B' (South - North) Cross Section



PRELIMINARY

Figure 2-4 - E-E' (West - East) Cross Section

A previous study (IT 1993) has noted that in addition to clay, lacustrine sediments also can consist of silt, sand, and gravel. The most significant coarse-grained unit is a large sand, and silty sand body in the northern portion of the basin fill called the NS sand. It is postulated (IT 1993) that this material represents a heterogeneous body of outwash clay, silt, sand, and gravel that was deposited by glacial runoff streams that entered the basin from the north in the vicinity of a recessional moraine in the waste storage area. The majority of the lacustrine sediments are oxidized, and thus are brown in color. This coarse-grained, sandy unit is water-bearing and may represent a significant pathway for lateral flow from the production area to Paddys Run.

6) Loess: Loess, an aeolian-derived silt deposit, is regionally pervasive. However, much of it has been stripped or regraded in the production area (IT 1993). In other portions of the model area, however, it is expected to be present in thicknesses ranging from 3 to 8 feet. Because it is deposited by wind, loess typically is a homogeneous, silty sediment.

2.3 Hydrogeologic Setting

Important hydrogeologic characteristics include the determination of hydrostratigraphic units (defined in Section 2.3.1), the morphology of the water table or the potentiometric surface in critical units, an understanding of how groundwater flows through the system, and a qualitative understanding of the site's water balance.

2.3.1 Hydrostratigraphic Units

A hydrostratigraphic unit (HSU) consists of geologic unit(s) possessing similar hydrogeologic properties. For the purpose of modeling the glacial overburden in the FEMP area, each of the stratigraphic units described in Subsection 2.2 can be evaluated with respect to its hydrogeologic properties. Once the lateral and vertical distribution of these unit is determined or estimated, an appropriate hydraulic conductivity value will be assigned to each of these units. There are six hydrostratigraphic units which will be included in the GO/UGMAS model. From the surface downward these are 1) recent alluvium, 2) loess & fractured till, 3) lacustrine silts, 4) lacustrine sand, 5) glacial till, and 6) unsaturated GMA outwash.

Although loess and fractured till are not at all the same genetically, they will both be assigned high vertical permeability and therefore grouped together. Both the glacial till and lacustrine deposits are heterogeneous geologic units. As previously discussed, each contains discrete, coarse-grained, conductive sand bodies within larger volumes of fine-grained clays and silts. Because little is known about the distribution of sand bodies within the till, other than that such sand bodies are relatively uncommon, the till will be treated as one hydrostratigraphic unit. However, the lacustrine sediments have been found to contain a volume of sediments which are characteristically more sandy. As a consequence, the

lacustrine deposits will be split into two hydrostratigraphic units: one for the area containing the sandier deposits, another for the remainder of the deposits. The surficial alluvial sediments occupy a completely different stratigraphic position than does the GMA outwash. They will therefore be made two distinct HSUs.

2.3.2 Artificial Features

In addition to proper HSU identification and delineation, any man-made features that impact the FEMP hydrogeologic system must also be included in the development of the conceptual and numerical model. Five obvious features are the subsurface storm sewer system, the amount of paved area within the former production area, lined waste management units, lined stormwater retention basins, and the cellar of Plant 6 (Figure 2-2). These features will need to be represented in the model.

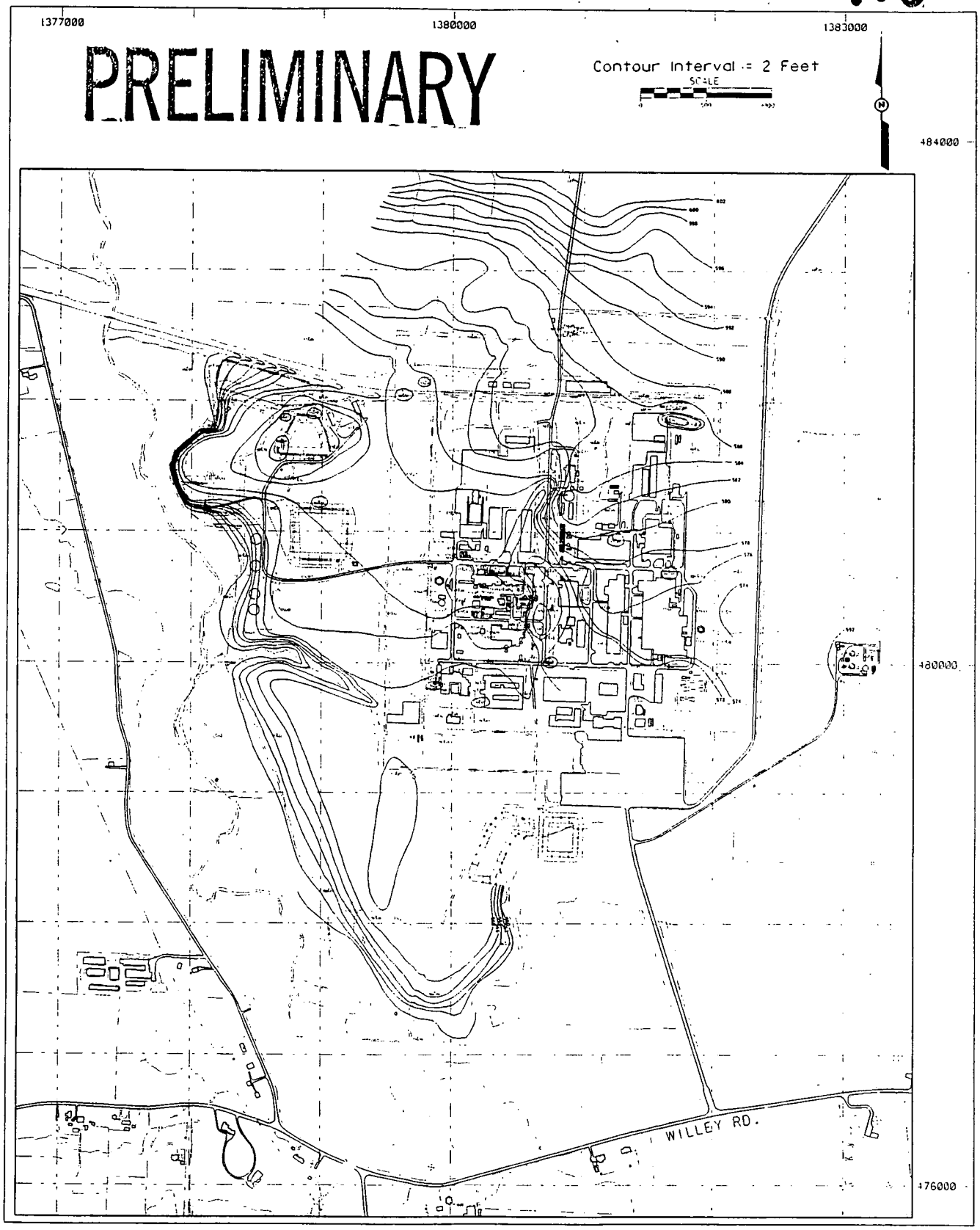
2.3.3 Groundwater Flow

To date, one set of water level maps has been generated from wells completed in the glacial overburden. Figure 2-5 is the plot based on averaged groundwater levels measured across a time span of more than one year. An inspection of this map shows that the water levels tend to mimic surface topography in the sense that the water level elevations drop westward across the site toward Paddys Run. The effects of the storm sewer drainage network, which is predominantly aligned in a north-south direction, are apparent on the surface, parallel to the main north-south road that bisects the production area into eastern and western sections.

An interpretation of how groundwater moves through the glacial overburden in the FEMP area is based on several types of information and concepts. Those concepts have most influenced the development of the conceptual model and will be included in the numeric model construction are:

1) The apparent distribution of saturated and unsaturated materials in the glacial overburden: There is uncertainty regarding how much of the glacial overburden is unsaturated and how much is saturated. The existing conceptual model conservatively assumes that the glacial overburden is continuously saturated across the study area, except for sediments lying above the water table, generally within 3-5 feet of the ground surface.

2) The probable distribution of transmissive sand bodies in the glacial overburden: At the time of this plan, there is still uncertainty regarding the distribution of transmissive sand bodies in the glacial overburden. Both the initial conceptual model and numerical model assume that only the sand-rich area in the lacustrine area contains a sufficient amount of interconnected, transmissive sand to represent it as a separate HSU.



LEGEND

— — Edge of Glacial Overburden

•566.04 Location of 1000-Series Well with Average Groundwater Elevation in Feet Above Mean Sea Level

NOTE

Wells With More Than 20 Observations Between January 1988 and July 1992

Figure 2-5 - Water Table Elevation Map for Glacial Overburden (Averaged, 1/88 - 7/92)

3) The differentiation of brown versus gray soils in the glacial overburden: It is recognized that brown soils are more likely to contain more rapidly flowing, oxygenated groundwater. This may relate to the possible presence of vertical fractures. As a consequence, brown soils will be assigned higher vertical conductivities in the model than gray soils.

4) A map of the water table in the glacial overburden: There have been several water table maps produced by project staff. While it has not been proven that a continuous water table is actually present in the glacial overburden, the model will assume that there is. An average water table map will be used for model calibration.

5) An evaluation of the distribution of dense till at the base of the glacial overburden: The model will assume that dense, low permeability till of varying thickness blankets all areas of the numerical model, excluding areas where it has been eroded along the southern portion of Paddys Run and the Outfall Ditch or where it has been removed by the addition of artificial features (see Subsection 2.3.2)

6) An evaluation of how the stormwater drainage system is influencing groundwater in the glacial overburden: The model will account for the presence of the stormwater drainage system in the former production area of the FEMP. Accordingly, recharge will be reduced in the areas affected by its presence, if appropriate. Other influences caused by this drainage system will also be considered and incorporated if they are considered significant.

7) The distribution of contamination in both the glacial overburden and the Great Miami Aquifer: Consideration will be given to contaminate distribution when constructing the model. Many of the areas where contamination is present in the underlying GMA are apparently related to locations where the till has been thinned by excavation or construction activities. While the model is being constructed, these locations will be identified. These excavated areas will be assigned much higher values of vertical conductivity, to represent these potentially significant pathways in the glacial overburden. However, where clay layers or liners have been placed at the base of any of these areas, conductivity will be lowered to account for their effect.

At this time, it is difficult to present a concise water balance or budget for the glacial overburden flow system. Factors which complicate such estimate include: the effects of natural unidentified heterogeneities, man-made influences, a lack of adequate field-measured recharge and stream gauging, and the fact that the overburden directly overlays the very permeable GMA outwash materials. On-going modeling exercises in the GMA indicate that as much as 6 inches of recharge (DOE 1993c) may be entering the GMA across the site. There is limited available information on the vertical and horizontal gradients across the site, but it is presently felt that given the presence of the low permeable basal till that blankets the model area, except in the select area where it has been excavated in the production area or incised along Paddys Run and the Outfall Ditch, there appears to be greater potential for lateral flow

discharge to Paddys Run and its alluvium than there is for downward flow and discharge through the base of the till into the underlying GMA outwash.

Information obtained from the Glacial Till/Vadose Zone Hydraulic Investigations (DOE document in progress) will provide more specific data on the hydraulic conductivity or the basal till which will improve the overall accuracy of the numerical model and any water balance analysis.

2.4 Contamination and Geochemical Conditions

The glacial overburden immediately underlies or surrounds the different waste areas at the FEMP. The fine-grained materials of the glacial overburden generally have great capacity for immobilization or retardation of contaminants due to adsorption, chemical precipitation, biodegradation, and radioactive decay (DOE 1993b).

The contaminant that is most abundant and widespread on site is Uranium-238. Uranium-238 will be used to calibrate the GO/UGMAS contaminant transport model. Other constituents may be simulated by defining appropriate source terms and model input parameters.

The FEMP has collected contaminant data and has developed a conceptual model for geochemical interactions. The conceptual model is based on infiltrating rainwater reacting with the minerals in the waste to form a leachate designated as Leachate A. Leachate A migrates through and reacts with the glacial overburden to form Leachate B. Parameter values are selected based upon a hierarchical method using direct data, if available, and using indirect data, if direct data is unavailable. Minerals in the waste are waste specific, generally based on chemical analysis of the waste. Minerals in the glacial overburden are reported to be predominantly quartz, smectite, illite, kaolinite, and smaller quantities of dolomite, calcite, feldspar, and iron-oxide minerals (DOE 1993b). The EQ3/6 codes (Wolery 1982a, b, and c) have been used to estimate the concentration of inorganic contaminants. EQ3/6 are geochemical codes that perform solubility, speciation, and reaction path calculations; however, EQ3/6 does not account for adsorption/desorption processes.

Adsorption/desorption have been accounted for with a retardation term in the ODAST transport code. The adsorption/desorption process is generally simulated in contaminant transport models with the distribution factor (Kd). To date, the site has relied on the calculation of the apparent Kd in the Great Miami aquifer solids. For the glacial overburden, the Kd for Uranium-238 is approximately 1.8 ml/g while in the aquifer material the Kd is approximately 1.4 ml/g (DOE 1993c).

Presently, a study of the Kd values is being conducted by FERMCO to better define and to possibly create zones of Kd values. This study will:

1) Review existing data to obtain additional apparent Kd values at locations where both soil and water have been sampled.

2) Obtain additional Kd data during the CRU2 and CRU4 supplemental investigation.

3) Obtain additional Kd data during CRU5 soil washing studies.

Results of these studies will be used to define Kd in the GO/UGMAS model.

2.5 Conclusions from the April 15-16, 1993, Industrial Workshop

On April 15-16, 1993, the University of Cincinnati organized a workshop for the FEMP which involved presentations from experts on glacial overburden characterization, monitoring, and modeling (DOE 1993a). The presentations created a focus for discussions ranging from the probable conditions at the time of the glacial overburden deposition through modeling methods which would best apply to the till and sand channel inclusions at the site. Although the proceedings from the workshop are not yet available, two conclusions can be drawn which directly affect the conceptual model.

The first conclusion involves the depth to the saturated zone. In the workshop, there was general agreement that the first saturated zone is near the land surface (within a few feet in places). The conceptual model should, therefore, include saturated till and sands overlain by unsaturated glacial deposits near the land surface (Figure 2-6). Because of the highly-fractured nature of the glacial overburden above the first saturated zone, downward flow velocities through the entire oxidized portion of these deposits are anticipated to be high. The frequency of fractures is anticipated to decrease with depth below the oxidized horizon reducing the downward flux (for example, McCay et al. 1993).

The second conclusion from the workshop was that it is nearly impossible to calibrate a fracture flow model even when a reasonably complete data base exists. The best modeling approach in light of the current data base involving fractures at the site is an equivalent porous media model. However, one participant recommended that a code should be available to explore the effects of fractures in the glacial overburden and compare fracture versus equivalent porous media approaches.

2.6 Expected Data from the Glacial Till/Vadose Zone Hydraulic Studies

A work plan for hydraulic studies of the glacial overburden has been prepared (PARSONS 1993a) with an objective of obtaining additional characterization information for the CRU5 Remedial Investigation/ Feasibility Study. This work plan has focused primarily on saturated flow conditions within the glacial overburden beneath the FEMP. Data from these investigations will be used to support GO/UGMAS model development.

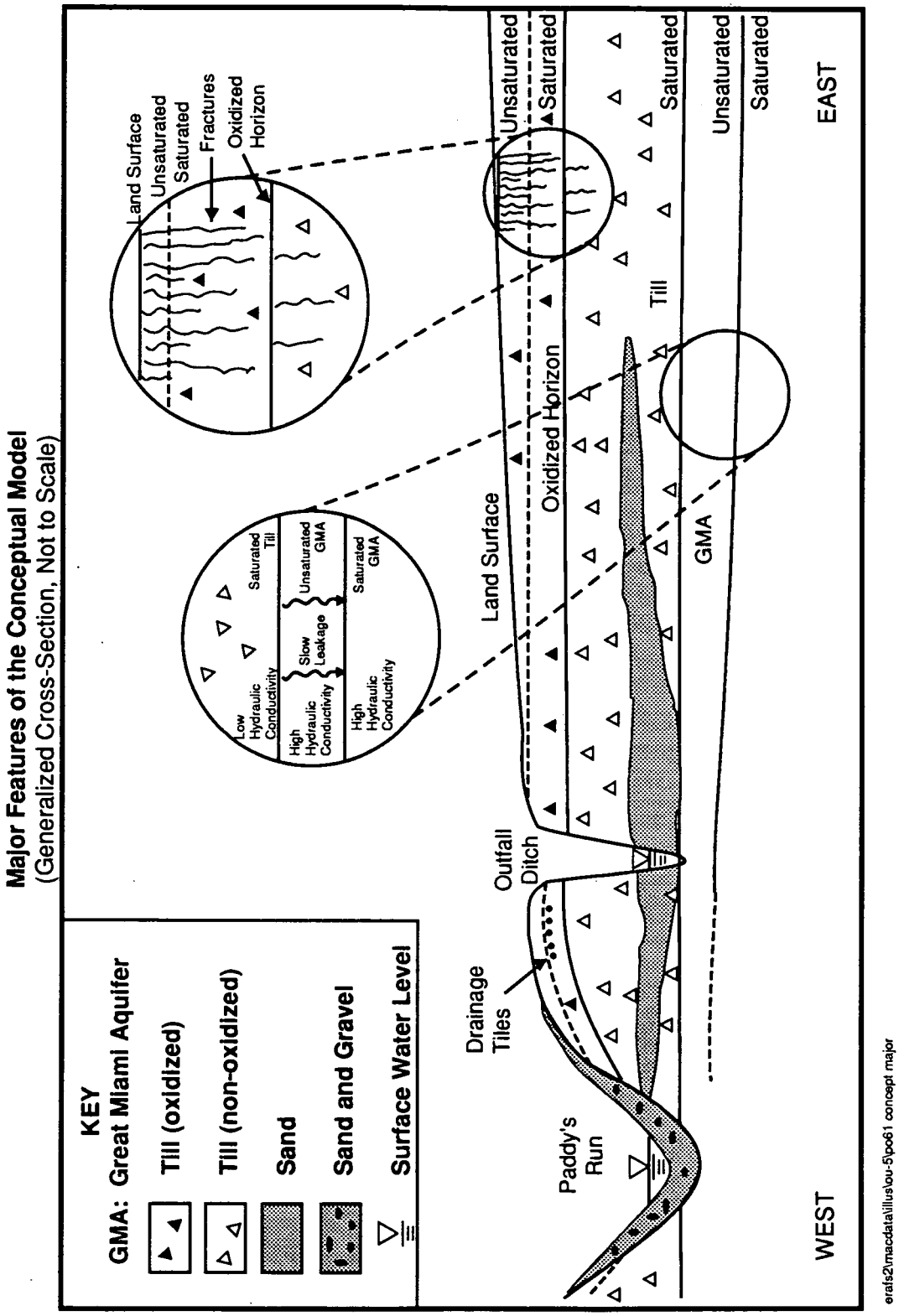


Figure 2-6 - Major Features of the Conceptual Model

Most of the saturated flow data will be used for calculating the hydraulic conductivity of the various lithologic and hydrogeologic units. Multiple methods of testing will be used across the same zones at the same locations thereby providing complementary measurements of the same data point. Hydraulic conductivity tests are being conducted on three operational scales based upon the volume of material sampled (Bradbury and Muldoon 1990). These operational scales are:

1) Small Scale Tests (< 1 m^3): Laboratory permeameter tests and particle size estimates.

2) Site-Specific Tests (1 m^3 to hundreds of cubic meters): Single well pumping tests, packer tests, and slug tests.

3) Local Tests (hundreds of cubic meters to thousands of cubic meters): Multiple well pumping tests.

Local scale hydraulic tests will be performed in the large sand unit that extends from the Plant 2/3 area to Paddy's Run. Site-Specific hydraulic conductivity tests will be performed in areas within and outside of the above described large sand unit. Small scale hydraulic conductivity tests (permeameter) will be performed at all new drilling locations where a suitable laboratory sample can be collected. Matrix conductivities will be compared to bulk hydraulic conductivities to assist in the determination of hydraulic interconnections.

Hydraulic conductivity and storativity will be calculated from the pumping tests in the large sand unit that extends from Plant 2/3 to Paddy's Run. Soil density, specific gravity, and moisture content will be measured in the laboratory tests. Three lysimeter clusters (two lysimeters to each cluster) will be installed to help determine the degree of saturation in the clay unit at the base of the glacial overburden as well as in the unsaturated portion of the Great Miami Aquifer (GMA). Groundwater from the pumping test wells will be analyzed for total uranium, volatile organic compounds, general chemistry (major anions and cations), and certain compounds on the FEMP hazardous substance list.

2.7 Definition of the Conceptual Model

Figure 2-6 depicts the major features of the conceptual model. This figure is based upon a generalization of the features of the GO/UGMAS identified in the discussion above. As the figure indicates, the generalized stratigraphy consists of an unsaturated layer of glacial overburden, a saturated layer of glacial overburden, an unsaturated horizon of the upper GMA, and finally, a saturated portion of the GMA. The glacial overburden is broken into an oxidized layer (brown clay) and reduced layer (gray clay). Based on the literature, a large number of fractures often appear in the oxidized layers of soft till; these fractures diminish with depth (McCay et al. 1993). Sporadic sand layers are located within the glacial overburden and may connect to the GMA at specific locations or may connect with surface ditches or Paddy's Run. As shown in Figure 2-6, water in the saturated glacial overburden slowly leaks into the

unsaturated upper GMA. Water transport occurs slowly through the unsaturated upper GMA due to the unsaturated or partially saturated conditions.

There are multiple potential pathways from any near-surface waste source downward to the GMA. These pathways include:

1) Vertical infiltration through the clay layers to the unsaturated GMA

2) Vertical infiltration through the clay layers to a sand lens, laterally along the sand lens which connects to the GMA

3) Vertical infiltration through the clay layers to a sand lens, laterally along the sand lens which connects to Paddy's Run (or the outfall ditch), and from the stream to the GMA

Subsurface boring and stratigraphic interpretation imply that sand zones are present in the glacial overburden. The presence of these sand zones may have control on the direction and enhance the rate of contaminant transport.

Figure 2-7 shows the conceptual model. The conceptual model is based on conclusions reached at the University of Cincinnati Industrial Workshop (see Subsection 2.5). This conceptual model represents a simplification from Figure 2-6 and is directed toward reasonably and conservatively simulating transport of constituents through the GO/UGMAS. The conceptual model consists of five layers. Layer 1 is the oxidized and fractured near surface glacial overburden (brown clay). This layer is included to provide a free surface for the saturated zone. However, this layer is ignored for contaminant transport since it does not provide a barrier to transport. Thus, contaminant sources are simulated to begin at the bottom of layer 1 (see Figure 2-7). Layer 2 consists of saturated glacial overburden below the oxidized horizon. Layer 3 represents a layer of either saturated sand or clay. Any lateral transport would primarily take place within this layer at identified, spatially varying sand lenses. Lateral flow along this layer may also contact surface water bodies (Outfall Ditch or Paddy's Run). Layer 4 depicts the lower glacial overburden which contacts the upper GMA. At specific locations, this layer may consist of more permeable soils (sand) representing a more permeable pathway to the upper GMA. Layer 5 is the bottom model layer consisting of unsaturated GMA sands. The GMA saturated zone is the bottom of this layer. Although layer 5 is thought to be unsaturated, it will be modeled conservatively as having saturated flow in the vertical direction only. The flux through the bottom of layer 5 will couple to the GMA Sandia Waste Isolation Flow and Transport (SWIFT) model in that it will form the upper boundary condition to the saturated GMA. This technique will build conservatism into travel times but, more importantly, will eliminate the calculational and conceptual problems of saturated and unsaturated flow boundaries.

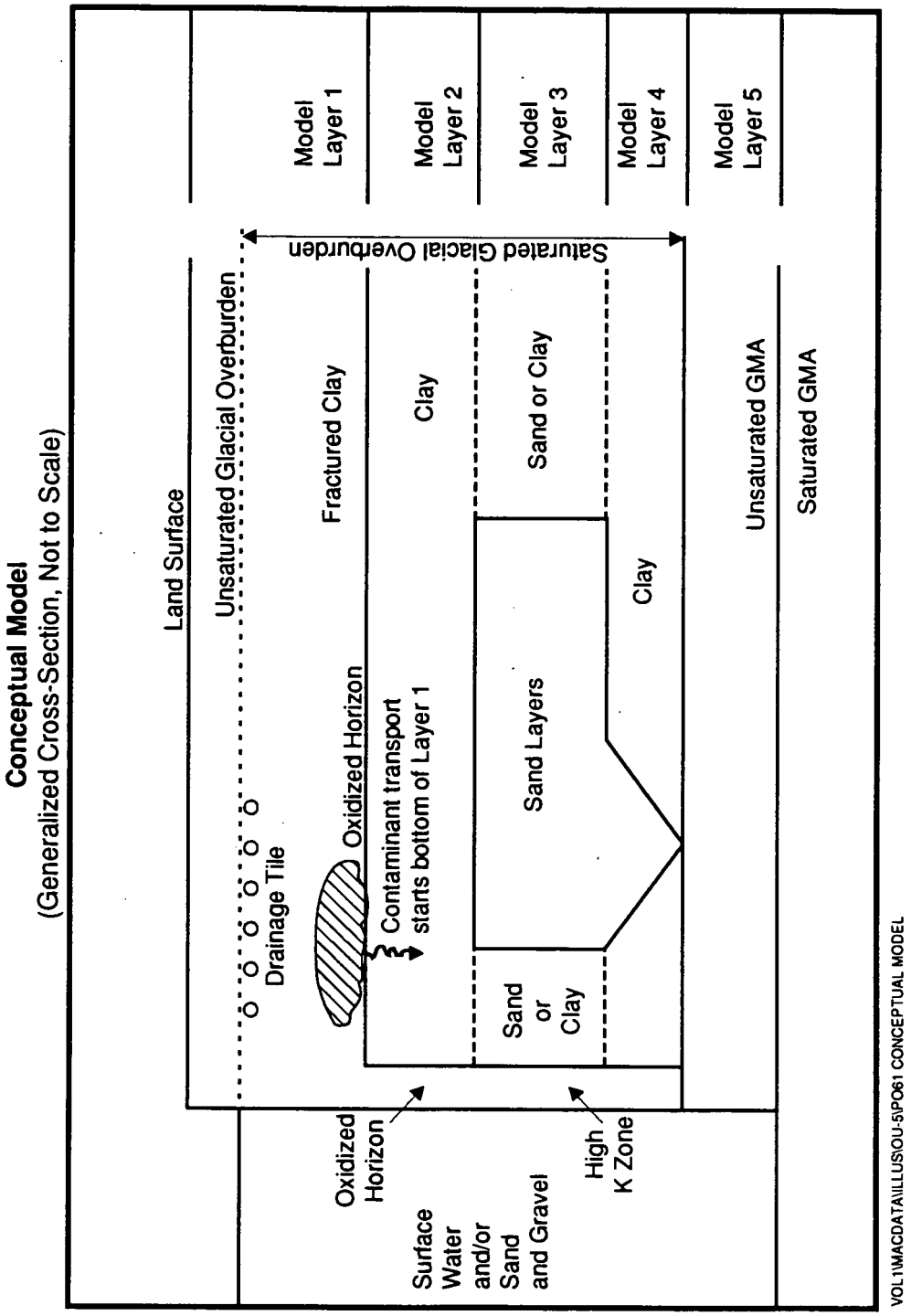


Figure 2-7 - Conceptual Model

Measurements from the Glacial Till/Vadose Zone Hydraulic Investigations field work will be used to refine the conceptual model. Data from slug tests, pumping tests, packer tests, and geotechnical laboratory tests will provide a better definition of the hydraulic characteristics of the various lithologic units and to help define the degree of interconnection (see Subsection 2.6). The anion/cation analysis from the wells and lysimeters may provide a specific "fingerprint" of groundwater types within different regions of the saturated and unsaturated zones. Sufficient measurements will be performed so that reasonable inferences can be made about the hydrogeology of the glacial overburden.

2.7.1 Primary Assumptions in the Conceptual Model

The conceptual model creates a simplification of the real system so that it can be effectively modeled. The primary assumptions used in creating the conceptual model include:

1) The Upper GMA sands are assumed to be fully saturated with only vertical transport. Since saturated transport is faster than unsaturated transport under similar conditions, this assumption is a conservative representation of flow and contaminant transport throughout the unsaturated zone. In essence, this layer represents a time delay between the overburden and the saturated GMA which can effectively be simulated with saturated conditions.

2) The upper oxidized zone (layer 1) is used only for allowing a free water surface in the model. Contaminant transport is simulated as beginning at the bottom of layer 1 because this layer may be highly fractured and will not provide an effective barrier to transport. Again, this is a conservative representation of the system since the model will assume no attenuation in this layer.

3) Equivalent porous media is substituted for potential fractures through the glacial overburden. The Industrial Workshop suggested it was impractical to calibrate a fracture flow model. The modeling objectives are on a large enough scale (time and space) that simulation of contaminants through porous windows can effectively meet the modeling objectives.

4) Steady state flow conditions can adequately represent flow conditions in the GO/UGMAS. Similar to 3 above, the modeling objectives are on a large enough scale (time and space) that simulation of contaminants moving under steady state flow conditions can effectively meet the modeling objectives.

Assumptions should be further checked during the model construction process.

2.8 Preliminary Boundary Conditions

The preliminary model domain and boundary conditions are shown in Figure 2-8. Figure 2-8 also shows the surface geology to help define these boundary conditions. The preliminary model domain covers an irregular rectangle approximately 10,000 feet by 6,500 feet with the long dimension oriented north-south.

On the west side, the model boundary will be along Paddy's Run. River node boundary conditions (head-dependent flux) will be used north of the silos where Paddy's Run rests on the glacial overburden. A no flow boundary will be used south of the silos where Paddy's Run has eroded through the glacial overburden into the GMA. The southern and eastern model boundaries will consist of a no flow condition coincident with the erosional edge of the glacial overburden or the edge of bedrock. The edge of bedrock to the north will be represented by either a no flow or lateral flux condition. Similarly, to the east and west of the northern bedrock, boundaries cut across the glacial overburden representing either a no flow or a lateral flux condition (from the upper reaches of the Paddy's Run watershed). A no flow condition will be imposed if uncertainty in flux across these boundaries is great. The bottom of layer 5 will consist of steady-state fixed head conditions consistent with the existing SWIFT GMA upper surface water level elevations.

Adjacent to certain model no-flow boundaries (typically glacial overburden margins or stream boundaries), the model will contain "draped zones." The draped zones will consist of model cells with higher hydraulic conductivities to allow downward flow to occur at the boundary. These zones represent either an oxidized zone along the bank of Paddy's Run or the erosional edges of the glacial overburden.

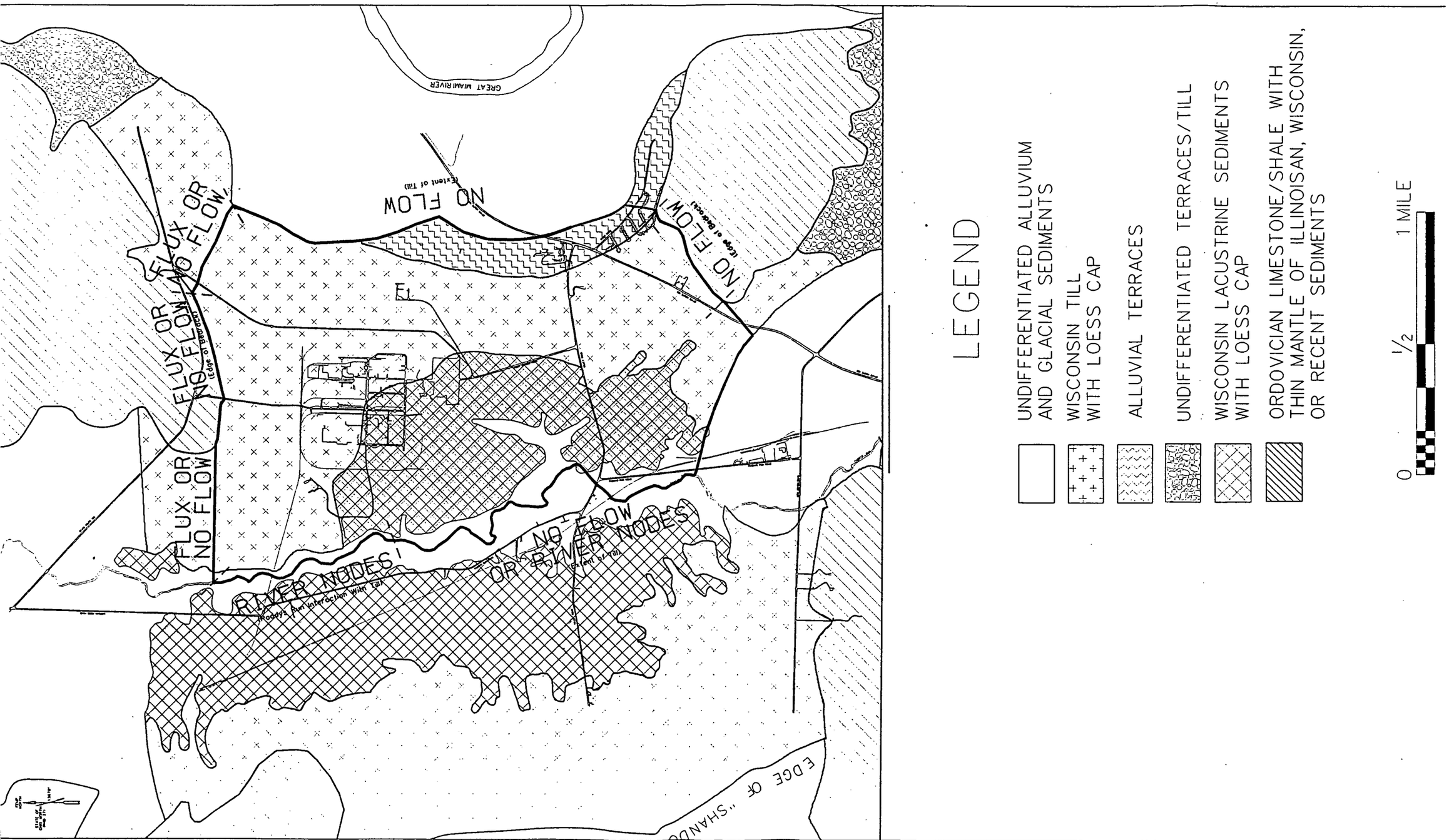


Figure 2-8 - Preliminary Boundary Conditions

SECTION 3

CODE SELECTION

Modeling in the GO/UGMAS must effectively reproduce the processes represented in the conceptual model in a reasonable yet conservative fashion.

To accomplish this, Section 3 presents the technical criteria for selection of the appropriate mathematical models for groundwater flow and contaminant transport through the GO/UGMAS at the FEMP. Following the presentation of these criteria, codes are selected that will meet the criteria and will most effectively perform the GO/UGMAS modeling.

As described in Subsection 1.3, two different codes will be utilized for preparing the GO/UGMAS model. The main code will build a three-dimensional representation of the GO/UGMAS. An auxiliary code will be used to build a two-dimensional cross-sectional model to support this representation by checking the assumptions of the main code. The auxiliary code will also be employed to help verify the main code. This section describes the selection process for the main code. The criteria and the selection of the auxiliary code is described in Appendix A.

3.1 Selection Criteria

The US EPA defines the code selection process as matching a detailed description of the modeling needs with well-defined characteristics of existing models. Therefore, the selection criteria presented herein are based on first identifying and analyzing the modeling needs for the GO/UGMAS and then simply matching these needs with an existing code that can provide an optimal solution to the problem. The final selection also considers the constraints in human and material resources available for the study.

To define the modeling needs, an understanding of the physical system is needed. This understanding was presented in Section 2, which described the development of the conceptual model. Selection criteria have been identified based on this conceptual model and other project needs. Both primary and secondary criteria are identified, as defined below:

1) Primary Criteria: Constitute the minimum requirements that are needed to perform groundwater flow and contaminant transport through the GO/UGMAS at the FEMP site.

2) Secondary Criteria: Include anticipated features that can be useful for current and future modeling efforts in the GO/UGMAS.

4776

3.1.1 Primary Selection Criteria

The primary code selection criteria consist of:

1) The code needs to effectively model the processes identified in the conceptual model. These processes include both heterogeneous and anisotropic conditions. Multiple layers are present in the conceptual model; therefore, the code needs to be three-dimensional. The simulated transport processes should account for advection, dispersion, adsorption, and source and solute decay.

2) The code must be able to perform transient flow simulations as well as steady-state conditions.

3) The code must be verified and peer reviewed. The verification process should have tested most of the functions and features available in the code. In particular, the published verification results for those features that are needed to perform the GO/UGMAS modeling should be available and compared with well-known analytical or numerical solutions. Further, the concepts, the theory (mathematical formulation), and the code documentation need to be peer reviewed.

4) The computer code must be flexible so it can interact with the SWIFT GMA model. A code that is in the public domain (with available source code) is preferred so that if coding changes are needed they can be easily incorporated to link the GO/UGMAS model with the SWIFT GMA model.

5) The code must be widely used and accepted by groundwater modelers.

3.1.2 Secondary Selection Criteria

The secondary criteria include:

1) The capability of the code to model both saturated and unsaturated flow.

2) The type of domain discretization (i.e., finite element or finite difference [FD]). This is mainly a preference on the modeler's part. Also, because the present GMA model (SWIFT) is an FD code, an FD model for the GO/UGMAS will simplify any linkage between models.

3) The ability of the code to account for fractured media as well as porous media.

4) Preprocessing and postprocessing capabilities of the code.

3.2 Selection of Codes

Two primary paths to code selection for the GO/UGMAS were considered. First, a new unsaturated/saturated code could be utilized which meets the selection criteria identified above. Second, SWIFT (a saturated code) could be used (i.e., the same code as is presently used for the GMA model).

These two options have certain advantages and disadvantages. The selection of a code with unsaturated capabilities allows an accurate depiction of both saturated conditions of the glacial overburden and unsaturated conditions in the upper GMA. However, the use of a new code will create a compatibility problem with the existing SWIFT GMA model. The two models will need to be linked for many applications. In addition, the introduction of a new code creates certain problems. These problems include the need to have trained staff familiar with the new code. As modelers work with a particular code, they develop pre- and post-processing routines to improve the efficiency of data transfers. These routines would have to be built for a new code.

SWIFT has all the capabilities identified in the primary and secondary criteria with the single exception of the ability to model unsaturated flow. Since SWIFT has been used for several years at the site, the use of SWIFT for the GO/UGMAS overcomes these practical problems of trained staff and support routines. The use of SWIFT also reduces any compatibility problems with the existing GMA model. It will be a relatively simple matter to link these models since they use the same code. SWIFT has been extensively verified and peer reviewed.

SWIFT seems to be the obvious choice except for the unsaturated flow issue. It is felt that this issue can be overcome through a simplification process. The unsaturated zone represents a vertical flowpath from the saturated glacial overburden to the saturated GMA. In effect, the unsaturated zone creates a time delay for transport from the glacial overburden to the GMA. This flowpath may be represented by assuming saturation, but with only vertical flow (horizontal hydraulic conductivity equal to zero). Another option may be to use a one dimensional code to simulate this time delay. The GO/UGMAS model could be set up so it could be coupled or decoupled with the GMA SWIFT model. Certain model applications may be more effective coupled to the SWIFT aquifer model (e.g., risk assessments) while other applications could be performed in a decoupled manner (e.g., groundwater recovery simulations).

3.2.1 Auxiliary Code

To support the development of the GO/UGMAS model using SWIFT, an auxiliary unsaturated code(s) will be selected and obtained. This code will be used to help derive a conservative representation of the key assumptions in the main model, including flow through the unsaturated upper GMA. This code will also be used to help solve other potential issues that may occur. The main objective of the auxiliary code

is to perform two-dimensional cross-sectional analysis that evaluates the impacts of the assumptions/simplifications used in the main GO/UGMAS model. These assumptions include:

1) The ability to effectively model the unsaturated zone. This supports the first conclusion of the workshop (Subsection 2.5). It also tests the assumption of having the bottom most layer of the GO/UGMAS simulated with 100 percent saturation and restricting flow to the vertically downward direction (see Subsection 2.3). Hence, the auxiliary code will provide a measure on the level of conservatism in travel times by assuming fully saturated media.

2) The effects of fractures on the predicted SWIFT results. The SWIFT model will use an equivalent porous media approach to incorporate the effect of fractures. The auxiliary code, in turn, will use the best available data on the existence and extent of the fractures to build a two-dimensional cross-sectional model and compare the results with the main model.

3) The effects of the steady state assumption. The SWIFT model will be built with steady state flow parameters. The impact of this assumption will be tested with the auxiliary code. Therefore, the auxiliary code needs unsaturated and transient capabilities.

The auxiliary code will also be used as a verification tool as described in Subsection 3.3. Therefore, a code with three-dimensional capability is needed.

Appendix A contains an evaluation of codes for the selection of this auxiliary unsaturated code. Auxiliary code selection criteria are identified and codes are screened to eliminate codes that are not three-dimensional and codes that simulated only flow and/or heat transport. After the initial screening, 13 codes are identified that could simulate three-dimensional unsaturated flow and transport. These codes are evaluated according to established criteria for unsaturated codes (see Appendix A). Based upon this evaluation process, the Multiphase Subsurface Transporter Simulator (MSTS) model is selected as the auxiliary code. MSTS will be obtained, verified, and used to support the GO/UGMAS model development.

3.3 Verification of SWIFT and MSTS

The SWIFT code has been verified in the literature, specifically for the FEMP project and in accordance with PARSONS' procedures. MSTS will be verified in two ways. First, input and output files from verification runs performed by the code authors will be obtained for the purpose of reproducing the runs on PARSONS' computer systems. This will include a number of runs for comparison with literature benchmark problems exercising as many of the code's options as is practical. The second verification step will consist of using the SWIFT and MSTS codes to perform the same benchmark run. An appropriate benchmark problem with a well-understood solution will be chosen from the literature. These problems should include analytical solutions and numerical solutions obtained with simpler (including two-

dimensional and one-dimensional), thoroughly tested codes. The code should produce a solution essentially the same as the established correct solution.

After the verification step, the code will be evaluated using run conditions anticipated in the GO/UGMAS. These will include low permeability layers, a large sand lens scenario with multiple migration pathways and contaminant source areas, and a small sand lens scenario with one migration pathway and a single contaminant source.

SECTION 4

TECHNICAL PLAN

4.1 Introduction

The SWIFT code will be used as the main code to build a three-dimensional representation of the conceptual model (see Figure 2-8). MSTS will first be used as a verification tool for the main GO/UGMAS model (using SWIFT). Then MSTS will be used to build two-dimensional cross-sectional model(s) to study the degree of conservatism of the key assumptions in the main model as described in Subsection 3.2. These key assumptions include:

1) Full saturation of the Upper GMA sands with only vertical transport
2) Elimination of the oxidized zone from the model domain
3) Substitution of equivalent porous media for potential fractures through the glacial overburden
4) Steady state flow conditions

4.2 Model Implementation

4.2.1 Initial Model Construction

Initial model construction will consist of specification of the grid scale, grid boundaries, hydrostratigraphic units and associated material properties, initial and boundary conditions, and sources or sinks in the interior of the calculation domain. These specifications will be made using the best data available at the time of the initial construction. The model obtained from the initial construction process will be refined periodically as new data from the glacial till/vadose zone hydraulic studies and other characterization efforts become available.

Grid scale will be arrived at through a tradeoff between the desired level of detail in modeling results and computational limitations (execution time and storage). The selection of grid scale will consider compatibility with the solute transport grid of the existing GMA model. The existing GMA model solute transport grid will be expanded as part of the SWIFT model improvement program (DOE 1993c); thus mesh development of the GO/UGMAS model will be integrated with these efforts. Regions with significant migration pathways through areally or vertically limited features such as sand lenses and fracture zones or to surface water such as Paddy's Run will be represented with refined gridding. Other regions with more homogeneous stratigraphy and primarily vertical transport will be represented with coarser gridding. The number of layers used in the vertical dimension will be chosen to accommodate relatively isolated features such as sand lenses with one or more vertically homogeneous layers. Based upon the present conceptual model (Figure 2-8), the model will have five vertical layers.

4770 Preliminary boundary conditions have been chosen to coincide with easily identifiable physical boundaries and boundary conditions (see Subsection 2.8). Examples include zero-flow and zero-flux conditions at locations where the porous medium meets bedrock or at a flow divide. These preliminary boundary conditions will be used for initial model construction. These boundaries may be updated based upon revisions in the conceptual model.

At the FEMP, a "telescoped" grid approach may be used for the flow portion of the problem. This consists of performing a single flow run with a coarse grid for a large area using zero-flow conditions at bedrock walls and flow divides. Subsequent fine-scale modeling runs use the coarse-scale results to establish specified head conditions at the boundary of the smaller area. A zero concentration gradient boundary condition may be used for the fine-scale solute transport run and the results will be valid provided the area of interest is not close to the boundary. The boundary at the base of the glacial overburden may have to be extended down into the saturated portion of the underlying aquifer to assure that the specified solute transport boundary condition does not exert undue influence on the solution at the glacial overburden/aquifer interface.

Discretization of the calculation domain into units representing the geometry and properties of glacial overburden hydrostratigraphic units will be heavily dependent upon results of the concurrent glacial overburden characterization effort. Data currently used for the one-dimensional GO/UGMAS modeling (ODAST) will be used where necessary for initial construction of the three-dimensional model. Soil characteristic curves of capillary pressure head and hydraulic conductivity versus moisture content will be used for checking the saturated flow assumption in the upper GMA. Either empirical correlations from the literature for similar soils will be used or, preferably, a parameter estimation algorithm will be used to determine curve coefficients based on site data generated by the glacial overburden characterization effort.

Initial conditions will be required for the solute transport calculations and for any transient flow calculations. It is anticipated that current concentration data, contoured from lysimeter and 1000 series well sampling results, will be used instead of a zero-concentration initial condition. Steady-state flow results corresponding to conditions at the start of a simulation will be used as initial conditions for transient flow runs.

038

4.2.2 "Calibration"/Comparison to Observed Conditions

Quantitative and qualitative criteria for the calibration effort will be defined. Quantitative criteria includes the definition of both target locations and statistical parameters (and acceptable ranges of these parameters) for calibration of the flow and transport models. In addition, qualitative comparisons between monitoring data and model predictions will be required. Qualitative criteria include evaluation of correspondence among model simulations and the physical structures of the hydrogeological system. Qualitative features include, but are not limited to, the pattern of heads and concentrations. The development of calibration criteria will consider the difficulties inherent in the GO/UGMAS.

The primary flow calibration of the GO/UGMAS model will be to steady state water elevation conditions. Head measurements in 1000 series wells will generally be used to calibrate the model in saturated regions. Recent water elevation data will be analyzed to select an appropriate time series of data to represent steady state conditions and for developing target head values. It is expected that quantitative criteria for the flow model will include measures of mean residual, maximum residual, variance of residual, and spatial correlation of residuals. Also, criteria for water mass balances will be defined.

Transient calibration will be performed by matching the model simulated and measured drawdown vs. time data measured during the glacial till pump tests. This transient calibration will be performed following the first successful steady state calibration. Since the transient calibration will need to adjust some hydraulic parameters that can also affect the steady state model results, the transient and steady state model calibrations will be an iterative process. The transient calibration will only be performed if pump test results from the glacial till/vadose zone hydraulic studies (PARSONS 1993a) are available.

The solute transport model will be calibrated with total uranium data only. The latest existing uranium data will be compiled and evaluated to define the solute transport calibration criteria. Both data range and 95 percent confidence interval of the mean for each monitoring well will be considered as the target range. An attempt will be made to balance two primary calibration targets: (1) concentrations at particular blocks representing location of measured data, and (2) total mass of contaminant in the aquifer.

Concentration data from sampling with lysimeters in the unsaturated regions and at 1000 series wells in saturated zones will be compared with calculated concentrations to determine the optimal transport parameters. It should be noted that because flow in large part determines solute transport, the transport calibration process may be used to make further adjustments to the flow parameters.

Geostatistical analysis will be conducted on an as-needed basis to understand and correlate the spatial distribution of key data sets. These data sets include the water elevation data, the uranium analytical data from the 1000 series monitoring wells, various layer thicknesses, and K_d. Calculations will include the sample semivariogram, and kriging and cokriging estimators along with their estimation variance. This

analysis will be used to help determine calibration criteria and to identify areas of the site where lower confidence exists in the analyzed data sets.

4.2.3 Sensitivity Analyses

Sensitivity analyses will be performed for flow and transport. Variation of flow and transport parameters across a range of reasonable values will allow identification of those having the greatest impact on predicted concentration plumes. Ongoing characterization studies can then become more efficient by focusing on the most important parameters. Likewise, variation of boundary conditions and parameters in the vicinity of inhomogeneities (Paddy's Run, sand lenses, fracture zones) may indicate local areas deserving special attention.

4.2.4 Linkage to Other Models

Since three-dimensional flow and transport codes typically do not explicitly address runoff and evapotranspiration, a water balance model (HELP or other) will be used to provide infiltration rates at the top of the GO/UGMAS. The surface will be subdivided into a number of relatively homogeneous regions and a water balance model run will be performed for each. The process of specifying surface infiltration rates to the GO/UGMAS model can be automated via a FORTRAN code for the initial model construction or later large-scale changes. Subsequent changes to infiltration rates over small areas of the grid may be done manually.

Concentration histories at the base of the GO/UGMAS will be used to calculate mass loading histories specified at the top of the saturated GMA model (SWIFT). This process will also be automated via a FORTRAN code.

4.2.5 Auxiliary Code

An auxiliary code MSTS will be used during SWIFT model development and during model performance evaluations. MSTS will be used to build two-dimensional cross-sectional model(s) to investigate the degree of conservatism of the key assumptions in the main model. The assumptions to be studied are:

1) Full saturation of the Upper GMA sands with only vertical transport
2) Elimination of the oxidized zone from the model domain
3) Substitution of equivalent porous media for potential fractures through the glacial overburden
4) Steady state flow conditions

4.2.6 Performance Evaluation

A performance evaluation (extended verification or "validation") simply uses the calibrated model to predict a totally independent set of field data measured over a longer period, at different times, that involve unique conditions. Unique conditions include different boundary conditions for water at the upper soil surface. These different boundary conditions may include a significantly different schedule of infiltration rates over time or a completely different type of boundary condition: constant potential, constant flux (for example, rainfall), or a mixed type. If the performance evaluation finds that the model cannot accurately predict the unique set of conditions, then recalibration is necessary followed by another performance evaluation until reasonable agreement is reached.

4.2.7 Post Audit Assessments

Post audit assessments compare model predictions with field data over long periods of time. The model that results from the calibration and performance evaluation should predict flow and transport conditions long after the periods used for calibration and performance evaluation. Collection of new field data at regular time intervals should determine and help interpret the discrepancies with previous predictions. The post audits should be conducted after several of the prediction intervals have passed to ensure that significant changes had time to occur. The evaluation of results of the post audit are similar to the methods used for the calibration and extended verification. The first post audits should be performed at least 5 years after calibration.

4.3 Test Simulations

Test simulations will be performed to check the functioning of the model for expected model applications. Expected model applications include baseline simple band risk assessments, alternatives evaluations for feasibility studies, and design support for the various OUs. To perform these applications, simulations will have to define the contaminant source terms, simulate flow and contaminant transport through the GO/UGMAS, and predict aquifer mass loadings for input to the groundwater flow model.

4.3.1 Contaminant Source Terms

The procedure for calculating contaminant leachate source terms will remain unchanged from the process described in Section 3 of the Fate and Transport Modeling Transition Report (PARSONS 1993b). The source mass flux into the GO/UGMAS will be assumed to be an exponentially decreasing function of time. The source depletion factor and time may be calculated as described in Section B-2 of Appendix B of the Fate and Transport Modeling Transition Report (PARSONS 1993b). However, IT has suggested an alternative procedure in which the source concentration remains at its solubility limit for a period of

776

time before depletion commences. This practice will be adopted once the suggested change is documented and reviewed.

4.3.2 Flow Simulations

Flow simulations will be performed under steady-state conditions. Flow simulations will include the simulation of pumping and particle tracking for capture zone analysis of theoretical pumping wells. The flow simulation will produce outputs that address the performance measures identified for a given calculation effort.

4.3.3 Transport Simulations

Transport simulations will take initial conditions of contaminant concentrations at some point in time with the derived source terms to predict contaminant transport through the GO/UGMAS. The transport simulations will be designed to address the performance measures of interest for the particular application.

4.3.4 Aquifer Mass Loading History Calculations

Aquifer mass loading history calculations will be automated via a FORTRAN code. This will consist of multiplying concentration histories at the glacial overburden and upper GMA interface by flow rate to obtain mass loading rates. Averaging must then be performed over specified time intervals and grid blocks and the results will be written to a file in the correct format for input to SWIFT.

4.4 Final Report

A final report will be prepared which will document the development of the GO/UGMAS model. This report will consist of sections describing:

1) Modeling Objectives and Approach
2) Conceptual Model
3) Code Selection and Verification
4) Model Construction
5) Parameter Selection
6) Model Calibration
7) Sensitivity Analysis

8) Test Simulations

9) Model Assumptions and Limitations

Figures will show input data sets and model output. Appendices will contain sample input and output files.

SECTION 5

MANAGEMENT PLAN

5.1 Hardware and Software Requirements

Both SWIFT and MSTS codes are written in the FORTRAN programming language. Both these codes have PC DOS based versions. These PC DOS applications will use existing hardware (Powerbox PC, 128 MB RAM, 1 GB hard disk) and software (Salford FORTRAN compiler, DBOS Memory Manager, PERUSE, and MULTIEDIT for file editing, SURFER and Intergraph's ERMA for post-processing). PARSONS has capabilities for running these codes on UNIX based platforms, if necessary. A Silicon Graphics Iris Indigo Workstation (VI editor, FORTRAN compiler, and post-processing software included) will be used. This system is currently on order. System selection will be based on obtaining reasonable execution times which are dependent on model size and the method of linkage to the existing GMA model. Dual DOS and UNIX capabilities will allow the greatest flexibility in coordinating with other modeling tasks and will allow GO/UGMAS modeling to proceed in the most timely fashion.

5.2 Quality Assurance

All quality assurance associated with the GO/UGMAS modeling and model development will follow the PARSONS Environmental Remedial Action (ERA) Quality Assurance (QA) Procedures Manual. This manual specifies procedures governing code verification, hand calculation, and computer modeling results documentation, and checking and review of hand calculations and modeling results. Appendix B reprints PARSONS Procedure ENG-006 "Preparation and Control of Calculations" (Revision 3) and PARSONS procedure ENG-012 "Verification and Validation of Engineering/ Scientific Codes" (Revision 1). PARSONS' QA Group performs independent audits of work governed by ERA procedures to assure compliance.

5.2.1 Peer Review and Oversight Committee

A peer review and oversight committee will be formed to check model development progress and modeling results, and to make recommendations for continuing model development. This committee will consist of FERMCO and PARSONS modeling personnel, Bill Sidle, PhD (DOE Technical Support), and Milovan Beljin, PhD (Technical Consultant).

5.2.2 Review Meetings

Meetings of the Review and Oversight Committee will take place as specific project milestones are completed. The first will be held after final selection and verification of the GO/UGMAS modeling code. The second will be held after construction of the model mesh and finalization of the conceptual model. A third meeting will take place after the model has been calibrated to observed conditions. A final meeting will be held after sensitivity analyses and test simulations have been performed and the preliminary glacial overburden model has been completed.

5.3 Project Team Organization

PARSONS has assigned a team of modelers to design and construct the GO/UGMAS model. An independent group of technical experts will be utilized to conduct peer reviews. Figure 5-1 provides a project organization chart.

5.4 Deliverables

PARSONS will provide the following deliverables to support the development of the improved GO/UGMAS model:

1) Draft Modeling Work Plan
2) Final Modeling Work Plan
3) Draft Modeling Report
4) Final Modeling Report

5.5 Schedule

The final calibrated model is scheduled to be completed in January 1994 and the final report is scheduled to be completed on February 1994.

Since field data collection is being conducted in parallel to model development, new data will be incorporated into the model up until final production runs commence.

Project costs will be closely monitored. When 60 percent of the budget is spent, FERMCO will be informed, and a meeting will be held to assess progress and to outline an approach to completion of the model.

Figure 5-1 - Organization Chart

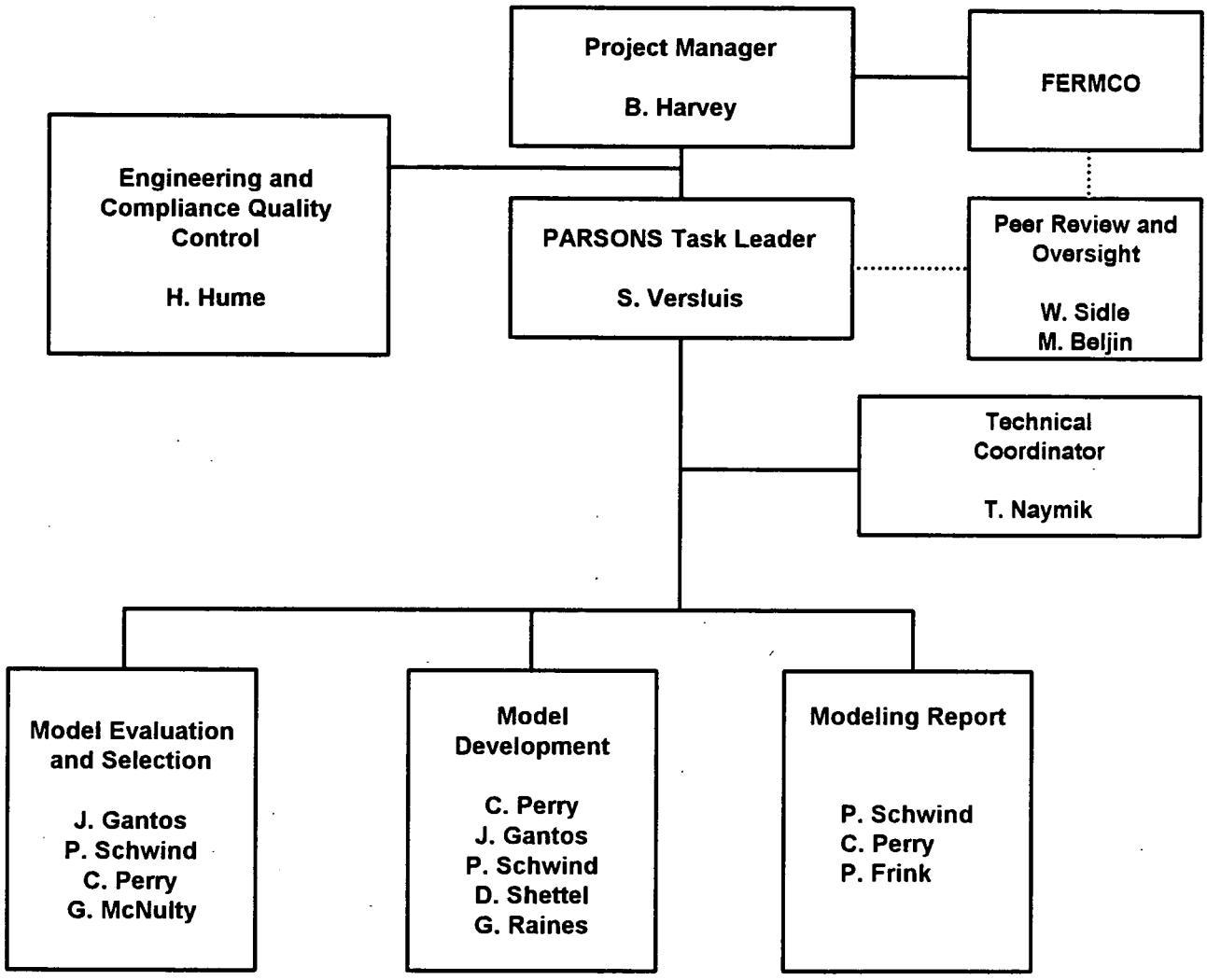


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Figure 5-1 - Organization Chart

SECTION 6

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APPENDIX A

AUXILIARY CODE SELECTION

APPENDIX A

AUXILIARY CODE SELECTION

1.0 INTRODUCTION

This section discusses the selection of the appropriate auxiliary code for supporting the construction of GO/UGMAS model. This model will be used for checking the assumptions in the main model and to support verification of the main model. The main model will use SWIFT to construct a three-dimensional model of the GO/UGMAS.

Section 2 presents a brief list of assumptions that will be used in constructing the main model. Section 3 provides a detailed discussion of the selection criteria and the basis for selecting these criteria. The selection process for the finalist codes is presented in Subsection 1.3.

2.0 ASSUMPTIONS IN CONSTRUCTING MAIN MODEL

The SWIFT code (three-dimensional saturated flow and transport) has been selected for the main code for construction of the GO/UGMAS model. The purpose of selecting an auxiliary code is to check the assumptions in the main model. The primary assumptions are:

1) The Upper GMA sands, unsaturated in the conceptual model, will be assumed to be saturated.

2) The oxidized zone will be eliminated from the model domain.

3) If necessary based upon field findings, equivalent porous media will be substituted for fractures through the glacial overburden.

4) Flow conditions will be steady state.

The selected auxiliary code needs to be able to check these assumptions.

3.0 SELECTION CRITERIA

The US EPA defines the code selection process as matching a detailed description of the modeling needs with well-defined characteristics of existing models. Therefore, the selection criteria presented herein are based on first identifying and analyzing the modeling needs and then simply matching these needs

with an existing code that can provide an optimal solution to the problem. Criteria are divided into primary and secondary, defined as follows:

1) Primary Criteria: Constitute the minimum requirements that definitely are needed to check the assumption of, and assist in verification of, the main model.

2) Secondary Criteria: Include anticipated features that can be useful for current and future modeling efforts in the unsaturated and saturated zone.

3.1 Primary Selection Criteria

The primary code selection criteria consist of:

1) The code needs to simulate both saturated and unsaturated flow.

2) The code needs to account for fractured media, as well as porous media.

3) The code needs to have three-dimensional and two-dimensional capability.

4) The code must be able to perform transient flow simulations as well as steady-state conditions.

5) The code must be verified and peer reviewed. The verification process should have tested most of the functions and features available in the code.

3.2 Secondary Selection Criteria

The secondary criteria include:

1) The transport processes simulated should account for advection, dispersion, adsorption, and source and solute decay. Advection and dispersion are the basic transport processes common to all the codes that were screened. Therefore, adsorption and decay were used to screen the codes.

2) The number of phases for which mass transport can be calculated.

3) The type of domain discretization (i.e., finite element or FD). This is mainly a preference on the modeler's part. Also, because SWIFT is an FD code, an FD model for the auxiliary code is preferred.

4) The concepts, the theory (mathematical formulation), and the code documentation have been peer reviewed.

5) The code must be widely used and accepted by groundwater modelers. The International Groundwater Modeling Center (IGWMC) ratings are utilized here to evaluate the extent of model use.

4.0 SELECTION OF FINALIST CODES

Only those codes that can handle unsaturated media were considered in the selection process. An initial list of unsaturated codes that were considered in the screening process is summarized in Table A-1. Table A-1 includes a comprehensive list of one-, two-, or three-dimensional codes that are specifically developed for unsaturated media to simulate flow, solute, and heat transport.

Table A-1 was assembled from several sources, which include:

1) Published reports such as van der Heijde (van der Heijde 1992), El-Kadi and Beljin (El-Kadi et al. 1987) and van der Heijde and Elnaway (in review).

2) US EPA Ada Lab

3) IGWMC

4) Colorado School of Mines

5) Waterloo Center for Groundwater Research

6) National labs (e.g., Los Alamos National Lab, Oak Ridge National Lab, and Battelle Pacific Northwest)

Table A-1 - A Comprehensive List of Unsaturated Codes

Model Name	Author(s)	Remarks
3DFEMWATER	Yeh, G.T.	3-D, UNS/SAT ANI. HETRO.
BIOSOL	Baek, N.H.	Biodegradation
CADIL/AGTEHM	Emerson, C.J.	Chemical Transport
CHAIN	van Genuchten, M.A.	MULTI-ION TRANSPORT
CHEMFLO	Nofziger, D.L.	1-D
CHEMRANK	Nofziger, D.L.	Ranking organic chain
CMIS	Nofziger, D.L.	Pesticide
CREAMS	Knisel, Walter G.	Agricultural
CTSPAC	Lindstrom, F.T.	Heat 1-D
CXFIT	Parker, J.C.	Parameter Estimation (P.E.)
DISPEQ/DISPER	Fluhler, H. and Jury, W.A.	No decay
DISSOLVED-CONSTITUENT TRANSPORT CODE	Duguid, J.O. and Reeves, M.	2-D
DRAINMOD	Skaggs, R.Wayne	1-D
FEATSMF	Neiber, J.L.	2-D
FEMTRAN	Martinez, M.J.	2-D
FEMWASTE/FECWASTE	Yeh, G.T. and Ward, D.S.	2-D, 3-D In Preparation
FEMWATER/FECWATER	Yeh, G.T. and Ward, D.S.	2-D (3-D)
FLAME	Baca, R.G.	2-D
FLAMINCO	Huyakom, P.S.	3-D
FLASH	Baca, R.G.	2-D
FLO/FLOW	Vandenberg, A.	2-D
FLOFIT	Kool, J.B.	Parameter Estimation
FLOTRA	Sagar, B.	2-D
FLOWVEC	Li, R-M.	3-D, Flow Analysis
FLUMP	Narasimhan, T.N.	2-D
FP	Su, C.	Parameter Estimation

Table A-1 - A Comprehensive List of Unsaturated Codes (Continued)

Model Name	Author(s)	Remarks
GASOLINE	Baehr, A.L.	1-D
GLEAMS	Leonard, R.A.	Agricultural
GRWATER	Kashkuli, H.A.	1-D
GRWATER	Sunada, D.K.	Flow Analysis
GS2	Davis, L.A. and Segol, G.	2-D
GS3	Davis, L.A. and Segol, G.	3-D
GTC	Yu, G.	Group Transfer Concentration
HYDROLOGIC CONTAMINANT TRANSPORT MODEL (HCTM)	INTERA Environmental Consultants, Inc.	3-D
HYDRUS	Kool, J.B.	Root uptake
INFGR	Craig, P.M.	Infiltration 1-D
INFIL	Vauclin, M.	Infiltration 1-D
INFILTRATING WATERSHEDS	Smith, R.E.	1-D
IRRIGATION RETURN FLOW MODEL	Gelhar, L.W.; Baker, A.; McLin, S.; and Updegraff, C.D.	Irrigation
LANDFIL	Korfiatis, G.P.	Landfil 1-D Ph.D.
LEACHMP	Wagenet, R.J.	Pesticide
MATTUM	Yeh, G.T. and Luxmoore, R.J.	No compartment method
MLSOIL/DFSOIL	Sjoreen, A.L.; Kocher, D.C.; Killough, G.G.; and Miller, C.W.	Soil
MMT-DRPW	Ahlstrom, S.W.; Foote, H.P.; and Serne, R.J.	3-D, Unsaturated/Saturated, Battelle PNL
MMT-ID	Kaszeta, F.E.; Simmons, C.S.; and Cole, C.R.	1-D, Battelle PNL
MOBIDIC	Couchat, P.H.; Lcardinal, G.; and Moutonnet, P.	2-D
MOISTURE TRANSPORT CODE	Reeves, M. and Duguid, J.O.	2-D
MOTIF	Guvanasen, V.	3-D Brine Transport

Table A-1 - A Comprehensive List of Unsaturated Codes (Continued)

Model Name	Author(s)	Remarks
MOUSE	Pacenka, S.	For Educational Purposes
MULTIMED	-	Analytical 1-D
MUST	De Laat, P.J.M.	1-D
NITRO	Kaluarachchi, J.J.	2-D
NITROSIM	Rao, P.S.C.	Transport and Plant Uptake
NMODEL	Selim, H.M. and Davidson, J.M.	1-D
ODMOD	Larson, N.M. and Reeves, M.	1-D
ONESTEP	Kool, J.B.; Parker, J.C.; and van Genuchten, M.Th.	Parameter Estimation
PC-SEEP	Krahn, J.	Seepage through Earth Dam
PERCOL	Serne, R.J.	Battelle PNL, No Decay
PESTAN	Enfield, C.G.	Pesticide
PISTON	Fluhler, H. and Jury, W.A.	?-D, Transport Only
PORFLOW-3D	Runchal, A.K.	Flow and Heat Transport
PRZM	Carsel, R.F.	Pesticide 1-D
PRZMAL	Wagner, J.	Pesticide
RETC	van Genuchten, M.Th.	Parameter Estimation (P.E.)
RITZ	Nofziger, D.L.	Regulatory
RUSTIC	-	Coupled PRZMT VADDFT
RZWQM	DeCoursey, D.G.	Root Zone
SALT TRANSPORT IN IRRIGATED SOILS	Dutt, G.R.; Shaffer, M.J.; and Moore, W.J.	1-D
SATURN	Huyakorn, P.S.	2-D
SBIR	Li, R-M	3-D Vector Processor
SEEP	Barends, F.	Seepage
SEEPV	Davis, L.A.	Seepage, 1-D
SESOIL	Bonazountas, M.	?-D

Table A-1 - A Comprehensive List of Unsaturated Codes (Continued)

Model Name	Author(s)	Remarks
SIMERO	Degallire, R.	Analytical Model
SIMGRO	Querner, E.P.	Quasi 3-D
SOHYP	van Genuchtn, M.Th.	Parameter Estimation
SOIL	El-Kadi, A.I.	Parameter Estimation
SOILMOP	Ross, D.L. and Morel-Seytoux, H.J.	Ponding Time, 1-D
SOILPROP	Mishra, S.	Parameter Estimation
SOMOF	Wesseling, J.W.	1-D Vertical
SPLASHWATER	Christopher, P. and Milly, P.	Heat ?-D
STDY 2	Amerman, C.R.	2-D
SUMATRA-1	van Genuchten, M.Th.	1-D
SUMMERS	Summers, K.	Analytic
SUPERMOCK	Reed, J.E.; Bedinger, M.S.; and Terry, J.E.	?-D, Flow Only
SUTRA	Voss, C.I.	2-D, Cannot Handle Unsaturated
SWACROP	Wesseling, J.G.	1-D
SWATRE, SWATR-CROPR	Feddes, R.A.	Cropped Soil Water Balance
TARGET-2DU	Moreno, J.L.	2-D
TARGET-3DU	Moreno, J.L.	3-D, Proprietary, License
TDFD1O	Slotta, L.S.	2-D
TFISUD	Vauclin, M. and Khanji, J.	2-D
TOUGH	Pruess, K.	3-D, With Heat
TRACR3D	Travis, B.J.	3-D, Two-phase
TRANS	Walker, W.R.	2-D
TRIPM	Gureghian, A.B.	2-D
TRUST	Narasimhan, T.N.	Flow Only
TWO-PHASE UNSATURATED FLOW	Green, D.W.; Dabiri, H.; Wienaug, C.F.; and Prill, R.	1-D
UNFLW	Kapuler, I.	1-D

Table A-1 - A Comprehensive List of Unsaturated Codes (Continued)

Model Name	Author(s)	Remarks
UNSAT	Khaleel, R.	1-D
UNSAT-H	Fayer, M.J. and Gee, G.W.	1-D, For Hanford
UNSAT1	van Genuchten, M.Th.	1-D
UNSAT1D	Gupta, S.K. and Simmons, C.S.	Battelle PNL
UNSAT2	Neuman, S.P.	2-D
VADOFT	Huyakom, P.S.	1-D
VADOSE	In Situ, Inc.	3-D, Unsaturated, Flow Only
VADOSE	Sagar, B.	2-D
VAM2D	Huyakorn, P.S.	2-D
VAM3D	Huyakorn3, P.S.	3-D, Decay?
VIP	Stevens, D.K.	Oily Stuff
VLEACH	Turin,, J.	Volatiles
VS2D/VS2DT	Lappala, E.G.	2-D
VSAFT2	Yeh, T.C.J.	2-D
WATERFLO	Nofziger, D.L.	1-D, Richards Eqt.
2-D INFILTRATION MODEL	Brutsaert, W.F.	2-D
3-D SATURATED-UNSATURATED FLOW MODEL (SOFM)	Verge, M.J.	O.K.
3-D SATURATED-UNSATURATED TRANSPORT MODEL (3-D SUTM)	Segol, G. and Frind, E.O.	3-D

Table A-1 was first screened to eliminate codes that are not three-dimensional and codes that simulated only flow and/or heat transport. Initial screening remarks are shown in Table A-1. After the initial screening, a number of codes were identified that could simulate three-dimensional unsaturated flow and transport. These codes include:

1) 3-D SUFM, 3-D SUTM
2) 3DFEMWASTE, 3DFEMWATER
3) FLAMINCO
4) FRAC3DVS
5) GS3
6) HCTM
7) MMT-DPRW
8) MOTIF
9) MSTS
10) SBIR
11) TARGET-3DU
12) TRACR3D
13) VAM3D

Then these codes were entered into Table A-2, which lists the primary and secondary criteria in matrix form so we can compare the capabilities of the codes in one table and be able to select the codes that have met the primary criteria and most of the secondary criteria.

Based upon a review of Table A-2, MSTS is recommended as the auxiliary code. MSTS met all the primary and secondary criteria. In addition, pre- and post-processors are available and support is directly available through Battelle.

Table A-2 - 3-D Unsaturated Flow and Solute Transport Codes

CODE			PRIMARY CRITERIA					SECONDARY CRITERIA							
Name	Author	Organization/Year	Sat/ Unsat	Frac-ture	Frac-Matrix Diffus	Tran-sient Flow	Verified	Peer Review	Adsorp	Decay	Code Avail-ability	Number of Phases	Domain Discret-ization	Model Users	Notes
3-D SUFM	Segol	Univ. of Waterloo, Canada, 1975	Y	N	—	Y	Y	U	—	—	U	1	U	U	
3-D SUTM	Segol	Univ. of Waterloo, Canada, 1976	Y	N	—	Y	Y	U	Y	Y	U	1	U	U	
3DFEMWASTE	Yeh	ORNL, 1992	Y	N	—	Y	U	U	U	U	Y	1	FE	U*	Good support for 2-D version. Extensive verification.
3DFEMWATER	Yeh	ORNL, 1987	Y	N	—	Y	Y	Y	—	—	Y	1	FE	U*	No pre-processor or post-processor for 2-D or 3-D version.
FLAMINCO	Huyakorn	Geotrans, Inc., 1985	Y	N	—	Y	Y	Y	Y	Y	N	1	FE	F	Needs a license. No support. No pre-/post-processor. Extensive verification.
FRAC3DVS	Therrien	Univ. of Waterloo, Canada, 1992	Y	Y	Y	U	Y	N	U	U	Y	1	FE/FD	N/A	PhD thesis, just completed.
GS3	Davis	Water, Waste & Land, 1985	N	N	—	Y	Y	Y	N	N	Y	U	FE	F	No support available. Limited verification.
HCTM	—	INTERA Envir. Consult., Inc., 1975	Y	N	—	Y	U	U	Y	Y	U	U	U	U	
MMT-DPRW	Ahlstrom	Battelle, PNL, 1976	Y	N	—	Y	Y	Y	Y	Y	Y	Multi	FD	U	Not being used currently at Battelle.
MOTIF	Guvanasen	AECL, 1986	Y	Y	Y	U	Y	N	N	Y	N	1	FE	U	More suitable for fracture flow/heat transfer. Needs a license.
MSTS	White	Battelle, PNL, 1992	Y	Y	Y	Y	Y	Y	Y	Y	Y	2	FD	N/A	New code. Good support. Pre-processor and post-processor.
SBIR	Li	U.S. Bureau of Reclamation, 1987	N	N	—	U	Y	N	U	U	U	1	FD	U	Vector process for solution. Extensive verification.
TARGET-3DU	Moreno	Dames & Moore, 1985	N	N	—	Y	Y	N	Y	N	N	1	FD	U	Needs a license. Good support. Pre-/post-processor provided.
TRACR3D	Travis	LANL, 1984	U	Y	U	Y	Y	Y	Y	Y	Y	2	FD	U	Limited verification.
VAM3D	Huyakorn	Hydrogeologic, Inc., 1986	N	N	—	Y	Y	Y	Y	Y	N	1	FE	F	Needs a license. Limited support. Extensive verification.

*IGWMC lists many users for the 2-D version.

Key: Y = Yes, N = No, U = Unknown, FE = Finite Element, FD = Finite Difference, F = Few, N/A = Not Applicable

APPENDIX B

APPLICABLE PARSONS PROCEDURES

PARSONS
ERA PROJECT

ERA PROJECT PROCEDURES

Procedure No.:	ENG-006
Page:	1 of 17
Date of Issue:	Oct. 1991
Date of Revision:	Feb. 1993
Revision No.:	3
Approved By:	

Procedure Title: Preparation and Control of Calculations

REFERENCE COPY

OBJECTIVE

The purpose of this procedure is to provide instructions for preparing, reviewing, approving, controlling, revising, and retaining engineering calculations and to assure that those calculations are accurate and documented sufficiently to be understood and repeatable by others.

APPROVALS

This procedure is approved by the ERA Project Director.

REQUIREMENTS AND GENERAL INFORMATION

1. This procedure applies to engineering and scientific calculations prepared by PARSONS staff on all activities affecting quality performance on the ERA Project. Its scope includes calculations done manually and calculations performed using computers.

2. Engineering calculations furnish the basis for design, expressed in drawings, models, reports, or documentation for procurement (specifications and inspection or test requirements). Many calculations and experience-type choices can be made without supporting calculations. Data extracted from tables, graphs, standards, textbooks, or handbooks are not considered to be engineering calculations, etc. These items are considered to be support documentation for the calculations.

3. Calculations are performed in a planned, controlled, and documented manner. The calculation documents are legible and in a form suitable for production, filing, and retrieval. The contents are such that a technically qualified person can review and understand them without consulting the originator. The calculations are identifiable by number, title, subject, originator signature, and date. All manual calculations shall be performed on PARSONS Calculation Paper (see Exhibit 7).

4. Specific data and equations used in the calculations shall be identified, and references to applicable data sources, codes, standards, and assumptions shall be listed. All answers or conclusions shall be clearly marked. If the calculations are complex, subconclusions shall be summarized at the end of each of the subcalculations, with overall conclusions stated at the end.

5. All calculations directly pertaining to a design shall include a "Title and Summary Sheet" (see Exhibit 3). This lead sheet clearly identifies and describes the context of the following computation sheets. All calculations shall also include a "Calculations Basis Sheet" (see Exhibit 4).

6. Previously prepared calculations shall be reviewed for applicability prior to use on a new project. If applicable, a new "Title and Summary Sheet" shall be prepared with appropriate project numbers and approval sign-offs.

7. The Project Manager shall approve any decision to use support group services or outside consultants for performing calculations and must assure that data from these sources have been checked. Calculations or calculation results, supplied by specialist groups, consultants, suppliers, or other outside agencies, may be accepted by PARSONS if:
   a. The Lead Discipline Engineer (LDE) is satisfied that adequate checking has been performed, or
   b. The checker has reviewed the calculation or calculation results and considers them acceptable.

8. All calculations pertaining to design shall be logged on a "Design Calculations Index" (see Exhibit 5) which will be maintained by each discipline for each project order. Preliminary and scoping calculations do not need to be logged until their completion. At that time, all records are transferred to Document Control.

9. Revisions to completed calculations shall be identified as follows:
   a. Completed calculations shall have a numeric designator.
   b. Revision within a calculation sheet shall be clearly identified in the right margin or adjacent to the revised material. A triangle or vertical line with revision letter/number shall be used. The revision number or letter of the sheet shall be revised and that sheet shall contain the identity of the originator and checker of the revision and the date the sheet was revised. The revision shall be recorded on the calculation Title and Summary sheet.
   c. If a revised calculation sheet is to be substituted for an existing sheet, the revised sheet needs to have the next revision letter/number, the name of the originator, checker initials, and date. For a revision requiring additional sheets, new sheets must have the same revision number as the original calculation, plus an alphabetic indicator beginning with "a," for example, "Sheet 24a."

d. For revisions requiring that sheets or portions of sheets be voided, superseded, or deleted, a box shall be drawn around the voided portion of the sheet and marked with cross-hatched or x-marking. Erasing of original signed and checked calculations is not permitted.

e. The revision number and initials of originator and the checker are recorded on each revised sheet of the calculation.

10. Calculations generated from computer programs shall be identified by name of the computer program (and owner in the case where the program is proprietary) and provide an effective date and brief program description to permit the checker to ascertain its applicability.

11. The first page of calculations performed by computer shall be the "Computer Calculation Title and Summary Sheet" (see Exhibit 6).

12. Desktop-developed computer programs shall be verified prior to approval for use (see Engineering Procedure ENG-012, "Verification and Validation of Engineering/Scientific Computer Codes"). Spreadsheet calculations shall include an attached printout of formulas used in the spreadsheet.

13. Computer calculations generally shall be performed in accordance with the procedures governing hand calculations. Multiple-page computer runs only need signatures and dates on the cover sheets.

14. Computer calculations shall be documented as follows:

a. Computer input data and output files are identified and marked with a calculation number. Calculations based on computer output should be cross-referenced.

b. Computer printouts retained but not included in the calculation are cross-referenced to their corresponding calculations package and filed in the same manner as hand calculations.

c. Appropriate headings on the initial pages of the computer printouts shall be included when the standard programs used do not include header printout. All units of the numerical values shall be identified.

d. Computer calculations shall be culled to eliminate unnecessary paper.

e. Disks or tapes of final data and output files shall be saved as part of the project record.

15. Checking of manual and computer calculations may be performed by comparison with alternate calculation methods. The alternate method used for comparison may be a simplified

approach, using approximations to determine the reasonableness of the answer. When alternate calculations are performed, the checker shall address the validity and appropriateness of the assumptions, data, and method used in the original calculation.

16. Calculations which have been superseded or which are no longer relevant to the project shall be voided but shall remain in the calculation files.

17. The originals of calculations shall be maintained by the LDE while a project is active. When a project is completed, original calculations shall be transmitted to Document Control for retention. A reference set of the Preliminary and Final calculations may be kept by the LDE for general use.

18. A checklist is provided (see Exhibit 2) to remind calculation originators and checkers of steps that should be taken in preparing and checking calculations.

PROCEDURES

Person Responsible	Actions
Lead Discipline Engineer	1. Designate the individuals to perform and check the calculation. 2. Provide appropriate instructions for performing and checking calculations. 3. Determine the need for and type of design calculations, including whether manual or computer program computations are required. 4. Ensure that data produced by support groups or outside consultants are reviewed to ensure design consistency and result credibility. 5. Ensure that calculations are checked, signed, and approved before a. using the results for input or other calculations. b. issuing drawings for construction or issuing equipment specifications for purchase. c. issuing other documents for use outside the ERA Project.
Chief Discipline Engineer	6. Ensure that the Calculation Index (Exhibit 5) for the discipline is maintained.

Person Responsible		Actions
Lead Discipline Engineer	7.	Review preliminary calculations.
	8.	Approve preliminary calculations used to support a deliverable product (such as Scope of Work) prior to issue.
	9.	Review and approve design calculations within discipline.
Originator	10.	List applicable criteria, design assumptions, codes, design bases, standards, specifications, and other references used in the calculations. References include edition, issue date or revision, page numbers, and the source of equations not in common usage.
	11.	Fold and properly identify special sheets such as coordinate paper, logarithmic paper, or large sketches for filing with the calculation sheets.
	12.	Prepare a "Title and Summary Sheet" (Exhibit 3) according to its instructions for hand calculations. Prepare a "Computer Calculation Title and Summary Sheet" (Exhibit 6) for calculations performed by a computer.
	13.	Prepare an "Engineering Calculations Basis Sheet" (Exhibit 4) according to its instructions.
	14.	Number each sheet. Each page has a unique page number, such as "Page 1 of 13." If calculations are divided into logical subdivisions, each may have its own unique page numbering system.
	15.	Perform Calculations.
		CHECKING
Checker	16.	Review the application of the design and obtain access to information sufficient to perform the check.
	17.	Make copies of the original calculations and perform checking activities on the copies.
Checker and Originator	18.	Resolve any differences in results. The alternate calculations, if they are used, are documented and retained with the check prints. A revision is not required.
Lead Discipline Engineer	19.	Ensure that a thorough, final check of all calculations and the associated design is made as soon as practical after all input data are available.

REFERENCE COPY

Person Responsible	Actions
	20. Review calculation inputs to verify conformance with specific technical requirements of the project.
	21. Review validity of assumptions, appropriateness of analytical methods, attainment of required mathematical accuracy, compliance with design criteria, and adequacy of output data.
Lead Discipline Engineer	22. Initial and date all calculation sheets after all changes or corrections have been made. If applicable, attach an initialed alternate calculation.
	23. Confirm that computer programs used for calculations have been authorized for use on the project.
	24. Confirm that computer programs used are applicable to the problem.
	25. Determine the checking method and process. Acceptable methods of checking include the following: a. Detailed review of and concurrence with the original calculations b. Performing alternate calculations The checking process, as a minimum, shall consist of the following: a. Procedure implementation check b. Arithmetic check c. Determination of the applicability of the computer program (if used).
Checker	26. Sign and date the original calculations after checking and corrections have been incorporated into the original.
	27. Assess input data and assumptions when alternate calculations are performed. The alternate calculations are attached to the original calculations.
	28. Add initials and date in the CHECKED block of each page when the checking process is complete.
Lead Discipline Engineer	29. Ensure that calculations are in proper order and complete in all respects with all cover sheets completed and signed by the originator and checker. Place the proper file index number in the upper right corner of the cover page. Transmit the original calculations and check copy to Document Control for inclusion in the project records after the Project Order is closed.

REFERENCE COPY

Person Responsible		Actions
		REVISIONS
Lead Discipline Engineer	30.	Check, review, and approve revisions in the same manner as for the original calculations. Only those parts of the calculation which are affected by the revision need to be checked, although the entire original calculation should be reviewed to determine which parts are affected. Interfacing or reference documents affected by the revision shall be modified to ensure alignment. All revisions made after the calculations have been issued should be made on the original calculation sheets. The revision block shall be marked with the appropriate revision letter, dated, and signed by the originator and the checker.
Lead Discipline Engineer	31.	Ensure that a true copy of the original calculation is on file in Document Control prior to revising the calculation.
Document Control	32.	Retain a copy of each numeric revision provided by the LDE. At the conclusion of the project order, all records will be maintained by Document Control.

EXHIBITS

Exhibit 1 - Definitions
Exhibit 2 - Calculation Checklist
Exhibit 3 - Engineering Calculations Title and Summary Sheet (2 pages)
Exhibit 4 - Engineering Calculations Basis Sheet (2 pages)
Exhibit 5 - Design Calculation Index (2 pages)
Exhibit 6 - Computer Calculation Title and Summary Sheet
Exhibit 7 - Calculation Sheet

REFERENCES

ENG-012, "Verification and Validation of Engineering/Scientific Codes"

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Exhibit 1
Definitions

REFERENCE COPY

1. ALTERNATE CALCULATION: Calculation or analysis performed by a method other than the one originally used. The appropriateness of the assumptions, input data used, the computer program (if applicable), and the calculation method used for the original calculation are also reviewed.

2. CHECKER: The person who examines the calculations for correctness, completeness, and applicability. That person has the responsibility of informing the originator of errors, omissions, or defects found during the examination.

3. COMPUTER APPLICATION PROGRAMS: Those programs which are verified, documented, and controlled in accordance with the engineering procedure on computer usage for engineering calculations.

4. FINAL CALCULATIONS: Calculations which form the basis of drawings, specifications, or other design documents which are used to construct or operate the facility, or to provide the design basis for change to the facility. The entire procedure governs for final calculations (see variation for preliminary calculations - #6).

5. GENERAL REFERENCE or ASSUMPTION: A reference or assumption that is applicable to the entire problem.

6. PRELIMINARY CALCULATIONS: Calculations made to develop concepts or estimates and not intended for direct use in the final design document. They may be based on incompletely substantiated assumptions or preliminary data, or they may employ simplified analytical methods. Summary sheets are not required for preliminary calculations.

7. SPECIFIC REFERENCE or ASSUMPTION: A reference or assumption that applies to a specific calculation or a portion thereof and, as such, is identified in the calculations.

8. VERIFICATION OF COMPUTER PROGRAMS: The testing and documentation of a computer program to ensure that the established engineering assumptions agree, the program is numerically accurate, and the program logic is correct (see procedure ENG-012, Verification and Validation of Engineering/Scientific Computer Codes).

REFERENCE COPY

CALCULATION CHECKLIST

The following checklist is intended to serve as a reminder of the requirements for calculations and does not replace the detailed requirements in pages 1 to 8 of this procedure.

1. Is every space/box on the applicable title and summary sheet filled in? (Non-applicable items should be marked N/A.)

2. Are Codes and Standards listed? (If none are referenced, enter N/A.)

3. Is status of calculation identified?

4. Are revisions also shown at the bottom of the Title and Summary sheet with date and signatures, including Lead Discipline Engineer?

5. Is every page numbered?

6. Is every page signed and dated by the originator (except on computer runs)?

7. Is every page signed and dated by the checker (except on computer runs)?

8. Is revision number on every page (except on computer runs)?

9. Are attachments identified by name?

10. Are attachments paginated?

11. Are handwritten changes in the calculation initialed and dated?

12. Are revisions clearly identified by revision triangle or line?

13. Is the checking method identified?

14. Has the completed calculation been reviewed by the LDE and then signed to indicate final approval?

PARSONS
ERA PROJECT

ERA PROJECT PROCEDURES

Procedure No.:	ENG-006
Page:	10 of 17
Date of Issue:	Oct. 1991
Date of Revision:	Feb. 1993
Revision No.:	3
Approved By:	

Procedure Title: Preparation and Control of Calculations

Exhibit 3
Engineering Calculations Title and Summary Sheet
(Page 1 of 2)

REFERENCE COPY

PARSONS
ERA PROJECT

ENGINEERING CALCULATIONS TITLE AND SUMMARY SHEET

Date _____

Sheet 1 of _____

Proj. Order No._____ Calculation No._____

Project Title _____

Calculation Subject _____ Date Checked/Verified _____

STATUS: PRELIMINARY _____ FINAL _____ SUPERSEDED _____ VOID _____

STATEMENT OF PROBLEM	
SUMMARY OF CONCLUSIONS	**Originator's Signature and Date**
CHECKING METHOD	**Checker's Signature and Date**
1. Review ____ 2. Alternate Calculation ____	
	Lead Discipline Engineer's Signature and Date

Rev. No.	Sheet No.	Description	Reviser's Signature/Date	Checker's Signature/Date	Approved by Signature/Date

11/92 ENG080

REFERENCE COPY

INSTRUCTIONS FOR ENGINEERING CALCULATION TITLE AND SUMMARY SHEET

1. Project Order Number
2. Calculation Number: the unique identifier assigned to the calculation. For example, "41-01."
3. Project Title
4. Calculation Subject: the subject or objective of the calculation, including the identification of the affected discipline structure, system, component, or service.
5. Date verified
6. Status: a check mark to indicate the calculation status designation. Write the number of the superseding calculation on the cover sheet when checking "SUPERSEDED."
7. Statement of Problem: brief statement describing the function of the item and the objective in making the calculations, avoiding repetition where possible. This may also be used to list attachments when a Table of Contents is not used. Indicate method of analysis used and if computer program was used.
8. Summary of Conclusions: brief statement summarizing conclusions.
9. Identify checking method used.
10. Revision: sequential numbers, starting with "0" for the original are assigned to calculation revisions.
11. Description: the purpose of the revision and identification of the changes. For example, "Revised page 3."
12. Reviser's Signature: the initials of the originator(s) of the revision and the date initialed.
13. Checker's Signature: the initials of the checker(s)/verifier(s) of the revision and the date initialed.
14. Approved by Signature: the initials of the lead discipline engineer and the date initialed.
15. Sheet Numbering: the number of the last sheet in the calculation package.

PARSONS
ERA PROJECT

ERA PROJECT PROCEDURES

Procedure No.:	ENG-006
Page:	12 of 17
Date of Issue:	Oct. 1991
Date of Revision:	Feb. 1993
Revision No.:	3
Approved By:	

Procedure Title: Preparation and Control of Calculations

Exhibit 4
Engineering Calculations Basis Sheet
(Page 1 of 2)

REFERENCE COPY

PARSONS
ERA PROJECT

ENGINEERING CALCULATIONS BASIS SHEET

Revision No. _____
Sheet 2 of _____

Proj. Order No._____ Calculation No._____

Project Title _____

Calculation Subject _____ Date Checked/Verified _____

Performed By: _____ Checked/Verified By: _____

Date _____

SUMMARY OF INFORMATION SOURCES - CODES - ASSUMPTIONS

08/92 ENG098

INSTRUCTIONS FOR ENGINEERING CALCULATION BASIS SHEET

Summary of Data Sources - Codes - Assumptions

1. Complete title information (see Exhibit 4).

2. Information sources
   List all pertinent sources of information used in the calculations. Identify by date and revision number. Sources may include the following:
   a. Basic data
   b. Scopes of work
   c. Other calculations
   d. Text books
   e. Journals
   f. Drawings
   g. Test results
   h. Field surveys
   i. Reports

3. Codes and Standards
   List all pertinent codes and standards used in the calculations. Identify by date and revision number. Sources may include the following:
   a. Nationally recognized codes and standards
   b. FERMCO standards
   c. US EPA guidelines
   d. USNRC guidelines
   e. State Environmental Agency Guidelines
   f. FEMP guidelines
   g. DOE Orders
   h. Other

4. Assumptions
   List all significant assumptions.

Exhibit 5
Design Calculation Index
(Page 1 of 2)

REFERENCE COPY

PARSONS
ERA PROJECT

DESIGN CALCULATIONS INDEX

Discipline _____ Project Order No. _____

CRU Number: _____

CALCULATION NO.	SUBJECT	COMPUTER GENERATED (Y/N)	ORIGINATING AUTHOR	CHECKED BY	REV. NO./ DATE

APPROVED _____ DATE _____ APPROVED _____ DATE _____
Project Discipline Engineer Lead Discipline Engineer

12/92 ENG023

Exhibit 5
Design Calculation Index
(Page 2 of 2)

REFERENCE COPY

INSTRUCTIONS FOR DESIGN CALCULATION INDEX

1. Discipline (civil, structural, mechanical, etc.)

2. Project Order Number

3. CERCLA/RCRA Unit Number

4. Calculation number should be according to number of back of time sheets.

Examples:		
	Civil	15 (optional) - 01 (sequential)
		15-02
		15-03
	Piping	32-01
		32-02
	Electrical	40-01
		40-02

CRU Project Manager/Engineer shall attach prefix of project number and Document Control filing number per ERA Project Procedure PRO-010, "Preparing and Numbering Project Documents."

5. Approvals: Signature of LDE for project/discipline and Chief Discipline Engineer (if applicable)

6. Indicate current status of calculation (revision no./date should be the same as the Engineering Calculations Title and Summary Sheet).

7. Indicate software used, if any; otherwise, enter N/A.

8. Originating author's name and date of calculation (date should be the same as on the Engineering Calculations Title and Summary Sheet).

9. Checker's name and date checked (date should be the same as on the Engineering Calculations Title and Summary Sheet).

Exhibit 6
Computer Calculation Title and Summary Sheet

REFERENCE COPY

PARSONS
ERA PROJECT

COMPUTER CALCULATION SUMMARY SHEET

CRU: _____ PO: _____ Job Number: _____

Computer Code: _____ Version: _____

Code Verification Status: _____

Description of Program: _____

Source of Data: _____

Purpose/Description of Calculation: _____

Run Performed By: _____

Date/Time of Run: _____

Computer Time of Run: _____

Input Filename: _____

Output Filename: _____

Files Saved to Diskname: _____ Disk Location: _____

Results: _____

Performed By: _____ Date: _____

Checked By: _____ Date: _____

Approved By: _____ Date: _____

12/92 ENG095

Exhibit 7
Calculation Sheet

REFERENCE COPY

PARSONS
ERA PROJECT

CALCULATION SHEET

REV	BY	DATE	CK	DATE	TITLE			
								CRU
					AUTHOR	SHEET	OF	PO

REFERENCE COPY

OBJECTIVE

This procedure provides procedural instructions for verification and validation of engineering/scientific computer codes used on the PARSONS ERA Project.

APPROVALS

This procedure is approved by the PARSONS ERA Project Director.

REQUIREMENTS AND GENERAL INFORMATION

1. This procedure applies to engineering/scientific computer codes used at PARSONS in support of the ERA project. Verification is required for all codes except widely distributed general-application software packages such as LOTUS, DBASE, SURFER, Harvard Graphics, WordPerfect, etc. Validation is only required for codes to be used in support of critical decisions as determined by the responsible manager.
2. For a very complex code, it may be desirable to verify a portion of the code, so that it may be used before the entire code has been verified. In this case, the verification plan will have to specify which parts of the code will be approved for use on completion of the verification, and which parts of the code may not be used until another verification plan has been developed and executed.
3. If the code verification involves a comparison between computer runs and hand calculations, one staff member may do both if the results are reviewed by a reviewer.
4. If, after a code has been verified, the code is moved to another computer system, an example problem used in the verification procedure will be run on the new computer system. If the same results are obtained, then the code will be considered verified on the new computer system. Documentation of such procedure consists of a memorandum written by the staff member briefly describing the confirmation procedure and attaching the applicable output. If the same results are obtained, then the code is verified on the new computer system in accordance with the requirements described below.
5. The retention, filing, processing, and subsequent turnover of the QA records shall be in accordance with the ERA Project QA requirements.
6. Calculations used in conjunction with verification or validation shall be checked in accordance with the appropriate sections of ERA Procedure ENG-006, Preparation and Control of Calculations.

4776

REFERENCE COPY

7. This procedure only pertains to verification and validation of existing codes. It does not cover the development of in-house codes. However, codes developed in house will have to be verified and validated in accordance with this procedure.

PROCEDURES

I. VERIFICATION

Person Responsible	Actions
Responsible Manager	1. Determine that code verification is required and assign responsibility for code verification to a staff member.
Staff Member	2. Prepare a brief verification plan for the code to include the following (see Exhibit I): a. Identification of the computer code to be verified (name and code version number). b. Outline of the approach to be followed to verify the code. c. Definition of the documentation to be required in the verification report to assure the specified verification has been completed. d. Description of the mathematical models and numerical methods used in the code. e. User instructions. f. Benchmark problems. 3. Submit the verification plan to the responsible manager for review and approval.
Responsible Manager	4. Review the verification plan. 5. Approve the verification plan and assign a staff member to perform the verification when review comments have been resolved.
Staff Member	6. Perform the verification as required by the verification plan.

REFERENCE COPY

Person Responsible	Actions
Staff Member	7. Prepare a verification report. The report shall be written as specified in the verification plan, and at a minimum will consist of: a. Completion of the "Computer Code Verification Summary Sheet" for each trial run (see Exhibit 2). b. Written description of the verification results. c. If the verification was unsuccessful, describe how the code must be modified to correct the error(s) discovered. Modifications to the code must be documented. 8. Determine if the verification is successful, and then describe a. The conditions for which the code has been verified (run options and ranges of input, where appropriate). b. Any conditions for which the code remains unverified (code segments, run options, and ranges of input which have not been tested). c. For codes that have been previously verified by the code's author or owner, and for which documentation of such verification exists, the above requirements are waived. 9. Submit the report to the responsible manager for review and approval.
Responsible Manager	10. Review the submitted results report. 11. Approve the verification report after the comments are resolved. 12. Transfer the verification plan and the verification report to Document Control.
	II. VALIDATION
Responsible Manager	13. Determine the need for validation of a particular code application and assign responsibility for validation to a staff member.

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Person Responsible	Actions
Staff Member	14. Prepare a brief validation plan for the code. The plan will include the following: a. Identification of the computer code to be validated (name, code version, number). b. An outline of the approach to be followed to validate the code c. Definition of the documentation required in the validation report to assure that the specified validation has been completed. d. For a complex code, specify the code functions or parts to be validated. The validation plan will be designated as an interim or final plan if the complexity of the validation efforts warrants a multistage approach. 15. Submit the validation plan to the responsible manager for review and approval.
Responsible Manager	16. Review the validation plan. 17. Appoint a validation panel to perform a detailed review of the validation plan if warranted by the complexity of the validation efforts. The validation panel will include: a. The responsible manager, who will chair the panel b. The staff member who developed the plan c. Other individual(s) with relevant expertise who were independent of the code development effort. 18. Approve the validation plan and assign a staff member to perform the validation when review comments have been resolved. 19. Perform interim or final validation as required by the validation plan.
Staff Member	20. Prepare a validation report at the end of the validation effort. The report is written as specified in the validation plan, and at a minimum shall include the following: a. The computer code and model application(s) for which an attempt at validation was made (name and code version number).

REFERENCE COPY

Person Responsible	Actions
Staff Member	b. The validation method. c. Results and success of the validation. d. The conditions for which the code and model have been validated (run options and ranges of input, where appropriate). e. Any conditions for which the code and model have been validated (code segments, run options, and ranges of input which have not been tested). 21. Submit the report to the responsible manager for review and approval.
Responsible Manager/ Validation Panel	22. Exercise the appropriate level of review. After the comments have been resolved, approve the validation report. 23. Transmit the validation plan and the validation report to Document Control.
	III. RECORD KEEPING
Document Control	24. Maintain records of the following when complete: a. Verification or Validation Plan b. Verification or Validation Report c. Internal Review d. Associated calculations packages e. Memoranda with applicable attachments for previously verified codes or for relocating codes. These documents are considered QA records.

EXHIBITS

Exhibit 1 - Computer Code Verification Plan
Exhibit 2 - Computer Code Summary Sheet
Exhibit 3 - Definitions

REFERENCES

NUREG-0856, "Final Technical Position on Documentation of Computer Codes for High-Level Waste Management"
ENG-006, "Preparation and Control of Calculations"

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Exhibit 1
Computer Code Verification Plan

REFERENCE COPY

PARSONS
ERA PROJECT

Computer Code Verification Plan

Discipline: _____

Computer Code: _____ Version: _____

Outline of the Approach to Follow to Verify the Code: _____

Definition of the Documents Required for Verification: _____

Description of the Mathematical Models and numerical Methods Used in the Code:

User Instructions: _____

Benchmark Problems: _____

Performed By: _____ Date: _____

Approved By: _____ Date: _____

06/92 ENG079

REFERENCE COPY

PARSONS
ERA PROJECT

Computer Code Summary Sheet

Computer Code: _____ Version: _____

Code Developed By: _____

Purpose/Description of Verification Run: _____

Run Performed By: _____

Date/Time of Run: _____

Input Filename: _____

Output Filename: _____

Serial Number of Computer Used: _____

Files Saved to Diskname: _____

Results of Verification Run: _____

Performed By: _____ Date: _____

Checked By: _____ Date: _____

10/91 ENG091

REFERENCE COPY

Exhibit 3
Definitions

Benchmarking	Comparison of the results of a computer code calculation to the results of calculations of other computer codes developed to perform the same type of analysis. The particular problem for which this comparison is made is called a BENCHMARK PROBLEM.
Computer Code Validation	"Assurance that a model as embodied in a computer code is a correct representation of the process or system for which it is intended." (NUREG-0856). This is usually accomplished by comparing code results to (1) physical data, or (2) a validated code designed to perform the same type of analysis (benchmarking with a validated code). A peer review may be used for code validation if it is the only available means for validating a code.
Computer Code Verification	"Assurance that a computer code correctly performs the operations specified in a numerical mode" (NUREG-0856). This is usually accomplished by comparing code results to (1) a hand calculation, (2) an analytical solution or approximation, or (3) a verified code designed to perform the same type of analysis (benchmarking).
Engineering/Scientific Computer Code	A computer code based on scientific or engineering principles that produces technical results. System-supported software packages such as SAS and IMSL, and languages such as FORTRAN and BASIC are not engineering/scientific computer codes as used in this procedure. Computer codes which are used as management tools for financial calculations such as LOTUS 1-2-3 are also not considered engineering/scientific codes.
Responsible Manager	The manager who has the authority to approve a particular computer code for use.
Simple Code	A code which performs functions that can easily be verified by hand calculation. It may stand alone or be part of a larger system of codes, but it does not usually contain external subroutines. External subroutines are a series of program steps to perform a specific calculation or to assist in the program operation, which are called from a main program.
Version Number	The number of the form X.Y used to identify the version of the computer code. For minor modifications (e.g., those that do not change the structure or capabilities of the code), the Y digit is increased by one. For major modifications, the version number is increased to the next highest X.O. This number is an integral part of each code and any analyses using the code must reference the code version number.