A two-stage multivariate approach to identifying ocean outfall plumes based on temperature and salinity profiles

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ABSTRACT

Ocean outfall plumes are often mapped using CTD profiles, but the extent to which particulate plume parameters, such as bacteria, behave like the physical parameters measured by CTDs has not been well tested. Additionally, interpretation of CTD data for plume mapping is typically based on subjective judgment of where physical parameters differ from those of surrounding waters. Here, we present monitoring data spanning two years in which bacterial concentration and CTD profiles were collected simultaneously near a large treated wastewater outfall. These data were used to assess the effectiveness of temperature-salinity (T-S) plots for describing bacterial plume dilution and to test a statistical model for predicting bacterial concentration from T-S data. Elevated bacterial concentrations were found to be consistently associated with subsurface low salinity deviations. We also found that this deviation could be quantifiably defined using a two-stage multivariate approach based on cluster analysis followed by principal component analyses (PCA). Due to the considerable natural variability in T-S relationships, the extent to which this approach can be used as a plume tracer was dependent on the level of detection required. T-S relationships were reliable for identifying the plume when bacterial concentrations were several times water quality standards and were also effective at defining areas from which the plume was absent. The T-S relationships were inconsistent in defining those areas where plume dilution reduced bacterial concentrations to moderate levels, including those approximately equal to that of the water quality standard.

INTRODUCTION

Many types of freshwater effluents, such as those from wastewater treatment or industrial facilities, are discharged into coastal ocean waters because these waters are believed to provide sufficient dilution to minimize environmental harm. This presumption is assessed using a variety of techniques that measure physical, chemical and biological responses. Conductivity-temperature-depth profilers (CTD) collect continuous water-column measurements of physical variables, such as temperature and salinity, to identify plume location and concentration. Physical parameter measurements are often used in lieu of direct measurements of bacteria, nutrients, or other contaminants because CTDs provide continuous measurements with depth and the results are viewable in real-time when connected to a shipboard data acquisition system. Grab sample measurements taken at discrete depths are less spatially descriptive, require additional time to analyze, and are more costly than CTD profiles.

One concern with CTD profiles is that many plume parameters of interest, such as bacteria and viruses in wastewater effluents, can adsorb to particles and may not disperse similarly to soluble constituents such as salinity. Viruses and bacteria have been shown to adsorb onto suspended particles in the marine environment (Chung and Sobsey 1993, MEC and AOS 2001), but it is unclear whether these small particles disperse similarly to the dissolved components or by a separate particle-dependent process. Some work suggests that bacterial association with particles contributes to the sinking losses, where the rate of sinking is a function of the size class of particles (Auer and Niehaus 1993). Particle adsorption and sinking would tend to separate the dispersion of particles from the dispersion of soluble components. With time and distance away from the source, the bacterial abundance could then be offset vertically from the low salinity signature of the outfall plumes. This would also result in horizontal separation due to the vertical shear of currents often observed in the coastal region. On the other hand, dissolved natural fluorescent tracers have been found to correlate with the bacteria concentrations in nearshore regions in Australia, consistent with the bacteria dispersing similarly to the dissolved components (Kaye and Haddad 1992). Recent analyses of the particles dis-

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charged from the Orange County Sanitation District (OCSD) ocean outfall indicate that the sinking rates of discharged particles are extremely small (SAIC 2003). Previous studies from other outfalls have indicated a close association between suspended particles and low salinity associated with the outfall plume (Wu *et al.* 1994).

Adding to the concern about using CTD data to describe a particle-laden plume is that CTD data are typically interpreted based on subjective judgment of where physical parameters appear to differ from those of the unaffected ambient waters. In a few instances, statistical algorithms have been used to define background conditions or the relationship between deviation from background and plume strength. Oceanographers typically evaluate water masses using a Temperature-Salinity (T-S) diagram. These diagrams are not typically evaluated statistically, but rather by comparison with water types having known T-S characteristics. In the case of outfall plumes, the T-S characteristics away and preferably upcurrent from an outfall discharge are used to define the ambient or background T-S characteristics, and the plume mixed with seawater is differentiated from the ambient T-S on the basis of salinities that are below the background levels for a given temperature (Washburn *et al.* 1992, Petrenko *et al.* 1998, Jones *et al.* 2002). However, subjective delineation of the plume can be problematic from a regulatory standpoint. Another approach taken by the City of Los Angeles' monitoring group is to create a depth-dependent average T-S profile and calculate an anomaly based on the difference between the individual measured profile and the depth-averaged profile (City of Los Angeles 2003).

Here, we present a study in which bottle samples for bacterial concentration were collected simultaneously with CTD profiles near a large treated wastewater outfall. These data are used to assess the effectiveness of using T-S relationships to describe bacterial distribution and dilution near the outfall. We also present and assess a statistical approach for predicting bacterial concentration from these T-S data.

METHODS

Our study was based on data collected over two years from a grid of stations surrounding the OCSD outfall, which is located approximately 7 km offshore of the Santa Ana River in southern California (Figure 1). The grid consisted of 17 core stations spaced at 4 km intervals in the along-shore direction
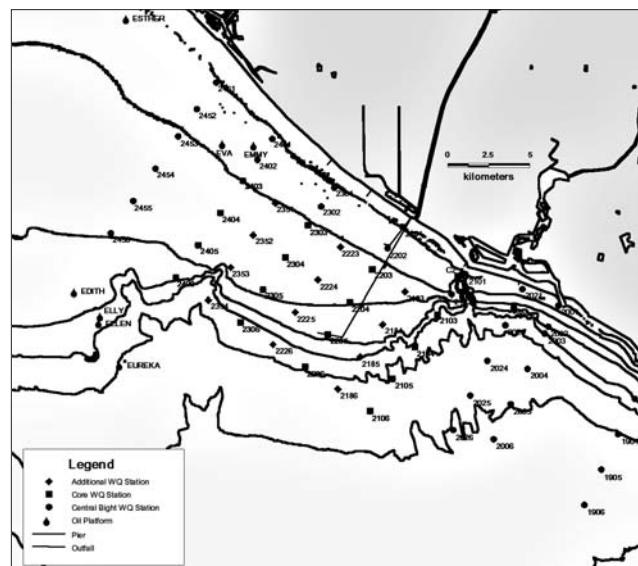

Figure 1. Map of sampling grid superimposed on shoreline.

and at 2 km intervals in the cross-shelf direction. At each core station, continuous CTD profiles were collected throughout the water column and averaged to 1 m depth intervals, and discrete water samples were collected for bacteria analysis at 5 to 15 m depth intervals. CTD profiles were also collected at up to 24 additional stations on some sampling dates. Sampling in 1999 consisted of one survey each month in February and April, two surveys in May, and one survey each month in March, August, and November. Sampling in 2000 consisted of one survey in February, two surveys in March, and three surveys each in May, August, and November.

CTD profiles were obtained using either a Sea-Bird (SBE) 911 or 911plus CTD recording at 24 Hz, or a SBE 25 CTD logging at 8 Hz. Recorded data included temperature, conductivity, pressure, dissolved oxygen, pH, chlorophyll fluorescence, beam transmission at 660 nm (25 cm path length), and photosynthetically active radiation (PAR). Salinity was calculated from conductivity, temperature, and pressure (Fofonoff 1985), and depth in meters was calculated from pressure. Discrete water samples were collected at 5 to 15 m intervals using a multi-bottle carousel water sampler (SBE 33) equipped with PVC bottles and analyzed for *Escherichia coli* (*E. coli*) using the Colilert™ chromogenic substrate technique.

A two-step multivariate approach was used to analyze the T-S data set statistically for the presence and discrimination of the effluent plumes. The first step utilized cluster analysis to parse the data into

hydrographic layers. A non-hierarchical clustering algorithm (SAS FASTCLUS procedure) was used because it allows the number of clusters to be specified prior to application (for a detailed description, see SAS/STAT User's Guide; SAS Institute, Inc. 1989). Three clusters were specified because three distinct layers (near-surface water, a transitional layer comprising the thermocline, and deeper water) were identifiable in the survey data. Prior to clustering, all of the T-S profiles collected on a given day were pooled into one array and standardized to their respective z-scores.
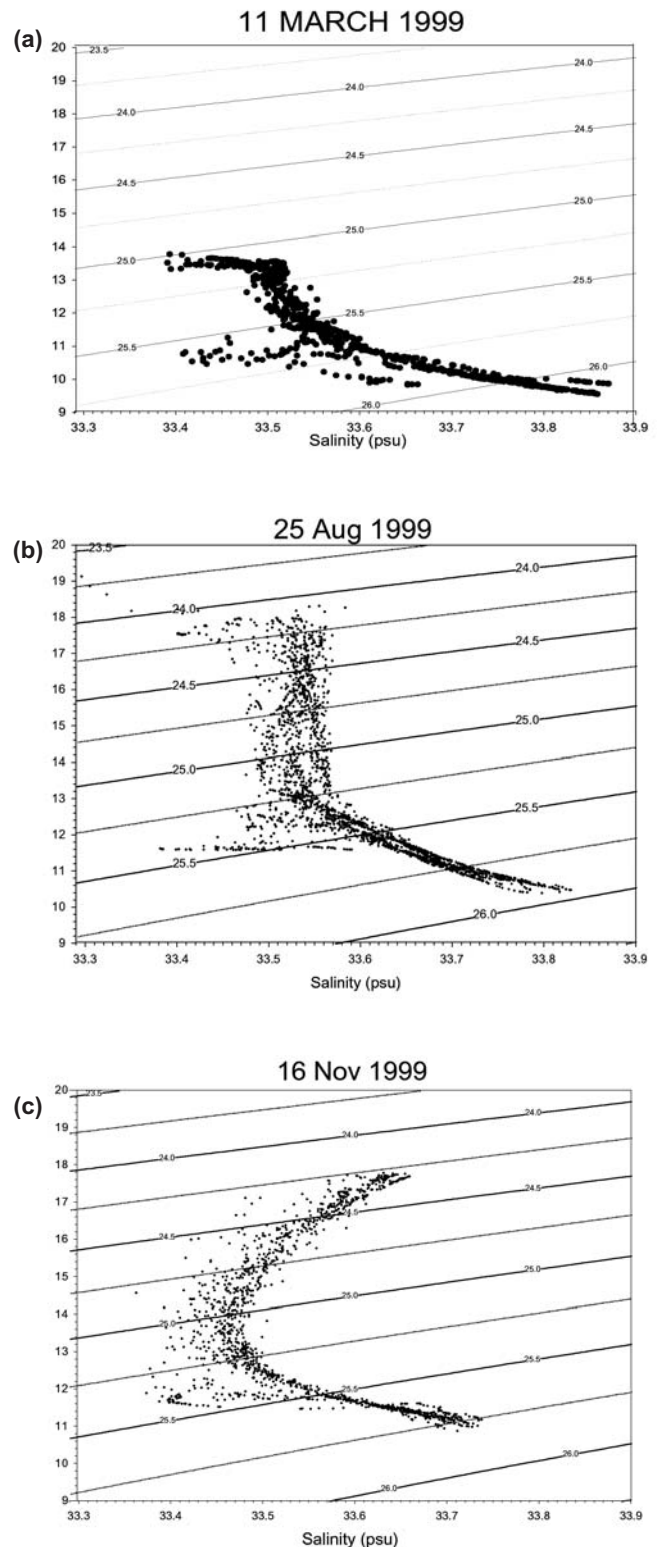
The second step used PCA to distinguish the freshwater effluent from the ambient water based on T-S. PCA was applied only to observations from the transitional (cluster 2) and deeper layers (cluster 3); surface samples (cluster 1) were excluded because previous studies have shown that the thermocline typically serves as a natural barrier that traps the effluent subsurface (Petrenko *et al.* 1998, Wu *et al.* 1994). This was confirmed with bacteria data, which showed that measurable bacteria concentrations rarely occurred near the surface.

RESULTS

Relationship between indicator bacteria and T-S structure

Three types of T-S relationships, corresponding to season, were observed (Figure 2a - c). During the late winter and early spring, surface salinities were generally lower than those found throughout the rest of the year, due to a combination of winter cooling and mixing, coastal runoff, and early upwelling (Figure 2a). During late spring and summer, an isohaline upper layer typically extended from the surface down to the 13°C isotherm. In the August 1999 example, the upper layer salinity ranged from 33.5 to 33.55 psu above temperatures of 13°C (Figure 2b). Subsurface salinity decreased later in the summer, probably due to an increase in low salinity California Current water advecting from the north (Hickey 1979). In the late fall (Figure 2c), surface salinity also tended to increase, possibly associated with warmer, saltier subtropical water advecting from the south (Reid *et al.* 1958). Nearshore, northward flow typically occurs in the late fall and winter associated with the Davidson Current (Hickey 1979).

In all seasons, the T-S relationships partitioned into three distinct depth zones. The first consisted of a surface layer of warm water above the thermocline, which

Figures 2. Examples of three types of temperature and salinity relationships (a - c).

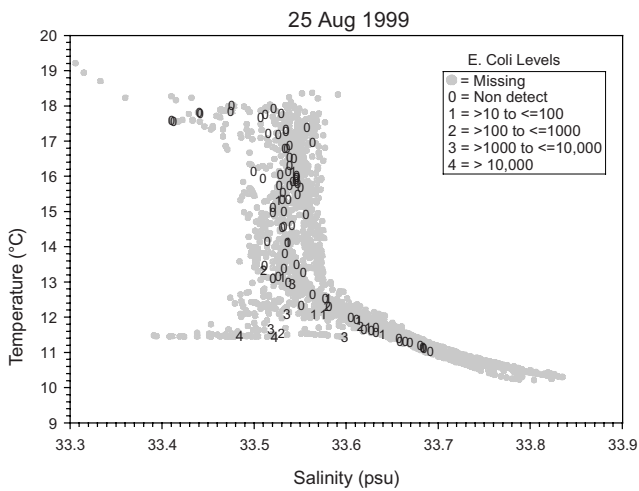was differentiated largely by temperature. The second was a transitional water region of lower surface layer

Figure 3. Temperature and salinity with _E. coli_ concentration.

and deeper water surrounding the thermocline. The third was a deeper region where salinity increased and temperature decreased with increasing depth.

The elevated bacterial concentrations were consistently associated with a low salinity deviation in the second and third layers (Figure 3). In most cases, the maximum salinity deviation (at a particular temperature) was more than 0.2 psu. This compares to a background salinity range at any given temperature of less than 0.1 psu in the upper layer and less than 0.02 psu in the lower layer for the portion of the T-S curve that did not contain bacterially affected water.

Low salinity anomalies were also occasionally apparent in the warmest portion of the surface layer, which is consistent with land-based runoff that remained near the surface due to buoyancy of the low salinity water (Figure 2 a - b). High bacterial concentrations were not observed in this near-surface low salinity water.

Statistical analysis of the T-S distribution

Cluster analysis effectively partitioned the three depth-related water mass regions observed in the T-S plots for both years (Figure 4a - 4b). Cluster 1 had the highest temperature and consisted predominantly of surface waters at depths between 5 and 10 m. Cluster 2 contained the mid-depth samples, centered at depths between 25 and 30 m. Cluster 3 contained the deepest and coldest water, centered at depths between 55 and 60 m. The depth distributions within clusters were nearly identical in 2000 and 1999.

The PCA effectively defined the bacterial concentration gradients observed in the T-S plots. The

first principal components axis corresponded to natural vertical density gradients in the water column (Figure 5). The second axis, more parallel with the density surfaces, was negatively correlated with bacteria concentration ($r = -0.6$). Large negative values along this second axis signaled the largest deviations in T-S values and were associated with the highest bacterial concentrations.

While values along the second principal component axis were correlated with bacteria concentrations, the predictive value of the relationship was better near the ends and poorest near the middle. For the 1999 data, samples with PC2 scores <-0.5 almost universally had elevated bacterial concentrations and almost all of the samples with PC2 scores $>+0.5$ had non-detectable bacterial concentrations (Figure 6). However, the correla-
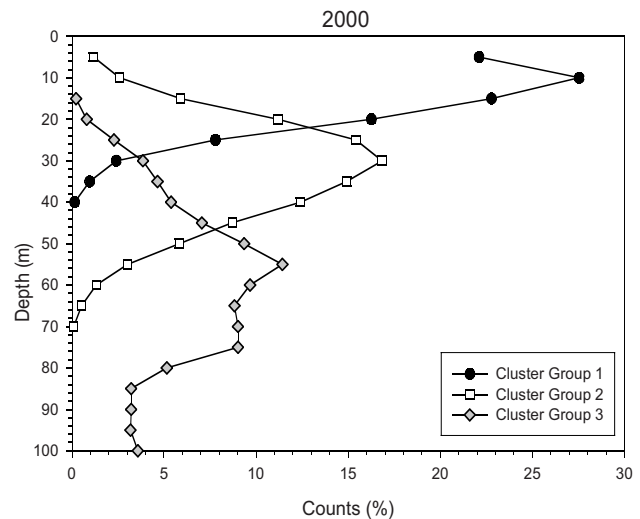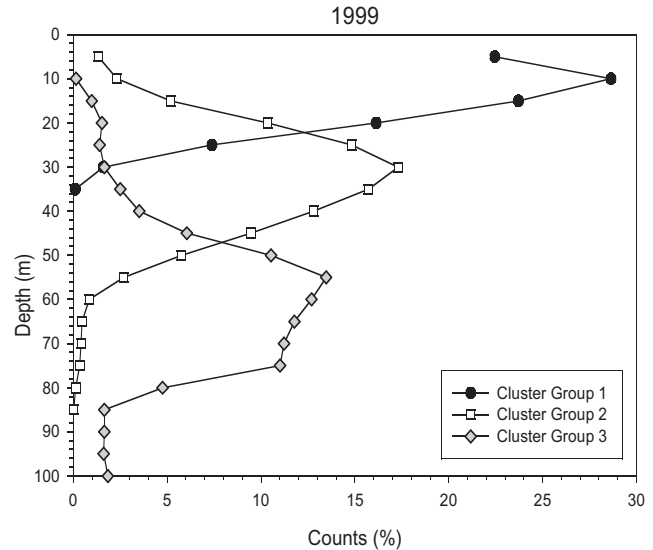
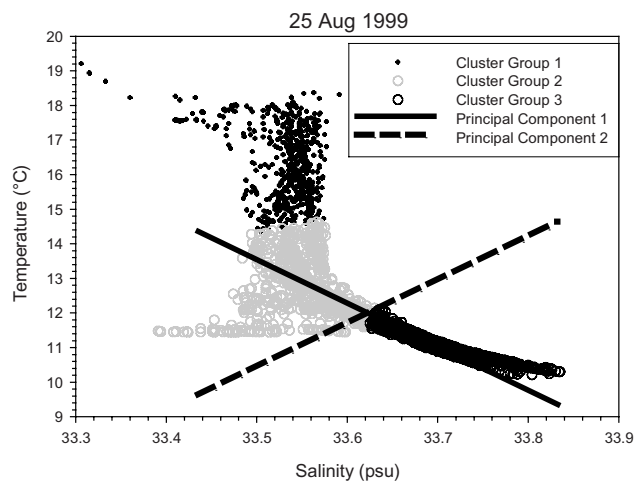

Figure 4. Cluster by depth.

Figure 5. Cluster analysis and principal component axes.

tion with bacterial concentration was weak for PC2 scores between -0.5 and +0.5.

To investigate whether these same PC2 cutoffs could be used to predict high and low concentrations in subsequent surveys, we applied the rule (PC2 <-0.5 and PC2 >+0.5) to the 2nd and 3rd clusters of bacteria data collected the following year. The majority of samples predicted to be elevated in 2000 did, in fact, have high bacteria concentrations (Figure 7). Of the samples having PC2 scores less than -0.5, around 85% had levels exceeding 500, compared to around 10% for those predicted to have low concentrations of bacteria (PC2 >0.5). Only a very small fraction of those samples predicted to be elevated (around 5%) had non-detectable levels of *E. coli*. In contrast, over 65% of the samples having PC2 scores greater than 0.5 were non-detectable values.
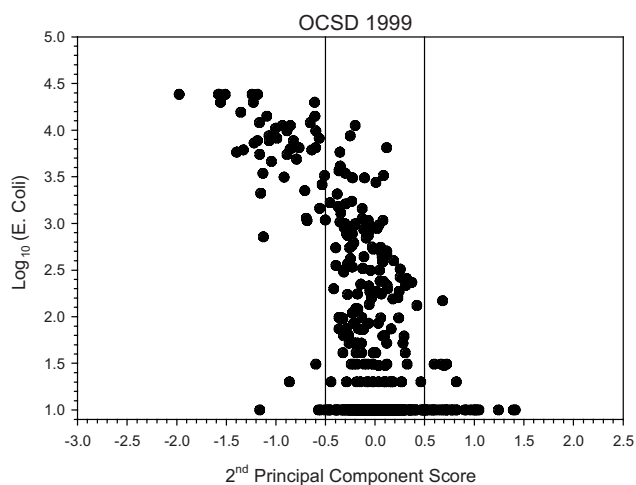

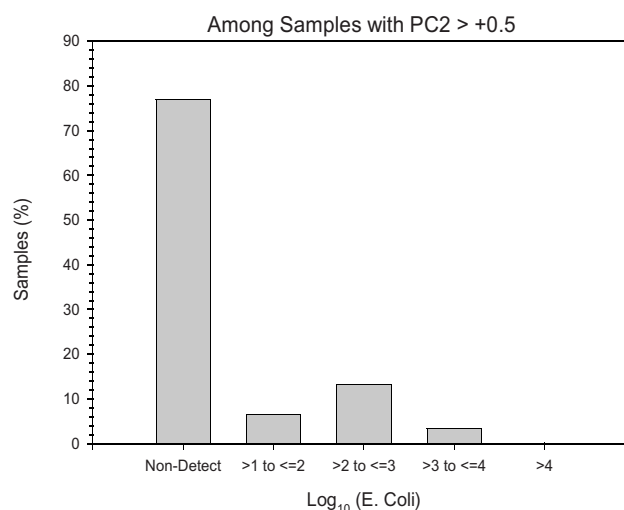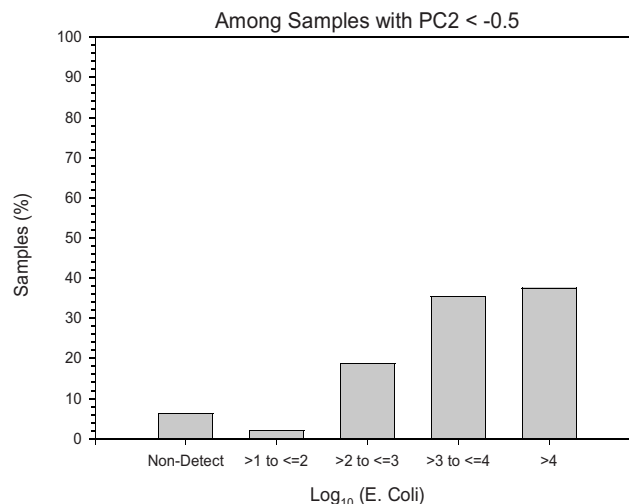Figure 6. Second PC score vs. *E. coli* (1999).

Figure 7. Distribution of *E. coli* using PC2 <-0.5 and PC2 >0.5, validation year 2000.

DISCUSSION

The T-S plots were found to be an effective tracer of plume bacteria, although there was considerable variability in the shape of the curve and the width of the portion corresponding to background condition. The greatest variability was among different months, driven by seasonal changes in air temperature, rainfall, and coastal advection (Figure 2a - 2c). More problematic, though, was the variability we observed within a given survey, as this limits sensitivity of these surrogate measures. Much of this variability appears to be due to the naturally occurring variability that is present in the upper layer. For instance, in Figure 2b, a low salinity bulge in the T-S distribution is seen between 17 and 19°C and between 33.3 and 33.6 psu. This variability is often observed in the spatial distribution of the upper layer

T-S in southern California and likely results from the complexity of coastal mixing and interleaving that occur (e.g., MEC and AOS 2001).

Because of this variability, the extent to which T-S relationships can be used as a tracer depends on the level of detection required. The T-S relationships were reliable for identifying the plume when bacterial concentrations exceeded water quality standards by several fold. It was also effective at defining areas from which the plume was absent, but was inconsistent in defining areas where plume dilution reduced bacterial concentrations to levels near the water quality standard. Part of this difficulty may be due to measurement variability for the bacteria, which can be as high as 50% of the measured value at concentrations near the water quality standard (Noble *et al.* 2004a). However, most of the limitation results because natural variability in temperature and salinity relationships confounds the plume signal at low dilutions, causing a decline in precision for bacterial concentration predictions.

The analysis of T-S relationships using the combination of cluster and PCA is not the usual approach for distinguishing water mass variability. However, PCA provides a means of describing deviation on multiple axes and allows differentiation of natural depth-related gradients from the anthropogenic influences on salinity and temperature from ocean outfall. PCA also has the advantage of quantifying this deviation, allowing development of relationships between deviation and pollutant concentration. While PCA has not been previously applied to distinguishing anthropogenic from natural water masses, it has been used to determine modes of variability in coastal oceanographic hydrographic data sets using not only T-S, but also nutrients, oxygen, and chlorophyll pigments (Blasco *et al.* 1980, Boyer *et al.* 1997).

Transmissivity and chlorophyll are other continuously measured parameters that have previously been found to be useful for identifying plumes (Washburn *et al.* 1992, Wu *et al.* 1994, Petrenko *et al.* 1998). These parameters are associated with particles, which might be advantageous for predicting particulate pollutants such as bacteria. However, we found that they were ineffective tracers for the OCSD plume and did not add predictive power when added as parameters in the PCA. The particulate loading in the OCSD outfall has been reduced in recent years. With the reduced particulate concentra-tions, other sources of suspended particulate matter such as sediment resuspension, phytoplankton growth, terrigenous runoff, and aeolian inputs contribute suspended particles to the water column that confound the particulate signal from sewage effluent. The only case we identified where chlorophyll fluorescence provided a noticeable source signal was in a tropical, oligotrophic environment where ambient chlorophyll was very low and where water clarity was sufficiently high that photosynthesis could occur at the depth of the plume (Petrenko *et al.* 1998). This is not the case in southern California, where effluent plumes typically reach density equilibrium beneath the subsurface chlorophyll maximum (MEC and AOS 2001, Jones *et al.* 2002, Noble *et al.* 2004b).

While we found statistical analysis of T-S relationships to be effective for the OCSD outfall, it is unclear whether they would be equally effective elsewhere. The ability of the method to work in other regions will depend on the nature and stability of the T-S relationships. T-S relationships appear to be stable in southern California, as the relationships we observed in Orange County are similar to those observed near Los Angeles (Washburn *et al.* 1992, Jones *et al.* 2002). It is also likely to work well in regions such as Mamala Bay, Hawaii, where the effluent plume provides a distinct perturbation on the ambient T-S structure (Petrenko *et al.* 1998). The limitations will depend on the depth of the outfall diffuser, the complexity of freshwater sources feeding into the coastal ocean, and the amount of stratification that separates the surface freshwater sources from the submerged outfall discharge. However, ocean outfalls are generally designed to release water below the thermocline, where salinity and temperature are most homogeneous and plume-generated deviations are most likely to be apparent.

Other scientifically based approaches to differentiating outfall effluent plumes from the ambient water have been attempted by other water quality monitoring agencies. The City of Los Angeles Hyperion Treatment Plant (HTP) monitoring group has used depth-averaged profiles of salinity to compare with individual CTD profiles of salinity in the evaluation of a salinity anomaly for detection of the plume. A salinity anomaly is calculated using the formula:

$$SA_i = (1 - S_i/Sx_i) \times 100$$
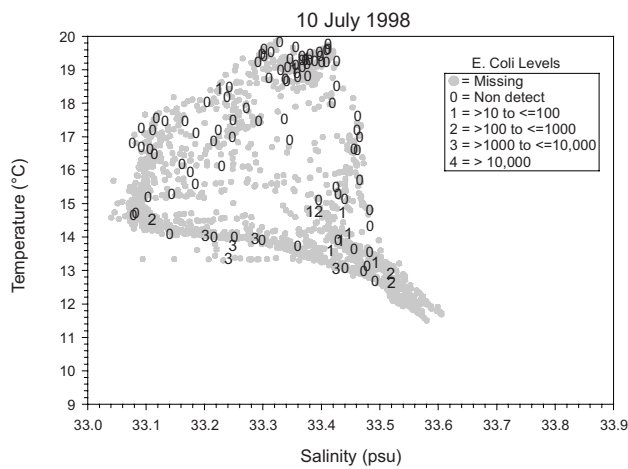
where S_i is the measured salinity in a profile at depth

Figure 8. Temperature vs. salinity with *E. coli* concentrations (El Nino - July, 1998).

interval i; Sx_i is the mean salinity at depth interval i; and SA_i is the calculated salinity anomaly.

Applying the depth-averaging approach poses several problems. First, the approach assumes that the isopycnal surfaces are relatively flat within the sampling grid. However, several oceanographic processes can tilt isopycnal surfaces. When isopycnal surfaces are tilted, the depth-averaged approach may provide misleading results. Second, coastal upwelling, eddies, geostrophically balanced along-shore currents, and internal tides can all contribute to tilting of the isopycnal surfaces over the shelf. In such cases, using a depth-averaged profile salinity to compare with individual profiles could lead to erroneous indications of the plume. Using the T-S relationship eliminates the potential problems of tilted isopycnal surfaces. An alternative approach to the HTP depth-averaging approach would be to average the salinity at fixed-density intervals rather than fixed-depth intervals, eliminating possible biasing due to tilted isopycnal surfaces. Further research is needed to quantify differences between the depth/density-average approach and the approach taken here.

Regardless of the approach, the use of T-S relationships has greater variability under unusual oceanographic conditions (such as El Niño or strong rain events), which cause stormwater to mix deeply in the water column. For instance, 1998 was an El Niño year in southern California and the T-S relationships near the OCSD outfall were different than in 1999 or 2000 (Figure 8). Low salinity water can also intrude into deeper waters from natural offshore sources. For example, naturally occurring salinities

of <33.4 are often observed in the southward flowing California current water (Lynn and Bograd 2002). If this water impinges on the coast, it may create ambiguity in the local T-S structure, and may be responsible for variations in the elbow seen in the ambient T-S relationship around 13°C (Figure 3). While T-S relationships can be confounded by potential ambiguities, T-S relationships should provide an effective method for mapping the effluent plumes in a stratified coastal ocean under most circumstances. The primary requirements are: (1) the water column should be somewhat stratified and (2) the observational program should have sufficient spatial coverage, so that observations outside of the influence of the outfall discharge are included within the data set.

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