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Deborah A. Bush

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3-D GEOSTATISTICAL LITHOFACIES MAPPING OF PLEISTOCENE FLOOD DEPOSITS IN A PORTION OF THE HANFORD NUCLEAR SITE, RICHLAND WASHINGTON

by

Deborah A. Bush

B.S. The University of Montana, Missoula 2003

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for the degree of

Master of Science

The University of Montana

May 2006

Approved by:

Chairperson

Dean, Graduate School

Date
The complexity of large-scale Pleistocene catastrophic flood deposits of the Hanford formation in the Pasco Basin (Washington State) presents challenges for constructing reliable flow and transport models for predicting contaminant migration. Previous hydrogeologic models of the Hanford formation in the 200 West Area of the Hanford Site relied on traditional sequence stratigraphy deduced from boreholes and outcrops to produce a 'layer cake' representation of hydrogeologic properties. Those models are limited in that heterogeneity and uncertainty within each layer is not adequately addressed.

Indicator geostatistics provides a tool for stochastic simulation of the heterogeneity of the sediments within each stratigraphic sequence and a quantification of the uncertainty in the distribution of lithofacies. This study classified the glacial flood deposits into five lithofacies: silty sand, fine sand, coarse sand, gravelly sand, and sandy gravel using data retrieved from the Hanford Borehole Geologic Information System. Borehole data from the study area provide data on the vertical heterogeneity of the subsurface sediments but only limited information on the lateral heterogeneity. Excavation sites near the study area provided a qualitative assessment of the lateral heterogeneity of the lithofacies.

Indicator variogram models were developed to characterize the spatial continuity of each lithofacies. Conditional indicator simulation techniques were applied to produce realizations of the distribution of lithofacies. Analysis of the realizations allowed for the quantitative assessment of uncertainty in the spatial distribution of the lithofacies. The realizations can be used as input for flow and transport modeling choosing the extreme lithofacies distributions and the modal distribution to capture the range of behavior in flow and transport predictions. Hydraulic conductivities were assigned to each lithofacies based on frequency distributions of measured hydraulic conductivity data from each lithofacies. The resulting 3-D geostatistical models of hydraulic conductivity provide an improved understanding of the heterogeneity of Hanford formation sediments and also provide geologically plausible constraints on flow and transport modeling of the study area.
ACKNOWLEDGMENTS

I would like to extend my gratitude to my family, my colleagues at the University of Montana, and the many people at Pacific Northwest National Laboratory who made this project possible. In particular, the members of my thesis committee and research mentor, Dr. Nancy Hinman, Dr. Marc Hendrix, Dr. David Patterson, Dr. Christopher Murray, and George Last. I would like to extend a special thanks to Pacific Northwest National Laboratory, U.S. Department of Energy, and Fluor Hanford for supporting my research.
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INTRODUCTION

The complexity of Pleistocene catastrophic flood deposits of the Hanford formation in the Pasco Basin of Washington state presents challenges for constructing reliable flow and transport models for predicting contaminant migration. Previous hydrogeologic models of the Hanford formation in the 200 West Area of the Hanford Site relied on traditional sequence stratigraphy inferred from boreholes and outcrops to produce a ‘layer cake’ representation of hydrogeologic properties. Those models are limited in that heterogeneity and uncertainty within each layer are not addressed. The use of geostatistical methods to construct a model provides a quantitative assessment of the uncertainty associated with the estimated values of properties.

Geologic Setting

The Hanford Site is located in south-central Washington (Fig. 1) within the Pasco Basin. The Pasco Basin is situated within the central Columbia River Plateau (Reidel, Campbell et al. 1994). The Pasco Basin is structurally bounded on three sides by anticlines of the Yakima Fold Belt. Neogene sediments of the Pasco Basin are confined mainly to the synclinal valleys. The sediments unconformably overlie Miocene basalts of the Columbia River Basalt Group. Figure 2 illustrates the general surface geology of the Pasco Basin.
Figure 1. Location map of the Hanford Nuclear Site in South-central Washington State
Figure 2. Geologic Map of the Pasco Basin (reprinted from Reidel et al. 1992).
History of the Hanford Site

In the early 1940's, the U.S. Army Corps of Engineers established the site as a nuclear reactor and chemical separation facility for the production of weapons-grade plutonium. The chemical methods used to process the plutonium resulted in aqueous waste containing radioactive and organic contaminants. Until 1973 the aqueous waste was discharged into shallow buried "cribs" (Fig. 3) that dispersed the waste directly into the sediments below (Price, Kasper et al. 1979). In 1989 the Tri-Party Agreement between the U.S. Department of Energy, U. S. Environmental Protection Agency, and the State of Washington Department of Ecology shifted the focus of the Hanford Site from plutonium production to environmental remediation and monitoring (www.hanford.gov/tpa).

Figure 3. Schematic the study area 216-Z-1A buried crib structure (from Rohay et al. 1994).
Purpose of Study

Over the last fifty years numerous borehole logs (driller's and geologist's logs), grain size analyses, geophysical surveys (e.g., seismic, ground penetrating radar, electromagnetic, resistivity and others), mineralogy and bulk rock geochemistry data were collected. The data were collected for specific project needs and qualitatively used to support subsurface geologic modeling. This study will more fully integrate all relevant geologic data from a small portion of the Hanford Site to produce a quantitative three-dimensional subsurface lithofacies model of the 216-Z-1A waste disposal site located in the 200 W Area (Fig. 4).

Figure 4. Location of 216-Z-1A study area in the 200 West operational unit within the Hanford Nuclear Site (reprinted from Price et al. 1979).
Previous geologic models for the area were based primarily on qualitative interpretations of the data in a "layer-cake" fashion with poor representation of the variability within the layers (Price, Kasper et al. 1979; Rohay, Last et al. 1992; Rohay 1993; Rohay 1994; Piepho and Inc. 1996). During groundwater flow modeling, such variability causes difficulty in predicting the flow and transport of contaminants to the environment. Herein, recently developed lithofacies mapping techniques are applied to produce a quantitative description of the subsurface geology. Geostatistical methods used for modeling in this study incorporate quantified, direct observations of sediments within each layer obtained from core and subsurface samples from the study site. The uncertainty for predicting contaminant fate and transport in the environment is believed to be decreased by incorporating the sediment variations.

Two hypotheses were tested in this study:

1. Although much of this area was deposited by Pleistocene cataclysmic floods, the facies distributions throughout the boreholes will contain non-random sequences. This hypothesis is tested using indicator geostatistical methods that have been widely applied to the analysis of sequences of stratigraphic data.

2. The second hypothesis is that the fine-grained stratigraphic units have greater horizontal continuity (i.e., they can be correlated over greater distances) than the coarse-grained units. This hypothesis is tested by examination of outcrops and the construction of cross sections using borehole data. Testing this hypothesis will provide information on the horizontal correlation lengths needed for the geostatistical simulations.
The project provides an important building block in the construction of a quantitative three-dimensional lithofacies model for the entire site. This building block provides a detailed methodology for quantitative geologic three-dimensional modeling for future flow and transport modeling of contaminants.

Approach

The overall conceptual geologic model for the Pasco Basin is assembled from previous studies of the regional geologic history and stratigraphy. Traditional geologic methods and geostatistics were used to build a site specific model from historical (e.g., previously collected) geological data.

GEOLOGIC BACKGROUND

Regional Structure

The structural complexity of the Columbia Plateau is attributed to post-Paleozoic tectonic development and evolution in the Pacific Northwest (Reidel, Campbell et al. 1994). Assemblages of exotic terranes accreted onto the North American craton during the Mesozoic and Cenozoic (Orr 1996). The accreted terranes form the geologic framework for the Cascade and the Blue Mountain ranges. The Columbia Plateau incorporates three main subprovinces; the Palouse, Yakima Fold Belt and the Blue Mountains (Fig. 5). The Palouse slope is the old continental margin and forms the eastern boundary of the basin (Swanson and Wright 1976). The Blue Mountains are a northeast trending anticlinorium that covers 250 km² from the Oregon Cascades to Idaho, and forms the southern boundary of the Columbia Plateau (Reidel, Fecht et al. 1989).
The Yakima Fold Belt extends eastward from the Cascade Range to the Palouse slope and southward to the Blue Mountains. The Yakima Fold Belt is a series of primarily east-west trending anticlines and synclines as a result of north-south compression (Reidel, Fecht et al. 1989).

Figure 5. Location of the Pasco Basin in relationship to the Palouse, Yakima Fold Belt, and Blue Mountains structural-tectonic subprovinces of the Columbia Basin, and location of the Olympic Wallowa Lineament and the extent of the Columbia River Basalt Group (from Reidel et al. 1994).
Columbia River Basalt Group

The stratigraphy of the Columbia Plateau records the depositional environment as well as the structural-tectonic events during the time of emplacement. Prior to the eruption of the Columbia River flood basalt the Yakima Fold Belt area was a subsiding basin filling with continental sediments derived from the ancient Cascade Range and the Palouse slope. The basin continued to fill with the eruption of the Columbia River Basalt Group (CRBG). The CRBG is a sequence of tholeiitic flood basalt flows erupted from north-northwest trending fissures in north-central and north-eastern Oregon, eastern Washington and western Idaho from 17-6 Ma (Swanson, Wright et al. 1979) (Fig. 6). The enormous volumes of basalt obliterated stream drainage systems that created ponds and lakes where water backed up. The topographic relief of the basin was sufficient for larger drainage systems inhibited by the basalt flows to re-establish new networks. The sedimentary interbeds of the Ellensburg Formation represent the obliteration and establishment of new drainage networks (Fecht, Reidel et al. 1987).
Figure 6. Illustration of the stratigraphy of the Pasco Basin from 17.5 Ma to Recent (from Lindsey 1995).
STRATIGRAPHY OF THE PASCO BASIN

The sediments of the Pasco Basin are located in the central Columbia Plateau, and overlie Miocene basalts of the Columbia River Basalt Group (Fig. 6). The Pasco Basin is structurally bounded on three sides by anticlines of the Yakima Fold Belt. The Saddle Mountains anticline form the northern boundary, the Hog Ranch-Naneum Ridge anticline creates the western boundary, Rattlesnake Mountain and Rattlesnake Hills anticlines on the south (Fig. 2). The Palouse slope forms the eastern boundary (Fig. 5). Sedimentation within the Pasco Basin is largely confined to synclinal valleys (Lindsey 1995). The Cold Creek syncline is located between Umtanum-Gable Mountain and Yakima Ridge anticlines (Fig. 2). The Cold Creek depression developed along the Cold Creek syncline as a deep structural low and greatly influences the sedimentation of the area (Reidel, Campbell et al. 1994).

Ringold Formation

The Ringold Formation disconformably overlies basalt dated at 8.5 to 10.5 Ma (Fig. 6) (Fecht, Reidel et al. 1987). The Ringold Formation is best described by sediment-facies associations and distributions (Lindsey and Gaylord 1990; Lindsey 1991; Lindsey 1991). The Ringold Formation is divided into five facies associations based on lithology and stratification; I) fluvial gravels, II) fluvial sands, III) overbank and paleosols, IV) lacustrine, and V) alluvial fans (Table 1) (Lindsey 1995).
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<td>Interbedded silt, silty sand, and fine- to medium-grained sand</td>
<td>Fsc, Fl, Sh, Sr, Sg</td>
<td>Laminated sand consisting of Sr, Sg, Fl, and Fsc commonly form tabular fining up beds &lt; 5 cm to 3 m thick that combine to form coarsening up intervals up to 10 m thick</td>
<td>Mixed deposition from suspension and minor sediment gravity flow in front of prograding delta</td>
<td></td>
</tr>
<tr>
<td>V</td>
<td>Matrix and lesser clast-supported basaltic gravel with high mud content</td>
<td>Gms, Gm, Gp</td>
<td>Stratification usually lacking or poorly defined; rare Gp</td>
<td>Sheet-like tabular sheets dominate</td>
<td>Debris flow, sheet flood, and minor fluvial deposition in proximal to distal fan environment</td>
</tr>
</tbody>
</table>
The alluvial and lacustrine sediments of the Ringold Formation record the structural evolution of the basin as changes in depositional style and as lateral distribution of facies. The depositional style of the basin from 10 to 6 Ma is one of a gravelly braided plain with localized alluvial fans and overbank deposits (Fig. 7A) (Reidel, Campbell et al. 1994). The depositional style of the basin changed between approximately 6 to 5 Ma to a sandy braided alluvial system (Fig. 7B). Lacustrine deposits dominated the depositional environment from 5 to 3.4 Ma (Fig. 7C). The lacustrine style deposits ended around 3.4 Ma with a regional incision of the Columbia River system draining the low-lying topography (Reidel, Campbell et al. 1994). The Ringold Formation is followed by a period of erosion or lack of sedimentation except for the localized Cold Creek unit (DOE 1988; DOE 2002).

Cold Creek Unit

The informal Cold Creek unit (CCU) is principally confined to the Cold Creek syncline and disconformably overlies the Ringold Formation (Fig. 8). The CCU records sediments deposited approximately 3 to 2 Ma constrained by the incision of the Ringold Formation around 3.4 Ma (Fecht, Reidel et al. 1987) and the beginning of the Pleistocene cataclysmic flood deposits approximately 2.5 to 1.5 Ma (Bjornstad, Fecht et al. 2001).
Figure 7. General stratigraphy during the three stages of Ringold Formation deposition in the Pasco Basin. Figure 7A represents a gravelly braided river plain and overbank depositional environment from approximately 10 to 6 Ma. Figure 7B signifies the deposition of a sandy braided river system from 6 to 5 Ma, and figure 7C illustrates the transition to a lacustrine depositional environment from 5 to 3.4 Ma (after Reidel et al. 1994).
Cold Creek Unit (CCU) Facies [depositional environment]

- [lam-msv] (overbank/eolian)
- [calc] (calcic paleosol)
- [ml] (mainstream alluvium)
- [rnd-bas] (sidestream alluvium)
- [ang-bas] (colluvium)
- CCU Eroded Away or Not Deposited

Upland Area

Paleochannel

Figure 8. Map of the facies distribution of the Cold Creek Unit in the Pasco Basin. Note the course to fine grained calcic paleosol is the principal facies present in the 200 West Area which provides a distinct marker bed for the study area (modified from DOE 2002).
The Cold Creek unit is divided into five facies differentiated by grain size, roundness, petrologic/mineralogic composition, sedimentary structure, and pedogenic alteration (Table 2) (DOE 2002).

- The **coarse-grained polylithic facies** of the CCU signify the period of downcutting and base level stabilization of the ancestral Columbia-Clearwater-Salmon River system.

- The **fine- to coarse-grained CaCO₃-cemented facies** is interpreted as a highly weathered paleosurface.

- The **coarse-grained, rounded, basaltic facies** is identified by the occurrence of greater than 50% basalt clasts. This facies is interpreted as locally derived side stream alluvium (Slate 1996; Slate 2000).

- The **coarse-grained, angular, basaltic facies** is interpreted as colluvium and slope-wash deposits based on the lack of stratification and the angularity of the clasts (DOE 2002).

- The **fine-grained laminated to massive facies** is interpreted as weakly developed paleosols and overbank deposits.

The Cold Creek fine-grained facies is differentiated from the fine grained facies in the Hanford formation by the moderate to high CaCO₃ content and comparatively high natural gamma activity.
Table 2. Cold Creek Unit facies distributions as determined from grain size, roundness, petrologic/mineralogic composition, sedimentary structure, and pedogenic alteration (modified from DOE 2002).

<table>
<thead>
<tr>
<th>Facies or Facies Association (abbreviation)</th>
<th>Principal Lithology (Folk Classification)</th>
<th>Subordinate Lithology (Folk Classification)</th>
<th>Depositional Process</th>
<th>Typical Sequence Thickness</th>
<th>Matrix color</th>
<th>Structure</th>
<th>CaCO$_3$ (wt%)</th>
<th>Natural-Gamma Response</th>
<th>Other Characteristics</th>
</tr>
</thead>
<tbody>
<tr>
<td>Laminated to Massive Fine-Grained (f(lam-msv))</td>
<td>Fine sand, silt, and/or clay (S, mS, sM, M)</td>
<td>Thin, weakly developed paleosols</td>
<td>Fluvial and/or Eolian</td>
<td>0-15 meters</td>
<td>Buff, pale to dark brown</td>
<td>Laminated and bedded to massive</td>
<td>5-20</td>
<td>Consistently high</td>
<td>Micaceous; weakly to moderately calcareous</td>
</tr>
<tr>
<td>Carbonate-Cemented Coarse- to Fine-Grained c-f(calc)</td>
<td>Calcium-carbonate cemented clay, silt, sand, and/or gravel (msG, smG, gmS, mgS, mS, gsM, sgM, gM, sM, M)</td>
<td>Intercalated beds of noncalcareous silt, sand, and gravel (msG, smG, gmS, mgS, mS, gsM, sgM, gM, sM, M)</td>
<td>Calcic Paleosol Sequence</td>
<td>0-15 meters</td>
<td>White to light gray</td>
<td>Massive to platy, bioturbated, rhizoliths</td>
<td>6-67 (Slate 2000)</td>
<td>Erratically low to moderate</td>
<td>Highly variable and laterally heterogeneous</td>
</tr>
<tr>
<td>Multilithic Coarse-Grained C(ml)</td>
<td>Sandy gravel (sG) to silty sandy gravel (msG)</td>
<td>Light gray to white, well sorted, medium to coarse grained sand (S) to pebbly sand (gS)</td>
<td>Mainstream Fluvial</td>
<td>Few meters to tens of meters</td>
<td>Light gray to olive gray, &quot;whitish&quot; or &quot;bleached&quot; clast coatings</td>
<td>Unknown since unit is has only been described from drill cuttings</td>
<td>0-5</td>
<td>Consistently low to moderate</td>
<td>Multilithic gravels; unaltered to slightly altered, locally carbonate cemented</td>
</tr>
<tr>
<td>Angular Basaltic Coarse-Grained C(ani-bas)</td>
<td>Gravel with sand and silt (G, sG, msG, smG, gS, mgS, gmS)</td>
<td>Calcic soils</td>
<td>Colluvial</td>
<td>0-10 meters</td>
<td>Dark gray to black</td>
<td>Massive to steep inclined bedding</td>
<td>0-30</td>
<td>Consistently low</td>
<td>Highly basaltic</td>
</tr>
<tr>
<td>Rounded Basaltic Coarse-Grained C(md-bas)</td>
<td>Gravel with sand and silt (sG, msG, smG, gS, mgS, gmS)</td>
<td>Calcic soils</td>
<td>Sidestream Fluvial</td>
<td>0-20 meters</td>
<td>Dark gray to black</td>
<td>Massive to bedded and laminated</td>
<td>0-30</td>
<td>Consistently low</td>
<td>Highly basaltic</td>
</tr>
<tr>
<td>Laminated to Massive Fine-Grained F(lam-msv)</td>
<td>Fine sand, silt, and/or clay (S, mS, sM, M)</td>
<td>Thin, weakly developed paleosols</td>
<td>Fluvial and/or Eolian</td>
<td>0-15 meters</td>
<td>Buff, pale to dark brown</td>
<td>Laminated and bedded to massive</td>
<td>5-20</td>
<td>Consistently high</td>
<td>Micaceous; weakly to moderately calcareous</td>
</tr>
</tbody>
</table>
Hanford formation

Myers and Price (1979) informally named the flood deposits in the Pasco Basin as the ‘Hanford formation’. The Hanford unit was determined by Bjornstad et al., (2002) that the unit does not fit the International Stratigraphic Guide for a formalized stratigraphic unit (Bjornstad, Last et al. 2002). Herein the informal Hanford “formation” is referred to as the Hanford unit. The Hanford unit records the cataclysmic Pleistocene “Ice Age” floods generated by the rupture of ice-dammed glacial lakes (Baker and Bunker 1985) (Fig. 9). The failure of the ice dams associated with the Cordilleran Ice Sheet resulted in large volumes (estimated discharge $2 \times 10^3$ km$^3$, Baker 1973) of water gushing over the landscape. Shaw et al., (1991) suggested an alternative hypothesis that the Scabland Floods were produced by large scale outbursts of subglacial water from beneath the Cordilleran Ice Sheet (estimated discharge $10^5$ km$^3$, Shaw 1999) (Shaw 1999). The enormous discharge and velocity of the water carved deep coulees and channels into the Palouse Formation (e.g., loess) and underlying basalt bedrock. The scarred landscape left behind is the ‘Channeled Scabland’ of eastern Washington (Baker and Nummedal 1978) (Fig. 9). The flood-waters converged in the Pasco Basin where they formed the short-lived Lake Lewis (Allison 1933) that was caused by the hydraulic constriction at Wallula Gap. The flow transported large volumes of sediment ranging from house-size boulders to clay particles (O’Conner and Baker 1992).

The first Ice Age floods are thought to have occurred in the early Pleistocene from 1.5 to 2.5 Ma. (Bjornstad, Fecht et al. 2001). Episodes of early (>780 ka) to middle (>130 ka) Pleistocene cataclysmic flood deposits were identified based on paleomagnetic evidence and radiometric age dating (Baker, Bjornstad et al. 1991; Bjornstad, Fecht et al.
The glacial Lake Missoula floods occurred during the period from at least 19.2 ka to perhaps 16 ka from OSL geochronology on clay laminae (Levish 1997). The number and frequency of floods during this time is still under debate (Waitt 1980; Baker and Bunker 1985; Atwater 1986; Waitt 1994).

In general, the glacial Lake Missoula floods in the Pasco Basin are interpreted to have produced a series of sedimentary packages characterized by erosion followed by deposition (Baker, Bjornstad et al. 1991). The initial phase was one of erosion where a
torrent of flood water stripped away older flood and Ringold deposits. The secondary phase was one of deposition. The massive amounts of sediment transported by the flood water created huge sub-fluvial depositional features. The flood waters were constricted through Sentinel Gap and expanded though the Priest Rapids area around Umtanum Ridge and into Cold Creek valley, creating giant expansion bars (Fig. 10). The Priest Rapids and Cold Creek expansion bars are the result of the rapid decrease in flow velocity from Sentinel Gap into the Pasco Basin. The characteristics of an expansion bar are similar to a prograding delta (Maizels 1997). The turbulent flows producing the expansion bars deposited a mix of boulders, gravel, and sand. The expansion bars consist of large-scale gravel-cobble foreset-beds associated with the downstream accretion of the bar front. Horizontally laminated gravel-cobble beds as well as giant current ripples are also common in expansion bars (Maizels 1997).

The formation of Lake Lewis caused poorly-sorted gravels to rapidly aggrade in the flood channels. Plain-laminated sand was deposited away from the flood channels that blanketed the central basin. Interbedded sand and silt were deposited in back-flooded valleys and along the margins of the basin (Baker, Bjornstad et al. 1991) (Fig. 11). The lake is thought to have existed for only a few days or weeks (O'Conner and Baker 1992). The final phase is the waning Lake Lewis phase (Baker, Bjornstad et al. 1991). The flood waters formed a network of anastomosing channels through the basin as Lake Lewis began to drain. Re-worked flood gravels were deposited in narrow gravel trains from Sentinel Gap to Wallula Gap as the final flood waters drained (Baker, Bjornstad et al. 1991).
The Hanford formation consists of three facies associations: gravel-dominated, sand-dominated, and interbedded sand and silt-dominated (DOE 2002). Each facies association has been further sub-divided based on textural and structural features. Table 3 describes each of the eleven Hanford formation lithofacies. “The Hanford unit includes minor fluvial, colluvial, and/or eolian deposits interbedded with the flood deposits” (DOE, 2002). The eleven Hanford formation lithofacies designations include these deposits (Table 3). The sediments of the Hanford formation are primarily unconsolidated and don’t generally crop out well. Fortunately a large number of boreholes pierce the Hanford unit throughout the Hanford study site, providing information on the grain size and composition of the sediments at specific elevations. The drilling operation usually does not preserve the sedimentary structures needed to classify the sediments into one of the eleven lithofacies classifications. Therefore this study used the nineteen sediment classifications for unconsolidated sediments modified from Folk (1968) to classify sediments in a borehole environment where sedimentary structures are not recognizable (Fig. 12)(Folk 1968). The classification scheme provides a measure of grain size as well as the general proportion of each grain size in the sample. The classification scheme can be broadly related to the eleven outcrop lithofacies scheme. It was proven difficult to apply to this study due to the similar characteristics of grain size classifications for distinguishing lithofacies. This study focuses on the Folk classification scheme because it does not introduce relationships to the sedimentary architecture of the deposit that cannot be observed in boreholes.
Figure 10. Map showing Cold Creek and Priest Rapids expansion bars, general paleoflow direction of the cataclysmic floods through the Pasco Basin, and deposit types (modified from DOE 2002).
Hanford Formation

- Gravel-Dominated Flood Deposits
- Sand-Dominated Flood Deposits
- Interbedded Sand- and Silt-Dominated Flood Deposits
- Above flood level (>380 m elev.)

Figure 11. Hanford formation facies distribution and thickness map, and general paleoflow directions of flood waters in the Pasco Basin (modified from DOE 2002).
Table 3. Eleven Hanford formation lithofacies designations as interpret from sedimentary structures and other attributes (modified from DOE 2002).

<table>
<thead>
<tr>
<th>Litho­facies Code</th>
<th>Grain Size</th>
<th>Sorting</th>
<th>Color</th>
<th>Primary Sedimentary Structure</th>
<th>Mineralogy</th>
<th>Depositional Environment</th>
<th>Rate of Deposition</th>
<th>Common Facies Transitions</th>
</tr>
</thead>
<tbody>
<tr>
<td>Fm</td>
<td>Silt and fine sand</td>
<td>Poor to moderate</td>
<td>Pale brown to light gray</td>
<td>None</td>
<td>Quartzo-feldspathic</td>
<td>Bioturbated slackwater flood deposits and/or inter-flood eolian, fluvial, or slopewash deposits</td>
<td>Slow</td>
<td>FI</td>
</tr>
<tr>
<td>Fl</td>
<td>Silt and fine sand</td>
<td>Moderate to well</td>
<td>Pale brown to light gray</td>
<td>Wavy to horizontal laminations</td>
<td>Quartzo-feldspathic</td>
<td>Slackwater flood sedimentation into hydraulically ponded, relatively still water</td>
<td>Slow to moderate</td>
<td>Sr</td>
</tr>
<tr>
<td>Sm</td>
<td>Silty sand</td>
<td>Poor to moderate</td>
<td>Pale brown to light gray</td>
<td>Massive</td>
<td>Quartzo-feldspathic</td>
<td>Bioturbated flood deposits and/or interflood eolian, fluvial, or slopewash deposits</td>
<td>Slow to moderate</td>
<td>Sr, Fl, Fm</td>
</tr>
<tr>
<td>Sr</td>
<td>Silty very fine sand to fine sand</td>
<td>Moderate to well</td>
<td>Pale brown</td>
<td>Ripple cross-lamination to climbing and wavy ripple laminations</td>
<td>Quartzo-feldspathic, micaceous</td>
<td>Mixture of traction and suspension load under low to moderate flow regime in slackwater environment or waning flood stage</td>
<td>Moderate</td>
<td>Sh, St</td>
</tr>
<tr>
<td>Sh(f)</td>
<td>Silty fine to medium sand</td>
<td>Moderate to well</td>
<td>Pale brown</td>
<td>Planar to low-angle cross stratification</td>
<td>Quartzo-feldspathic</td>
<td>Superconcentrated plane-bed deposition atop washed-out, subaqueous dunes away from or above elevation of main flood channels</td>
<td>Rapid</td>
<td>Sh(c), Sr</td>
</tr>
<tr>
<td>Sh(c)</td>
<td>Medium to coarse sand to granule-pebbly sand</td>
<td>Moderate to well</td>
<td>Gray</td>
<td>Planar to low-angle cross stratification</td>
<td>Mixture of quartzo-feldspathic and basaltic sand lithic fragments</td>
<td>Superconcentrated plane-bed deposition atop washed-out, subaqueous dunes away from or above elevation of main flood channels</td>
<td>Rapid</td>
<td>Gm, Gh, Gp, Sh(c)</td>
</tr>
<tr>
<td>Sp</td>
<td>Medium to coarse sand to pebbly sand</td>
<td>Moderate to well</td>
<td>Gray</td>
<td>Planar-tabular cross stratification</td>
<td>Mixture of quartzo-feldspathic and basaltic sand lithic fragments</td>
<td>Planar-tabular cross-bedded sand deposition associated with straight-crested dune migration</td>
<td>Rapid</td>
<td>Gm, Gh, Gp, St</td>
</tr>
<tr>
<td>St</td>
<td>Medium to coarse sand to pebbly sand</td>
<td>Moderate to well</td>
<td>Gray</td>
<td>Trough to tabular cross stratification</td>
<td>Mixture of quartzo-feldspathic and basaltic sand lithic fragments</td>
<td>Trough cross-bedded sand deposition associated with sinuous-crested dune migration</td>
<td>Rapid</td>
<td>Gm, Gh, Gp, Sp</td>
</tr>
<tr>
<td>Lithofacies Code</td>
<td>Grain Size</td>
<td>Sorting</td>
<td>Color</td>
<td>Primary Sedimentary Structure</td>
<td>Mineralogy</td>
<td>Depositional Environment</td>
<td>Rate of Deposition</td>
<td>Common Facies Transitions</td>
</tr>
<tr>
<td>------------------</td>
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<td>--------------------------------</td>
<td>----------------------------------------------------------------------------</td>
<td>------------------------------------------------------------------------------------------</td>
<td>--------------------</td>
<td>--------------------------</td>
</tr>
<tr>
<td>Gm</td>
<td>Silty sandy pebble to boulder gravel</td>
<td>Poor to moderate</td>
<td>Dark gray to dark brown to black</td>
<td>Massive; no contrasts in grain size/sorting</td>
<td>Sand fraction mostly a mixture of quartz, feldspar and basalt; gravel fraction mostly basalt lithic fragments detrital caliche clasts</td>
<td>Disorganized flood flow and rapid deposition within or near axis of flood channel</td>
<td>Very Rapid</td>
<td>Gh, Gp</td>
</tr>
<tr>
<td>Gh</td>
<td>Silty sandy pebble to boulder gravel</td>
<td>Poor to moderate</td>
<td>Dark gray to dark brown to black</td>
<td>Grain size/sorting variations produce horizontal to subhorizontal bedding</td>
<td>Sand fraction mostly a mixture of quartz, feldspar and basalt; gravel fraction mostly basalt lithic fragments detrital caliche clasts</td>
<td>Plane-bed deposition atop washed out subaqueous dunes within or near axis of flood channel</td>
<td>Very Rapid</td>
<td>Gm, Gp</td>
</tr>
<tr>
<td>Gp</td>
<td>Silty sandy pebble to boulder gravel</td>
<td>Poor to moderate</td>
<td>Dark gray to dark brown to black</td>
<td>Planar-tabular, large-scale foreset beds of contrasting grain size/sorting show dip of beds up to 30 degrees</td>
<td>Sand fraction mostly a mixture of quartz, feldspar and basalt; gravel fraction mostly basalt lithic fragments detrital caliche clasts</td>
<td>Planar-tabular, large-scale foreset beds deposited on lee sides of migrating giant current ripples within or near axis of flood channel</td>
<td>Very Rapid</td>
<td>Gm, Gh</td>
</tr>
</tbody>
</table>
GEOLOGY OF LOCAL STUDY AREA

Location

The 216-Z-1A study area is located in the south-central portion of the 200 West Area of the Hanford Site in the Pasco Basin (Fig. 4). The 200 West Area is located within the Cold Creek expansion bar (Fig. 10).
History

The 216-Z-1A crib was constructed in 1949 to receive the overflow of aqueous waste from adjacent cribs from the Z-plant analytical and developmental laboratory. The crib received overflow from 1949 to 1959. The use of all four of the crib structures including 216-Z-1A ceased after this ten-year period. In 1964 aqueous waste was routed directly to the 216-Z-1A crib. The crib received aqueous and organic waste from the re-processing of plutonium. In 1969 the use of the 216-Z1A crib was permanently discontinued. Table 4 describes the type of waste the crib received during its time of service. Several studies over the years have been conducted to try to determine the nature and extent of contamination under the crib.

Table 4. Possible constituents discharged into the 216-Z-1A crib from 1949-1959, and 1964-1969.

<table>
<thead>
<tr>
<th>Radionuclide</th>
<th>Inorganic Constituents</th>
<th>Organic Constituents</th>
</tr>
</thead>
<tbody>
<tr>
<td>Pu</td>
<td>HNO₃</td>
<td>CCl₄ - Carbon tetrachloride</td>
</tr>
<tr>
<td>U</td>
<td>Al(NO₃)₃</td>
<td>TBP - Tributylphosphate</td>
</tr>
<tr>
<td>²⁴¹Am</td>
<td>AlF(NO₃)₂</td>
<td>DBBP – Dibutylbutylphosphonate</td>
</tr>
<tr>
<td>⁹⁰Sr</td>
<td>Mg(NO₃)₂</td>
<td>TCE - Trichloroethane</td>
</tr>
<tr>
<td>¹⁰⁶Ru</td>
<td>Ca(NO₃)₂</td>
<td>PCE – Perchloroethene</td>
</tr>
<tr>
<td>¹³⁷Cs</td>
<td>NaNO₃</td>
<td>DCM - Methylene Chloride</td>
</tr>
<tr>
<td>⁶⁰Co</td>
<td></td>
<td>MEK - Methyl Ethyl Ketone</td>
</tr>
<tr>
<td></td>
<td></td>
<td>Triolene – lard oil</td>
</tr>
</tbody>
</table>

Previous Investigations

There have been numerous investigations around the 216-Z-1A waste site. The investigations were focused on determining the location and type of contaminants present (Price, Kasper et al. 1979; Rohay, Last et al. 1992; Rohay 1993; Rohay 1994; Piepho and Inc. 1996; Rohay and McMahon 1996; Swanson, Rohay et al. 1999). The investigations
characterized the subsurface geology by applying layered stratigraphy determined from borehole logs and outcrop studies.

Price et al. (1979) completed a study to characterize the distribution of plutonium and americium in the sediments below the 216-Z-1A crib. Seventeen boreholes were drilled to determine the geological character of the sediments and the distribution of actinides. Sediment samples obtained during the drilling operations were analyzed for plutonium and americium content. Selected sediment samples were quantitatively analyzed using granulometric techniques. The data were used to construct geologic cross sections and isopleth maps of the distribution of plutonium and americium in the subsurface. Several detailed cross sections were completed for the study area. The cross sections provide a stratigraphically layered characterization of the sediments. Price et al. (1979) provided an invaluable overview of the history of the waste site and contaminants received as well as a well-constructed geologic characterization of the sediments.

Additional investigations around the 216-Z-1A crib include investigations conducted for the 200 West Carbon Tetrachloride Expedited Response Action (ERA) and the Volatile Organic Compounds – Arid Integrated Demonstration (VOC-Arid ID). The focus of these investigations was to determine the nature and extent of carbon tetrachloride contamination and implement remediation strategies. Rohay et al. (1992, 1993, and 1994) conducted site characterizations of the area contaminated with carbon tetrachloride. Two additional boreholes were drilled in the 216-Z1-A area during this time period. Piepho (1996) constructed a numerical flow and transport model for an area near the 216-Z-1A crib using the data acquired from the characterization efforts. The
model was based on hydrogeologic properties derived from a geologic ‘layer cake’
representation of the subsurface. Characterization and remediation efforts in this area
are on-going and lead to the present study which aims to provide an improved geologic
model for the implementation of flow and transport modeling.

NUMERICAL-CONCEPTUAL MODELS FOR FLOW AND TRANSPORT

Traditional Approaches

Traditional mapping techniques used for flow and transport modeling create
smooth “layer cake” maps that represent the stratigraphy of the study area. Traditional
numerical models are created from a conceptual model of the study area. The conceptual
model organizes field observations and data to provide an illustrative representation of
the study area. The purpose of a conceptual model is to simplify natural systems
observed in the field so they can be used as input boundary conditions for subsequent
numerical modeling. Several common data sources for building the model include
geologic maps, cross sections, geophysical data, well tests, and hydraulic conductivity
measurements. Traditional modeling techniques disregard the small-scale variability
often present within each layer of the model. However, the small-scale variability within
a layer may be essential to modeling flow and transport and for assessing the uncertainty
present in the system caused by geologic heterogeneity. The inherent uncertainty in
modeling natural systems is inadequately addressed with traditional modeling techniques
that ignore the internal heterogeneity and treat each layer as a homogeneous unit.
Geostatistical Approaches

Introduction

Geostatistical methods were developed to address the need to produce consistent and reproducible modeling methods that capture the spatial dependence of the data; can incorporate large amounts of data at different scales and precision; and can express the variability (uncertainty) within the modeled system (Deutsch 2002). The underlying concept in geostatistics is based on the random function model. The random function model considers the unknown value or random variable RV(Z) as spatially dependent. A random variable (Z) may have any number of probable outcomes as defined by a probability distribution. The random function concept models the probability that an attribute (e.g., random variable) takes a particular value at a certain location, denoted Z(u), where u is a vector location. Although the values of geologic variables in the subsurface (e.g., lithology or porosity) are already fully determined, there are never sufficient data to know what the true values are throughout the subsurface. There are only samples from a limited number of locations to estimate the value of a geologic attribute at all locations in the subsurface. Therefore, although the subsurface geologic attributes are already fixed and determined, the uncertainty of the attribute at a given location is modeled as a set of possible outcomes or realizations of a random variable. Isaaks and Srivastava (1989), provide a detailed discussion of the random variable and random function concepts and probabilistic models. Geologic properties can be modeled as continuous or categorical variables. Examples of continuous variables modeled using geostatistical methods are porosity, permeability, and concentration where the possible outcome of the random variable is a continuous value from zero to a given maximum.
Stratigraphic units or facies can be modeled as categorical variables, for example, siltstone, sandstone and limestone are defined as categories.

One major difference between geostatistics and traditional statistics is that traditional statistics assumes that the measurements of a variable at different spatial locations are independent of one another. However, this is often untrue for geologic variables that result from geologic processes that have some spatial organization (e.g., the deposition of clastic sediment by fluvial processes and the tendency for channel and floodplain facies to be separable in terms of their lithofacies and distribution). The action of continuous geologic processes implies that points closer to one another are usually more similar to one another than pairs of points that are further away from one another. The application of geostatistical methods to geological processes recognizes and quantifies the spatial continuity between pairs of points as a function of the distance between the sample pairs. The calculation of an experimental semi-variogram provides a measurement of the spatial continuity between data points according to:

$$\gamma(h) = \frac{1}{2} E(Z(u) - Z(u + h))^2$$

where $\gamma(h)$ is one half the expected squared difference between samples separated by the vector $(h)$ (i.e., lag distance) (Isaaks and Srivastava 1989). The experimental semi-variogram is modeled to provide a mathematical representation of the spatial continuity between any two points. The range identifies the distance over which the data have some degree of spatial correlation. Points are uncorrelated if they are separated by distances larger than the range (Fig. 13). The sill represents a constant value beyond the range that is usually equal to the total variance of the random variable. The nugget can be used to model short range variability at the origin present that represent independent error,
measurements error, or spatial variations at distances less than the sampling interval (Murray 1993; Deutsch 2002) (Fig. 13). Examples of mathematical models used for modeling experimental semi-variograms are spherical, exponential, and Gaussian. Isaaks and Srivastava, (1989) provide a detailed description for each of these models. The semi-variogram models are essential for estimation techniques such as Kriging and geostatistical simulation because those estimation techniques require calculation of the semi-variance for any separation vector distance within the model domain, including vector distances for which few, if any, pairs of data points exist.

Figure 13. General calculated experimental semi-variogram and model explanation. The experimental semi-variogram provides a measurement of the average squared difference between two pairs of data values separated by a specified lag distance. The semi-variogram model enables estimation of values at locations where data is not present. The range identifies the distance over which the data have some degree of spatial correlation. Points are uncorrelated if they are separated by distances greater than the range. The sill represents a constant value beyond the range that is to the total variance. The nugget can be used to model short range variability at the origin (reprinted from Murray 1992).
The semi-variogram model provides the basis for estimation or simulation of values at locations where the value is unknown. Normally, this estimation or simulation is performed on a regular grid (Deutsch 2002). A grid is designed for the type of model desired (e.g., 1-D, 2-D, or 3-D). For example, a 3-D model requires the X, Y, and Z grid spacing to be defined. Grid spacing is typically determined by the geometry of the study area and the location of the sample data, and by the requirements of any subsequent modeling processes (e.g., a flow and transport model) that will use the geostatistical grid as input.

The estimation method known as Kriging is a collection of generalized linear regression techniques used for interpolation that are based on minimizing an estimation variance defined from a prior model for a semi-variance. Kriging methods are valuable interpolation methods because they minimize the difference between the true value and the estimator as well as minimize the variance of the estimation error (Deutsch 2002). At each unsampled point where an estimate is needed, a value is estimated by a weighted linear combination of nearby data according to the following equation:

\[ Z^*(u) = \sum_{\alpha=1}^{n} \lambda_{\alpha} \cdot Z(u_{\alpha}) \]

where \( Z^*(u) \) is the estimate at location \( u \), and \( \lambda_{\alpha} \) are the weights applied to the available data points \( (Z(u_{\alpha})) \). The weights are calculated from the simple Kriging system (SK):

\[ \sum_{\alpha=1}^{n} \lambda_{\alpha} C(u_{\alpha} - u_{\beta}) = C(u - u_{\alpha}), u_{\alpha} = 1, \ldots, n \]
where $C$ is the covariance function of a separation vector $(u-u_a)=h$. The covariance function is linked to the semi-variogram model described previously by the relation: $C(h) = C(0) - \gamma(h)$. The variance of the estimation error is calculated by:

$$\sigma^2_{sk}(u) = C(0) - \sum_{a=1}^{n} \lambda_a C(u-u_a)$$

The Kriging variance provides a measure of uncertainty for the estimate at each unknown point. Several forms of Kriging have been developed to address the estimation needs of different types of data and models to be constructed. Isaaks and Srivastava (1989), provide a comprehensive discussion of the different types and usage of each form of Kriging. A negative aspect of Kriging is that it tends to smooth out extreme values. Conditional simulation techniques account for the extreme values by honoring their proportion and spatial correlation.

Because Kriging is a form of linear regression, it tends to provide a smooth representation of the interpolated data that does not represent the true variability present in the data (Deutsch 2002). For certain applications, e.g., estimation of contaminant concentrations, this does not present problems. However, for data that are being used as input to flow and transport modeling, this smoothing can produce highly biased estimates of transport rates. Conditional simulation is an alternative geostatistical method that generates equally probable outcomes or “realizations” that reproduce the critical attributes of the variable (e.g., the global histogram and semi-variogram model).

Sequential simulation is a conditional simulation method that reproduces the spatial dependence of a variable by calculating the conditional probability for each grid node using the semi-variogram model and all available data, and then drawing a value from the conditional probability distribution. The principal concept of sequential
simulation is that previously simulated values are considered as data during the simulation of subsequent nodes, which leads to the reproduction of the spatial correlation model between all of the simulated values. Each grid node is simulated on a random path using a pseudo-random number generator and a random number ‘seed’. Large numbers of realizations of the spatial distribution of a variable can be simulated by using different random number seeds. The uncertainty of the simulated values for any location is quantifiable by simulating multiple realizations and then examining the simulated values at that location.

Direct estimation or simulation of hydraulic properties

Models of direct simulation of properties are used to estimate the hydrogeologic properties of a study area when the spatial distribution of a variable is relatively homogeneous, i.e., that the variable is stationary (Chiles and Delfiner 1999). Stationarity implies that the mean and the semi-variogram model of a variable can be applied to the entire estimation domain. In many geologic applications this is not the case. For example, the mean and semi-variogram of permeability will be quite different for sand and shale sediments. For non-stationary (heterogeneous) study areas a combination of cell-based methods (e.g. Gaussian and Indicator) followed by direct estimation of properties are used (Deutsch 2002), as discussed below.

The Gaussian method is widely used in geostatistics for direct estimation of hydraulic properties. The method is “simple, flexible, and reasonably efficient” (Deutsch 2002) and is often used for estimating continuous random variables such as porosity, permeability and concentration. The multi-Gaussian approach is parametric in that the
conditional cumulative distribution function is completely determined by the parameters
of the mean and semi-variogram models. Assumptions of the multi-Gaussian approach
include the idea that the mean is known and the global distribution is stationary, i.e., that
the mean doesn’t exhibit a trend where the mean is a function of location (Isaaks and
Srivastava 1989). The method involves transformation of the original data to a standard
normal distribution with a mean of zero and a variance of one. The data are transformed
first by ranking them in ascending order then calculating the sample cumulative
frequency by: \[ p_k = \frac{k - 0.5}{n} \]. The resulting quantiles are then converted to normal
scores by assigning the value from a standard Gaussian distribution associated with the
quantile of each data value (Deutsch and Journel 1998). Once the data are transformed to
a univariate standard normal distribution the data must be checked to ensure the
multivariate spatial distribution is also normal (Goovaerts 1997). For sequential
Gaussian simulation (SGS), simple Kriging (SK) is performed in random order for each
grid node. A simulated value is then randomly drawn and used to condition the
simulation of subsequent nodes. The process is repeated until all the nodes are simulated.
Sequential Gaussian simulation provides a simple and fast method to model the
spatial distribution of geologic properties. One disadvantage of the multi-Gaussian
method is that it is not always appropriate for geologic variables. The Gaussian model is
a maximum entropy model, which implies that values near the mean of the distribution
have the greatest spatial structure, i.e. values near the mean have greater spatial influence
on the model, and extreme values have very little spatial structure. The consequence is
that the extreme values of the distribution cannot be connected. The Gaussian method
may not be appropriate if the data contain extreme values whose spatial continuity is
essential to the model. For example, if continuous mud layers with very low hydraulic conductivity are present, sequential Gaussian simulation will not generate simulations that capture the continuity of those low conductivity layers.

The Indicator model provides an alternative to the Gaussian model. The indicator model directly estimates the conditional probability distribution for un-sampled locations with no Gaussian assumptions. The indicator model requires transformation of the data into binary indicators based on several thresholds of the data. The number of thresholds is usually between 5 and 11, and the deciles of the data (i.e., 10th percentile, 20th percentile, etc.) are commonly used as thresholds to bin the data (Deutsch 2002). Indicator transforms are completed for each threshold according to:

\[ i(u_a; z_k) = \begin{cases} 1, & \text{if } z(u_a) \leq z_k \\ 0, & \text{otherwise} \end{cases} \]

where \( i \) is the indicator and \( z_k \) is the variable at \( k \) threshold, at location \( u_a \). The spatial dependence of the variable is obtained by calculating and modeling the experimental semi-variograms for the indicator data associated with each threshold. The indicator Kriging (IK) estimation procedure requires a semi-variogram model for each threshold. IK estimates the conditional cumulative distribution function (ccdf) of a variable by estimating the probability of a series of thresholds by:

\[ \mathbb{E}\{I(u; z)\} = 1 \cdot P\{Z(u) \leq z\} + 0 \cdot P\{Z(u) > z\} = P\{Z(u) \leq z\} = F(z) \]

The ccdf at any location can be modeled by determining the conditional expected values for all indicator thresholds. The IK approach can be extended to simulation using the sequential simulation algorithm described above. At each node, a simulated value is drawn at random from the ccdf obtained using IK. The process is repeated until all the
nodes have been visited in random order and all grid nodes have been simulated.

Advantages of the indicator model over the Gaussian model are: 1) the indicator model is non-parametric which allows estimation of each indicator threshold according to conditional probability distributions derived from the data; 2) the spatial continuity is described for each threshold from the corresponding semi-variogram model, so that the spatial continuity of extreme values can be modeled correctly; and 3) the indicator method has greater flexibility for combining hard and soft data (Deutsch 2002).

Cell Based Approaches – Stratigraphic Units or Facies

Cell based indicator modeling is similar to the models described previously in that the estimates are made for equal-sized grid nodes. However, the cell-based approach models the spatial distribution of categorical variables, such as the stratigraphic unit or lithofacies, rather than continuous properties like permeability or porosity. The method directly estimates the spatial uncertainty for the distribution of a defined category. The data for each category are transformed to an indicator $k = 1, \ldots, K$ where $K$ values are mutually exclusive categories by:

$$i(u_a; z_k) = \begin{cases} 
1, & \text{if facies } k \text{ is present at } u_a \\
0, & \text{otherwise}
\end{cases}$$

Experimental semi-variograms are calculated and modeled for each of the indicator categories. Indicator kriging for categorical variables requires a semi-variogram model for each category to estimate the conditional probability distribution function. The related technique of sequential indicator simulation involves searching for nearby data or previously simulated values, and then constructing the conditional probability distribution using indicator kriging for each node. A simulated value is drawn randomly from the
probability distribution for each node. The estimation procedure is repeated on a random path until all nodes are simulated.

The facies or categorical approach to modeling provides the overall architecture of the deposit that can be used to constrain the simulation of hydrogeologic properties described below under the Combined Approach section. One drawback to the facies approach is the large number of variograms required to define the spatial correlation of each facies. In addition, the sequential indicator simulation approach does not capture the relationships between facies, unless indicator co-kriging is employed. Sequential indicator simulation using co-kriging is extremely demanding, requiring the calculation and modeling of cross semi-variograms between each facies in addition to the semi-variogram modeling of the facies themselves required for standard sequential indicator simulation (Carle and Fogg 1997). For this reason, the co-kriging approach is rarely employed. The transition probability approach is an alternative developed by Carle and Fogg (1997) that has the ability to model the relationships between geologic facies. Transition probability models determine the probability that a certain facies will continue in three-dimensional space as well as the probability that another facies will be present instead.

Combined Approach

The combined approach to geostatistical modeling of hydrogeologic properties is implemented when major changes in stratigraphy are observed and must be accounted for before modeling hydrogeologic properties (e.g., permeability and porosity). Major changes in stratigraphic units demonstrate significant control over the saturation properties of the study area. For example, saturation properties change significantly at
the contact between sandstone and a mudstone. That stratigraphic change would be associated with a significant change in hydrogeologic properties and require a combined modeling approach. Cell-based models such as the indicator or Markov transition probability simulation methods are applied to simulate the spatial distribution of the stratigraphic facies, as described above. Direct simulations of properties (e.g., porosity and permeability) are then modeled for each stratigraphic unit or facies using the Gaussian or indicator techniques as described above. Then, the hydraulic properties for each grid node are chosen from the relevant direct simulation using the simulated facies as a template. The combined approach to geostatistical modeling assists in reducing the uncertainty of the model by first simulating the overall geometry of the geologic units then simulating the direct properties for each unit. The main benefit of the combined approach is that it only requires the assumption of local stationarity, i.e., that the hydraulic properties are relatively homogeneous within each facies (Deutsch 2002).

METHODS

Many geologic data have been collected in the study area over the last fifty years. The data were in several different formats and range in quality. The data used for this study include a combination of borehole logs, particle size (grain size), CaCO₃, and gamma logs compiled from previous work. These data provide the framework for sediment classification for application of geostatistical methods as well as traditional geologic approaches (e.g., construction of stratigraphic sections and cross sections). Additional data were collected in field sites near the study area to better understand and apply the historical data (Fig. 14).
Figure 14. Flow chart of methods consisting of hard copy and electronic data manipulation, field observations, vertical logs, stratigraphic cross-sections, geostatistical analysis and simulation, and application of hydraulic conductivity to simulations utilized to complete the study.
Original methods of collection – Historical Data

Borehole logs

The borehole logs within the study area vary in quality. Borehole logs were completed based on a driller’s or geologist’s qualitative description of the sediments encountered during drilling operations. The drilling method used throughout the study area was primarily the cable-tool percussion method. The method involves lifting and dropping a string of heavy drilling tools. The weight of the tools forces the drill bit into the ground with minor rotation. The drill and sample method used have an effect on the observed grain size and sediment classification. Three cable-tool drilling and sampling methods were used (Fig. 15). The first method uses a bit attached to the drill stem and is designated “hard tools” in the driller’s log. The rotating action of the bit, drill stem, and added water crushes rocks and loosens sediments to form a slurry of sediments. The slurry is removed from the well at regular intervals with a bailer. This drilling and sampling method tends to decrease the grain size observed in samples due to the crushing action of the bit. The second method uses a core barrel or “drive barrel”, a meter long pipe attached to the drill stem. The core barrel is driven into the ground and then pulled from the well. Sediments accumulated in the core-barrel are retrieved by striking the core-barrel with a hammer. This method provides a better representation of grain size encountered during drilling. The third method is a split-spoon sampler. The split-spoon sampler is a specialized core-barrel designed to obtain comparatively undisturbed samples. The split-spoon consists of an outer barrel, head, drive shoe, and an inner barrel. The operation of the split-spoon is the same as the core-barrel. The sampler is broken open to retrieve the sediments in the inner barrel. The inner barrel is then cut
open to observe the sediments. The inner barrel is replaced each time a sample is taken. The split-spoon sampler preserves the sediment sample, but was found to be too time consuming and expensive to be widely used in this study area (Price, Kasper et al. 1979). Boreholes in the study area were primarily drilled with “hard-tools” and “drive-barrel” (Fecht and Price 1977).

Drill Logs

In 1949 eleven boreholes were drilled using the hard-tool sampling method. It is not clear if the drillers followed a specified procedure, but the qualitative descriptions of the sediment samples are consistent for these wells. The drillers provided a qualitative description of the sediments they retrieved from a sample depth of every 1.5 meters (5 feet). Changes in the lithology encountered between sample intervals were described in the same manner. The qualitative descriptions include, particle sizes present and occasionally descriptors for percentage of a certain particle size (Appendix A). The descriptions sometimes included color or petrologic composition, for example, black and white sand, or basalt gravel. The drillers placed a sediment sample from each of the 1.5 meter depth intervals into labeled glass jars that were saved for future analysis. The size of the glass jar limits the maximum clast size of sampled sediments to small cobble (<6.4 cm).

In the 1960’s twelve boreholes were drilled in the study area using a combination of drive-barrel and hard-tool sampling methods. The driller’s logs were similar to the 1949 logs with some containing additional descriptors of sand size or maximum particle size. Sediment samples were collected and stored for most of the boreholes drilled during this time.
Figure 15. Illustrations of the three cable tool drilling methods used for boreholes in the 216-Z-1A study area (illustration by George Last).
Seventeen boreholes were drilled in the 1970’s using primarily the drive-barrel sample method with small sections of split-spoon or hard-tool sampling. The driller’s descriptions for the seventeen boreholes drilled in the study area during the 1970’s provide a greater variety of qualitative information. The logs consist of the particle size data with descriptions of sand and gravel size, petrological composition, color and moisture. It is not clear if specified procedures were followed for the drilling and sampling of sediments. Most of the sediments collected during this period were contaminated with radionuclides and/or chlorinated solvents. The samples retained for further analysis were handled as ‘hot samples’.

Geologists Logs

Last and Liikala (1987) prepared a field guide for geologists that specified observations to be recorded during drilling (Last and Liikala 1987). The procedures were set forth to create consistency in how and what observations were to be made. Two boreholes used for this study were drilled during this time using the drive-barrel sample method with small sections of split-spoon or hard-tool sampling. The geologist’s logs provide grain-size and percent, roundness and shape, gross mineralogy, color, reaction to 10% HCl, and consolidation. The geologist’s logs also include sketches of the geologic materials encountered during the drilling operation (Appendix A).

Particle size and CaCO₃

Two sources for grain size data were used in this study: 1) ROCSAN- a historical database consisting of laboratory particle size and calcium-carbonate percentage for sediment samples, 2) Smith and Additon (1980) – laboratory particle size for sediment samples contaminated with radionuclides. Sixteen boreholes used in this study have
laboratory particle size and CaCO$_3$ weight percent available in the ROCSAN database. The laboratory methods used for analyzing the samples from those boreholes were not documented in the database. The laboratory procedures of Fecht and Price (1977) are from the same time period in which these samples were analyzed and may have been used for the samples. Particle sizes for two boreholes used in the study were analyzed using the procedures documented in (Smith and Addition 1980). Due to time constraints for this study it was not possible to complete laboratory sieve analysis for archive borehole samples not included in the database.

**Gamma Logs**

The gamma logging procedures for the boreholes used in this study vary over the years. Last and Horton (2000) provide a summary of geophysical characterization methods used at the Hanford Site relative to the time the data was collected (Last and Horton 2000).

**Data Collection**

**Classification of Borehole logs**

Borehole logs for each well in the study area were acquired from files located at Pacific Northwest National Laboratory, Richland, Washington. The borehole logs were converted initially to an electronic worksheet to enable data analysis. The sample depth, drill and sample method, and sample description were crucial for this study. Each borehole log was entered verbatim into a worksheet from the paper copy following procedures outlined in PNL Procedure DO-7 (Appendix B). Sediment classification for
each depth observation (sample description; Folk, 1968) was assigned based on the order in which the driller listed the sediments. For example, if the driller documented the sediment as sand, silt (mud), and gravel, it was assumed the first type of sediment was the greatest percentage of the sample, and decreased in order listed (Fig. 12). Some of the drill logs were more detailed than others and therefore permitted finer classification of the sample. Additional indicators of sediment percentages in the sample such as the qualifying terms “lots”, “very little”, “trace of”, “some”, “slightly”, “sparse”, and grain size indicators like “small gravel”, and “medium-coarse sand” allowed the observation to be more tightly classified. The borehole sediment classification data from the drill logs (hereafter referred to as drill log data) provided a qualitative assessment of the type of sediment present in each sample.

Laboratory Particle Size and CaCO₃

Particle size distribution was one of the most valuable forms of data used in this study. Laboratory particle size provides a quantitative data source with which to classify sediments. Particle size data for sixteen wells in the study area were available in the ROCSAN database. The data were directly imported into a worksheet from the database. The ROCSAN database provided laboratory measurements of particle size, total gravel, sand, mud, and CaCO₃ weight percent. The sample depth, number, and sediment classification also were provided.

The particle size data for two boreholes in the study area were taken from Smith and Additon (1980) as the weight percent for sediment retained on each sieve. Normalized percentages of gravel, sand, and silt, as well as the cumulative weight percent
of the sample all were determined in a spreadsheet and used to classify the sediments according to Folk's (1968) scheme (Fig. 12).

**Gamma Logs**

Gamma logs were useful in estimating particle-size distribution through the borehole when laboratory or field estimates were not available. Gamma logs also were used to help identify stratigraphic units with distinct geophysical characteristics. Nineteen of the boreholes in the study area had digital gamma logs. There were several gamma logs for each well logged. The study was located in an area contaminated with radionuclides that can mask the natural gamma signature of sediments. This study uses gross gamma and spectral gamma logs that were conducted at the time of emplacement of the well or relatively soon after (e.g., oldest digital) emplacement. The logs were obtained from two database sources; PNNL Log Database (http://boreholelogs.pnl.gov) for wells logged between 1989 and 2002, and the Hanford Geophysical Logging Project Database (http://gi.em.doe.gov/hanf) for geophysical logs collected from 2001 to present.

**Field Studies**

An analog outcrop was chosen near the study site to examine different lithofacies and to provide an improved understanding of the sediments described in borehole logs (Fig. 16). Photos and field notes from an additional field site also were considered. The outcrops were excavation sites where heavy equipment stripped away sediment to reveal the horizontal sedimentary architecture. The excavation pits are referred to by pit number or project number. Pit 30 consists mostly of the Hanford gravel facies association and the IDF trench consists of the Hanford sand facies association.
Figure 16. Digital elevation map displaying the location of field sites in relationship to the 216-Z-1A study area.
Vertical Logs - 1D Visualization of Data

The worksheets with borehole logs, grain size, CaCO$_3$, and geophysical data were imported into a geologic database (Hanford Borehole Geologic Information System (HBGIS)). One feature of the database was to provide output files of the cumulative data from each borehole in tabular format. The output files were used to plot a one-dimensional representation of the data as a vertical log.

The completed logs were used to qualitatively estimate the position and lateral expression of stratigraphic contacts. Contacts were chosen using a combination of particle-size data, sediment classification, CaCO$_3$, and gross or spectral gamma in order of significance. Boreholes with the greatest amount of data were used to assist in the determination of stratigraphic contacts in nearby boreholes with limited data. The stratigraphic contacts identified in the borehole logs were used to construct a set of two-dimensional cross sections.

Cross Sections – 2D Visualization of Data

Hand-drafted cross sections were completed using all 19 of the borehole-log sediment classifications, grain size and CaCO$_3$ content. North-south and roughly east-west cross sections were constructed (Fig. 17). Stratigraphic correlations made between boreholes were based on the identification of large packages of sand, silt or gravel. The original cross-sections revealed the need to group the 19 different classes of lithofacies in order to better determine the stratigraphic correlations.
Figure 17. Diagram showing the location of the East-West and North-South borehole cross sections through the 216-Z-1A study area (modified from Rohay et al. 1994).
The 19 sediment classifications were reduced to eight classifications based on borehole-log sediment classification, grain size and percent CaCO₃. The Hanford formation was the focus of the study. Therefore classifications for the Cold Creek unit and Ringold Formation were grouped by formation and maker facies. The grouped lithofacies included silty sand (mS), fine sand (fS), coarse sand (cS), gravelly sand (gS), sandy gravel (sG), Cold Creek silty facies (Uz), Cold Creek calcic facies (Uc), and the Ringold Formation (R) (Table 5). The classification of lithofacies from laboratory particle size provided a quantifiable cut-off between lithofacies. The silty sand facies was only used for samples that consisted of greater than 25% silt. Sand size distinctions were determined by the amount of each sand size present. The sandy gravel facies was assigned to samples with greater than 30% gravel. The grouped lithofacies were used to re-construct the cross sections in Adobe Illustrator. Stratigraphic correlations were made based on the grouped lithofacies present in the cross-sections.

Table 5. Grouped lithofacies designations from the 19 modified Folk (1968) sediment classifications.

<table>
<thead>
<tr>
<th>Lithofacies</th>
<th>Description</th>
<th>Characteristics</th>
<th>Modified Folk (1968)</th>
</tr>
</thead>
<tbody>
<tr>
<td>HmS</td>
<td>Hanford — silty sand</td>
<td>&gt; 25% silt</td>
<td>mS, sM</td>
</tr>
<tr>
<td>HfS</td>
<td>Hanford — fine sand</td>
<td>mostly v.fine-fine sand, &lt; 25% silt</td>
<td>S[vf-m], (m)S, mS, (g)mS</td>
</tr>
<tr>
<td>HcS</td>
<td>Hanford — coarse sand</td>
<td>mostly med.-coarse sand, ≤ 10% gravel</td>
<td>S[m-vc], (gm)S, (g)S</td>
</tr>
<tr>
<td>HgS</td>
<td>Hanford — gravelly sand</td>
<td>mostly med.-coarse sand, with 10-30% gravel</td>
<td>gS, (m)gS, mgS</td>
</tr>
<tr>
<td>HsG</td>
<td>Hanford — sandy gravel</td>
<td>gravel with 20-70% sand</td>
<td>sG, msG, G</td>
</tr>
<tr>
<td>CCUz</td>
<td>Cold Creek Unit — silty facies</td>
<td>silty sand 5-20% CaCO₃ content</td>
<td>S, mS, sM, M</td>
</tr>
<tr>
<td>CCUc</td>
<td>Cold Creek Unit — calcic facies</td>
<td>fine-coarse grained 6-67% CaCO₃ content</td>
<td>msG, smG, gmS, mgS, mS, gsM, sgM, gM, sM, M</td>
</tr>
<tr>
<td>R</td>
<td>Ringold Formation undifferentiated</td>
<td>mud, sand, sandy gravel differentiated by decreased CaCO₃</td>
<td></td>
</tr>
</tbody>
</table>
Geostatistical techniques were applied to the borehole sediment classification data in order to generate a high-resolution 3-D lithofacies model. The cross sections provided the basis for geologic interpretation. The original 19 sediment classifications grouped as eight lithofacies provide an intermediate modeling scale (Table 5). The grouped lithofacies capture the significant sediment heterogeneities within the study area based on the observed sorting and particle size distribution within the field sites.

Two datasets were used for geostatistical analysis, the qualitative borehole sediment classification (drill-log data) and the quantitative laboratory particle-size sediment classification (particle-size data). The particle-size dataset was considered the ‘hard data’ for statistical analysis and the drill-log dataset as ‘soft data’ to provide data where there were no particle-size observations. A cross tabulation was performed between the drill-log data and the particle-size data for sample locations where both were available in order to determine the quality and usefulness of the drill-log data (Table 6).

Table 6. Cross-tabulation of Drill log sediment classification vs. Particle size sediment classification to determine the quality and usefulness of the Drill log data as “soft” data for statistical analysis.

<table>
<thead>
<tr>
<th>Particle Size</th>
<th>mS</th>
<th>fS</th>
<th>cS</th>
<th>gS</th>
<th>sG</th>
<th>N</th>
<th>Total %</th>
</tr>
</thead>
<tbody>
<tr>
<td>Drill Log</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>mS</td>
<td>82.1</td>
<td>3.6</td>
<td>0</td>
<td>10.7</td>
<td>3.6</td>
<td>28</td>
<td>100</td>
</tr>
<tr>
<td>fS</td>
<td>55.8</td>
<td>35</td>
<td>0</td>
<td>6.7</td>
<td>2.5</td>
<td>120</td>
<td>100</td>
</tr>
<tr>
<td>cS</td>
<td>12.2</td>
<td>9.7</td>
<td>24.4</td>
<td>31.7</td>
<td>22</td>
<td>41</td>
<td>100</td>
</tr>
<tr>
<td>gS</td>
<td>6.1</td>
<td>2.4</td>
<td>9.8</td>
<td>45.1</td>
<td>36.6</td>
<td>82</td>
<td>100</td>
</tr>
<tr>
<td>sG</td>
<td>0</td>
<td>0</td>
<td>5.3</td>
<td>38.6</td>
<td>56.1</td>
<td>57</td>
<td>100</td>
</tr>
<tr>
<td>Total N</td>
<td>100</td>
<td>49</td>
<td>21</td>
<td>83</td>
<td>75</td>
<td>328</td>
<td></td>
</tr>
</tbody>
</table>
Examination of the data distribution with elevation (Figures 18 and 19) showed that the vast majority of the data were collected within the Hanford unit at elevations greater than 170 meters, so the geostatistical modeling was restricted to that formation. Only five of the 8 grouped lithofacies occur within the Hanford unit and were included in the geostatistical analysis.

Figure 18. Graph of data density by elevation.

Figure 19. Graph of grouped lithofacies data density by elevation.
Experimental semi-variograms were calculated for each of the 5 lithofacies within the Hanford unit. Vertical semi-variograms were calculated for both the particle size and the drill-log datasets using GSLIB’s GAMV program (Deutsch and Journel 1998). Indicator transforms of the lithofacies categories were prepared for each observation, coded as one if the lithofacies was present, or zero if they were not. The GAMV program requires certain parameters to calculate semi-variograms, one of the most important being the lag distance between pairs of observation. The lag is the separation vector, $h$, between the head and tail values. The number of pairs available for calculation of the semi-variogram value for a given lag is dependent on the lag distance and the tolerance. The objective was to have the greatest number of pairs in the calculation while limiting the lag separation and tolerance to preserve as much detail as possible. The vertical lag spacing was based on the average spacing between samples in the boreholes, which was 5 feet or 1.52 meters. The lag tolerance was set to 0.76 meters which is $\frac{1}{2}$ of the lag spacing. The azimuth angle, tolerance angle and horizontal bandwidth parameters are essentially ignored for the vertical semi-variogram calculations. To force the calculation of a vertical semi-variogram, the dip angle was set to 90°, the dip tolerance was set to 1°, and a vertical bandwidth of 1m was used to limit the search area within one meter of the vertical. Figure 20 provides a graphical representation of these parameters. The GAMV program was used to calculate a vertical semi-variogram for each of the defined variables (i.e., one vertical semi-variogram for each lithofacies).
Figure 20. Illustration of vertical experimental semi-variogram calculation parameters, including the vertical lag distance $h$, lag tolerance, angle tolerance, and bandwidth (reprinted from Deutsch 2002).

The GAMV output file was imported into a worksheet for modeling. Graphs for each lithofacies were created from the semi-variogram calculations, and a spherical variogram model was fit to the experimental semi-variogram data. The spherical variogram model is defined by:

$$
\gamma(h) = c \cdot Sph \left( \frac{h}{a} \right) = \begin{cases} 
1.5 \frac{h}{a} - 0.5 \left( \frac{h}{a} \right)^3, & \text{if } h < a \\
0, & \text{if } h \geq a 
\end{cases}
$$

where $h$ is the lag separation vector, $a$ is the range, and $c$ is the sill. A theoretical sill was calculated for each of the five lithofacies according to the equation $c = p \cdot (1 - p)$ where $p$ was the proportion of each lithofacies within the total number of samples. The
experimental semi-variograms were modeled with an attempt to fit the experimental semi-variogram points as closely as possible, especially for the shorter lag distances, while preserving the theoretical sill. The parameters used for modeling a spherical semi-variogram model include the sill, nugget, and range. The nugget effect is the "discontinuity" at the origin of a semi-variogram which includes both measurement error and short range geologic variability (Deutsch 2002). Sparse data can increase the apparent nugget effect (Deutsch 2002). The range is a measure of spatial continuity within the variable. The vertical variograms were modeled using only one nested structure by varying the nugget and range to provide the best fit of the experimental semi-variogram. Experimental semi-variogram points that were based on a small number of data pairs (less than about 30 pairs) often form outliers near the origin and maximums, and were not honored in the model-fitting process.

Horizontal semi-variograms often do not have sufficient data to provide a useful spatial model, especially when well spacing is sparse (Deutsch 2002). The sparse particle-size dataset was of particular concern for this study (Fig. 21). Horizontal semi-variogram calculations were performed using both the particle-size and drill-log datasets. The procedures for calculating horizontal semi-variograms were essentially the same as for the vertical semi-variograms with a few additions (Fig. 22). A horizontal lag separation distance of 10 meters and a tolerance of 5 meters were determined based on the spacing of the boreholes to maximize the number of pairs for each separation vector \( h \). The horizontal semi-variogram calculations were limited to be nearly horizontal by setting the dip to zero with a dip tolerance of 1° and a vertical bandwidth of 1 meter.
Figure 21. Map showing the distribution of boreholes with Particle size data in the study area.
Five horizontal semi-variograms were calculated, an omni-direction (e.g., all directions) semi-variogram plus four different directions in order to determine a possible direction of maximum continuity in the horizontal. The omni-directional semi-variogram calculation surveys the entire horizontal field without regard to horizontal anisotropy. However, paleoflow directions from previous studies suggest that the maximum horizontal continuity direction in the Hanford unit should be approximately north-south through the study area. Field measurements of foreset bedding in Pit 30 indicated an apparent transport direction of 165°, which fit with those previous estimates. Four directional semi-variograms were calculated to examine the horizontal anisotropy for this study. They included 0° (N-S), 45° (NE-SW), 90° (E-W), and 135° (NW-SE) azimuth angles. The tolerance angle for the four directional semi-variograms was set at 22.5°.

Figure 22. Illustration of horizontal experimental semi-variogram calculation parameters, including the horizontal and vertical; lag distance \( h \), lag tolerance, angle tolerance, and bandwidth (reprinted from Deutsch 2002).
The modeling process for the horizontal semi-variograms was the same as for the vertical except there were five semi-variograms to model for each variable (omni-directional plus 4 directional semi-variograms). The particle-size and drill-log horizontal semi-variograms were graphed and then reconciled with the vertical variograms to develop an integrated model that accounted for the difference in spatial continuity (i.e., the anisotropy) between the horizontal and vertical data.

**Indicator Simulation**

The required input data for sequential indicator simulation included Particle Size 'hard' dataset, i.e., the sediment classification based on the particle size data and a 'soft' dataset, the Drill Log Data, i.e., the sediment classification derived from the drill-log data. The input file for the 'soft' dataset required additional information. Because the dataset was considered 'soft' each lithofacies designation from the Drill Log dataset must include calibration values, which provided an estimate of the probability that each facies was present, given a reported occurrence of a facies in the Drill Log dataset. The calibration values were estimated from the comparison of Particle Size and Drill Log sediment classifications included as Table 6.

The cell-based sequential indicator simulation method discussed previously was used to simulate the spatial distribution of facies values in the study area on a regular grid with one meter vertical and five meter horizontal increments where, \( nx = 32, ny = 24, nz = 44 \). GSLIB's SISIM (sequential indicator simulation) program was used to generate the simulations. The program required a parameter file which includes the global cdf or pdf, 'hard' dataset, 'soft' dataset with calibration values, the
number of realizations, grid parameters, random number seed, and the variogram model for each of the categorical variables (see Deutsch and Journel 1998 for a detailed description of all parameters). Calculation of one hundred realizations was chosen to provide a quantitative measure of the uncertainty of the estimated values at each grid node.

Post Processing

Post processing of the one hundred realizations was conducted to obtain the mean, median, and mode of the lithofacies simulations. The GSLIB software package provided a post-processing program (postsim) for the mean and median of the realizations. The mode of the lithofacies simulations was calculated by counting the number of times each lithofacies was present at a specific location and then choosing the lithofacies with the greatest number of occurrences for that location. Ties between the modal lithofacies were broken randomly. The mode calculation provided the most useful analysis of the realizations in that it conveyed the lithofacies simulated most often for each node in the grid.

Individual simulations with the minimum and maximum number of three lithofacies expected to have a major influence on hydraulic flow and transport (mS, and gS combined with sG) were selected from the suite of simulations. Counts of the number of times each lithofacies were present for each simulation were tabulated and used to determine the minimums and maximums.

The reproduction of both horizontal and vertical semi-variograms was examined for a small suite of output simulations. The five minimum and maximum simulations
described above were used for variogram reproduction as well as five additional randomly drawn simulations. The semi-variograms were calculated using GSLIB’s GAM program for regularly spaced data (Deutsch and Journel 1998). The semi-variogram results for the ten simulations were plotted and compared to the input semi-variogram models.

Hydrologic properties were simulated for several of the lithofacies simulations using previously estimated probability distributions of hydraulic conductivity in the 200 West Area for the relevant lithofacies (Last 2004). Hydraulic conductivity values were generated for the five simulations that include the minimum and maximum simulated values for mS, combined gS and sG, as well as the modal simulation. Each lithofacies was randomly assigned a lognormal hydraulic conductivity value using Gaussian probability models calculated by Last and others (2004) using laboratory hydraulic conductivity measurements for each lithofacies (Table 7). These values were then converted to hydraulic conductivity using the exponential function.

<table>
<thead>
<tr>
<th>Facies Designation (Last et al. 2004)</th>
<th>Lognormal Ks Mean (cm/s)</th>
<th>Lognormal Ks STD (cm/s)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Lith_1 (mS) Hanford silty sand_200-ZP-1</td>
<td>-11.936</td>
<td>1.000</td>
</tr>
<tr>
<td>Lith_2 (fS) Hanford fine sand_200-ZP-1</td>
<td>-9.449</td>
<td>1.446</td>
</tr>
<tr>
<td>Lith_3 (cS) Hanford coarse sand_200-ZP-1</td>
<td>-6.512</td>
<td>2.361</td>
</tr>
<tr>
<td>Lith_4 (gS) Hanford gravelly sand_200West</td>
<td>-8.354</td>
<td>2.074</td>
</tr>
<tr>
<td>Lith_5 (sG) Hanford sandy gravel_200-ZP-1</td>
<td>-5.651</td>
<td>2.359</td>
</tr>
</tbody>
</table>
Visualization

A 3-D visualization program was used to create plots of selected simulations. 3-D plots were created for the modal simulation, as well as for the minimum and maximum lithofacies simulations. Several slices through the 3-D plots were constructed through areas of densely populated borehole data. Probability maps were created to display the probability of each lithofacies being present at a given grid node. The simulations of hydraulic conductivity for the minimum, maximum, and mode simulations were also displayed in 3-D.

RESULTS

Field

Field study of analogous outcrops provided an improved understanding of the descriptions of sediments in the borehole logs. Three lithofacies are identifiable from the Hanford gravel facies in Pit 30; coarse sand, gravelly sand, and sandy gravel (Table 8). The Integrated Disposal Facility (IDF) trench includes three recognizable lithofacies of the finer grained Hanford sand facies; silty sand, fine sand, and medium-coarse sand (Table 8).

Pit 30 is located within the Cold Creek expansion bar. It provides an opportunity to view the sedimentary architecture in the Hanford gravel facies. Large scale foreset-bedded gravels dominate the architecture of the pit. The foreset beds have lateral continuity of approximately ten meters. The gravel beds are interstratified, grading from imbricated open framework gravels to poorly sorted sandy gravel (Fig. 23). The gravel
beds grade upward to moderately-sorted horizontally laminated beds that truncate the foreset beds (Fig. 24).

Table 8. Qualitative descriptions of characteristics of sediment samples collected at Pit 30 and IDF.

<table>
<thead>
<tr>
<th>Hanford Facies</th>
<th>Sediment Composition</th>
<th>Particle Size</th>
<th>Petrologic Composition</th>
<th>Sorting</th>
<th>Structure/Fabric</th>
</tr>
</thead>
<tbody>
<tr>
<td>Pit 30 Gravel</td>
<td>100% gravel</td>
<td>v.fine-peb - sm.cobble</td>
<td>70% basalt</td>
<td>moderate to well</td>
<td>open-framework</td>
</tr>
<tr>
<td>Gravelly Sand</td>
<td>40-50% gravel</td>
<td>70% v.fine peb</td>
<td>60% basalt</td>
<td>moderate</td>
<td>foreset &amp; Horizontal beds</td>
</tr>
<tr>
<td>&lt; 1% silt</td>
<td>80% v. coarse</td>
<td>20% med</td>
<td>80% basalt</td>
<td>poorly</td>
<td>foreset &amp; Horizontal beds</td>
</tr>
<tr>
<td>Sandy Gravel</td>
<td>90% sand</td>
<td>85% v. coarse-coarse</td>
<td>60% quartz &amp; feldspars</td>
<td>moderate to poorly</td>
<td>Horizontally laminated gravels</td>
</tr>
<tr>
<td>Coarse Sand</td>
<td>80% coarse</td>
<td>85% v. coarse-coarse</td>
<td>60% quartz &amp; feldspars</td>
<td>moderate to v. poorly</td>
<td>Horizontally laminated</td>
</tr>
<tr>
<td>IDF Coarse Sand</td>
<td>80% coarse</td>
<td>85% v. coarse-coarse</td>
<td>60% quartz &amp; feldspars</td>
<td>moderate to v. poorly</td>
<td>Foreset beds</td>
</tr>
<tr>
<td>Fine Sand</td>
<td>80% sand</td>
<td>90% v.fine-fine</td>
<td>90% quartz &amp; feldspar</td>
<td>well sorted</td>
<td>Foreset &amp; Horizontal beds</td>
</tr>
<tr>
<td>Silty Sand</td>
<td>75% sand</td>
<td>90% v.fine-fine</td>
<td>90% quartz &amp; feldspar</td>
<td>well sorted</td>
<td>Horizontally laminated and lenses</td>
</tr>
</tbody>
</table>
Figure 23. Photograph of foreset bedded interstratified gravels grading from imbricated open framework gravels to poorly sorted sandy gravel in Pit 30.

Figure 24. Photograph of sedimentary architecture of gravel beds in Pit 30. Foreset beds truncated by moderately sorted horizontally laminated gravels, topped by another succession of foreset beds.
The sedimentary structures observed in Pit 30 provide a record of the flow regime and depositional environment. There are at least two distinctive depositional events recorded in the gravel facies. The first is observed in the lower set of foreset beds followed by horizontally laminated gravels beds. A second set of foreset beds truncates the underlying horizontal and foreset beds (Fig. 24). The flow regime is interpreted as upper part of the lower flow regime transitioning into the upper flow regime. The coarse sand facies present at Pit 30 is a result of a third time-stratigraphic event. The flow regime that deposited that facies is interpreted as the upper part of the lower flow regime from the apparent large or “mega” ripple structure observed (Fig. 25). The particle-size distribution and relative thickness of the unit indicate a change in sedimentation. The coarse sand facies can be interpreted as deposited during a smaller scale flood event.

![Figure 25. Panoramic photograph of the poorly sorted coarse sand “mega” ripple structure at Pit 30.](image)

The IDF trench provides a record of the sediment deposition about 4-5 km downstream. Sediment samples and photographs taken during the construction of the IDF trench provide a visual representation of the sand and silt facies of the Hanford unit. The sedimentary structures observed are similar to Pit 30 except in finer sediments (Fig. 26). The foreset beds range in lateral continuity from meter scale to tens of meters. The sediments in the foreset beds are interstratified, alternating from coarse sand to fine sand.
with some local silt lenses. The IDF trench displays an apparent unconformity at the base of the horizontally laminated sand. The horizontally laminated sands and silt range in lateral continuity from tens of meters to hundreds of meters. Individual beds in the horizontally laminated sands and silt are centimeter scale (Fig. 27). The laminated sands and silts appear to follow fining upward sequences throughout much of the exposure except where reverse grading was noted. The sediments deposited in the IDF trench area are interpreted to have been deposited during downstream aggradation of the Cold Creek expansion bar.

Figure 26. Photograph of the architecture of sand and silt at the IDF site. Large-scale foreset beds are truncated by horizontal beds of very fine to silty sand.
Figure 27. Photograph of horizontally laminated sand and silt deposits at the IDF field site. Individual beds of sand and silt range from millimeter to centimeters in thickness.
Vertical Logs

The logs provide a visualization tool to determine stratigraphic contacts in the 216-Z1-A study area using all the data accumulated for each borehole. The Hanford unit consists of three main facies associations; gravel dominated, sand dominated, and interbedded sand and silt dominated (DOE 2002). The Cold Creek Unit in the study area consists of two facies: coarse- to fine-grained CaCO$_3$-cemented and fine-grained laminated to massive facies. Most boreholes in the study area penetrate only the very top of the Ringold Formation; therefore it was not subdivided into stratigraphic units for this study. Contacts for each stratigraphic unit and sub-unit were interpreted from the vertical log plots.

The boreholes with drill logs, laboratory particle-size data, CaCO$_3$, and gross gamma logs, and the geologist logs with CaCO$_3$, moisture, gross gamma and/or spectral gamma provided the most information with which to estimate the position of stratigraphic contacts (Appendix C). There are recognizable patterns of stratigraphic sequences within the vertical log plots. The vertical log plot for Borehole A7541 (299-W18-58) provides an example of the sequences. The upper sequence, approximately 15 meters, consists, in ascending stratigraphic order, of sandy gravel transitioning to gravelly sand followed by coarse sand then fine sand. The middle sequence, approximately 15 meters, consists of fine sand and interbedded silt. The lower sequence is considered the base of the Hanford unit, and consists of approximately 5 meters of gravel. The Cold Creek fine-grained facies (approx. 5m) is present below the last Hanford gravel sequence and is distinguished from Hanford fine sand by the increased CaCO$_3$ content or increased gross
gamma signature. The stratigraphic patterns observed in the vertical log plots provide a
general understanding to apply to cross sections.

Cross Sections

The Pleistocene flood deposits are traditionally correlated in large packages of
similar lithofacies (e.g., gravel, sand or silt). The Hanford unit in the north-south cross
section (Plate 1) consists of several sequences of sandy to silty-sand facies with large
discontinuous lenses of gravelly sand facies. The east-west cross section (Plate 2) is very
similar to the north-south cross section. The sandy facies are more laterally continuous
than the gravelly facies in both cross sections. However, Plates 1 & 2 illustrate that the
distribution of lithofacies is very heterogeneous within those sequences.

Geostatistics

Calibration of Drill-Log and Particle-Size Data

The cross-tabulation between the quantitative particle size and qualitative drill log
provides statistical information that can be used to calibrate the hard and soft data. Table
6 displays the results of the cross-tabulation that were used to establish the calibration.
The results are fairly consistent for some facies. For example, samples classified as
muddy-sand (mS) facies using particle size data were also classified as mS by the drill-
log classification 82% of the time. However, the agreement between the particle-size and
drill-log classifications is not as good for several of the facies. For example, for the fine
sand (fS) facies, the particle-size data only classified samples the same as the drill-log
data 35% of the time (Table 6). Although the classification of fS from the drill-log data
was often incorrect, the calibration still provides valuable information about the correct classification that was incorporated in the soft data file generated for the geostatistical simulations. For example, if the drill log at a particular location suggested that fS was present, then the soft probabilities associated with each facies were 56% that the location was actually mS, 35% that it was actually fS, 6.7% that it was gS, and 2.5% that the sediment at the location was actually sG. Similar soft probabilities were derived from Table 6 for the classification of each facies by the drill log. The calibration results allow the use of the drill-log data as ‘soft data’ with a measurable degree of confidence.

Particle-Size Semi-variogram Models

Figures 28a-e displays the experimental vertical semi-variogram models for the particle-size data as well as the model’s fit to those experimental semi-variograms. The silty sand facies appears to have no effect apparent spatial correlation and could be interpreted as a pure nugget (Fig. 28a). However, the proportion of samples for the silty sand facies comprises only 8.3% of the total, so the apparent pure nugget could be a result of insufficient data to determine spatial correlation (Deutsch 2002). The fine-sand facies experimental semi-variogram displays evidence of cyclicity (Fig. 28b). The alternating negative and positive correlations represent cyclic geologic depositional patterns, such as sediments that coarsen upward then transition to fining upward (Deutsch 2002). The semi-variogram model for the fine-sand facies supports the patterns observed in cross sections through the study area. The vertical range of 6.5 meters is consistent with the observed thickness of approximately 10 meters seen in the cross sections. The model for the coarse-sand facies contains a relatively high nugget effect of approximately...
50% (Fig. 28c), indicating a relatively high amount of spatial variability in the coarse-sand distribution. The gravelly sand facies semi-variogram demonstrates a normal semi-variogram model in that the variability increases from the origin and levels out at the theoretical sill (Fig. 28d). The vertical range of 5.5 meters is consistent with the observed thickness of approximately 5 meters in cross section. The model for the sandy gravel facies is similar to that of the coarse-sand facies (Fig. 28e), with a relatively high nugget effect of approximately 50%. The range of 5.5 meters is equivalent to the thickness noticed in cross section of approximately 5-6 meters.

Figures 29a-e are the horizontal semi-variograms for the particle-size dataset. The particle-size horizontal semi-variograms did not have enough data pairs for points near the origin to constrain the models for those semi-variograms. Therefore, the horizontal range and anisotropy ratio for the “soft” or secondary drill log, as described below, were used to constraint the horizontal semi-variogram models for the particle-size dataset shown in Figure 29a-e.
Figure 28. Experimental vertical semi-variograms and model for the particle-size dataset. a) The silty sand facies appears to have no apparent spatial correlation. b) The fine-sand facies displays evidence of cyclicity. c) The model for the coarse-sand facies contains a relatively high nugget effect of approximately 50%. d) The gravelly sand facies demonstrates a normal semi-variogram model in that the variability increases from the origin and levels out at the theoretical sill. e) The model for the sandy gravel facies is similar to that of the coarse-sand facies, with a relatively high nugget effect of approximately 50%.
Figure 29. Horizontal experimental semi-variograms and model for the particle-size dataset. The particle-size horizontal semi-variograms did not have enough data pairs for points near the origin to constrain the models.
Drill-Log Semi-variograms

Figures 30a-e displays the vertical semi-variogram models for the qualitative drill-log data. The silty sand experimental semi-variogram appears to have a slight cyclic pattern (Fig. 30a). The silty sand vertical range of 9 meters is consistent with the observed thickness in cross section of approximately 10-15 meters. The semi-variogram for the fine-sand facies is similar to that of the experimental semi-variogram for the particle-size fine-sand facies model, in that it displays a slight cyclicity (Fig. 30b). The proportion of samples identified as fine sand in the drill-log data is less than the proportion of fine sand in the particle-size dataset, which may be responsible for the lower level of cyclicity observed in the drill-log semi-variogram. The semi-variogram model for the coarse-sand facies (Fig. 30c) has a range of 7 meters, which is slightly larger than the observed thickness of that facies observed in cross sections of approximately 5 meters. The vertical semi-variogram for the gravelly sand facies (Fig. 30d) has a range of 6 meters; that is consistent with the range for gravelly sand in the particle-size dataset (5.5m) and also the thickness of 5-6 meters observed in cross sections. The sandy gravel facies semi-variogram demonstrates a slight cyclicity (Fig. 30e). The vertical range of 8 meters is greater than that observed for the sandy gravel facies in the particle size dataset of only 5.5 meters. The proportion of samples for the sandy gravel facies in the drill-log dataset is greater than the proportion for the particle-size dataset, which may account for the differences in the semi-variogram models for that facies in the two datasets.

The drill-log horizontal semi-variograms for the silty sand and fine sand facies were well defined (Fig. 31 a & b) which was expected given the larger number of
boreholes with drill log data. The horizontal range for the silty sand is 40 meters and 45 meters for the fine-sand facies. The horizontal ranges are consistent with the observations made for the fine-grained facies observed at the IDF trench of tens of meters to hundreds of meters. The horizontal semi-variogram model for the coarse-sand facies model is not well constrained (Fig. 31c), as the data points near the origin are based on an insufficient number of pairs to consider them as reliable data points. The gravelly sand facies model has two outlying data points near the origin that greatly influenced the horizontal variogram (Fig. 31d). The horizontal range of 7 meters is inconsistent with the continuity of tens of meters seen in the gravelly sand facies at Pit 30 (Fig. 31d). The horizontal semi-variogram model for the sandy gravel facies has a range of about 10 m, which coincides with the horizontal continuity observed in the gravel facies in Pit 30.

Nested Horizontal and Vertical Variograms

Fitted (e.g., nested) models were developed that reconcile the vertical and horizontal semi-variogram models for both the particle-size and the drill-log datasets. The resulting models provide the semi-variogram models needed for lithofacies simulation. Figures 32 and 33 display the semi-variogram models for drill-log and particle-size data. Table 9 displays the horizontal and vertical range and the anisotropy for each lithofacies for indication simulation. The finer grained facies (e.g., silty sand and fine sand) are more continuous in the horizontal than the vertical. The semi-variogram models progressively decrease in anisotropy as the grain size increases with the exception of the sandy gravel facies. Both the particle-size and the drill-log models for the coarse sand and gravelly sand facies are isotropic or nearly isotropic.
Figure 30. Vertical semi-variograms and models for the qualitative drill-log dataset. a) The silty sand experimental semi-variogram appears to have a slight cyclic pattern and its vertical range of 9 meters is consistent with the cross section thickness of approximately 10-15 meters. b) The fine-sand facies displays a slight cyclicity that is similar to that of the experimental semi-variogram for the particle-size fine-sand model. c) The semi-variogram model for the coarse-sand facies has a range of 7 meters, which is slightly larger than the observed thickness of that facies observed in cross sections of approximately 5 meters. d) The semi-variogram for the gravelly sand facies has a range of 6 meters which is consistent with the range for gravelly sand in the particle-size dataset of 5.5 meters and the thickness of 5-6 meters observed in cross section. e) The sandy gravel facies semi-variogram demonstrates a slight cyclicity. The vertical range of 8 meters is greater than that observed for the sandy gravel facies in the particle size dataset of 5.5 meters.
Figure 31. Horizontal experimental semi-variograms for the drill log dataset. a & b) Horizontal semi-variograms for the silty sand and fine sand facies were well defined given the larger number of boreholes with drill log data. c) The semi-variogram model for the coarse-sand facies model is not well constrained, as the data points near the origin are based on an insufficient number of pairs to consider them as reliable data points. d) The gravelly sand facies model has two outlying data points near the origin that greatly influence the horizontal variogram. e) The semi-variogram model for the sandy gravel facies has a range of about 10 m, which coincides with the horizontal continuity observed in the gravel facies at Pit 30.
Figure 32. Nested semi-variogram models for the Drill log dataset. a) The vertical range for the silty sand facies is 9 meters, and the horizontal is 40 meters. b) The fine sand facies has a vertical range of 4 meters and a horizontal range of 18 meters. c) The vertical and horizontal range for the course sand facies is 8 and 13 respectively. d) The vertical and horizontal ranges for the gravelly sand facies are 7 meters. e) The sandy gravel facies has a vertical range of 9 meters and a horizontal range of 12 meters.
Figure 33. Nested semi-variogram models for the Particle size dataset. a) The vertical range for the silty sand facies is 5 meters, and the horizontal is 22 meters. b) The fine sand facies has a vertical range of 6.5 meters and a horizontal range of 29.5 meters. c) The vertical and horizontal range for the course sand facies is 4.5 and 8 respectively. d) The vertical and horizontal ranges for the gravelly sand facies are 7 meters. e) The sandy gravel facies has a vertical range of 9 meters and a horizontal range of 12 meters.
Table 9. Horizontal and vertical semi-variogram model parameters by lithofacies utilized for indication simulation. The anisotropy values indicate the finer grained facies are more anisotropic and progressively decrease as the grain size increases.

<table>
<thead>
<tr>
<th>Lithofacies</th>
<th>Vertical Variogram</th>
<th>Horizontal Variogram</th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>Nugget</td>
<td>Sill 1</td>
<td>Sill 2</td>
</tr>
<tr>
<td>Silty Sand (mS)</td>
<td>0.035</td>
<td>0.031</td>
<td>0.010</td>
</tr>
<tr>
<td>Fine Sand (fS)</td>
<td>0.080</td>
<td>0.120</td>
<td>0.030</td>
</tr>
<tr>
<td>Coarse Sand (cS)</td>
<td>0.050</td>
<td>0.042</td>
<td>0.016</td>
</tr>
<tr>
<td>Gravelly Sand (gS)</td>
<td>0.100</td>
<td>0.080</td>
<td>0.014</td>
</tr>
<tr>
<td>Sandy Gravel (sG)</td>
<td>0.050</td>
<td>0.080</td>
<td>0.012</td>
</tr>
</tbody>
</table>

Lithofacies Simulations

Individual realizations displayed in two and three dimensions are visually noisy. Figure 34 is an example of an individual realization displayed in 3-D. The facies seem somewhat erratic, but provide a visual representation of the spatial variability seen in the lithofacies data. Figure 35 is the post-processed mode of all one hundred simulations. The mode presents a measure of the most frequently simulated lithofacies for a vector location, and represents the most probable facies at each grid node.

Reproduction of Lithofacies Proportions and Variogram Models

The input semi-variogram models were generally well reproduced for the lithofacies that have relatively high sample proportion. Figures 36 and 37 compare both the vertical and horizontal semi-variogram model used as input to the simulation program with the results from ten simulations. The semi-variograms of the silty sand facies do not reproduce the input model very well. The silty sand facies was simulated as having thinner layers than the input semi-variogram models suggested. This probably occurs
because that lithofacies contains the smallest proportion of samples in the dataset (Table 10), so there were few data to constrain the variogram modeling for that facies. The model for the coarse sand facies was also constrained by a small proportion of samples. The simulations provide a fair representation of the input model, although the simulations suggest a greater proportion of the simulated volume falls into this facies as well as a more continuous range in the horizontal. The semi-variograms for the simulated fine-sand facies, on the other hand, do a good job of reproducing the input semi-variogram model, although the simulation results appear to have a slightly longer range and a slightly lower proportion of fine sand facies than the input models. The gravelly sand facies simulations also provide a good representation of the input semi-variogram model. The simulations do suggest a greater proportion of samples are gravelly sand than the input model implies (Table 10). The sandy gravel simulations provide the best representation of the modeled semi-variogram. The horizontal simulations suggest a slightly longer range for the sandy gravel facies. Some of the observed differences are possibly due to the influence of the soft data. The soft data have different spatial heterogeneity and different proportions than the hard data. Overall, the simulations appear to provide a good representation of the input semi-variogram models, and thus reproduce the spatial heterogeneity of the facies observed in the data.

Table 10. Proportions for Drill log and Particle size datasets vs. simulated proportions.

<table>
<thead>
<tr>
<th>Lithofacies</th>
<th>Proportion Drill Log</th>
<th>Proportion Particle Size</th>
<th>Mean Simulated Proportion</th>
<th>Min Simulated Proportion</th>
<th>Max Simulated Proportion</th>
</tr>
</thead>
<tbody>
<tr>
<td>Silty Sand (mS)</td>
<td>0.175</td>
<td>0.083</td>
<td>0.075</td>
<td>0.043</td>
<td>0.107</td>
</tr>
<tr>
<td>Fine Sand (fS)</td>
<td>0.252</td>
<td>0.359</td>
<td>0.241</td>
<td>0.191</td>
<td>0.289</td>
</tr>
<tr>
<td>Coarse Sand (cS)</td>
<td>0.164</td>
<td>0.124</td>
<td>0.197</td>
<td>0.153</td>
<td>0.252</td>
</tr>
<tr>
<td>Gravelly Sand (gS)</td>
<td>0.242</td>
<td>0.261</td>
<td>0.306</td>
<td>0.252</td>
<td>0.366</td>
</tr>
<tr>
<td>Sandy Gravel (sG)</td>
<td>0.167</td>
<td>0.172</td>
<td>0.181</td>
<td>0.139</td>
<td>0.221</td>
</tr>
</tbody>
</table>
Modal Simulation Slices

The modal simulation slices provide a look at the most likely simulated value for a given area. Figures 38 and 39 are north-south and east-west slices, respectively, through the three-dimensional mode of all one hundred simulations. The slices were cut through the general location of the wells used for the cross sections. They reveal the heterogeneity within the sediment in the study area. Figure 38 (north-south) consist of an assortment of discontinuous lithofacies. There are several large packages that grade upward into finer-grained facies that are contained within an overall sandy gravel facies. Figure 39 (east-west) provides a more continuous assignment of facies through the study area. There are several successions of somewhat continuous fining-upward sequences. The most probable lithofacies tend to show the same gross distribution of lithofacies packages seen in traditional cross sections (compare with plates 1 and 2). However, the distribution of lithofacies is very heterogeneous within those packages.

Minimum and Maximum Simulation Slices

Figures 40-45 are north-south and east-west in the same locations as the modal simulation slices in figures 38 and 39. The facies distributions within individual simulations seem somewhat erratic, but they provide a visual representation of the spatial variability identified by semi-variogram analysis of the lithofacies data. Figures 40 and 41 are slices from the individual simulation with the greatest proportion of silty sand. Figures 42 and 43 are slices from the individual simulation with the smallest proportion of silty sand. Figures 44 and 45 are slices through the individual simulation with the highest proportion of sandy gravel values simulated. The individual simulations with the
minimum and maximum simulated values for muddy sand and the maximum simulated values for sandy gravel provide a range of lithofacies simulations that should have very different hydrogeologic properties for flow and transport modeling.

Simulation of Hydraulic Conductivity

Figures 46-51 are the minimum and maximum silty sand lithofacies simulations transformed to a realization of hydraulic conductivity. Figures 46 and 47 (max mS) are the hydraulic conductivity slices for the maximum silty sand simulation. The hydrofacies are predominately in the moderate range with small areas of very low hydraulic conductivity (Table 7). The minimum silty sand hydrofacies simulation (Figures 48 & 49) depicts a larger range of hydraulic conductivity values. There are three small areas with the largest hydraulic conductivity values and several areas with moderately high values (Table 7). Figures 48 and 49 also include areas of very low hydraulic conductivity where the silty sand facies is concentrated in small areas. Figures 50 and 51 are the simulated hydrofacies for the maximum sandy gravel simulation. This simulation is very similar to the minimum silty sand hydrofacies simulation. The areas with high hydraulic conductivity values are larger than those for the minimum silty sand hydrofacies. There are larger areas of higher hydraulic conductivity values throughout the simulation. The simulation also includes small areas with very low hydraulic conductivity. Overall, the simulations vary only slightly except within localized areas where the extreme hydraulic conductivity values are simulated.
Figure 34. Illustration of an individual realization displayed in 3-D.

Figure 35. Three dimensional illustration of the post-processed mode of all hundred simulations.
Figure 36. Graphical comparison of vertical semi-variogram input model to the simulated results of ten simulations. a) Silty sand facies. b) The semi-variograms for the simulated fine-sand facies. c) The model for the coarse sand facies. d) The gravelly sand facies simulations also provide a good representation of the input semi-variogram model. e) The sandy gravel simulations provide the best representation of the modeled semi-variogram.
Figure 37 Graphical comparison of horizontal semi-variogram input model to the simulated results of ten simulations.
Figure 38. North-south slice through the three-dimensional mode. The slice consists of an assortment of discontinuous lithofacies.

Figure 39. East-west slice through the three-dimensional mode. The slice provides a more continuous assignment of facies through the study area than the north-south slice.
Figure 40. East-west slice through the maximum silty sand 3D simulation cut through the general location of the wells used for the cross sections. The slice is from the individual simulation with the greatest proportion of silty sand simulated. This represents the simulated maximum silty sand which provides an upper limit of fine grained facies for flow and transport modeling.

Figure 41. North-south slice through the maximum silty sand 3D simulation.
Figure 42. East-west slice through the minimum silty sand 3D simulation cut through the general location of the wells used for the cross sections. The slice is from the individual simulation with the smallest proportion of silty sand simulated. This represents the simulated minimum silty sand which provides a lower limit of fine grained facies for flow and transport modeling.

Figure 43. North-south slice through the minimum silty sand 3D simulation.
Figure 44. East-west slice through the maximum sandy gravel 3D simulation cut through the general location of the wells used for the cross sections. The slice is from the individual simulation with the greatest proportion of sandy gravel simulated. This represents the simulated maximum sandy gravel which provides an upper limit of course grained facies for flow and transport modeling.

Figure 45. North-south slice through the maximum sandy gravel 3D simulation.
Figure 46. East-west slice through maximum silty sand lithofacies 3D simulation transformed to a realization of hydraulic conductivity (e.g. hydrofacies). The hydraulic conductivity values are predominately in the moderate range with occasional small areas of very low hydraulic conductivity.

Figure 47. North-south slice through maximum silty sand hydrofacies. The hydraulic conductivity values are predominately in the moderate range with a fair number of small areas of very low hydraulic conductivity and occasional areas of higher conductivity.
Figure 48. East-west slice through minimum silty sand lithofacies 3D simulation transformed to a realization of hydraulic conductivity.

Figure 49. North-south slice through minimum silty sand hydrofacies. The minimum silty sand transformed simulation depicts a larger range of hydraulic conductivity values.
Figure 50. East-west slice through maximum sandy gravel lithofacies 3D simulation transformed to a realization of hydraulic conductivity. This simulation is very similar to the minimum silty sand hydrofacies simulation.

Figure 51. North-south slice through maximum sandy gravel hydrofacies.
DISCUSSION

Classification Schemes

The classification schemes for both the drill-log and particle-size datasets introduce uncertainty in lithofacies designations. The drill-log classifications are based on the sediment type the driller listed first as the dominant grain size of the sample. Further classification into lithofacies groups relied upon the amount of information the drill log recorded. If the drill log recorded sand and silt the interval was categorized into the silty sand lithofacies without indication of how much silt was present in the sample. Other drill logs recorded qualitative indications of silt content such “a trace”, “or lots of silt”. More complete sample descriptions decreased the uncertainty associated with the lithofacies groupings. The coarse sand facies designation was made only if the drill log stated the sand to be coarse, otherwise it was assumed to be fine to medium sand. Designations between gravelly sand and sandy gravel were made by which was stated first in the log.

Drill-log classifications were also affected by the type of drilling and sampling method used. A large number of the boreholes in the study area were drilled using the “hard tool” drilling and sampling method. The hard tool tends to decrease the grain size of the samples by the pulverizing action of the bit. The addition of water while drilling also increases the possibility of mixing of sediments from previous samples. Most of the samples collected while drilling were placed into glass sample jars. The circumference of the jars was less than cobble-sized sediments. Consequently larger particles were excluded from laboratory analysis because they did not fit into the sample jar. The result
was uncertainty introduced as to whether the sample was representative of the subsurface sediment.

Calibration

The results of the calibration between the drill-log and particle-size datasets suggest there is better correlation between certain facies than others (Table 6). The silty sand facies has an 82% correlation rate. However, this facies was classified from the drill logs only by whether silt was mentioned along with sand. There were relatively few qualitative descriptions that allowed for more accurate division between silty sand, and fine sand or even coarse sand. The result is a high correlation for this facies, but appears as poorer correlation with the sand facies (Fig. 36 and 37 a-b). For example, both the fine sand and the coarse sand have much lower correlation rates at 35% and 24% respectively as a result of the inability to make the distinction from the drill logs. The gravelly sand and sandy gravel calibration appears to reflect the restriction of the size of the sample jar on the particle size. Field observations at Pit 30 suggest a greater proportion of samples are sandy gravel than gravelly sand. The sandy gravel samples correlated only 56% of the time and 39% of the samples were classified gravelly sand. The differences in classifications shown by calibration results are reflected throughout the variograms, and introduced uncertainty into the lithofacies simulations.

Variograms

The vertical semi-variograms support the hypothesis that the flood deposits contain non-random sequences. The variograms contain distinct structures with well
defined spatial correlation which indicates the sediments are not randomly distributed. The particle-size dataset vertical variograms for the fine sand, gravelly sand and sandy gravel facies display a cyclic pattern (Fig. 28 b, d and e). The silty sand, fine sand, gravel sand, and sandy gravel drill-logs dataset also display cyclicity (Fig. 30 a, b, d and e). The cyclicity represents geologic patterns of deposition. The cyclic nature of the variograms confirms the alternating sequences of fine to coarse grained sediments observed in cross section. There is only one variogram that could possibly be interpreted as a pure nugget, i.e. random, and that is the vertical particle size silty sand lithofacies. The sample proportion for this facies in the particle-size dataset is very low at only 8.3%. The true nature of the facies is not regarded to be represented by the small proportion of samples. It is uncertain if this conclusion is accurate due to uncertainty in drill-log classifications and field observations. The drill-log variogram for the silty sand facies is based on a greater proportion of samples. The uncertainty introduced by facies classification generated a larger number of silty sand observations than might be accurate. In that case the facies appears to be cyclic, but could actually be a random distribution of lenses throughout the study area. Field observations of the sandy silt facies appear as lenses in the IDF pit, but are also observed as thin laterally continuous horizontally laminated beds.

The horizontal semi-variograms confirm the hypothesis that the lateral continuity of the fine-grained facies tends to be greater than the coarse-grained facies (Fig. 29 and 31). The silty sand facies has a horizontal range of approximately 25 meters and the fine sand around 30 meters. The coarse sand and gravelly sand facies show substantially shorter horizontal continuity of 8 and 7 meters respectively. The sandy gravel facies
range is somewhat unexpected in that it is slightly less than the silty sand facies at approximately 20 meters. This could be the effect of a larger proportion of samples for the sandy gravel than gravelly sand in the drill-logs dataset. The horizontal range observed in Pit 30 for the gravelly facies was approximately 50 meters. The difference noticed between the observed and the modeled range is influenced heavily by data points honored near the origin of the variogram. By excluding the somewhat outlying data points in both the gravelly sand and sandy gravel facies the horizontal range would be closer to that of the observed of approximately 40-45 meters. If the horizontal range for the sandy gravel were 40-45 meters, then the hypothesis that the fine-grained facies are more laterally continuous would be rejected.

Variogram Reproduction

The reproduction of variograms from simulated values emphasizes the differences between the hard and soft datasets (Fig. 36 and 37). The silty sand facies was simulated as more laterally continuous than the input model suggests. This was most likely the result of the small proportion of hard data points to constrain the simulations. The larger proportion of samples for the soft data silty sand facies greatly influenced the simulations. The drill log semi-variogram for silty sand depicts the facies as more laterally continuous. The simulations reproduce the spatial structure of the silty sand facies classified from drill logs more accurately than the particle-size dataset. The coarse sand facies is similar to that of the silty sand facies in that the input model was constrained by a small proportion of samples and heavily influenced by the soft dataset.
The differences in the model inputs and the simulations are a direct result of the soft data influence. Comparing the proportions of hard data with the simulated proportions reveals the relationship of the soft data to the simulation results. For example, the proportion of silty sand facies are low and fine sand facies is high for the hard dataset. The soft dataset proportions are higher for the silty sand and lower for the fine sand, thus reflected in the simulations as a higher proportion of samples as silty and lower proportion for the fine sand facies. The coarse sand and gravelly sand facies are similarly represented in the simulations. The qualitative grouping of the drill-logs classification scheme tends to dictate the distribution of facies in the simulations.

3D Model
Individual Simulations

The facies distributions within individual simulations appear to have a random distribution at first look. The distributions of facies are not random as identified by semi-variogram analysis of the data. Closer examination of the borehole data, cross sections and field observations also reveal the heterogeneity within large packages of sediments. The individual simulations represent the variability seen in the geologic data. The facies inter-finger with one another or grade to another. Re-examining the photographs taken at Pit 30 reveals a similar complex and erratic distribution of facies. Most geologists tend to smooth out differences in facies distributions without even realizing they are doing so. Geostatistical methods rely on the data to draw the picture, which is sometimes different than what is perceived. The end result is much different than ‘layer cake’ stratigraphy, but provides a better representation of how the sediments are distributed spatially.
Multiple realizations allow for consideration of many different possible facies distributions. The visualization for many different realizations enables the geologist to see how the facies distributions change spatially. For example, the minimum and maximum realizations for silty sand display similar distributions in specific areas where they were constrained by nearby borehole data. The distribution of silty sand in the maximum realization is somewhat evenly dispersed throughout the study area. The distribution of the silty sand in the minimum realization is more concentrated spatially. The generation of multiple realizations provides a quantitative estimate of the spatial uncertainty in the lithofacies distributions produced by geologic heterogeneity given the available data.

Modal Simulation and Stratigraphic Cross Section

The stratigraphic cross section was correlated in large packages of similar lithofacies. The need for geostatistical analysis was apparent when comparing the layers to the heterogeneity within the layers. The facies within the layers are notably different, but capturing the heterogeneities within the cross section was difficult. The modal simulation also captures the heterogeneity that the traditional ‘layer cake’ cross section does not. The overall distribution of sediments is somewhat similar to that in the traditional cross section. The differences are within the spatial structure of the lithofacies. The traditional method defines layers that have significant heterogeneities, but does not portray the heterogeneity within the layer. The modal simulation allows for the facies to be spatially independent of one another with no pre-defined layering, thus creating a more realistic representation of the heterogeneity of the sediments and their spatial distribution.
Compare with Previous Models

The individual realizations are considerably different than previous models of the study area. The detailed geologic cross sections constructed by Price et al (1979) provide a stratigraphically simple layered characterization of the sediments. However, the modal simulation is similar to the cross sections created by Price et al (1979). Comparable to the cross sections created for this study, the Price cross sections smooth out heterogeneities within the layers. Price attempts to capture some of the heterogeneities within the layers by including lenses in the cross section where sediments are notably different from the stratigraphic layer.

The flow and transport model constructed by Piepho (1996), for an area near the 216-Z-1A crib, was based on hydrogeologic properties derived from a geologic ‘layer cake’ representation of the subsurface. The model is similar in nature to that of the Price et al. (1979) geologic model. As a result the heterogeneities with in the stratigraphic layers were not captured for flow and transport modeling.

Hydraulic Conductivity Simulations

The geostatistical simulations were used as the basis for generation of hydraulic conductivity simulations by assigning a distribution for each lithofacies. The result is a hydrofacies distribution that to some extent mimics the distribution of extreme lithofacies (e.g., silty sand or sandy gravel). The overall distribution of hydraulic conductivity is somewhat similar, but areas of extreme conductivity values will dictate flow models. These simulations reflect the heterogeneity within the sediments which will enable a more accurate flow and transport model. For example, the minimum silty sand
hydrofacies simulation captures both high and low areas of hydraulic conductivity in a relatively small area. Traditional flow and transport modeling would combine this area into one or the other hydraulic conductivity value. Although the areas with different hydraulic conductivity values seem to be relatively small, they are positioned in the center of the crib. This is significant in that the majority of the waste was distributed through a pipe in the center of the crib. The hydrofacies simulations are believed to provide a more accurate model to determine the distribution of those wastes through the sediments.

The gravelly sand and sandy gravel horizontal variogram range models were strongly influenced by often questionable data points near the origin. This greatly reduced the horizontal range of the variogram models. The study would benefit from testing alternative models for the horizontal variograms for the gravelly sand and sandy gravel facies and generation of new simulations with the new model parameters. This would allow for comparison of the two simulation groups and would allow testing of the effect of a longer horizontal range for coarse sediments on flow and transport modeling.

CONCLUSIONS

The calibration results demonstrated the usefulness of the drill-log classifications as soft data. The calibration of lithofacies classes from different sources was used to derive estimates of the probability distributions relating "soft" drill-log data to the "hard" particle-size data. This enabled the use of drill-log data as soft indicator data in the indicator simulation process with a measurable degree of confidence. The uncertainty associated with the soft data classifications were influenced by the drill and sample
method used during the drilling operation as well as the qualitative nature of the sediment descriptions by the driller’s.

The study would benefit from particle-size analysis of archived borehole samples to decrease the uncertainty associated with the qualitative classification of drill logs for the silty sand, fine sand and coarse sand facies. Then re-calculate semivariograms with the new data to determine if the range and structure is consistent with the initial qualitative classifications. If new semi-vario-grams are substantially different from the original drill log semi-vario-grams re-run the simulations utilizing the new data.

Traditional ‘layer cake’ stratigraphy often used in flow and transport modeling does not capture the heterogeneity within the Hanford formation sediments. Individual geostatistical simulations express the spatial heterogeneity of the lithofacies identified by semi-variogram analysis. The spatial variability identified in the lithofacies data is conveyed through multiple realizations. The most probable lithofacies simulation, based on the mode of all one hundred simulations, is comparable to the interpretive stratigraphic cross section of the study area. The generation of multiple realizations provides a quantitative estimate of the spatial uncertainty in the lithofacies distributions.

The realizations will provide an improved geologic model for contaminant flow and transport modeling of the study area. The use of multiple realizations will provide an estimate of the uncertainty caused by geologic heterogeneity in flow and transport predictions.
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