Heterogeneity of Sedimentary Aquifers: effect on microbial dynamics at successive spatial scales as revealed by geophysical imaging: Final report to the Department of Energy on Award DE-FG02-9ER62478

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Introduction

This report describes the geological component of the interdisciplinary study of the experimental aquifer at Oyster, Virginia, by the NABIR program, Department of Energy (Natural and Accelerated Bioremediation Research), between 1997 and 2003, as conducted by the Sediment dynamics group of Old Dominion University.

The Oyster Study was a m,ultidisciplinary study designed to 1) develop new insights into the basic processes that control bacterial transport in aquifers, and 2) extend this experience to metal-contaminated DOE sites. A pristine site was sought for initial field experiments to elucidate the basic mechanisms controlling field-scale transport before transitioning to contaminated sites where this basic understanding could be applied. To meet these needs, the Oyster Scientific Team selected an appropriate field site, are developing procedures for selecting bacteria strains from in situ communities, developed new procedures for tracking bacteria, tested scale-up approaches, and generally designed strategies to facilitate the transport of bacteria within heterogeneous Fe and Al oxyhydroxide-bearing subsurface systems where so much toxic metal and radionuclide contamination resides. To test the hypotheses of bacterial transport in the field, flow cell locations were located at the Oyster site where aerobic and suboxic groundwater exist in proximity within approximately the same hydrogeological unit.

The Geological component of the Oyster study was designed to 1) predict patterns of physical heterogeneity in sedimentary aquifers that control groundwater flow by application of geological first principles, 2) determine the geophysical imaging signatures of these patterns, and 3) relate patterns of physical heterogeneity thus sampled to observed microbial populations. The geological study began in 1997 at the North Oyster site, but in 2002, moved to the south oyster site.

This report summarizes the information generated by the geological component. The information has been published in two papers (Swift et al., 2003; Parsons et al., 2003), Further information can be found in a paper in revision (Muller et al., in revision) and further information being prepared for a fourth paper (Green et al. , in preparation).

Quaternary Facies Assemblages and their Bounding Surfaces, on Virginia’ Eastern Shore peninsula: An approach to Mesoscale Stratigraphic Analysis

A study of the regional setting of NABIR's experimental aquifer on Virginia's Eastern Shore Peninsula of Virginia sheds new light on the relationship between mesoscale stratigraphic units (facies assemblages or "depositional systems") and the bounding surfaces from which they have been formed Swift et al. 2003; Parsons et al.,, 2003). These units were deposited by the coast-parallel progradation of the Pleistocene barrier spit (Eastern Shore peninsula) during successive Quaternary highstands. As a consequence, each segment of the spit complex has been produced by the coast-parallel translation of a relatively small growth area at the spit tip. The distal end of the present (Holocene) barrier system appears to closely resemble the Pleistocene highstand growth area, and this environment consequently serves as a partial analog for interpreting the depositional environment of the fossil highstand deposits.

The many facies patterns present in the spit complex can be reduced to four kinds of facies assemblages (depositional systems), adopting a process-based model (facies template). In this scheme, definitions of both "facies" and "facies assemblage" are more limited than is the case in most textbook definitions in that the facies of a given assemblage are systematically related to each other by grain size and stratal pattern, and also related to a bounding surface ("source diastem") which is the immediate source of sediment for the facies assemblage. Vertical transitions between individual facies are easily identified in outcrop, but the horizontal gradients of facies change are too gentle to be observed over the short dimensions of the borrow pits, and do not have sufficient acoustic contrast to appear on ground-penetrating radar records. However, the facies assemblages, both in the borrow pits and on radar records, stand out by virtue of their sharply defined bounding surfaces (source diastems). The facies assemblage either buries its source diastems or is capped by it.

The assemblages in the spit complex are, in ascending stratigraphic order: (1) several tidal shoal deposits, each underlain by a channel-base diastem, (2) Two shoreface systems separated by a channel-base diastem, (3) an upper shoreface assemblage capped by a surf diastem, and (4) a beach-strandplain assemblage, underlain by the same surf diastem. All of these systems prograded southward as the nose of the spit prograded, and while they did so, zones of erosion cut the bounding surfaces that separate them. Two important bounding surfaces are "conjugate" surfaces, which nourished both the facies assemblage above and the assemblage beneath. As each surface advanced, erosion at their leading edge spilled sediment forward, down the nose of the spit, while sediment was also swept backward, aiding in the burial of the surface. A conjugate surface creates a "sandwich" structure, in which two facies assemblages are separated by the generating surface. Proximal facies are back-to-back across these sediment-spreading boundaries.

Episodic progradation of the spit tip by development of successive, recurved, beach ridges has overprinted the horizontal first-order reflectors (separating facies assemblages) with gently dipping second-order reflectors that separate successive growth increments of the spit. Although less clearly defined, these growth increments are essentially high-frequency autocyclic sequences, and constitute the next higher scale of spatial organization above the depositional systems scale. The manner in which facies have been organized into depositional systems in the late Pleistocene highstand deposits of the Eastern Shore is specific to this estuary-mouth setting. These assemblages are, however, local expressions of a facies “template” that can be generalized to many other settings.

Stratal Architecture of Sedimentary facies at the North Oyster: Relationship to grain size and permeability

A study of the late Pleistocene section of the Eastern Shore Peninsula of Virginia indicates that problems of reservoir and aquifer analysis can be illuminated and simplified by merging sedimentological and hydrological traditions. The Butlers Bluff Member of the Nassawadox Formation is a barrier spit deposit of late Pleistocene age (Isotope Stage 5e) that prograded across the mouth of Chesapeake Bay in a high mesotidal setting, lead to a shoaling-upward, coarsening, and thickening, stratal sequence. In this sequence, baymouth tidal shoal deposits were successively overrun by lower shoreface deposits, marginal shoal deposits, upper shoreface deposits, and strandplain deposits. These successive deposits can be shown to comprise diastem-bounded depositional systems (facies assemblages) that are various arrangements of a few basic facies types (Shelly Gravelly Sand Facies, Cross-Stratified Sand Facies, Horizontally Stratified Sand Facies, and Micro Cross-Stratified Sand Facies).

A review of existing stratigraphic classifications suggests that the critical linkage in resolving the spatial organization of the Butlers Bluff Member is the equating of the smallest mesoscale unit of classical stratigraphy (facies assemblage or depositional system) with the largest unit of the small-scale (stratal) classification scheme, the strata coset, This identification allows petrographic descriptions undertaken at small spatial scales to be extrapolated to larger stratigraphic scales. Strata cosets (equivalent to facies assemblages) are bounded above and below by erosional surfaces, but within the strata coset, successive facies pass one into another through gradual, horizontal facies change. The simple statistical analyses presented in this paper (analyses of variance) demonstrate that for both grain size and permeability, there is greater variance between cosets that within cosets, and correspondingly greater variation among sets than within sets, and that these levels of stratal organization are useful ones for mapping granulometric attributes. Spatial continuity analyses (variograms) detect, but do not fully resolve, stratal geometries through these two scales of organization.

The most useful stratigraphic identification that emerges from this study of littoral and shallow marine sands is the recognition of strata cosets (small scale, or event stratigraphic term) as the equivalent of a depositional system or facies assemblage (mesoscale, or systems stratigraphic terms), allowing petrographic descriptions undertaken a small spatial scales to be extrapolated at larger spatial scales. Such strata cosets (facies assemblages) are bounded above and below by erosional surfaces, but within the strata coset, successive facies pass one into another through gradual, horizontal facies change. Consequently, a strata coset may at a given location be a unique facies body (lithosome) as well as a portion of a facies assemblage (depositional system). The cosets of the oyster pit exhibit a second characteristic behavior of facies assemblages; autocyclic repetition. Cosets A and B are autocyclic repeats of the marginal shoal depositional system. Coset D has been treated as a single facies assemblage for the purposes of this study, but there is reason to believe that in fact the several included “sets” are autocyclically repeated cosets of a distal shoreface facies, whose set structure is so uniform as to be indistinguishable. The spatial scale at which such repetition occurs is the scale at which sequence architect becomes apparaent.

Physical characterization of subsurface heterogeneity at the South Oyster VA, Site: A statistical approach

General,--The closely-spaced data collected in the course of the North Oyster, Virginia, study reveal a more complex stratigraphy than does the regionally oriented study of Mixon (1985). Comparison of cores collected along the centerlines of the flow cells with ground-penetrating radar profiles reveals a succession of high-frequency sequences, apparently the consequence of sea level oscillations during late Pleistocene time. The first two units (here designated the Narrow Channel Sequence and the South Oyster Sequence) form a offlapping succession indicating oscillatory sea level fall, but are overstepped by a third high-frequency sequence, which extends back to the foot of the Mappsburg scarp. The earliest unit, the Narrow channel Sequence, apparently formed a mainland beach “welded” to the Mappsburg scarp, so that no lagoon formed in the back-beach area, as did the later overstepping sequence. The south Oyster sequence, however, developed a back-barrier swale in which salt marshes developed between washover episodes, so that Spartina peat alternates with sand.

As a consequence, the sediments of the Narrow Channel flow cell sediments consist of relatively uniform sand. The upper parts of the cores consist of poorly to moderately sorted, medium-grained, quartz sand. In the middle part of the cores, the sediments consist of an oxidized, orange-gray, medium to very coarse sand, interbedded with gravelly sand. Below the gravelly layer, the sediment is a well-sorted, fine sand with heavy minerals lamina.

At the South Oyster flow cell, the sediments are considerably more heterogeneous. In this area, medium-grained sand, and medium-gray gravelly, medium- to coarse-grained sand layers are interbedded with peat . A very fine micaceous sand with lenses of silt and clay occupies the lower half of the core. The sediments of the Narrow Channel Area correspond to the upper unit of the Wachapreague Formation as defined by Mixon (1985), while in those of South Oyster area both of Mixon’s (1985) units are present. In terms of grain size, permeability distributions, amount of fine-grained material (clay and silt), and organic matter present, the South Oyster Area possesses greater heterogeneity than does the Narrow Channel Area

Defining lithofacies.-- Earlier investigations of the Oyster aquifer (Parsons et al., in press; Swift et al., in press; Mueller et al., in review) have focused on the more heterogeneous Butlers Bluff Member of the Nassawadox Formation. These studies have suggested that a single genetic lithofacies is present in this unit; the amalgamated sand lithofacies, a component of a regressive shoreface-shelf lithofacies assemblage. They have further concluded that this genetic lithofacies can be broken down into several subfacies developed in tidal shoal and inner shelf settings. The amalgamated sand lithofacies is formally designated by both its stratal pattern (beds are poorly discerned to sand-on sand contacts; are amalgamated) and its grain size (sand), and the subfacies are likewise identified by both stratal pattern and grain size. However, lithologic variation is significantly more restricted in the portions of the Wachapreague Formation sampled at the narrow Channel and South Oyster flow Cells. Because its lower altitude (below the Mappsburg Scarp) and the resulting proximity of the water table, it is not possible to develop observation trenches more than one to two meters deep, and stratal patterns are not well resolved in cores. Consequently, we have begun the process of resolving facies by cluster analysis of grain size distributions.

On the basis of the cluster analysis, seven clusters (hereafter called lithofacies) were identified in the South Oyster Site. Perhaps the most important feature of the dendogram is that grain size and organic matter content are the most fundamental parameters in discriminating among lithofacies. The cluster analysis for the fine to gravelly sand sediments of the Narrow Channel Area shows four lithofacies. For South Oyster Area, three additional lithofacies were identified, corresponding to zones of fine sand, or to the peat layers.

In the absence of sedimentary structures (often difficult to resolve in cores), the grain size parameters mean and sorting are the principal elements in the lithofacies classification. At Narrow Channel, the four lithofacies identified are: 1) Poorly sorted Medium-grained Sand (PSM, mean size between 1.0 and 2.0 phi with sorting between 1.0 and 1.5 phi), 2) Moderately sorted Medium-grained Sand (MMS, mean size between 1.0 and 2.0 phi but sorting between 0.5 and 1 phi), 3) Well sorted Fine-grained Sand (WFS, mean size between 2.0 and 3.0 phi with sorting between 0.4 and 0.75 phi) and Poorly sorted Gravelly, medium-gained Sand (PGS, mean size between 1.0 and 3.0 phi, sorting between 1.5 and 2.0 phi, and percent gravel greater than 5%). The Poorly Sorted Gravelly Sand is probably deposit of the alongshore trough (surf zone), with the Poorly sorted Medium Sand, and the Moderately sorted Medium Sand deposited in beach or near-beach settings, and the Well sorted Fine Sand deposited a little further offshore. These lithofacies comprise Mixon's Upper Unit of the Wachapreague Formation (Mixon, 1985).

At South Oyster, three additional lithofacies occur; 5) Well sorted Very Fine Sand (WVFS, mean size between 3 and 4 phi, sorting less than 0.5), 6) Silty sand (S, mean size finer than 4 phi, sorting better than 1, more than 15% silt) and 7) Peat (P, between 0 and 50 % organic matter content). WVFS and S correspond to the lower unit of the Wachapreague Formation. and were probably deposited in a shallow inner shelf setting, while the peat layers were dep[osited in a back-barrie, wsahover flat.

The ANOVA tests indicate that the mean values of the mean diameter measurements are significantly different, as well as the mean values of each criteria used for the cluster analysis (sorting, percent gravel, percent silt, and percent of organic matter content) are significantly different.

Converting Lithofacies to Hydrofacies.-- The hydraulic conductivity values of Oyster facies range between 2 x 10-4 and 10 x 10-4 cm/s in the sand fraction. values of 0 K were assigned to the peat and silty sediments. The correlation of the granulometric attributes (mean grain size and sorting) with hydraulic conductivity (K), is not uniformly high. For example samples of the WVFS (well sorted very fine-grained) lithofacies define a narrow and distinct range of ln K values when compared to samples of the other lithofacies. Alternatively, samples of the PGS (poorly sorted gravelly sand) exhibit a wide range of K values. In the sandy fraction, phi moment standard deviation (sorting) varies directly with phi moment grain size. Finer samples are better sorted (WVFS and WFS). However, sorting is strongly correlated with percent of gravel (PGS) in that as the percentage of gravel increases, the sorting is poor. Since hydraulic conductivity is in part a function of grain size, it also shows a positive linear correlation. However, the hydraulic conductivity is also function of the sorting, and the effect of the coarser grain size of the PGS is neutralized in part by its poorer sorting.

The ANOVA tests indicate that the lithofacies assignment is a significant factor in explaining the variance of hydraulic conductivity and helps to elucidate differences for the definition of hydrofacies. The following key results for K by lithofacies were noted: The P and S lithofacies are not significantly different from each others, but they are both different from all other lithofacies. The hydraulic conductivity values assigned to these lithoface is zero, so these two lithofacies constitute the impermeable hydrofacies. The same test results for other lithofacies. Other lithofacies can likewise be grouped on the basis of permeability. The PMS and WVFS lithofacies are not significantly different from each other, but they are both different from all other lithofacies.The associated hydraulic conductivity values vary from 1 x 10-4 to 3 x 10-4 defining a low permeability hydrofacies. The MMS and WFS lithofacies are not significantly different from each other, but they are both different from all other lithofacies. (space) The hydraulic conductivity values vary from 3 x 10-4 to 6 x 10-4 define a medium permeability hydrofacies. The PGS lithofacies is significantly different from all other lithofacies. This lithofacies presents the highest values of K ranging from 6 x 10-4 to 10 x 10-4 defining a high permeability hydrofacies.

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