Geologically based model of heterogeneous hydraulic conductivity in an alluvial setting

Graham E. Fogg · Charles D. Noyes
Steven F. Carle

Abstract Information on sediment texture and spatial continuity are inherent to sedimentary depositional facies descriptions, which are therefore potentially good predictors of spatially varying hydraulic conductivity (K). Analysis of complex alluvial heterogeneity in Livermore Valley, California, USA, using relatively abundant core descriptions and field pumping-test data, demonstrates a depositional-facies approach to characterization of subsurface heterogeneity. Conventional textural classifications of the core show a poor correlation with K; however, further refinement of the textural classifications into channel, levee, debris-flow, and flood-plain depositional facies reveals a systematic framework for spatial modeling of K. This geologic framework shows that most of the system is composed of very low-K flood-plain materials, and that the K measurements predominantly represent the other, higher-K facies. Joint interpretation of both the K and geologic data shows that spatial distribution of K in this system could not be adequately modeled without geologic data and analysis. Furthermore, it appears that K should not be assumed to be log-normally distributed, except perhaps within each facies. Markov chain modeling of transition probability, representing spatial correlation within and among the facies, captures the relevant geologic features while highlighting a new approach for statistical characterization of hydrofacies spatial variability. The presence of fining-upward facies sequences, cross correlation between facies, as well as other geologic attributes captured by the Markov chains provoke questions about the suitability of conventional geostatistical approaches based on variograms or covariances for modeling geologic heterogeneity.

Résumé Les informations sur la texture des sédiments et leur continuité spatiale font partie des descriptions de faciès sédimentaires de dépôt. Par conséquent, ces descriptions sont d'excellents prédicteurs potentiels des variations spatiales de la conductivité hydraulique (K). L'analyse de l'hétérogénéité des alluvions complexes de la vallée de Livermore (Californie, États-Unis), sur la base de descriptions de carottes relativement nombreuses et de données d'essais de pompage, montre que l'hétérogénéité souterraine peut être caractérisée par une approche des faciès de dépôt. Des classifications conventionnelles de la texture de la carotte montrent une corrélation médiocre avec K; toutefois, une amélioration ultérieure des classifications de texture en faciès de dépôt de chenal, de levée d'inondation, de coulée boueuse et de plaine d'inondation a fourni un cadre systématique pour une modélisation spatiale de K. Ce cadre géologique montre que le système est composé pour l'essentiel par des matériaux d'inondation à très faible perméabilité ; ceci laisse envisager qu'on ne peut pas supposer que K suit une distribution log-normal, sauf peut-être à l'intérieur de chaque faciès. Une modélisation par chaîne de Markov de la probabilité de passage, représentant la corrélation spatiale dans les faciès et entre eux, prend en compte les faits géologiques intéressants tout en fournissant une approche nouvelle pour une caractérisation statistique de la variabilité spatiale des faciès. La présence de séquences à faciès tronqués vers le haut, d'une corrélation croisée entre faciès, ainsi que d'autres caractères géologiques pris en compte par les chaînes de Markov conduisent à se poser des questions sur l'adéquation des approches géostatistiques conventionnelles utilisant les variogrammes ou les covariances pour modéliser l'hétérogénéité géologique.

Resumen La información respecto a la textura de los sedimentos y la continuidad espacial es inherente a las descripciones de las facies deposicionales sedimentarias. De este modo, estas descripciones se convierten en excelentes predictores potenciales de las variaciones espaciales de la conductividad hidráulica (K). El análisis

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Graham E. Fogg (✉) · Steven F. Carle
Hydrologic Sciences, University of California, 1 Shields Avenue, Davis, California 95616, USA
Fax: +1-916-752-5262
e-mail: gefogg@cicdavis.edu

Charles D. Noyes
Weiss Associates
5500 Shellmound St., Emeryville, CA

Present address: Steven F. Carle, Lawrence Livermore National Laboratory, P.O. Box 808, Livermore, California 94551, USA

de la heterogeneidad en un aluvial en el Valle de Livermore (California, EEUU), a partir de las relativamente abundantes descripciones de testigos y de datos de ensayos de bombeo es una muestra del método de la facies deposicional para caracterizar la heterogeneidad subsuperficial. Las clasificaciones texturales convencionales de los testigos muestran una correlación pobre con K; sin embargo, el posterior refinamiento de la clasificación en canales, diques, flujo de derrubios y llanura de inundación revela un marco sistemático para la modelización espacial de K. Este marco geológico muestra que la mayor parte del sistema está compuesto por materiales de la llanura de inundación, de muy baja permeabilidad, y sugiere que no debe asumirse que K tiene una distribución log-normal, excepto quizás para cada facies por separado. Un modelo de cadena de Markov, tanto para representar la correlación espacial en cada facies como la relación entre las distintas facies, capta las características geológicas más importantes, a la vez que presenta un nuevo método para la caracterización estadística de la variabilidad espacial de las hidrofacies. La presencia de secuencias de facies más finas hacia la superficie, la correlación cruzada entre facies y otros atributos captados por las cadenas de Markov cuestionan lo adecuado de los métodos geoestadísticos convencionales basados en variogramas y covarianzas para modelar la heterogeneidad.

Key words USA · alluvial · sediments · heterogeneity sediments · statistical modeling · hydraulic conductivity

Introduction

Hydrologists generally agree that detailed characterization of subsurface heterogeneity can substantially improve reliability of models of groundwater contaminant transport (e.g., Fogg 1986; Anderson 1987; Johnson and Dreiss 1989). The lack of tractable, proven methods for accomplishing this characterization, however, remains a formidable obstacle to progress in predictive transport modeling.

Inverse techniques (Hill 1992; Yeh 1986; Carrera and Neuman 1986) provide important information on the general trends in transmissivity or hydraulic conductivity (K) but not on the finer details of heterogeneity that can substantially influence transport (Fogg 1986). More recent approaches combining inverse methods as well as geophysical and hydrologic data (McKenna and Poeter 1995; Copty and Rubin 1995) show promise, but application of these techniques to real systems is still in developmental stages, and the relationships between hydrologic or geologic attributes (e.g., K or geologic facies) and the surface geophysical signal (e.g., seismic or electromagnetic) are still elusive. Statistical models of heterogeneity have become popular as a means of representing generic or theoretical heterogeneity in K (e.g., Freeze 1975; Gelhar and Axness 1983; Dagan 1990; Neuman 1995). These models are commonly based on assumptions that K is distributed log-normally and varies spatially according to an exponential covariance or power-law variogram representing hierarchical scales of heterogeneity. Applying this approach to typical field sites, however, is problematic because actual K data that are needed to support the assumed probability density function and covariance or variogram models are commonly lacking. Furthermore, as discussed herein, important structural patterns in K may not be adequately captured by covariance or variogram models.

Indicator geostatistical modeling techniques (Johnson and Dreiss 1989; Deutsch and Journel 1992; Ritzi et al. 1995; McKenna and Poeter 1995; Carle and Fogg 1996, 1997; Carle et al., 1998), which are capable of modeling K or geologic facies as categorical variables, provide a means of using the commonly rich information on geology or hydrostratigraphy to guide characterization efforts. In this approach, one attempts to categorize the heterogeneity in terms of hydrogeologic facies to which an effective value or a probability density for K can then be assigned. In hydrologic studies of unconsolidated systems, the chosen "facies" are typically based on sediment texture (e.g., sand, silt) rather than the local depositional environment (e.g., fluvial channel or overbank deposits). Depositional facies, which have characteristic geometries, provide theoretical basis for estimating plausible indicator covariance or variogram models using typically sparse data sets (Fogg 1986, 1990; Webb and Anderson 1996). Koltermann and Gorelick (1996) provide a comprehensive review of techniques for characterizing sedimentary heterogeneity.

Although more data are generally available for conditioning indicator methods as compared with methods based on continuously varying K, little research has been devoted to the problem of selecting facies that have characteristic K values and predictable spatial continuity. The geometric context inherent to depositional facies may provide the necessary spatial-predictive context, but few published demonstrations of the approach exist in the hydrology literature.

This paper presents a statistical model of heterogeneity based on alluvial depositional facies rather than textural facies or continuously varying K. Using geologic characterization created with abundant core descriptions and geophysical logs coupled with data on K from field pumping tests, we show how K varies within and among the facies. Geologic conceptual models then provide a logical basis for predicting lateral spatial variability, which is difficult to characterize because lateral extent of the facies tends to be significantly smaller than the borehole spacing. Furthermore, a transition probability approach to modeling spatial variability among the facies is outlined, including an example for the vertical direction. The transition probabilities are modeled with Markov chains that are rich in geologic information that is either not contained or difficult to incorporate into standard geostatistical models of the covariance or variogram. The results provoke questions about suitability of the presently widespread assumptions among hydrologists that a log-normal distribution can be tacitly assumed for K, and that simple covariance or variogram functions capture the relevant features of spatial variability in K.

Study Area

The subject of this study is a portion of Lawrence Livermore National Laboratory (LLNL), Livermore, California, USA, a Superfund site where volatile organic compounds trichloroethylene (TCE), tetrachloroethylene (PCE), and chloroform and fuel petroleum hydrocarbons, have contaminated the underlying groundwater (Webster-Scholten and Hall 1989). Locations are shown in *Figure 1*. The LLNL site represents one of the most extensive, densely sampled field sites in an alluvial-basin setting of the western United States. The data set includes many detailed geologic core descriptions from closely spaced wells, a large amount of archived core from both the saturated and unsaturated zones detailed soil-analysis data, and numerous hydraulic conductivity estimates from field aquifer tests. These data provide a unique opportunity to study the relationship between hydraulic conductivity and sedimentary facies. This study focuses on a subregion of LLNL known as the Treatment Facility A Area, which contains approximately 5500 m of core descriptions made by previous investigators.

The LLNL is located in the southeastern portion of Livermore Valley, an east/west-trending topographic and structural basin within the Diablo Range, part of the Coast Ranges (Carpenter et al. 1984). The younger sedimentary fill, consisting of fluvial and lacustrine sediments of Pliocene to Holocene age (CDWR 1966; Blume 1972; Dibblee 1980; Thorpe et al. 1990) contains the main aquifer systems of concern.

Most of the data shown herein come from shallow Quaternary-age alluvium and the Upper Member of the Livermore Formation (Pliocene–Pleistocene age), consisting predominantly of terrestrial gravel, sand, silt, and clay deposited in an alluvial-fan setting (CDWR 1974; Dibblee 1980; Thorpe et al. 1990). Total thickness of the valley fill locally exceeds 1200 m. Conventional analysis of geologic cross sections indicates that individual sand and gravel layers within the fan lobes are laterally discontinuous. Recent geostatistical and groundwater flow modeling by Carle (1996) and Carle et al. (1998), however, strongly suggests that the channel sand-and-gravel units are extensively interconnected in three dimensions.

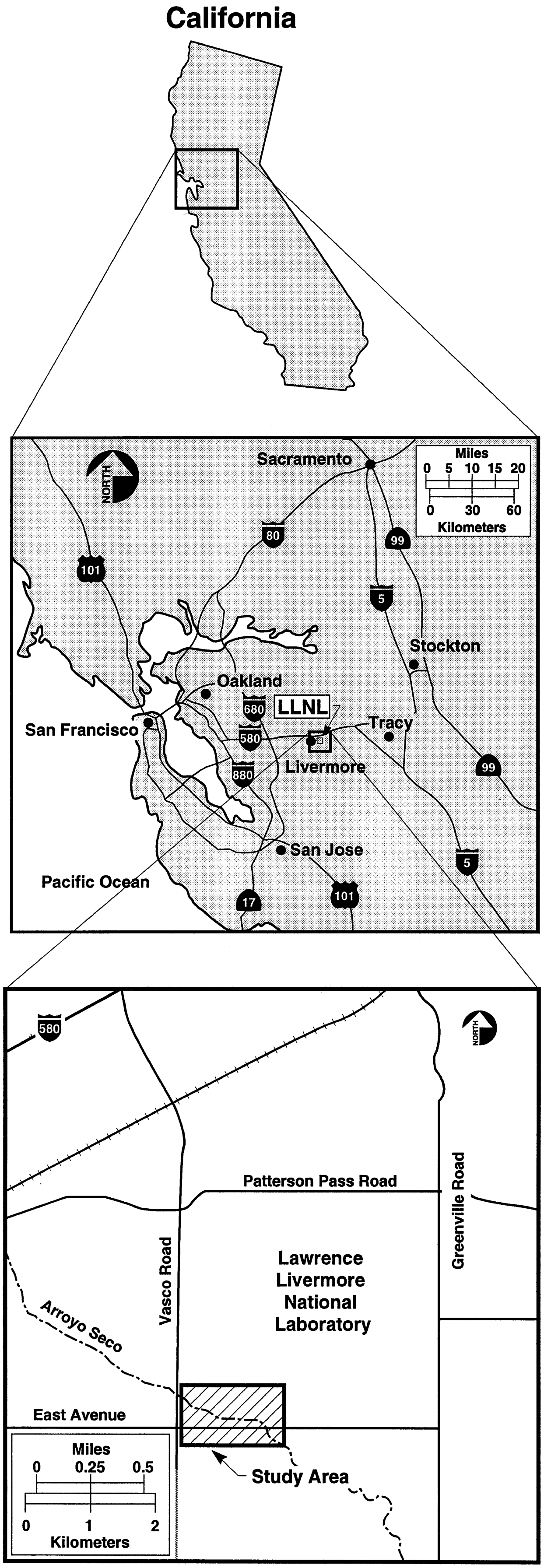

Fig. 1 Location of study area

Data

The geologic, hydrologic, and geophysical data were provided directly by LLNL or were obtained from Qualheim (1988) and Thorpe et al. (1990). Following the construction and development of LLNL monitoring wells, LLNL and its environmental contractor, Weiss Associates, performed pumping tests on each well. The pumping tests are of two types: "drawdown" tests (1-h pumping tests) and "long-term" tests (24- to 48-h pumping tests). The pumping-test interpretations (transmissivity and hydraulic conductivity) were obtained using the techniques of Theis (1935), Cooper and Jacob (1946), Papadopulous and Cooper (1967), Hantush and Jacob (1955), Hantush (1960), and Boulton (1963). Where a conventional pumping test could not be run in a monitoring well, a slug test was performed. The method of Cooper et al. (1967) was used to determine aquifer parameters where slug tests were run.

The investigators rated the hydraulic tests based on the "uniqueness" of the curve matches. An "excellent" rating means that the type curve match is considered to be unique; a "good" rating means some confidence exists that the curve match is unique; a "fair" match means low confidence exists that the curve match is unique; and a "poor" match means that a curve match could not be obtained. Preliminary screening of the data indicated the best correlations between textural facies and K occurred if the "poor" long-term data and all but the "excellent" short-term data were removed from the analysis.

Available LLNL monitoring-well composite logs are catalogued in the Well Log Report for the LLNL Ground Water Project (Qualheim 1988). The composite logs include geophysical logs (caliper, spontaneous potential, gamma ray, and resistivity), well-completion information, a graphic lithic log, lithologic descriptions and remarks, and well-construction data.

All sediment samples at the LLNL site, including the sedimentary sequences logged in monitoring wells, are described by LLNL and Noyes (1991) using the Unified Soil Classification System (USCS; ASTM 1986). Although the USCS was designed primarily for use in evaluating the engineering properties of soils, it is used widely by the environmental consulting industry to describe unconsolidated sedimentary sequences. The USCS system groups "soils" according to their grain size, grading, and Atterburg limits.

The USCS core descriptions provided by LLNL were made by geologists who characterized the core as it was being collected and later refined their descriptions mainly through visual inspection of archived core. To our knowledge, sieve analyses of grain size was not generally done, and the USCS classifications are based primarily on visual and tactile inspection. A significant amount of cored sediments from LLNL monitoring wells had been archived and was reexamined by Noyes (1991).

Objectives and Methods

The objectives are to elucidate relationships between depositional facies and K in alluvial materials and to demonstrate a technique for characterizing spatial variability of K based on the geologic architecture. Ultimately, the abundant core data together with the less abundant data on measured K are to be used in geostatistical modeling procedures to produce the best possible estimates of three-dimensional distribution of K in a $1.5 \times 1.5 \times 0.1$-km volume of the system with spatial resolution of 5, 10, and 0.5 m in the x, y, and z directions, respectively. Such fine resolution is desired for adequate representation of observed heterogeneities (Carle and Fogg 1997; Carle et al., in press) and of scale-dependent advective-dispersion and molecular-diffusion processes in long-term simulations of aquifer remediation. Molecular diffusion is potentially important in this as well as many other sedimentary systems because of the substantial volume of low-K silt and clay beds within and between the aquifer materials. The K measurements by themselves are inadequate for such a characterization, not only because of their sparseness but also because they represent primarily the non-aquitard materials, which form less than 45% of the system.

The general approach was to first examine relationships between K and textural facies and then between K and depositional facies. Textural facies had already been identified in the standard core descriptions. Identification of depositional facies required additional geologic interpretation based on reexamination of available core and on consideration of the overall environment of deposition. The initial step in this analysis involved determining whether the field pumping- and slug-test data on K could be used to identify characteristic K ranges for each of the predominant sedimentary textures present in the subsurface at the LLNL site. Because most of the screened intervals in test wells penetrated more than one sedimentary texture, each interval had to be assigned a dominant texture that could be logically ascribed to the measured K value. The principal assumption here is that hydraulic conductivities from pumping tests are predominantly a measure of the hydraulic conductivity of the highest K stratum in a screened interval. This assumption is valid when most of the flow is parallel to the strata, as would be expected in the study area.

Composite logs of LLNL monitoring wells (Qualheim 1988) were reviewed to identify screened intervals where only a single, relatively high-permeability sedimentary texture was present. The "relative" hydraulic conductivity of the sediments within a screened interval was evaluated using geophysical-log response and the well-site geologist's descriptions, as noted in the composite geologic logs. Examples of the selected sedimentary sequences include: (a) homogeneous sections composed of a single, relatively high-K sedimentary texture (these were rare); (b) sections in which the bulk of the interval consists of relatively low-permeability sediments with stringers of high-permeability sediments of one predominant texture (e.g., sandy gravel stringers within an interval of clayey, silty sand); and (c) sections where the bulk of the relatively permeable sediments consists of one dominant texture, but minor amounts of another relatively permeable texture are also present. In each of these instances, the hydraulic conductivity measured for the screened interval can be ascribed to a single sedimentary texture.

K was calculated for each selected well by dividing the transmissivity (T) by thickness of the high-K sediments within the screened interval. For the materials encountered, this method provided good K estimates of the high-K sedimentary texture in a screened interval as long as the K of this texture exceeded that of adjacent materials by a factor of two or three.

Statistical analysis of correlation between K and geophysical-log response (resistivity and gamma), as well as texture, yielded poor results (Noyes 1991). The more fruitful procedure proved to be an organization of the K values in terms of both textural and depositional facies.

After dividing the textural facies into two groups consisting of fine and coarse textures, and ranking the facies in each group according to average K and grain size, different populations became evident. Reexamination of available core samples then led to grouping of the textural facies into three different populations representing well known components of the alluvial depositional environment. Core representing the screened intervals of selected wells were described in detail with the aid of dilute hydrochloric acid, a pen knife, a hand lens, and a grain-size comparator chart. Rather than focusing solely on textural characterization, as in the USCS approach, sedimentologic attributes (sorting, texture, average grain size, sedimentary structures, bedding-contact morphology, clast composition, and diagenetic or pedogenic alteration; Reading 1978) were examined and described in a depositional context (Walker 1981). Since much of the sedimentary fill consists of very fine-grained sediments that were not field tested for K, a fourth depositional category, generally representing distal flood-plain deposition, was established.

Lastly, vertical spatial variability of the resulting four depositional facies was quantitatively assessed using transition probability geostatistics (Carle and Fogg 1996) and a large portion of the core-description database. Markov chain models of transition probability are then shown to provide a geostatistical description of spatial correlation and cross correlation along the vertical among the four categories (Carle and Fogg 1997).

Results

Correlation of K and Sediment Texture

Initial plots of K vs USCS texture for all 121 K measurements gave disappointing, noisy results; however, after screening out all the slug-test data, the "poor" long-term pumping-test data, and all but the excellent short-term pumping-test data, some interesting trends emerged, as shown in *Figure 2*. The slug-test data were dropped because they tended to yield K values on the low side and because they constituted a small percentage of the K database.

Sediment textures in *Figure 2* are shown in two groups labeled "fine" and "coarse," which contain the lowest and highest measured K values, respectively. The order of the textural categories within the "coarse" group is in terms of generally increasing grain size and sorting, or increasing expected K to the right. The order of the categories in the "fine" group is in terms of increasing average K values, because the relationship between K and grain size is much more difficult to anticipate in sediments containing amounts of significant fines.

All USCS texture codes for the data in *Figure 2* are from the original descriptions provided by LLNL, with the exception of two instances where intervals were recategorized from gravelly clay (CL) to sand (SP) and sandy gravel (GM), based on reexamination of the core. Benefiting from hindsight, we might have been able to improve on LLNL's descriptions; however, most of the core had already been discarded, so later use of the core descriptions for stochastically or deterministically modeling of K would have to rely on the original LLNL descriptions. Thus, we focused on un-

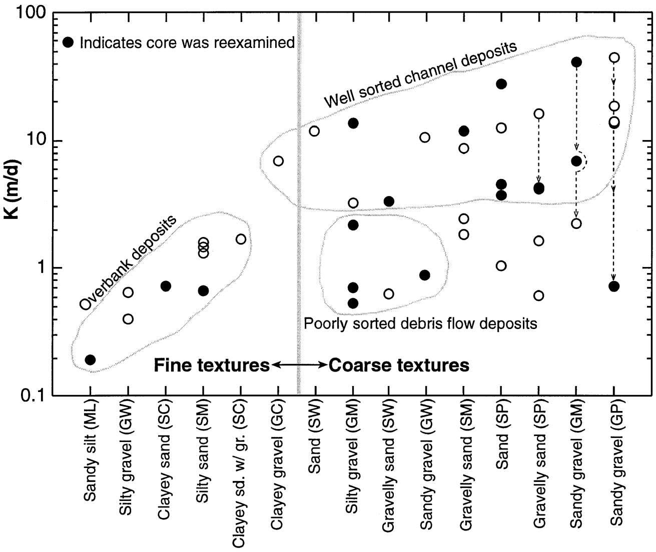

Fig. 2 Hydraulic-conductivity (K) values grouped according to textural facies (abscissa) and depositional facies (*circled*). Letters in parentheses on the abscissa are USCS codes. The first letter indicates the predominant grain size (*G* gravel; *S* sand; *M* silt; *C* clay), and the second letter indicates either grading (*W* well graded; *P* poorly graded) or presence of more than approximately 12% of silt (*M*) or clay (*C*). *Solid circles* indicate that the core was available and was reexamined by Noyes (1991). As used by the well-site geologists, "grading" means the opposite of "sorting" (e.g., "well graded" is the same as "poorly sorted")

derstanding the meaning of LLNL's core descriptions and composite logs in the context of the available K data.

Three data populations are evident in *Figure 2*. K values from the fine-grained textures show an approximately linear trend from higher silt and clay content and poor sorting (e.g., ML, GW) to coarser average grain size and slightly better sorting (e.g., SC, GC). The coarse-grained textures seem to contain two groups: relatively high K values whose maxima tend to increase with grain size and sorting, and significantly lower K values that show no hint of correlation with the textural descriptions.

Reexamination and Description of Cored Material

To determine whether geologic or sedimentologic processes were responsible for the high degree of variation in hydraulic-conductivity values measured in coarser-grained LLNL USCS textures, all available core representing screened intervals of long-term (2-day) pumping-test wells were examined and a detailed sedimentologic description, including facies analysis, was made. A total of 23 screened intervals totaling approximately 280 ft (85 m) of core were examined and described by Noyes (1991). The solid circles in *Figure 2* indicate which wells were studied. Cores for all the other wells were missing or had been discarded.

A close examination of the core material suggests that K variations within coarser-grained USCS textures are primarily a function of the following:

1. Limitations of the USCS description method. The method does not allow for adequate description of sorting, average grain size, and other depositional attributes that can affect K. In some cases, the original core descriptions emphasized the largest grain sizes present, overlooking the presence of dispersed fines that can dramatically reduce K.
2. Alteration of primary porosity by cementation (diagenesis and pedogenesis).
3. Compaction as a function of lithostatic overburden. The dashed lines for the three coarsest categories in *Figure 2* indicate cases where the reduction in K is coincident with increasing depth of the samples.

Other possible sources of noise in the K data are variations in lateral continuity of the cored materials and possible problems with well construction and well development. In the case of poor lateral continuity, the core descriptions would not be representative of the materials controlling flow to the well.

The sedimentary units are interpreted to have been deposited in an alluvial-fan setting. Fan-lobe switching, avulsion of stream channels within individual fan lobes, and other sedimentary processes have led to the formation of complexly interbedded deposits characterized by substantial lateral and vertical heterogeneity.

Hydrogeologic Depositional Facies

Based on Miall's classification scheme for fluvial deposits (Miall 1984), four depositional facies assemblages were recognized in the screened intervals described by Noyes (1991):

1. Well sorted, predominantly coarse-grained deposits composed of sandy gravels (GP, GM), gravelly sands (SP, SM), and sands (SP). These deposits generally fine upward with sharp, erosional bases, are poorly consolidated, and have predominantly grain-supported textures. The deposits sometimes form stacked sequences and only rarely exhibit small-scale cross bedding and other sedimentary structures. The absence of recognizable sedimentary structures may be due to the fact that these sediments are very poorly consolidated and begin to disaggregate upon handling. The deposits exhibit blocky to upward-fining gamma-ray and resistivity-log profiles. Typical sequence thickness ranges from 0.6–3 m. These sediments correspond to Miall's lithofacies Gms, Sp, St, Sr, and Ss and are interpreted to represent stream-channel deposits (channel lag, channel bar, etc.).
2. Poorly to very poorly sorted, predominantly coarse-grained deposits composed of sandy and silty gravels (GW, GM), clayey gravel to gravelly clay (GC, CL), and gravelly sands (SW, SC). In vertical sequence, these deposits have erosional bases and occasionally form upward-fining sequences. The gamma-ray and resistivity-log profiles tend to be highly variable in shape. The deposits are typically very well indurated, with muddy, matrix-supported textures completely lacking in sedimentary structures. Rip-up clasts were observed at the base of several sequences. Typical sequence thickness ranges from 0.6 to 2.4 m. These sediments correspond to Miall's (1984) lithofacies Gms and are interpreted to represent debris-flow deposits.
3. Very well sorted deposits composed of fine-grained sands (SP). This deposit, which was identified in only one screened interval, is characterized by a quartzose, fine-grained sand of extremely uniform grain size that is wholly disaggregated and thus exhibits no sedimentary structures. The sequence was estimated to be approximately 0.9–1.2 m in thickness. This deposit, which corresponds to Miall's lithofacies Sse and She, is postulated to be an eolian deposit. Because of the apparent small amount of this facies and our inability to recognize it on geophysical logs, it was not included as a facies category in the statistical analysis to follow.
4. Poorly sorted, finer-grained deposits composed predominantly of clayey and silty sands (SC, SW), and sandy silts (ML), silts (ML), and muds (silty clays) (ML to CL). These USCS sediments are characterized by (a) subdued resistivity profiles and relatively high gamma-ray responses, (b) occurrence of caliche, rootlets, and carbonaceous fragments, and (c) dense, well-indurated cores exhibiting a lack of sedi-

mentary structures other than mottling and mud (desiccation) cracks. The thickness of these deposits appears to be considerable, ranging from several feet to tens of feet in core. These sediments correspond to Miall's lithofacies Fl and Fm and are interpreted to represent overbank and flood-plain deposits.

More than half of the stratigraphic section consists of the ML and CL textures of item 4 above, but K of these materials was not measured. One could interpret the sandy, poorly sorted, finer-grained deposits as proximal flood plain (levee and crevasse splay) and the ML and CL textures as distal flood plain.

The groups of circled data in *Figure 2* summarize the general outcome of the core analysis. The fine-grained textures are interpreted to be primarily proximal overbank deposits, perhaps with some debris-flow and channel deposits. These overbank sediments would primarily include levee and crevasse-splay deposits, as shown by the fluvial facies model in *Figure 3*. Such deposits tend to be finer grained and less sorted than the channel sediments. The high-K, coarse-grained intervals are interpreted to be primarily well sorted channel deposits. As indicated by the solid circles in *Figure 2*, many cores were available to verify this interpretation.

The five points labeled "poorly sorted debris flow deposits" (*Fig. 2*) exemplify a potential drawback of the USCS system for hydrogeologic description of core samples. Compared with the higher-K values obtained for these same textures (silty gravel, GM; gravelly sand, SW; and sandy gravel, GW), these deposits contain more fines than indicated by the original descriptions and are matrix supported, i.e., the coarse-grained sizes that tend to dominate the descriptions are really floating in a poorly sorted matrix of silt and/or fine sands. Furthermore, the coarser material in the matrix is commonly angular; hence, these samples are interpreted to represent debris flows.

Causes of the low-K values for the seven uncircled points in *Figure 2* are unclear. Likely explanations are compaction and burial diagenesis for at least two of the points (see dashed lines in *Fig. 2*) or overemphasis of the coarser textures when the cores were originally described. Only one of these core samples was available for reexamination, and our description agreed with that of the original description. Unfortunately, despite the existence of abundant geophysical logs, we found no way of successfully separating the "coarse-grained channel deposits" from the "debris-flow deposits" except through examination of actual core.

Extensive diagenetic alteration appears to have masked the primary sedimentary texture of much of the coarser-grained sediments. In several instances, gravel-sized clasts were so severely altered that upon disaggregation, the core broke *through* the grains, not *around* them. This textural alteration made the classification of some of the core using the USCS system extremely difficult. Some USCS classifications may have been misidentified by well-site geologists and subsequently incorporated into the final LLNL composite core descriptions.

Operational Hydrogeologic Facies

The next step is the categorization of the entire geologic database (i.e., the composite descriptive and geophysical logs) in terms of hydrogeologic facies. Although the insight derived from the above-described analysis suggests ways that the geologic descriptions could be improved, we could not reinterpret this massive amount of raw borehole data, mainly because much of the core had been discarded. The goal then was to categorize hydrogeologic facies based on the composite logs and USCS descriptions while incorporating as much of the knowledge gained from the study of texture as well as K and depositional facies.

Analysis associated with *Figure 2* indicates that K is weakly correlated with sediment texture but more strongly correlated with interpreted depositional facies. Sediments that are clearly well sorted, unconsolidated channel deposits yield consistently high-K values, and the overbank deposits have substantially lower-K values. The debris-flow deposits tend to have K values intermediate between the channel and overbank materi-

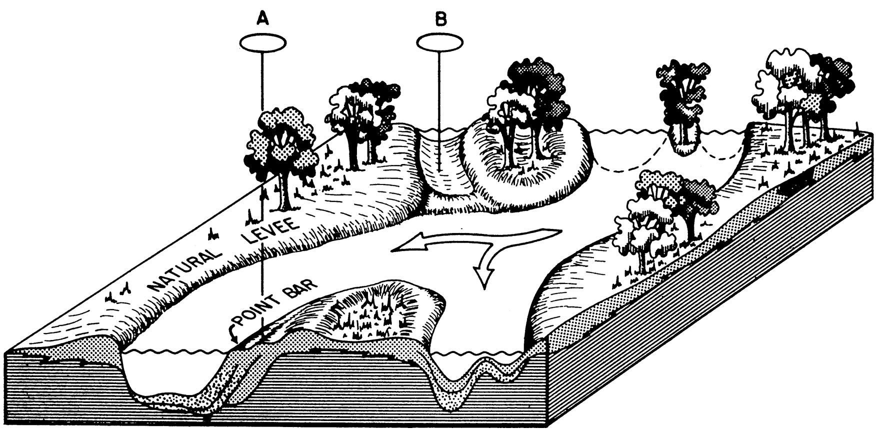

Fig. 3 Facies model for a fluvial depositional system. (From Galloway and Hobday 1983)

als. Perusal of the entire database shows that most of the geologic section comprising the Quaternary-age alluvium and Upper Livermore Formation is comprised not of the materials represented in *Figure 2* but rather of low-K silts and clays that can logically be ascribed to a flood-plain depositional environment. K of these materials is expected to be several orders of magnitude lower than K of the channel deposits; thus, the first priority of the hydrogeologic facies designations should be to represent the extreme K values of channel and flood-plain units. The other categories, i.e., the overbank deposits, debris flows, and the other, lower-K coarse-grained deposits (*Fig. 2*), should have intermediate K values.

Working from the information in *Figure 2*, Carle (1996) used the composite logs and USCS designations to arrive at the operational hydrogeologic facies described in *Table 1*.

The grain size and sorting are mainly from the USCS designations, whereas additional information on sorting, sedimentary structure, and angularity of grains was obtained from other descriptive notes provided in the composite logs. Angular grains are diagnostic of debris flows because they indicate rapid transport and deposition, with little reworking by flowing water.

As used in *Table 1*, "levee" refers to the proximal overbank facies, which is thought to include mainly levee materials. The flood-plain and levee facies were the easiest to determine from the available data. The flood-plain facies is typified by massive, fine-grained texture in cores and characteristic response in resistivity logs. The levee facies essentially corresponds to the overbank deposits in *Figure 2*, and these tend to overlie coarser-grained channel deposits as part of fining upward sequences that commonly occur in alluvial systems. The channel facies essentially corresponds to all the "coarse textures" in *Figure 2*, and the debris-flow facies was identified as intervals containing coarse, angular fragments supported in a poorly sorted matrix of mud (silt and clay undifferentiated).

The channel facies in this interpretation contains some coarse-grained debris-flow and other intermediate-K sediments. As discussed in the previous section, however, we have no way of distinguishing these materials except in those cases where grain angularity and existence of gravel in a mud or fine-grained matrix was indicated. The uncertainty in K of these channel facies can be handled by assuming that all the coarse-grained sediments occur in the vicinity of the actual channel sediments and then assigning K to this "channel" category stochastically, or by assigning an effective K representing a random composite of channel and associated debris-flow sediments. If the true channel sediments, coarse-grained debris-flow deposits, and diagenetically altered coarse sediments commingle, an effective K of approximately 2–8 m/day would be appropriate for the composite (*Fig. 2*).

The debris-flow facies recognized in the core may represent only the coarsest of the actual debris-flow sediments. Much finer-grained materials were probably also deposited by the debris flows and were presumably logged as flood-plain facies. As shown in *Table 1*, the volume of the system interpreted as debris flow is relatively small (7%). Lumping of the fine-grained debris-flow deposits with the flood-plain facies provides little loss of hydrogeologic information, as both facies have very low K. The main reason for distinguishing the coarse-grained debris flows was to separate out materials having primary grain size similar to that of the channels but having lower K values, owing to a high percentage of fines and poor sorting.

The hydrogeologic-facies analysis culminated in the K histogram in *Figure 4*. The K database for the channel, levee, and "other" categories is the same used in *Figure 2*, and "other" in *Figure 4* includes both the debris flows and other coarse-grained materials that registered low K's due to diagenesis, compaction, or possible data errors. The volume fractions of each category in the histogram were adjusted to reflect the "true" volume fractions derived from analysis of all the core *Table 1*. The schematic probability density function for the flood-plain category in *Figure 4* is based on reasonable estimates of K for silt and clay (Freeze and Cherry 1979) and is consistent with more recent K data measured on core (personel comm., A.F.B. Tompson, 1997).

Geometry and Juxtaposition

The depositional-facies approach to designating hydrogeologic facies has two key advantages. Firstly, depositional facies have characteristic geometries. For example, the channel, levee, and debris-flow facies are expected to be elongate, and geomorphic models are available for estimating the width of channel facies based on channel depth (Etheridge and Schumm 1978; Fogg 1990). Secondly, depositional facies point to logical juxtapositional relationships. The levee facies tends to be laterally adjacent to the channels, and the flood-plain facies tends to fill in the areas not occupied by

Table 1 Hydrostratigraphic facies (Carle, 1996)

Facies	Grain size	K (est.)	Sorting	Angularity of grains	Volume fraction
Flood plain	Clay/silt	Low	–	–	0.56
Levee (proximal overbank)	Silt/sand	Moderate	–	–	0.19
Channel	Sand/gravel	High	Moderate/well	Rounded	0.18
Debris flow	Mud/gravel/sand	Moderate	Poor	Some angular	0.07

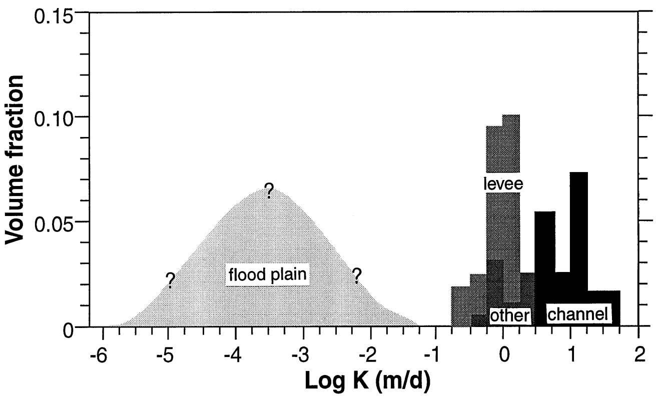

Fig. 4 Histogram showing hydraulic conductivity (K) of the operational hydrogeologic facies. *Other* refers to debris flows and other materials that were described as predominantly coarse grained but yielded K values that were somewhat low. All frequencies were adjusted so that the relative areas represented by each facies correspond to their field volume fractions

channel*s*. Debris flows may tend to deposit in the channels themselves; however, preservation potential of debris flows is probably greater outside of the channels. Thus, locations of the debris flow*s* that are identified are probably somewhat independent of locations of the other facies.

Given that geologic deposition tends to obey Walther's Law (Reading 1978), horizontal juxtaposition provides information on vertical juxtapositional tendencies, and vice versa. In particular, one can anticipate that levee deposits tend to overlie channel deposits, which in turn tend to form sharp, erosive contacts with underlying flood-plain facies. Indeed, such patterns are evident in the descriptive and geophysical logs. The fining-upward sequence is typical of fluvial deposits and should be accounted for in a spatial model. Hydrogeologic significance of such juxtapositional relationships is discussed later in the text.

Transition Probability Model of the Hydrogeologic Facies

Carle and Fogg (1996, 1997), and Carle et al. (1998) developed a transition probability approach for statistical modeling of spatial variability of cross-correlated facies. The approach is based on representation of the spatial structure with the transition probability t rather than the variogram or covariance:

$$t_{jk}(\mathbf{h}) = \Pr\{k \text{ occurs at } \mathbf{x}+\mathbf{h} \mid j \text{ occurs at } \mathbf{x}\} \quad (1)$$

where k and j refer to categories or geologic units, $\mathbf{x}$ is a spatial location vector, and $\mathbf{h}$ is a separation vector (lag). Measurements of $t_{jk}(\mathbf{h})$ on the LLNL core data categorized into the above-described hydrogeologic facies are illustrated in *Fig. 5*. The solid line in *Figure 5* is a one-dimensional Markov chain model for the vertical (upward) direction calculated from

$$\mathbf{T}(h_z) = \exp[\mathbf{R}_z h_z] \quad (2)$$

where $\mathbf{T}(h_z)$ denotes a $K \times K$ matrix of transition probabilities ($K=4$ in *Fig. 5*), z represents the vertical direction, and $\mathbf{R}_z$ is a matrix of transition rates

$$\mathbf{R}_z = \begin{bmatrix} r_{11,z} & \cdots & r_{1,K,z} \\ \vdots & \ddots & \vdots \\ r_{K1,z} & \cdots & r_{KK,z} \end{bmatrix} \quad (3)$$

with entries $r_{jk,z}$ describing rate of change from category j to category k per unit length in the z direction. By differentiation of *Eq. (2)* with respect to h_z at $h_z=0$, the transition rates are related to transition probabilities by

$$r_{jk,z} = \frac{\partial t_{jk}(0)}{\partial h_z} \quad (4)$$

(Ross 1993). Values of $t_{jk,z}$ can be measured on spatially continuous (e.g., core) or discontinuous data by recording transitions between materials j and k (Carle and Fogg 1996). Importantly, the appropriate Markov chain model T(h_z) can be computed by either measuring the $t_{jk,z}$ values and computing $r_{jk,z}$ values, or from information that is commonly available in facies models, i.e., (a) volume proportions of the K categories, (b) mean lengths of certain categories in the chosen direction, and (c) juxtapositional tendencies of facies with respect to an estimated "independent" transition rate $\hat{r}_{jk,z}$, which can be calculated based on volume proportions and the mean lengths (Carle and Fogg 1997). Several approaches exist for calculating an "independent" or "maximum disorder" transition rate. In general, a lack of order in the juxtapositional tendency between facies j and k would be indicated by a measured transition rate equal to the calculated independent transition rate ($r_{jk,z} = \hat{r}_{jk,z}$).

The Markov chain model in *Figure 5* fits the data very closely, despite some of the rather irregular measured t curves. The key item that distinguishes the transition probability technique from standard geostatistical approaches which are based on variograms or covariances is that cross correlations and asymmetry of correlation (e.g., stacked, fining-upward sequences) as well as other geologic attributes are rigorously modeled and readily incorporated from either hard data, geologic conceptual models, or a combination thereof. Furthermore, the procedure of transition probability model building is simpler than construction of indicator cross-variogram or cross-covariance models, particularly when the number of categories exceeds two. In-depth discussion of this approach, including examples, is in Carle and Fogg (1997), Carle (1996), and Carle et al. (1998).

The measured and modeled $t_{jk}(h_z)$ for the channel-to levee transitions is noticeably above the "maximum disorder" curve representing $\hat{r}_{jk,z}$ in *Figure 5*. This is consistent with the observation that the levee facies tends to overlie channel facies. Carle (1996, 1997), and Carle et al. (1998) demonstrate a three-dimensional stochastic modeling procedure based on this transition

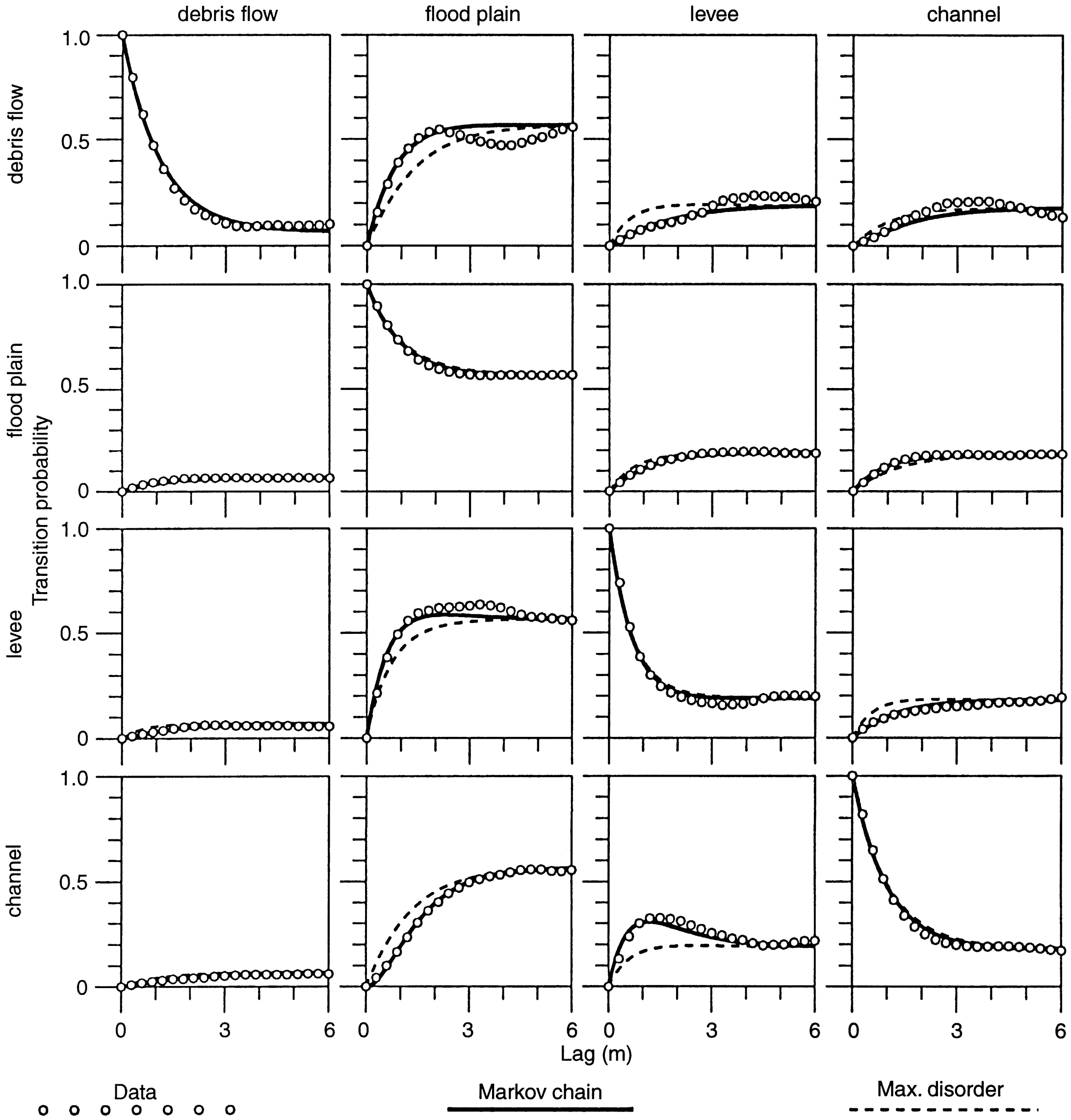

Fig. 5 Matrix of vertical-direction transition probabilities t_{jk}(h) for the operationally defined hydrogeologic facies; core data measurements (*dots*), and Markov chain model (*solid lines*). Maximum disorder (*dashed lines*) represents $\hat{r}_{jkz}$. Plots on the main diagonal represent auto-transitions between like facies, and plots off the main diagonal represent cross-transitions between different facies

probability approach for conditionally simulating spatial distribution of categorical data such as hydrogeologic facies.

Discussion

Models of Heterogeneity

The approach of characterizing subsurface heterogeneity based on categories of hydrogeologic facies is not without pitfalls. Some facies are undoubtedly misidentified. Variability within facies is not necessarily represented unless one makes special provisions to account for it, and expected K's of each facies are sometimes difficult to estimate. For perspective, however, it is useful to consider the alternatives. The approach of measuring K or T values and interpolating or kriging them would lead to an unrealistically smooth parameter field, especially since practically none of the facies can be correlated between wells that are as close as 3–10 m. Modeling the K field as a Gaussian random field with an estimated variogram to represent spatial correlation (e.g., Fogg et al. 1991) might be useful for preliminary analysis but lacks scientific basis in this case because (a) the system shows no indication of conforming to the assumption that K is distributed log-normally (*Fig. 4*), (b) K of the flood-plain facies was essentially not measured, and (c) the erosional contacts and other sharp boundaries would not be represented. Moreover, the horizontal correlation lengths used in the variogram would tend to be speculative and without geologic foundation. We expect the log-normal assumption for

K might be justifiable within individual facies but not over the entire stratigraphic section.

Importantly, the alluvial system studied here is not unique. Most alluvial sediments, with the possible exception of glacial outwash materials, contain a significant volume (20–70%) of variably continuous or lenticular, low-K silt and clay. Furthermore, most K data are collected preferentially from the high-K materials because of historical lack of interest in non-aquifer media and the difficulty of measuring K in tight formations. We can find no studies in the literature in which the entire spectrum of hydraulic conductivities that typify alluvial materials, ranging from clay to sand or gravel, have been measured in one formation or aquifer system and form a log-normal distribution. This leads us to question the legitimacy of the now-widespread assumption in groundwater hydrology that K is distributed log-normally. Indeed, it seems that the K data exhibiting log-normality in the literature are predominantly or entirely from the relatively high-K aquifer materials that form only a fraction of a more complex system. Jensen et al. (1987) present strong arguments based on data and theory that little foundation exists for tacitly assuming that K is distributed log-normally as a general rule.

Neglect of the low-K media when characterizing statistical and spatial distributions of K may be appropriate for analysis of groundwater flow processes as long as one can assume the aquifer media are extensively interconnected. For analysis of transport, however, the low-K media can significantly affect dispersion and matrix diffusion. Stochastic transport models that assume log-normality of K and attempt to model spatial distribution of K throughout the system may not be appropriate for sedimentary environments containing substantial volumes of fine-grained materials.

The excellent detail provided by the transition probability representation of spatial variability along the vertical (*Fig. 5*) indicates the existence of asymmetrical cross correlation (i.e., fining-upward sequences) that could not be captured by cross variograms (Carle and Fogg 1996, 1997). Similarly, studies of flow through structured arrangements of geologic facies by Webb and Anderson (1996) and Scheibe and Murray (1994) conclude that variograms and corresponding geostatistical simulations do not necessarily capture the important geologic heterogeneity. Again, this leads us to question the validity of the common assumption that spatial variability of K can be represented adequately with a variogram or covariance. Certainly, subsurface data often produce sample variograms that closely match exponential or other simple variogram models, but does this imply that such a model captures the relevant features controlling flow and transport? The existence in the LLNL data set of both abrupt transitions (e.g., channel eroded into flood-plain and levee sediments) and gradational transitions (e.g., fining-upward sequences from channel to levee), and the ability of the Markov-chain model of transition probability to capture these features, all suggest that alternatives to the simple variogram or covariance models of K should be considered seriously.

The fining-upward sequences can be quite relevant to transport processes in the subsurface, particularly when the contaminant is a NAPL. For example, an LNAPL in a fining-upward channel-to-levee sequence would tend to migrate upward into the lower-K upper-channel and levee deposits. Remediation efforts would then be exasperated by preferential flow of injected or pumped fluids through the more permeable, lower sections of the sequence, bypassing the LNAPL. Moreover, we anticipate field-scale connectivity of the high-K units and surface area of low-K (e.g., flood-plain) materials encountered by contaminants are partly functions of the facies juxtapositional relationships. Connectivity and surface areas of the low-K media are potentially important influences on the efficacy of remediation.

Role of Depositional Facies in Stochastic Modeling

Although the vertical Markov chain model in *Figure 5* fits the measured transition probabilities very well, well densities are seldom large enough to produce even remotely similar success in the lateral directions. In stochastic modeling, one must then produce a lateral spatial-variability model that is geologically plausible. The depositional-facies context provides the foundation needed to generate plausible lateral models, because the facies connote three-dimensional geometric and juxtapositional characteristics (Galloway and Hobday 1983). Carle and Fogg (1991) devise a geologically and statistically rigorous procedure for constructing three-dimensional models of transition probability. Carle (1996, 1997) and Carle et al. (1998) develop transition probability-based geostatistical procedures for stochastic simulation of cross-correlated geologic facies.

Stochastic models of subsurface hydrogeologic-facies distributions tend to neglect heterogeneities within the facies; however, such models better represent the major patterns in extremes of K that can dominate flow and transport processes. If desired, plausible log-normal K distributions can be assumed within individual facies.

Transferability of Approach

The value of detailed core descriptive data cannot be overestimated, and this study could not have been performed without such data. One might argue that the facies approach used herein is impractical without abundant core data. On the contrary, we believe the facies approach is feasible with substantially fewer data especially if the abundant information on depositional systems concepts (e.g., Galloway and Hobday 1983; Miall 1984; Walker 1981) is integrated into the characterization from start to finish, i.e., from the core-description phase through the modeling of heterogeneity. Although this approach is used routinely in the petroleum industry with substantial success, the concepts are still relatively new to the hydrologic community. The main requirements are (a) keen understanding of the geologic origins of the subsurface system, (b) experience collecting and interpreting core and geophysical information, and (c) stochastic modeling capabilities. In our opinion, as the integration of these concepts and skills becomes more routine, field characterizations of subsurface heterogeneity will become significantly more useful and reliable.

Conclusion

The facies approach to characterizing spatial variability of K provides a workable means of modeling subsurface heterogeneity. The set of alluvial data examined herein exhibit weak correlation between K, sediment texture, and geophysical log response, but fairly strong correspondence to depositional facies that were operationally defined as channel, flood plain, levee, and debris flow. The geometric and juxtapositional information inherent to these facies designations provides a scientific basis for realistic geostatistical modeling of spatial variability. The K data, geologic information, and transition probability models of facies spatial variability in the Upper Member of the Livermore Formation and Quaternary-age alluvium suggest that conventional stochastic models, which assume K is represented by a log-normal distribution and simple covariance, would not adequately represent this system.

The Unified Soil Classification System (USCS), widely used in site characterization by hydrologists, was designed for use by geotechnical engineers and soil scientists primarily to measure engineering properties, not to describe sedimentologic origin or hydrogeologic characteristics. Consequently, the USCS does not directly address influences on K such as sorting, porosity, fines, and diagenesis, or average grain size in detail. For example, a given USCS sedimentary texture, such as "sand (SP)," by definition includes sands ranging from moderately well sorted to very well sorted, and from fine to very coarse grained. From a geotechnical point of view, these sands may be indistinguishable from one another; however, from a sedimentologic or hydraulic point of view, they may be very different.

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