Ocean Circulation and Plume Dispersion Modeling Review, with Emphasis on Orange County Sanitation District's Offshore Outfall and Wastewater Plume

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September 2000

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EXECUTIVE SUMMARY

Overview of Paper

This paper reviews the state of ocean circulation and plume dispersion modeling, with particular emphasis on the application of such models to evaluate the fate of the wastewater plume that originates from the Orange County Sanitation District's outfall in the Southern California Bight. Two types of dispersion models were reviewed:

- **Near Field.** The near field models are used to predict initial dilution, plume height of rise, and dimensions of the initial mixing zone.
- **Far Field and Circulation.** These models are used to predict the and hydrodynamics and fate of reactive constituents in the plume (such as coliform organisms or ammonium-nitrogen) as such constituents migrate away from the zone of initial mixing and dissipate throughout the coastal ocean. These models have limitations such that they may not be valid in the near field.

Hence, there is a use for both types of models.

The circulation and plume dispersion models reviewed are three-dimensional models (rather than 2D or 1D models). This is because the problem of concern is inherently three-dimensional. Further, several quasi-analytical models were reviewed. While such models are simpler than the numerical models, nevertheless they are very useful in providing a practical means of addressing a very difficult and data-intensive problem using limited resources.

The circulation and plume dispersion models can be used in two quite different applications:

- **Diagnostic.** The diagnostic analysis is intended to answer "what if" questions, such as "What would be the coliform counts at bathing beaches should the plume surface and currents persist in the onshore direction?"
- **Prognostic.** The prognostic approach produces real time predictions of plume behavior for present conditions (nowcasting) and for future conditions (say during the next weekend when bathers will be using the beach).

History of Ocean Circulation Modeling

Ocean circulation modeling began in the 1960s at the Geophysical Fluid Dynamics Laboratory in New Jersey where ocean circulation models were developed for use with atmospheric models to study the influence of the oceans on climate. The models were far simpler and computers were far slower relative to today, so that months of computational time were needed to simulate a few years of real time. Consequently, grid resolutions were between two to five degrees latitude/longitude (very coarse) in order to allow simulations to proceed to completion. Many of these earlier models were related to the MOM (modular ocean model) series.

During the 1970's and 1980's a number of ocean circulation models were developed, including finite difference models that used curvilinear coordinates (e.g., POM), models that used constant density as a vertical ordinate (isopycnal models such as MICOM), and models that began to take advantage of parallel processing machines (POP). Also, a fewer number of finite element models were developed. The finite element models were developed primarily because they could more accurately simulate complex bathymetry and irregular shoreline boundaries. Gradually grid resolution began to decrease to about 1/10 degree, equivalent to about 10 km of distance. This allowed predictions to be made of more detailed features of the oceans' circulations, such as the meandering Gulf Stream.

Models Reviewed

As part of this review, organizations that develop ocean circulation models were identified, as well as more than 20 circulation models that are in use today. Also, URLs are embedded in the report so that more information on specific models or organizations can be accessed on-line.

Some of the circulation models have been in use for years, and their names have been changed to reflect new model generations (for example, MOM, MOM1, MOM2, and MOM3). Circulation models are predominantly finite difference models rather than finite element models. However, finite element models are actively being applied and developed, as well. It appears that the major impetus for developing circulation models is to study climate, and for military applications, rather than for wastewater plume dispersion studies.

In contrast to the many circulation models, there are fewer plume dispersion models that can simulate reactive and buoyant plumes. It is ultimately these models, used in conjunction with the ocean circulation models, that would be used to predict the fate of the District's plume (including the fate of discrete particles, if desired).

Model Applications

A number of model applications were reviewed and documented in this report, with emphasis on Pacific Ocean applications, Southern California Bight applications, and wastewater outfall applications. The ongoing work that appears most related to the District's application is the application of plume dispersion models to simulate the fate of the City of Boston's wastewater discharged into Massachusetts Bay.

As mentioned above, it is feasible to apply plume dispersion models to the District's outfall in a diagnostic mode, using either numerical or quasi-analytical models. As a matter of fact, more quasi-analytical model applications were found in the literature reviewed than purely numerical model applications. In one case (Mamala Bay), both types of applications were performed.

No prognostic applications to the fate of wastewater plumes released into the coastal environment were found. Certainly, circulation models applied in a prognostic mode have been documented for both the Pacific Ocean, including the Southern California Bight and in the coastal Atlantic Ocean. However, much finer resolution is required for the accurate forecasting of a wastewater plume's position and constituent concentrations. The prognostic applications may need a grid spatial resolution of approximately 100 times finer than now used by the ocean models to generate in appropriate detail the required open ocean boundary conditions. Further, linkage to an atmospheric model is needed in order to provide real-time and future surface forcing functions. At this small scale, accurate prediction of weather is still problematic.

Summary

As part of this review, a number of "Perspectives" are given at the end of the paper. These perspectives are intended to summarize the important information documented during this review that can assist the District as they consider how best to approach the modeling. These perspectives include:

- **State of Models**: Ocean circulation models and plume dispersion models are simplified representations of the physical, chemical, and biological processes that actually influence the fate and transport of wastewater plumes. Limited information is available to force or drive the models. Solution techniques are numerical (for the complex models being constructed today) and solve the imperfect equations imperfectly. These limitations should always be kept in mind.

- **Limitations** should be explicitly stated: For any modeling application, the assumptions employed in the modeling should be explicitly stated, as well as their implications on limiting the use of the model.

- **Case studies:** No case studies were found that convincingly show that the fate of wastewater plumes released in the coastal environment can be accurately predicted in either a prognostic or diagnostic sense.

- **Impetus for model development**: There is a surge in the ocean circulation model development and applications that appears to be largely driven by climatic and military applications, rather than wastewater plume modeling.

- **Most relevant studies**: Of the organizations reviewed that appear to have a major emphasis on simulating near shore processes are the Woods Hole Oceanographic Institute, with their involvement in the City of Boston's wastewater discharge studies, and the Naval Research Laboratory with their interest in coastal military applications, and especially in the Southern California Bight area.

- **Two types of models**: Both finite difference and finite element models of ocean circulation and plume dispersion models have been developed and are in use. The finite difference models are currently more widely used. There does not appear to be unusual agreement among modelers as to which type of model is superior.

- **Site specific calibration/verification**: Models should always be calibrated and verified for each site-specific application under a variety of conditions.

- **Model validation:** Extensive model validation studies (studies that answer the question "Is the code functioning correctly?") should always be conducted and documented. The degree that models are validated is typically not made clear in documentation available for the models.

- **Mass conservation**: Is mass conserved over the period of simulation of the numerical models? This is an important question that can only be answered for each site specific application.

- **Funding Opportunity**: The National Oceanic Partnership Program (NOPP) offers funding opportunities in such areas as "pollution problems in the coastal ocean".

Despite the major advances in ocean circulation modeling and plume dispersion modeling, truly prognostic plume modeling is not yet possible. More computer power, models with more complete equations that apply to the wastewater discharge problem, better local weather predictors, and more complete data sets and data assimilation techniques are all needed. However, models can now be applied in a "what if' mode, and such applications should provide great value.

Recommendations

Recommendations that have come out of this study include:

- More information about the relevant activities of the Woods Hole Oceanographic Institute and the Naval Research Institute should be gathered, perhaps by visiting and discussing how information might be shared between those organizations and the District.

- A proposal to the NOPP could be prepared and submitted on proposed plume modeling activities.

- Diagnostic models of the District's wastewater plume can be developed now that will provide useful information.

- Analysis of the District's data using three-dimensional visualization tools would be beneficial to better understand the spatial and temporal content of that data with respect to modeling needs.

White Paper for Dispersion Modeling of the Wastewater Plume Discharged into the Southern California Bight From The Orange County Sanitation District's Offshore Outfall

1.0 Background and Objectives of Paper

This paper has been prepared by Tetra Tech at the request of the Orange County Sanitation District (District) to evaluate the feasibility of using dispersion models to better understand the fate of the District's wastewater plume. Although the District has been performing extensive monitoring of the coastal environment around their outfall for years, there is still a need to better understand the fate of the plume, and how concentrations of constituents in the plume evolve over time and space. Since monitoring is expensive, and the informational content of the data collected are necessarily sparse in comparison to the information needed to completely describe the physical and chemical characteristics of the coastal environment, and the conditions under which monitoring occurs may not always coincide with critical conditions of concern, it is natural to ask if dispersion modeling can supplement monitoring and in what manner, to better understand the fate of the wastewater plume, selected constituents in the plume, or constituents that have become dissociated from the main body of the plume (e.g., floatables).

The major objective of this paper is to review the state of models and modeling as applied to the specific problem discussed above, and to discuss how such models could be used for the benefit of the District. While modeling generalities will by necessity be introduced and discussed, for the most part the discussion is intended to focus on this site-specific application.

Complex, three-dimensional numerical models are emphasized in this review (some limited discussions on a quasi-analytical three-dimensional models is also included because these simpler models can also be quite useful as screening-level tools). This means that one-dimensional and two-dimensional models are not evaluated. This is because three-dimensional models have now been around for a decade or more, and their range of application is growing along with the feasibility of using them as computational speed and memory capacity increase. Further, the wastewater plume under consideration here is a three-dimensional phenomenon. It spreads up and down coast, may move toward shore or off shore, and may remain trapped below the pycnocline or rise higher in the water column when stratification is weak. So, this paper is intended to be forward looking, and to focus on what is now the state of the modeling, and directions of new advances.

Second, dispersion modeling consists of both three-dimensional circulation modeling of coastal currents, water temperature and salinity fields, and most importantly the movement and fate of constituents within the plume and the plume itself. Those constituents may be present in the dissolved phase in very low concentrations or as small particles that are positively or negatively buoyant, or even larger objects that at times may be discharged with the waste water. The plume itself may retain its identity for a number of kilometers away from the outfall and for a period of several days. Thus this is the region of primary concern for dispersion modeling.

Third, dispersion modeling here is assumed to include the movement of neutrally buoyant constituents, as well as both floatable materials that may move along the surface in a direction different from the main plume body, or settleable constituents that may slowly migrate along the bottom or be resuspended to move more rapidly within the water column.

Ultimately the issue here is not really whether to apply modeling techniques to this site-specific application, but how best to go about doing it.

2.0 Environmental Setting

The Orange County Sanitation District discharges treated residential and industrial wastewaters through a 120-inch submarine outfall to the Pacific Ocean off Huntington and Newport Beaches in Southern California. Figure 2-1 shows the regional setting of the discharge. Treated wastewater is discharged through an outfall that extends 8.2 kilometers (5.1 miles) offshore into water at a depth of approximately 60 meters (200 feet). Figure 2-2 shows a more detailed view of the outfall and diffuser along with bathymetric contours. A second emergency outfall closer to shore is also shown. That outfall has a diameter of 78-inches, and has not been used to date. A third emergency outfall is in the Santa Ana River, and has also not been used. Appendix A provides more details of the regional setting for readers not familiar with the particular environmental setting.

The estimates of the initial dilution achieved by the discharge has ranged from 148:1 based on data available for the original 301(h) waiver to as high as 300:1 (Stolzenbach and Hendricks, 1997). The California State Water Resources Control Board determined a minimum initial dilution of 180:1, as reported in the District's 1989 permit reapplication.

To illustrate the approximate shape of the wastewater plume at the completion of near-field mixing, CORMIX was applied to the discharge for the conditions corresponding to July 1998. This time period was arbitrarily chosen as an example, and it is noted that the near-field mixing zone is dependent on the specific conditions simulated. The results for this particular set of conditions are shown in Figure 2-3. The initial dilution calculated was 210, which is within the range of dilutions reported earlier. For this application the water column was temperature and

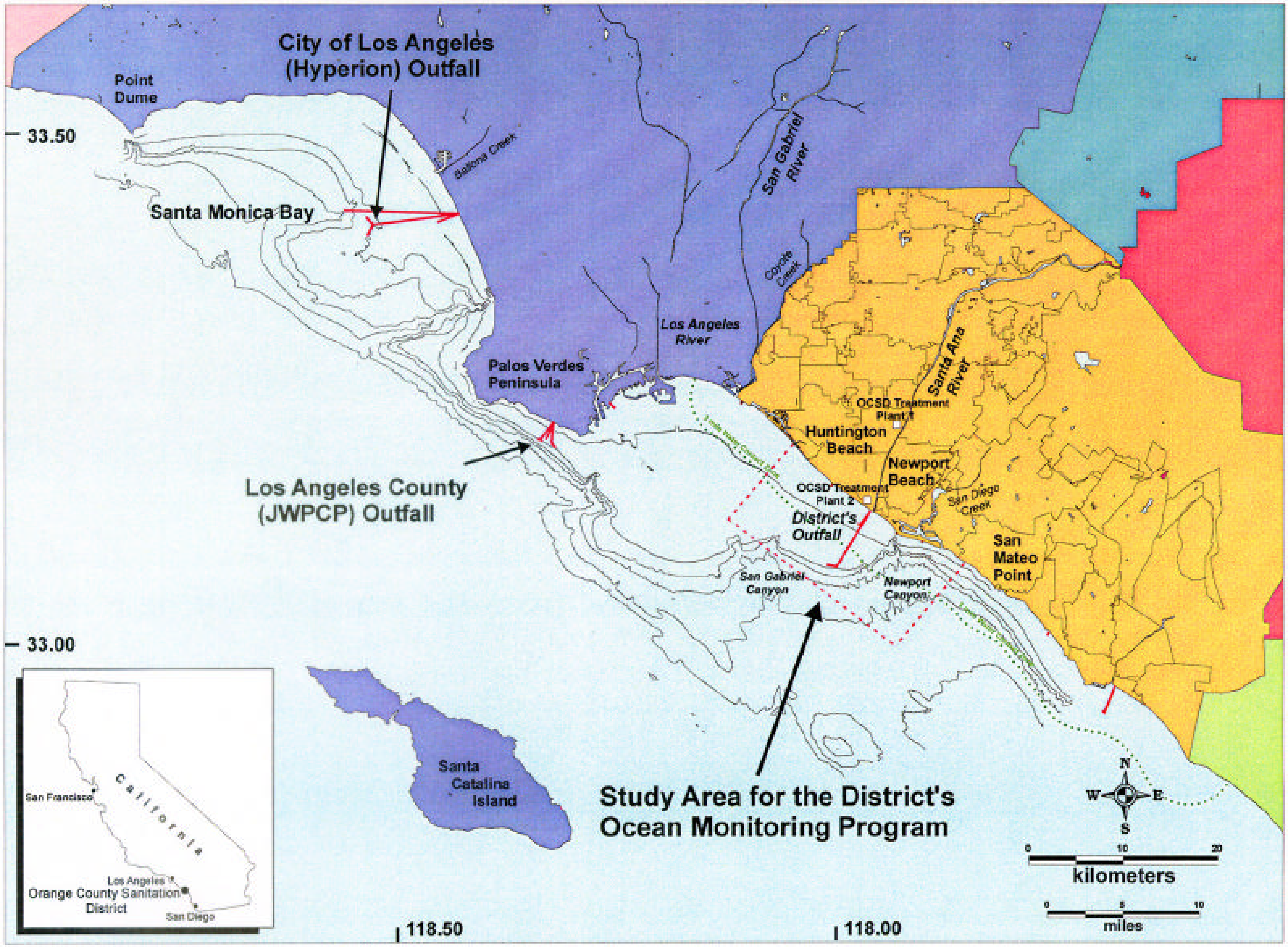

Figure 2-1. Regional setting for the district's ocean monitoring program.

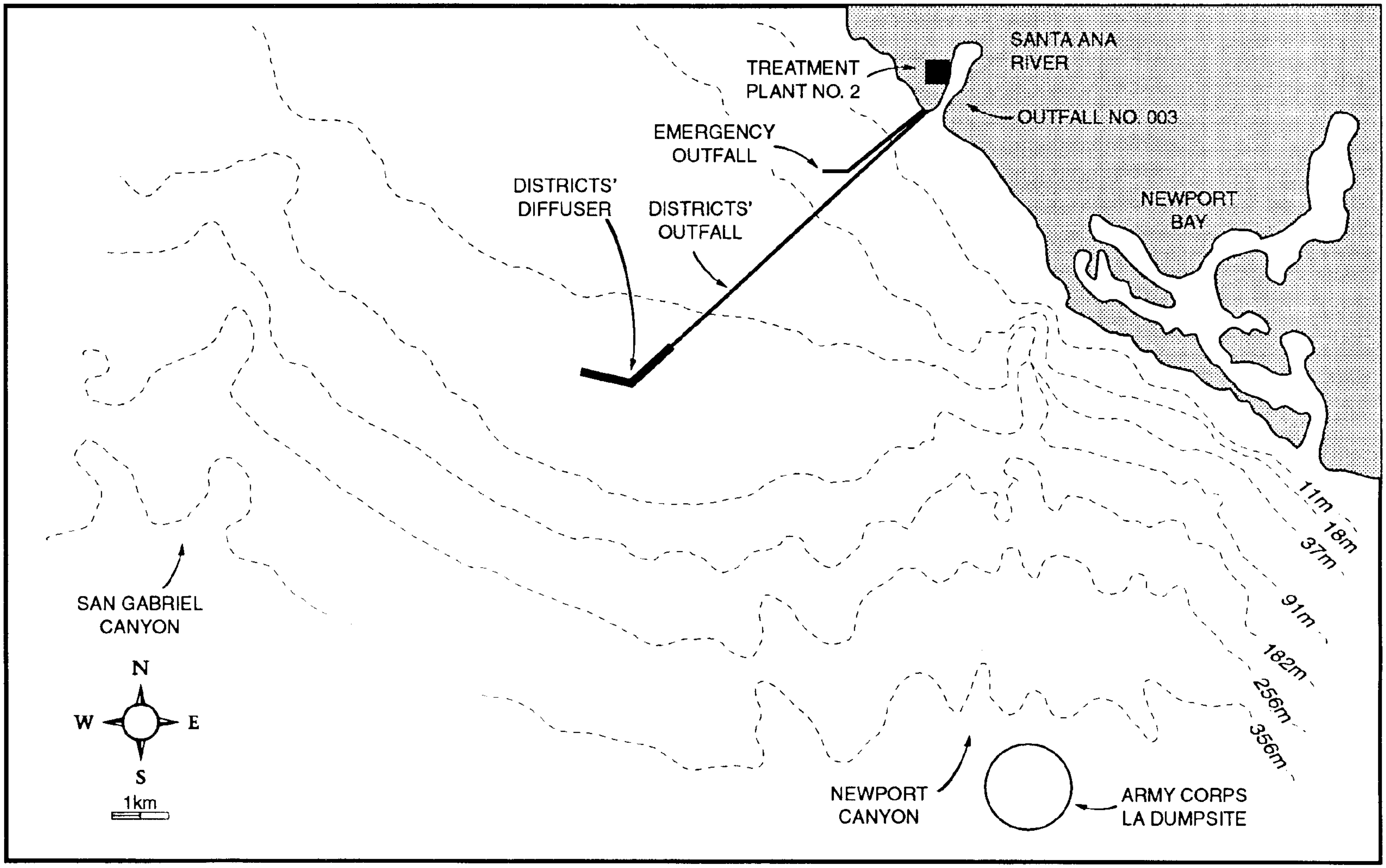

Figure 2-2. Location of Orange County Sanitation District plant No. 2, ocean outfall, and emergency discharge outfall.

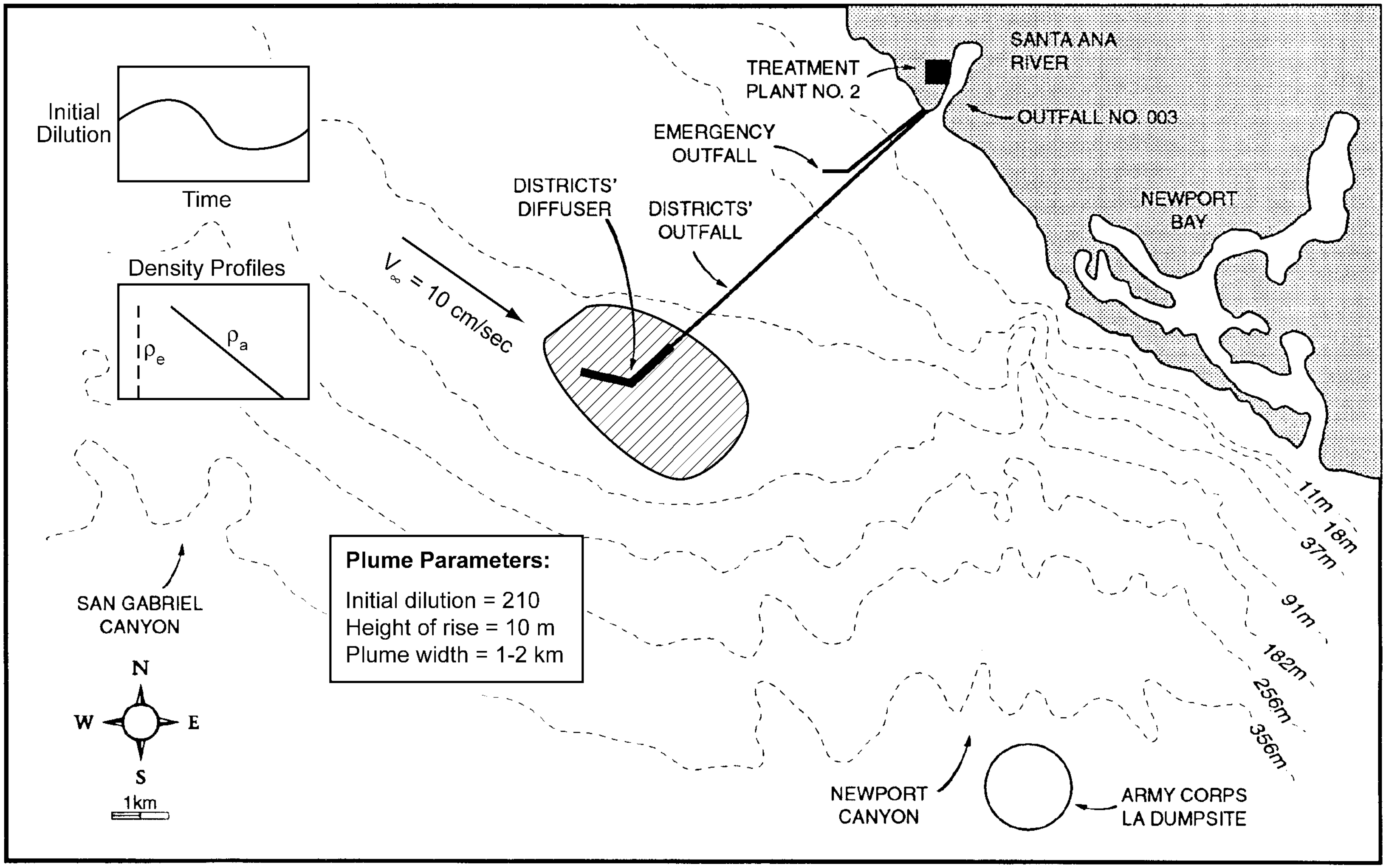

Figure 2-3. Location of Orange County, CA Treatment Plant No. 2, ocean outfall and emergency discharge points.

density stratified, so that the plume remained within about 10 meters of the bottom. This analysis is intended to illustrate the three dimensional nature of the plume. It is emphasized that Figure 2-3 is simply a “snapshot” in time. The initial dilution is continually changing over time as ambient currents and the receiving water/discharge conditions change. Additionally, the plume rendition shown in Figure 2-3 stops at the approximate boundaries of initial mixing. In actuality, the plume continues to migrate and disperse until all its characteristics are indistinguishable from the ambient. How the far-field migration of the plume can be predicted is the major topic of this paper.

To illustrate the influence of the initial dilution on ambient concentrations of selected constituents discharged in the wastewater, the dilution of 210 is used. Predictions are made at the completion of mixing and shown in Table 2-1. Notice that practically no changes are evident for dissolved oxygen and water temperature when compared to ambient levels. Some potential increases in ammonium-nitrogen, total coliform bacteria counts, and copper concentrations are evident.

It is possible that, as the plume migrates away form the zone of initial dilution, conditions may be conducive to current reversals such that the ambient water entrained into the plume in the initial mixing zone is partly wastewater that has been released during a previous tidal cycle. Should this happen, it is possible for higher concentrations of constituents such as ammonia to occur in and near the ZID. Figure 2-4 illustrates this, and assumes some reentrainment has occurred over several subsequent tidal cycles. The ammonia concentration increases to approximately 0.8 mg/L, about double what it would be without the reentrainment. While the above is a hypothetical exercise at this stage, it does illustrate immediately a use of a three-dimensional plume model: to determine if this can happen, and the condition when it would happen.

Table 2-1
Examples of Concentrations of Wastewater Constituents at Completion of Initial Dilution

Constituent	Effluent Characteristics	Ambient Concentration	Concentration at Completion of Near-field Mixing
Dissolved Oxygen, mg/L	1.4	5.0	4.98
Water temperature, deg-Celsius	26.9	10.5	10.6
Ammonium-nitrogen, mg/L	77.3	0.02	0.4
Total coliform bacteria, MPN/100ml	10^7	0	48000
Copper, ug/L	38	0.001	0.18
pH, su	7.15	7.4-7.9	–

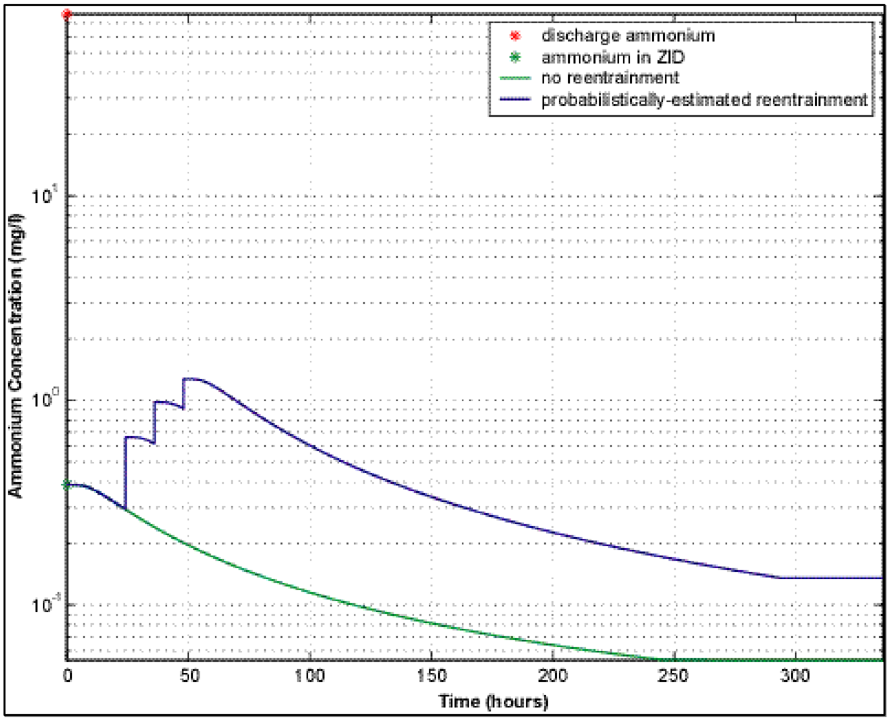

Figure 2-4. Ammonium concentration for District wastewater discharge into the Southern California Bight.

3.0 Why Model the Orange County Sanitation District Wastewater Plume?

The District has been monitoring the coastal environment in the vicinity of their wastewater discharge for many years to gain a better understanding of the extent of the plume under different ambient conditions, and the potential impacts of the plume on the coastal environment. The study area for the District's ocean monitoring program was shown on Figure 2-1. The approximate extent of up coast and down coast monitoring is 10 kilometers in each direction. Offshore monitoring extends several kilometers past the outfall, and onshore monitoring extends all the way to the shore. Monitoring stations are shown in Figure 3-1. Even with the extensive monitoring network and the length of time that monitoring has been conducted, understanding the plume's configuration at any moment in time, and how the wastewater plume actually migrates and dissipates in the coastal environment under continually evolving seasonal influences is not presently possible. One way to better understand the evolution of the wastewater plume is to simulate its fate by using an appropriate numerical model that accounts for influences such as the outfall configuration, characteristics of the discharge, bathymetry of the coastal environment, and ambient conditions and forcing functions. This approach would use monitoring data to help generate input to the model, and when all input to the model has been specified, the model would predict the spatial and temporal evolution of the plume under conditions of interest to the District. If there were a need to track the plume's evolution for a

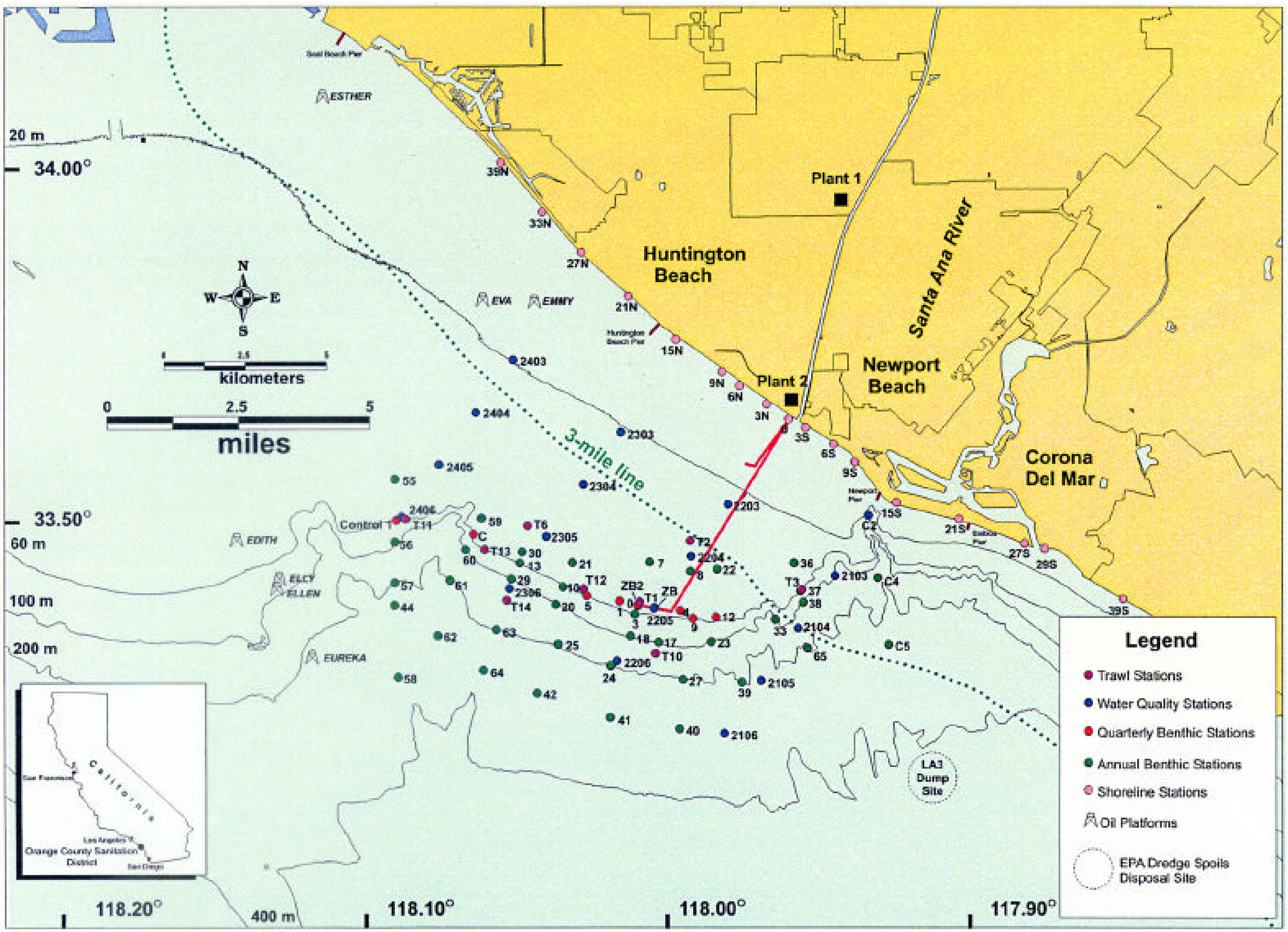

Figure 3-1. General location of the district's ocean monitoring program study area, including water quality, benthic, trawl stations, and other prominent features.

hypothetical two-week period, for example, then the input data that forces the plume's evolution and migration over that two-week period would be needed. The types of issues that could be addressed include:

- A visual display of the plume over the period of interest using appropriate three-dimensional software that displays the plume within the water column by the appropriate use of colors, with the bathymetry and coastal features visible for reference. The current field that forces the plume would be visualized as well.
- Determination of conditions that results in the plume moving back over the zone of initial dilution, and that might result in constituent levels in the ambient environment that are higher than expected.
- Examination of conditions that leads to the plume breaking apart (say due to vertical velocity shear), and could lead to parcels of the plume traveling in different directions, with discontinuous concentration fields.
- Evaluation of plume transport during conditions of special concern to the District, such as upwelling, storm events with large discharges of fresh water from the Santa Ana River near the outfall (see Figure 2-1 for the location of the river relative to the outfall), and minimal stratification that might cause the plume to surface.
- Should the plume surface, under what conditions, if any, would constituents such as coliforms reach the beach area in excessive concentrations?
- What is the fate of floatables, and do they reach critical locations, such as the shoreline?
- Determination of the assimilative capacity of the coastal waters.
- Predicting the changes in the wastewater plume as discharge flow rates increase substantially over the next 20 years, or potentially decrease because of water reclamation practices (See Appendix A for projected flow rates).
- Evaluating the impacts of infrequent emergency discharges through the shorter 72-inch discharge shown in Figure 2-1, or of discharging into the Santa Ana River during extreme flow rates associated with storms. What would be the levels of coliforms, ammonium-nitrogen, and grease, for example, from such discharges, and where would the plume go.
- Distinguishing the impacts on the coastal waters from the multiple sources of constituents that may originate from other wastewater discharges, for example. Figure 2-1 shows the Los Angeles County and City of Los Angeles outfalls, both of which are located up coast.
- Distinguish impacts between other sources, such as storm water runoff.

To answer the above questions, an appropriate plume modeling framework and sufficient historical and real-time data would be needed. In a sense, then, the above issues are intended to be plausible scenarios to recreate situations in the past, or to examine plausible future scenarios (diagnostic analysis). However, there is another type of question that may be of concern to the District that is not addressed above. "That question is: "What is now happening with respect to the plume's evolution and what is expected to happen in the next few days?" This may be of interest when weather forecasts are such that a large storm event is predicted, and the short-term fate of the plume is in question. This type of analysis is known as nowcasting, and short-term forecasting. To implement this approach requires that real time forcing data be fed into the model, and the model is able to execute and present results in a manner that is useful for the purpose at hand (prognostic analysis). Both of these types of applications (diagnostic and prognostic analyses), and issues associated with their implementation, are discussed in subsequent sections.

4.0 General Overview of Components of Dispersion Modeling

4.1 Introduction

As discussed previously, dispersion models are intended to simulate the fate of neutrally buoyant constituents (often called scalars), such as coliform organisms or ammonium-nitrogen, positively buoyant scalars such as floatable materials, negatively buoyant scalars such as suspended materials, biota such as plankton or fish, and to provide input to seabed models that simulate the fate of settled materials. Even though dispersion models have been around in one form or another for more than 30 years, and three-dimensional models for more than a decade, the need for improvements in such models still drives the development of better models. Some general issues and limitations of dispersion models will be discussed in more detail later in Section 4.4. In general, it should always be remembered that models are simplifications of reality that allow us to make predictions that hopefully have a beneficial use. However, it should not be assumed that just because a model appears to "work", that the results are representative of the real world. Proof that a model works as desired is really application (or site) specific, and a model's predictive ability should be verified as often as possible, and under different conditions.

4.2 How Dispersion Modeling Components can Interact for the District's Open Ocean Boundary Modeling Application

Potential plume modeling components are conceptualized in Figure 4-1. The figure consists of four parts:

- Data Requirements: information required to run the model.
- Modeling components: The various models needed to make the desired predictions over the time and spatial scales of concern.
- Output: The predicted results generated by the models, which may not be in a form most amenable to being understood.
- Post processing: The use of state-of-the-art GIS and visualization tools used to display complex three-dimensional model results.

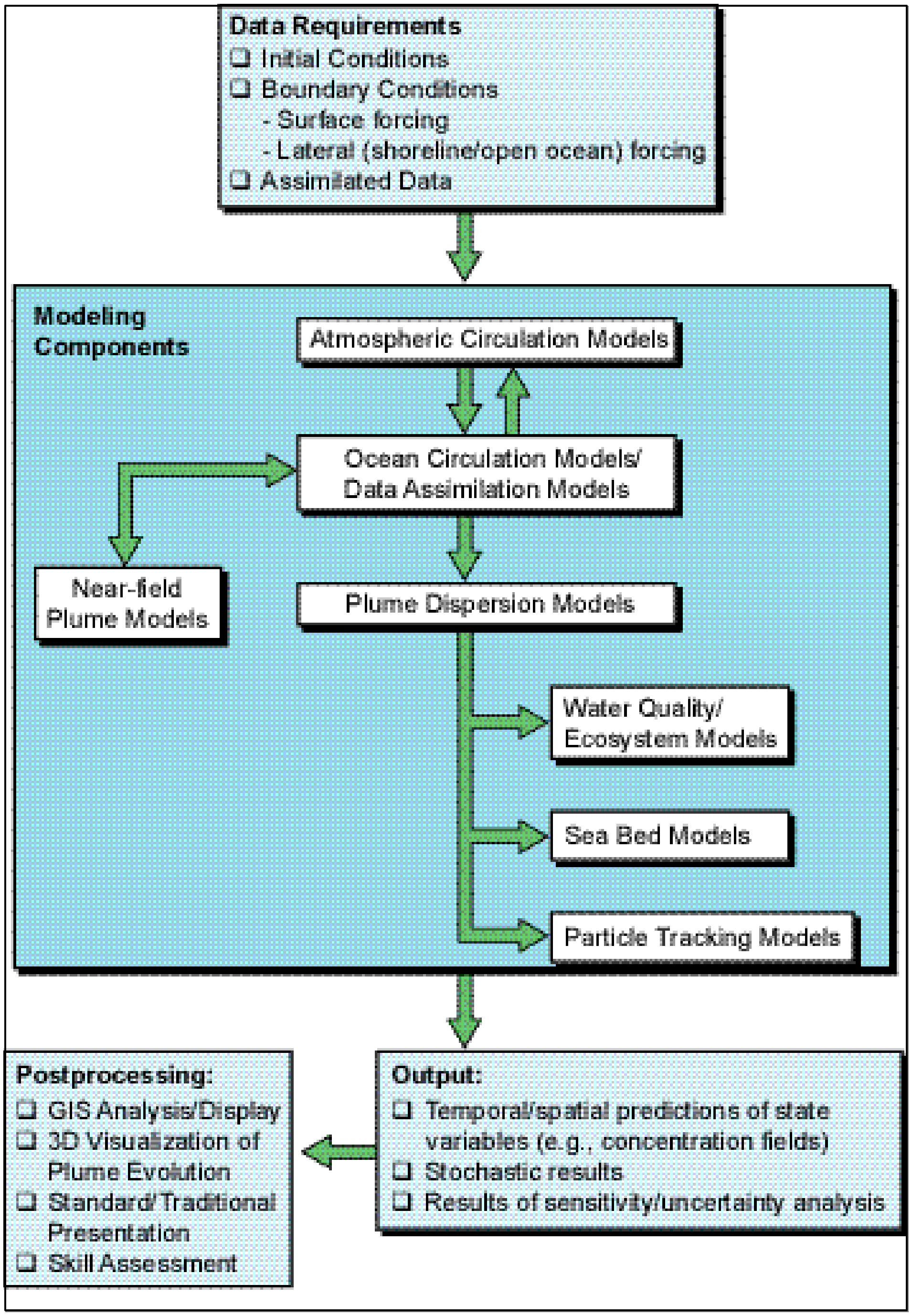

Figure 4-1. Potential Plume Modeling Components.

The framework depicted is very general, and is intended to be applicable to either diagnostic or prognostic modeling, both of interest to the District. However, such a framework today probably does not yet exist, at least at the fine temporal and spatial scales needed for plume dispersion modeling. Thus the framework in intended to be forward-looking.

The information needed to run the model (data requirements) are expressed in terms of initial conditions, boundary conditions, and assimilated data. The initial conditions specify the state of the system to be simulated at the beginning of the simulation. This would include the spatial distribution of coliform organisms (if coliform organisms were to be simulated), for example. The boundary conditions would include the information specified along the boundaries of the system over the complete time frame simulated. Assimilated data are those data that are continuously fed into the model as it executes to make prognostic predictions. Such data are not needed for diagnostic simulations.

The model components box illustrates the range of sub-models that might be needed, depending on the ultimate goal of the District. The appearance of an atmospheric circulation model in the figure may be puzzling. In fact, it is expected that an atmospheric circulation model is not needed for present applications. However, in the future, it is likely that atmospheric circulation models will be coupled with ocean circulation models to allow more realistic exchanges that produce more accurate ocean circulation predictions (actually, this is now being done on a demonstration basis, as discussed in Section 5). In addition to the atmospheric and oceanic circulation models, a near-field plume model (such as CORMIX or Visual Plumes, for example) might be used to predict the near field plume dynamics so that accurate estimates of height of rise and initial dilutions can be calculated. This would require linking the ocean and near field dispersion models together. The results of the models mentioned so far would be to predict the water temperature, salinity, velocity, and density fields that are used by the plume dispersion model. The plume dispersion model simulates the passive scalars that do not influence the velocity or density fields. Further, plume models can be extended to predict water quality, ecosystem interactions, perform particle tracking, or provide input to models that predict changes in seabed characteristics.

The model output can be enormously large files of model predictions. They can include time series of predictions at user-specified locations, on snapshots of the spatial distribution of scalars for different times throughout the simulation period. Such output needs to be post processed so that the results are meaningful. Ultimately, either traditional approaches can be used, or newer visualization techniques can be used to display the data three-dimensionally. Visualization techniques are no longer luxuries; they are essential to help understand what the model has predicted.

Table 4-1 provides a brief overview of the models in terms of the scale that is typically simulated, the grid resolution, and information generated, and data required to implement the models. The grid resolutions are specified with the intention to capture the necessary information to make the applications meaningful, but not to be so resolved that the computational time is prohibitive and the problem is never solved. This remains an issue in practically all real-world applications, despite the rapidly increasing speed of computers.

Table 4-1 goes here

The modeling application to the District's wastewater plume that is discharged in the Southern California Bight requires the specification of an open ocean boundary condition. An open ocean boundary is the specified Pacific Ocean boundary of the modeling domain. That is, inside the boundary, the model simulates the relevant processes to predict the fate of the plume, and on the boundary the appropriate forcing information or boundary conditions are specified. Unfortunately, along the open ocean it is not possible to specify the required information with great accuracy. Thus, the presence of an open-ocean boundary condition is a real challenge to handle appropriately. One way to address the problem is by using nested grids of increasing resolution in the interior, at the region where specific predictions are desired (such as around the District's outfall). This concept is illustrated in more detail subsequently in Section 5.

4.3 Role of Stochastic Models in Plume Dispersion Studies

Plume dispersion modeling can either be deterministic or stochastic. Further, their equations can be solved numerically or analytically (if the equations are simplified enough). Deterministic models treat the problem in a purely deterministic sense. That is, variables are not considered as random variables, nor are the model simulations repeated multiple times within a Monte Carlo loop. Stochastic models, on the other hand, do accommodate random variables in some sense. Because of the computational expense associated with executing numerical plume dispersion models, most of the modeling that is done is deterministic. In other fields, (e.g., human health risk assessments) however, where much more simplified models can be used, Monte Carlo techniques are occasionally employed. For Monte Carlo techniques to be practical, the computational time to execute the model thousands of times (so that the solution has converged in the sense that all the information contained in the random structure of the model has been extracted) has to be manageable. For example, consider a simple plume model for a riverine discharge that takes 0.5 seconds to execute, and then is executed in a Monte Carlo loop 5000 times. This would require about 40 minutes to execute. Now, consider an ocean plume modeling scenario that requires 2 hours to simulate. Five thousand simulations would take over a year to execute, obviously a prohibitive amount of time. Thus, Monte Carlo techniques are only practical for the simpler analytical plume dispersion models, rather than the numerical models.

One type of relevant model that uses the concept of randomness is particle-tracking models. In this type of model, discrete particles are tracked, and a random dispersion component is used, so that multiple simulations of the release of the same particle (or alternatively, the release of multiple particles) result in the particles migrating to different locations. This type of modeling is sometimes used to predict whether spills will impact sensitive locations. Further these models case be run in a reverse mode in an attempt to estimate where an observed impact from the spill originated.

4.4 General Issues in Using Ocean Dispersion Models

In this section, a brief summary of some of the major issues associated with ocean dispersion models is introduced. Elaboration of some of these issues is provided in subsequent sections. These issues are:

- **Boundary Conditions.** Both locations and types of boundary conditions are important because the information specified on the boundaries ultimately propagates through the system and must be accurate in order for model predictions to be meaningful. Boundary conditions should be set at locations where the information at the boundaries is either known (such as at shorelines), or such that the boundaries chosen do not influence significantly the desired results in the model domain. For open ocean modeling, this can be very difficult to achieve. The types of boundary conditions that are specified can also be important. Generally, the presence of boundaries should not influence the transport of momentum, energy, or mass through them.

- **Initial Conditions.** The initial conditions define the state of the system at the beginning of simulation. Assuming the number of grid points in the dispersion model's grid is on the order of 10^4 to 10^6, then for an accurate depiction of initial conditions, data need to be available at all those locations, or plausible interpolation of available data are needed. Of course this may not be plausible, especially the initial plume configuration. Several options are available to handle this difficulty (in addition to more intensive sampling, which is not considered here). One, the model can be run for a period long enough so the results are independent of the initial conditions. Or two, the initial conditions are set to a plausible scenario that mimics a situation of concern to the District in order to follow the plume's response over time to that condition.

- **Mass Conservation.** It is important that the dispersion model conserve mass. That is, it not create or destroy mass artificially. An example of how mass could be lost could occur is by passage of the plume through the grid boundary, and return of the plume back into the domain that is simulated. The outward passage could be simulated by ignoring the turbulent flux (typically acceptable), but the inward passage would have difficulty in specifying the appropriate boundary condition. If it was specified that the incoming concentration were zero, then some mass could be lost on each cycle of velocity reversal. To minimize this or to avoid the effect may require a grid large enough that the plume never crosses the boundaries.

- **Model Assumptions.** The assumptions made in the models need to be carefully understood to be sure that the model does not assume away an important part of the problem. For example, it was stated earlier that only three-dimensional models would be evaluated here. Two-dimensional models assume an averaging over one spatial dimension that would not be appropriate here. A second example is that most three-dimensional models assume hydrostatic equilibrium in the vertical direction (that is, vertical accelerations are unimportant). This is typically true in the ocean environment, even in situations where upwelling is important, as in the District's application. However, models with these assumptions would have difficulty in simulating the near-field around the outfall itself, since vertical accelerations are very important (outfalls are designed to produce vertical accelerations to maximize initial mixing).

- **Model Physics and Process Representations.** One example of model physics (or lack of) was described above in terms of the hydrostatic assumption. In terms of process representations, the representation of turbulence is important. Many models use the Mellor-Yamada closure scheme for turbulence. This scheme and all others contain some empirically-derived information in them.

- **Model Numerics and Solution Approach.** Due to the computational time requirements needed to run these models, the most advanced numerical techniques with a proven record of performance are needed. Based on experience and discussion with numerical modelers, it does not appear that all models have made the best use of numerical and programming techniques to speed the execution of those models. The execution of different models on the same problem may take on an order of magnitude range, for example. This could mean the difference in a one-day vs. ten-day simulation time. The solution approach (where here the only finite difference and finite element techniques are considered) can also make a significant difference.

- **Model Grid.** One of the advantages of the finite element method that lead to its application to problems of the type examined here (where the boundaries can be quite irregular) is the ability of finite element models to accurately match those irregular boundaries. Finite difference techniques were viewed as inferior in terms of their ability to match these irregular boundaries. However, this has changed as finite difference techniques now employ better techniques to help match irregular boundaries. In the end then, the choice of a finite element vs. finite difference model for a specific problem may not be how accurate the boundaries can be approximated by the different techniques (they may be equally approximated), but how the speed of simulations compare for the same degree of accuracy.

- **Model Accuracy and Stability.** These are concepts pertinent not only to any model itself, but also to any application of that model. That is, because a model has performed well on an application in the North Atlantic Ocean, does not mean it will automatically perform well in a Pacific Ocean application. For each model application, the issues of accuracy and stability should be reevaluated.

- **Model Validation.** Model validation relates to model accuracy, but is not exactly the same. Model validation refers to confirming that the code is performing exactly as intended. That is, it is bug free. Generally models are validated by comparing the three-dimensional numerical model against simpler analytical solutions, or even against other models that have been thoroughly evaluated (but, might be simpler, for example). Since analytical solutions are the exact solutions this may be preferred. However, since only a few analytical solutions are available to the complicated problems addressed by the numerical models, typically many validation tests are required that may check various components of the model. This work can be time consuming, and the tendency may be to minimize this effort or not to document it. In fact, this is an important step in giving the model credibility, and should not only be well documented, but should be a continuing component of model quality assurance testing as the code is updated, and other test results become available.

- **Model Calibration and Verification.** Model calibration refers to the process of matching model results against an observed data set, and adjusting (within realistic limits) selected model coefficients until the match of observed data vs. model predictions is acceptable (typically, “acceptable” has to be defined). Then the model verification step follows, where model predictions are compared against an independent data set, where no further adjustments are made in model coefficients, and again a determination is made of whether the comparison is acceptable. There are not really a single set of rules on the process of calibration and verification. It is reasonable to establish the goals before the process is started, including acceptability criterion. Modelers may disagree as to whether the calibration/verification process is application specific (validation is not), but the most conservative approach is to calibrate and verify models for each site application, and to consider this an ongoing part of modeling at a site, as new data become available, or modeling objectives change.

- **Model Maintenance and Quality Assurance/Control.** It is important that models be maintained, and upgraded as the need arises. This can be costly to accomplish, and unless there is a continual source of funds available for this, models may soon become outdated and perhaps obsolete. For example, more efficient numerics that minimize numerical dispersion and make the codes execute faster and newer types of grids are typical examples of model updates that may be needed for many models developed a decade ago. The point is that unless models are continually upgraded, they will no longer reflect the current state of the knowledge in coastal plume modeling.

5.0 Examples of Modeling Applications to Coastal Oceans

5.1 Organizations That Develop and Apply Circulation and Plume Dispersion Models

Table 5-1 summarizes information on organizations that have developed and applied coastal ocean circulation and water quality models. The table is intended to provide an overview only; increasing levels of detail on the models is provided subsequently. Because the use of ocean circulation models is growing quite rapidly due to both concerns about the health of the oceans as well as other reasons such as related to military activity, Table 5-1 is not necessarily completely comprehensive. However, omission of relevant organizations is unintentional. Nevertheless the information in that table is thought to be representative of the universe of the pertinent activities. (Note that an internet contact is provided for each organization so that much more information can be obtained, as needs dictate).

Table 5-2 summarizes a number of the coastal circulation and water quality modeling studies that have been performed over the years. Based on some of the materials reviewed on the web sites, many hundreds of applications exist. However, it was not feasible to document all such applications (many likely appear in the gray literature and may have limited availability). A selected subset of the studies in the table is described in the section below. Those studies are intended to emphasize a range of applications, including plume modeling, embedded grids, nowcasting/forecasting, and Southern California Bight applications.

Table 5-1 goes here

Table 5-1 (continued) goes here

Table 5-2 goes here

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5.2 Examples of Applications to Pacific Ocean, Southern California Bight, and West Coast Estuaries and Bays

5.2.1 Early Model of the California Coastal Circulation [Blumberg, Kantha, Herring and Mellor (1984)]

This modeling effort was perhaps the first to develop and apply a model to the North Pacific Ocean to predict the circulation off the California coast. The model, called the General Circulation Model (GCM), is an early version of the Princeton Circulation Model (POM), which is still in wide use.

The area simulated by the models is shown in Figure 5-1. Note the boundaries of two modeling grids are shown. The grid boundaries for the GCM approximately span the western boundary of the state of California and extend offshore to nearly 500 kilometers. Within this grid the GCM is applied, and the grid used by that model is shown in Figure 5-1. The grid is an orthogonal curvilinear grid, and reflects a model advancement for this application because the GCM used a rectangular grid system prior to this application. The curvilinear grid permits a better fit to the bathymetry and coastline, and allows more detailed predictions near the shoreline. The grid is chosen to be large enough to encompass the spatial distribution of the California Current in the offshore direction. It is interesting to note that very fine near-shore resolution is still missing, however (see Figure 5-2). Thus, further refinement would still be required for application of the model to a localized phenomenon, such as a plume.

The purpose of the outer grid is to apply a simpler model over the larger domain in order to help generate information needed for the GCM's open ocean boundary condition. Once this is done, then the more complex GCM makes predictions. The reason for this nested grid/nested model approach is for computational savings that are needed. That is also the same reason a more highly resolved grid was used only in the near-shore part of the GCM grid.

A significant part of the modeling effort was devoted to acquiring and analyzing the comprehensive set of data needed to run the model (that is, to specify the model's initial and boundary conditions). Data were obtained from such sources as California Cooperative Fisheries Investigation (CALCOFI), National Oceanographic Data Center (NODC), and Fleet Numerical Oceanography Center (FNOC). The data were reduced to seasonal averages over a grid of 0.5 degrees by 0.5 degrees from southern Baja California to Vancouver Island, and to 1000 km offshore.

The model was applied in both diagnostic and prognostic modes. In the diagnostic mode, seasonal circulation was calculated with a water density field defined by the climatological data. Also, seasonal atmospheric forcing was induced for each of the seasons. The model was able to simulate seasonal features of the California Current and counter currents as well. In the prognostic mode the model simulated a one-year period, and synoptic rather than seasonal atmospheric forcing was needed. While the intent was to simulate a one-year period continuously, two model restarts were made during the simulation to keep the hydrographic fields in deep water from diverging from the climatology. Although this illustrates some uncertainties associated with model predictions, nevertheless, the model results showed anticipated circulation characteristics during the period of predication.

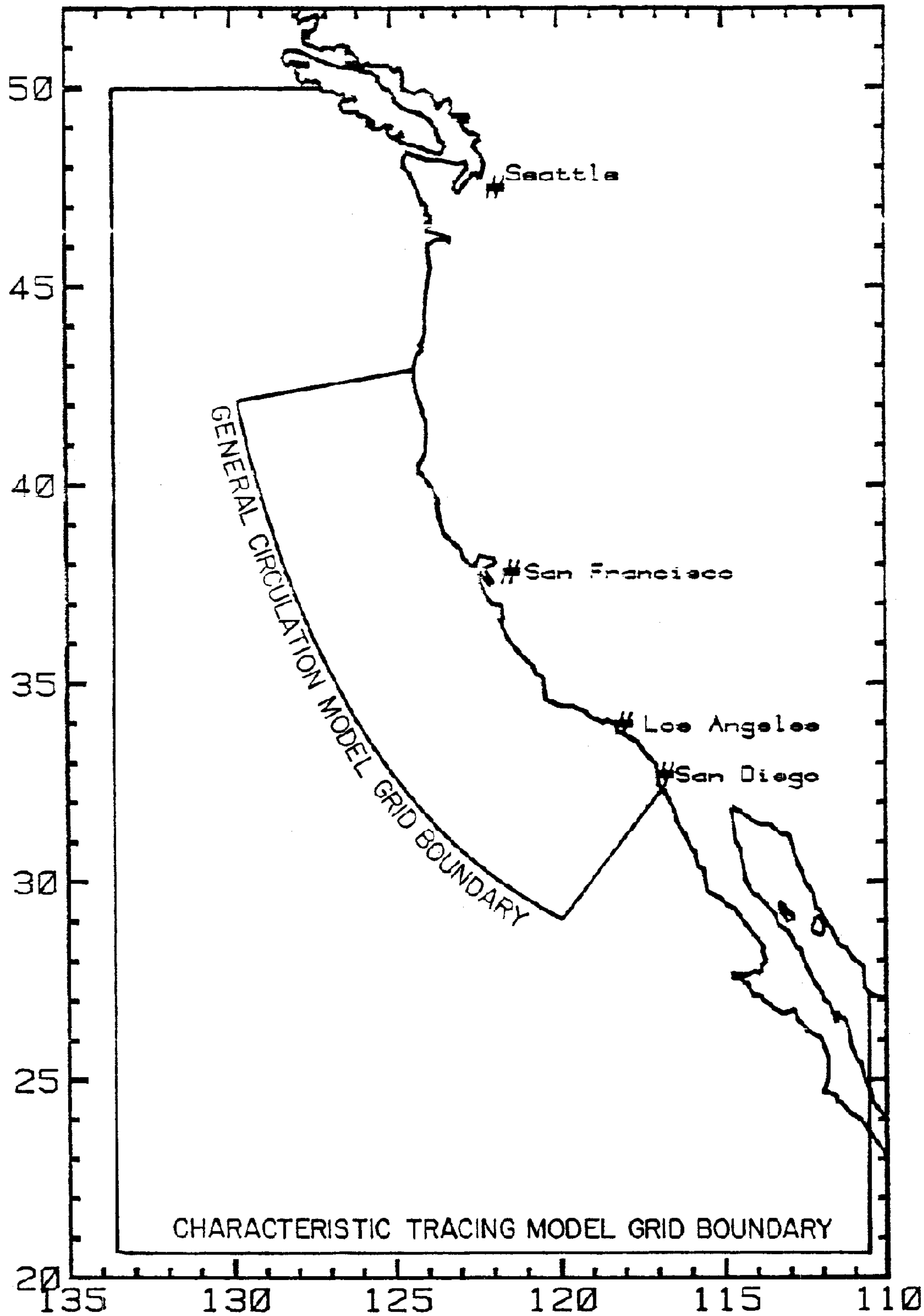

Figure 5-1. Location of the computational domains utilized in the 1984 California Coastal Circulation Model Study.

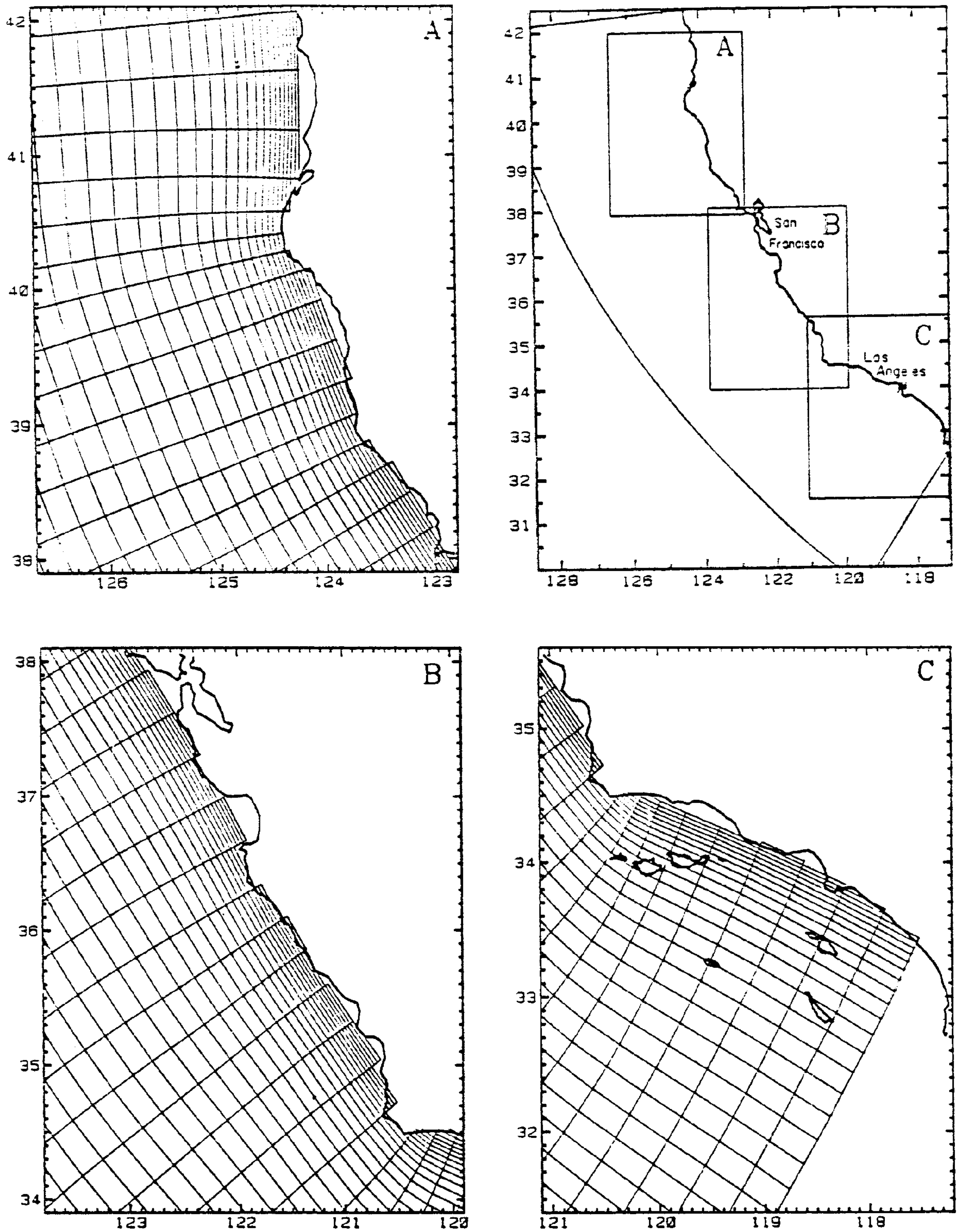

Figure 5-2. Illustration of the three subdomains used to plot magnified views of the nearshore region and the portion of curvilinear grid included in each.

In addition to the diagnostic and prognostic model applications, an extensive set of model validation exercises was performed prior to applying the model to its intended purpose. These were simplified applications that were intended to show whether the code was performing correctly by comparing the model results against simpler analytical solutions, or against situations where the general behavior of the model is known from physical principles. These exercises have lasting value in that they can be used to validate other models, as well.

Model sensitivity analyses were performed in order to establish confidence in the curvilinear coordinate system. This was done by comparing selected simulation results against an earlier version of the model that used a Cartesian coordinate system. Little difference was found in the two comparisons.

5.2.2 Plume Dispersion Study in Near San Clemente Island (Stacey et al., 2000)

Dispersion of a passive scalar released near the seabed at a depth of about 10 meters was experimentally analyzed, and then model predictions were made with both three-dimensional analytical and numerical models. The study site was on the eastern side of the San Clemente Island, which borders on the Outer Santa Barbara Channel. This study is unique in that a controlled dye release was passively (that is, without initial momentum or buoyancy) made into the coastal ocean environment. The spatial scale of the analysis is within 100-200 meters of the coast, and within a kilometer of the source. The temporal scale was on the order of hours. Thus the experiment simulates the fate of a small wastewater plume in the far field, after initial momentum and buoyancy are exerted.

One of the primary objectives of the study was to determine an appropriate expression for the lateral turbulent diffusion coefficient. It was found that the “4/3-law” was obeyed, consistent with earlier open-ocean experimental data. As a result of this finding, an analytical three-dimensional dispersion model was developed that accounted for the scale dependent turbulent diffusion process. The model was applied to the plume that resided below the thermocline. Additionally a three-dimensional finite difference model was also applied to predict concentrations within the plume. That model was able to simulate the general advective behavior of the plume, but was not able to predict the lateral scale-dependent dispersive process with accuracy. This study shows the importance of correctly characterizing the turbulence processes, a challenge that has been on-going for decades by generations of researchers. The importance to the District is that these small-scale processes must be correctly simulated in order to predict the evolution of their plume.

5.2.3 Mamala Bay, Hawaii, Outfall Modeling Study (Roberts, 1999a,b; Connolly et al., 1999)

Both the near field and far field behavior of the Sand Island, Hawaii, and ocean outfall plume were modeled. The near field modeling was conducted using a modified version of the Roberts-Snyder-Baumgartner (RSB) model, and far field modeling was conducted using a variety of models, as discussed below.

The Sand Island outfall discharges approximately 71 MGD, and varies between 45 to 89 MGD during a day. The total outfall length is 3811 meters, of which 1031 meters is the diffuser. The water depth at discharge ranges from 67 to 72 meters (see Figure 5-3).

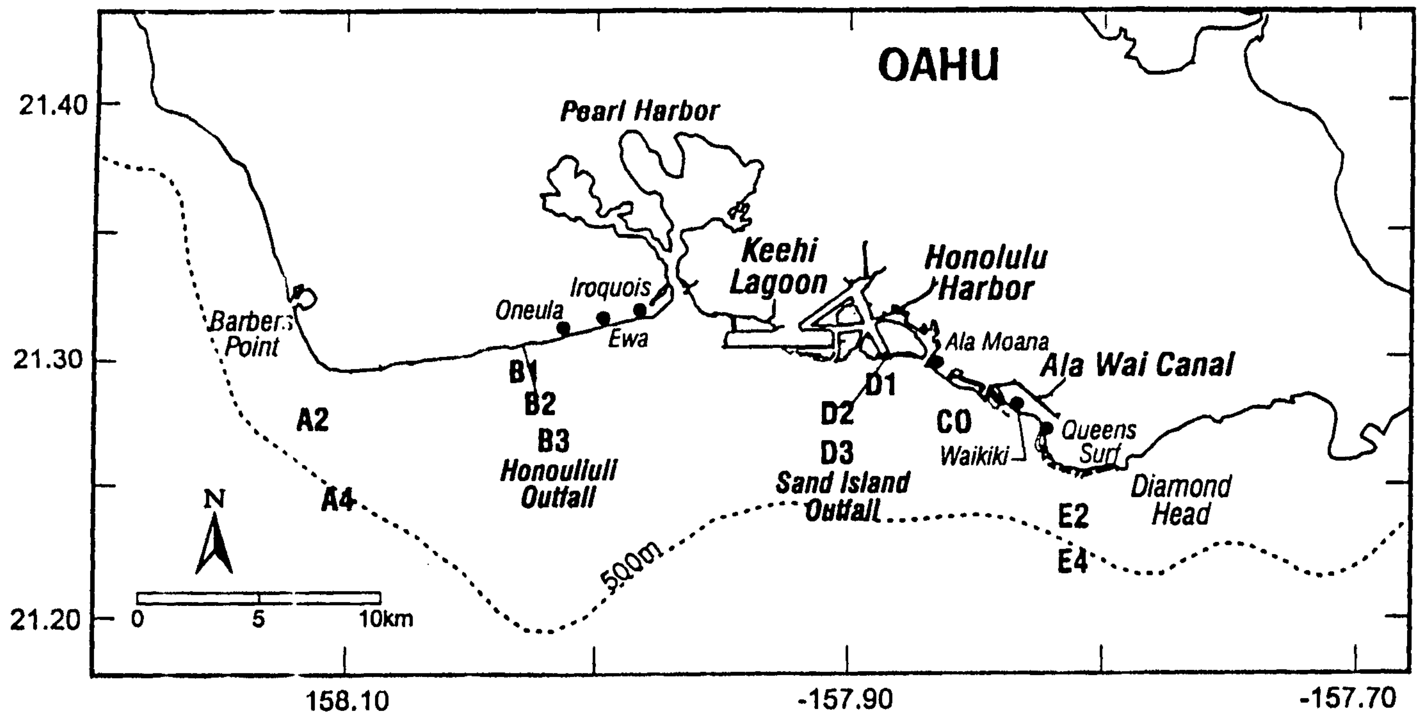

Figure 5-3. Location of Sand Island outfall in Mamala Bay, Oahu, HI.

Peak currents in the vicinity range from 100 cm/sec at Diamond Head to the east to about 40 cm/sec at the outfall. The principle directions of the currents are along local depth contours. Currents reverse twice daily, showing the strong semidiurnal tidal component. Both upwelling and downwelling occur in the vicinity of the discharge, due to the periodic convergence and divergence of currents in the vicinity of the outfall due to the movement of the M2 tidal component around the island. This phenomenon is important in affecting the strength of density stratification (the water column destratifies frequently).

The near field RSB model simulates for each time step requested by the user, the initial dilution, the height of rise of the plume, the plume's thickness, and the horizontal dimensions. Based on the large amount of data available, the model was run 20000 times to simulate the period June 5, 1994 to April 18, 1995. Dilutions during that time varied widely from about 100 to 4000; the median value was 320, and the mean value was 540. The plume was predicted to surface about 11 percent of the time. When comparisons were made between model results and field observations thickness and height of rise predictions were in good agreement; dilutions were overestimated by a factor of about two.

Two basically different far field modeling approaches were used: one by Roberts(1999) and the other by Connolly et al.(1999). Roberts took an approach simpler than the complex numerical simulation models, and cited a number of limitations of the three-dimensional numerical simulation models that include:

- Coastal circulation patterns are complex, and difficult to predict.
- The open ocean boundary condition introduces unknown conditions into the domain to be simulated.
- Uncertainties exist in the parameterization of the shear stresses as a function of degree of stratification.
- Unknown spatial and temporal variations in forcing functions exist.
- Uncertainties are introduced in modeling turbulent diffusion processes.
- Excessive numerical dispersion may result from using fixed grid Eulerian models.
- An inability exists to accurately verify the models due to undersampling of current fields, for example.

Roberts chose simpler far field models, and divided them into short-term and long-term far field components. For the short-term model, Roberts developed a diffusion model that obeys the 4/3-law of turbulent diffusion in the coastal environment. The total dilution calculated was found as the product of the dilution at the completion of initial mixing and the short-term far field model. Then the long-term model was used to generate a background concentration that was governed by the plume itself, and its movement in the local area. This was also an analytical model based on previous work by Csanady (1983). The models were applied to predict the fate of coliform organisms released from the diffuser. Contours of exceedance frequencies of coliforms in the vicinity of the outfall were calculated. Emphasis was on an area within 10 km of the outfall.

Independently, the three-dimensional circulation and water quality model ECOM was applied to predict the fate of pathogenic organisms in the vicinity of the outfall. Two numerical grids were generated for this application: one for the circulation model that extended around the island, and a grid for the fate and transport model that was more local in extent (see Figure 5-4). The more extensive circulation model grid was needed in order to correctly simulate the observed circulation patterns in Mamala Bay. The numerical grid consisted of cells between 2 to 4 kms on a side, with smaller grid cells within Mamala Bay (400 to 700 meters on a side). The grid extended into harbor areas to allow better representation of the impacts from sources of pathogens within those areas.

The water temperatures used by the model were not calculated directly, but were specified over the simulation period. This was done because the water temperatures exhibited such a complex pattern that it was not possible to simulate them.

ECOM was used jointly with the near-field model of Roberts (1999) described previously. The near-field model predicted plume height of rise and initial dilution on a continuous basis, and that information was fed into ECOM.

The model was calibrated based on data collected over a one-year period by comparing predictions to water surface elevations, current velocities, temperature, salinity, and a conservative tracer from a dye release. Predicted water level elevations were compared with measured values at five locations for a thirty day period. Relative errors were less than three percent.

Tidal current comparisons were made at six stations also for 30 day periods. While a quantitative measure of agreement was not given, the result “was quite reasonable given our level of understanding of the circulation physics”.

The ability of the model to predict pathogen concentrations was evaluated using both cumulative distributions and time series of data. The root mean errors were less for the probability distributions than for the time series.

A conclusion of the study was that the Sand Island discharge was a primary contributor of observed fecal coliform levels on eastern recreational beaches. Other sources were identified as important for other beaches, and during storm events.

5.2.4 Massachusetts Bay and Boston Outfall Coastal Modeling

For more than a decade, work has been ongoing to evaluate the potential impacts of an outfall from the City of Boston designed to extend 9 miles out into the Massachusetts Bay. The outfall will discharge approximately 455 MGD of treated effluent from the city of Boston. During that time nearly continuous model applications and further model developments have been made. A summary of that work is described here, from various papers and website postings.

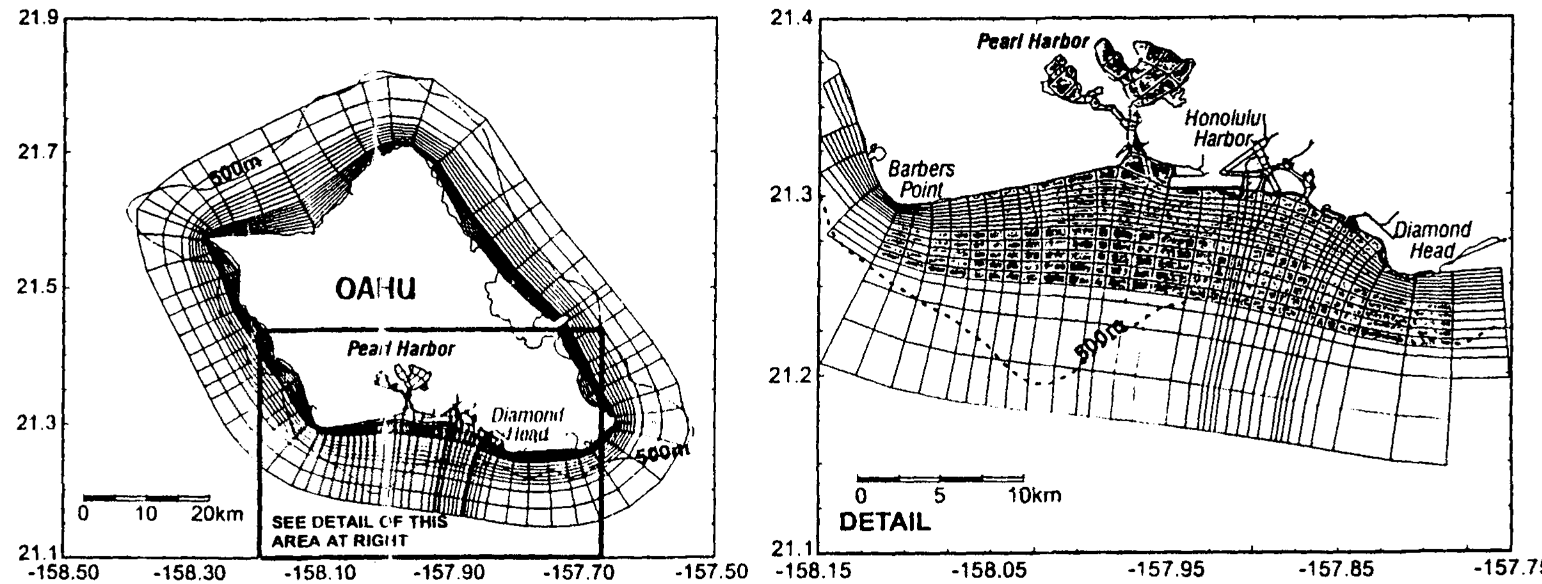

Figure 5-4. Circulation and water quality grids used for numerical models.

Blumberg et al. (1993) describes the application of ECOM to Massachusetts Bay (see Figure 5-5). That figure shows the locations of the present and proposed outfalls. Two existing outfalls are denoted by triangles in the figure, and both are located in Boston Harbor. The new outfall is shown in Massachusetts Bay, and is near the 40 m contour. The grid used is shown in Figure 5-6. Grid size ranges from 8 kilometers at the open ocean boundary to 600 meters in the near shore portions of the grid. The ECOM model employees an orthogonal curvilinear grid in the horizontal, and a sigma coordinate system in the vertical, where the number of layers is the same regardless of water depth. Ten sigma layers were used.

The modeling work reported in Blumberg et al. (1993) was largely exploratory, and addressed issues such as tidal and subtidal currents, the causes of the counterclockwise currents in the Bay, and outfall plume dynamics. However, the last topic was only briefly addressed in this paper. There was no discussion of how near-field plume dynamics were handled. Blumberg et al. discuss this topic in a subsequent paper (1996). By comparing ECOM predictions in the vicinity of the proposed outfall with ULINE, a near field plume model, it was shown that the model comparisons for height of plume rise and initial dilution were in general agreement. Subsequently, Zhang and Adams (1999) developed procedures for coupling near and far field models, so that the far field model simulates the correct dimensions and initial dilution of a plume.

More recent efforts at modeling the Massachusetts Bay circulation and the outfall plume dynamics are reported by the USGS Woods Hole Field Center at URLs such as http://crusty.er.usgs.gov/mbay/effluent.html, or, http://crusty.er.usgs.gov/mbay/modeling.html. A 1996 USGS Open file report (96-015) is included on the site. A conclusion of that report is that the model can represent the response of the bay during unstratified conditions and not during stratified conditions. Also discussed is the fact that the Gulf of Maine was also simulated using an expanded grid in order to provide the appropriate forcing. More detailed effluent modeling was performed, and comparisons were made with dilution simulations from existing and the proposed outfall.

5.2.5 Coastal Marine Demonstration Project for the U.S. East Coast

This is a two-year demonstration project conducted during the years 1999-2000. The project is a component of the National Oceanographic Partnership Program (NOPP), and focuses on providing oceanographic and atmospheric products for the Chesapeake Bay and surrounding coastal waters from approximately 70 degrees west to the coast (actually to the 10 meter depth contour), and from 32 degrees north to 42 degrees north. Figure 5-7a shows this area. The grid for the numerical ocean model used extends beyond this area, as shown in Figure 5-7b. Note that the grid extends to 50 degrees west, so that boundaries are well away from the interior of the domain where predictions are made.

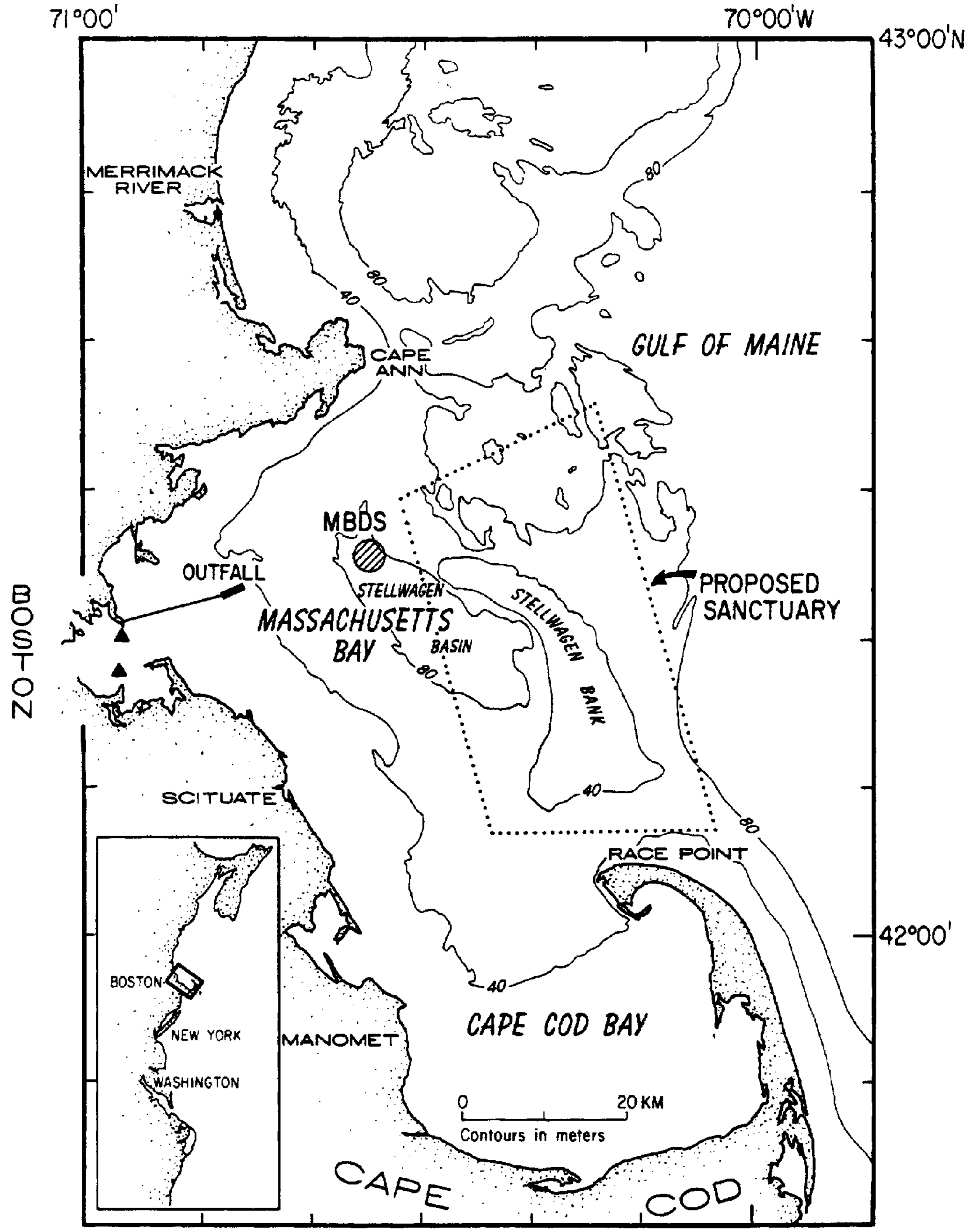

Figure 5-5. Bathymetric map showing Massachusetts and Cape Code Bays, present sewage outfalls in Boston Harbor (solid triangles), and location of new ocean outfall for treated Boston sewage in western Massachusetts Bay.

Massachusetts Bays Model Grid

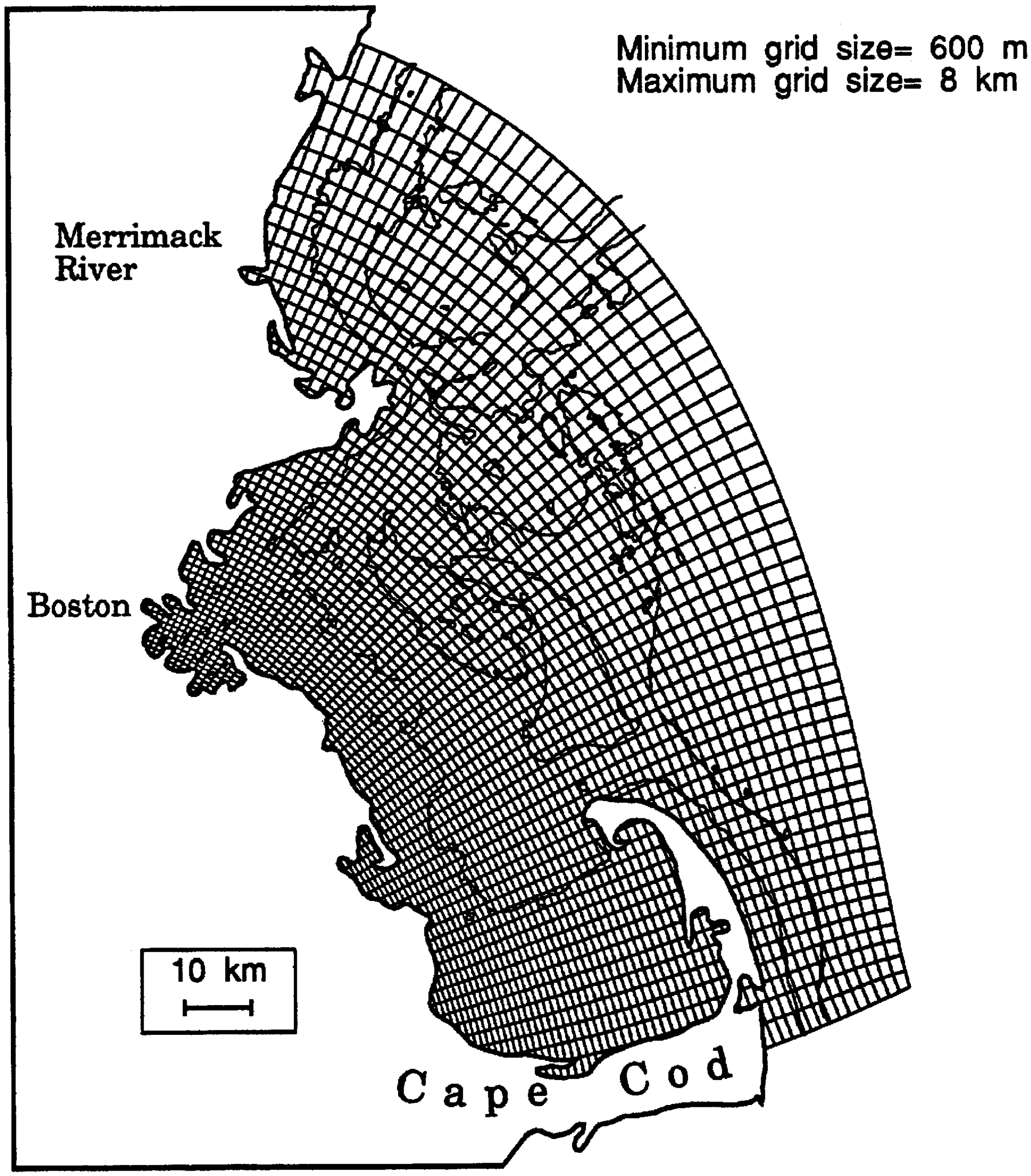

Figure 5-6. Model grid for three-dimensional circulation model, ECOM3D, of Massachusetts and Cape Cod Bays.

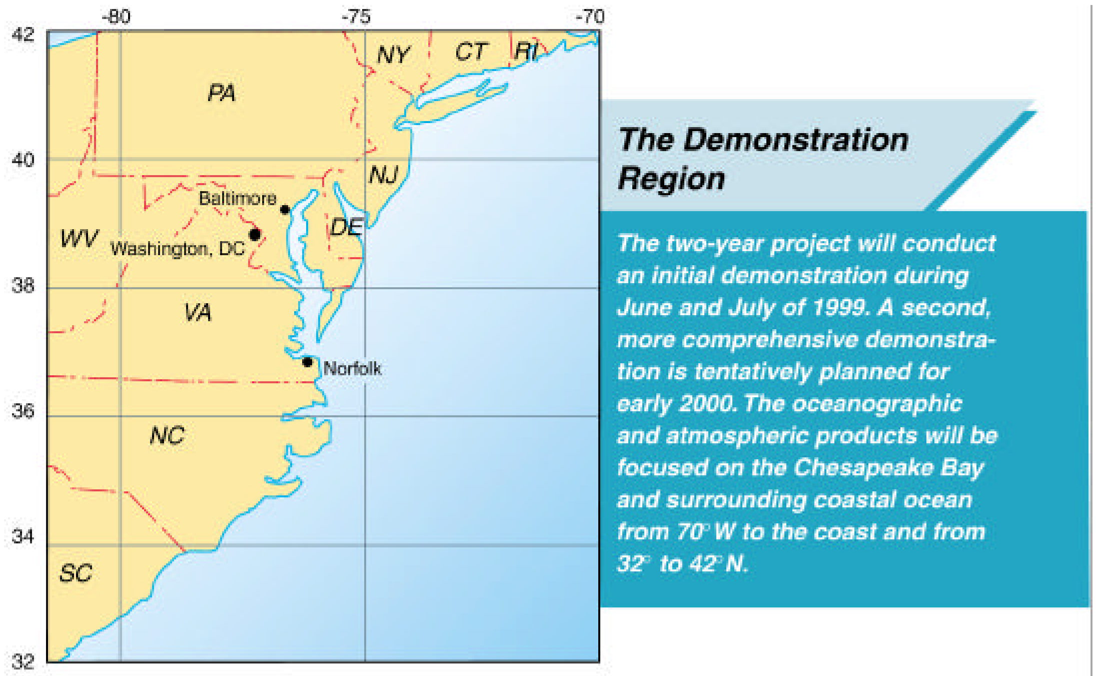

Figure 5-7a. Extend of coastal ocean where forecasting information made.

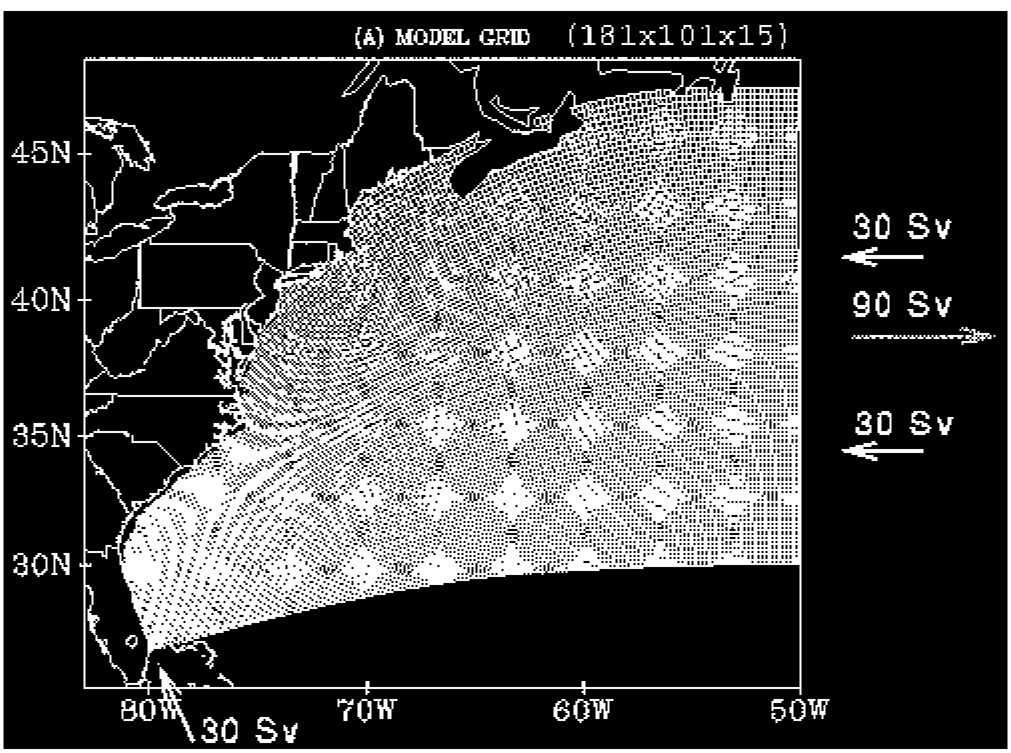

Figure 5-7b. Extent of ocean model grid used in ECOFS.

The long-term objective of the program is to develop a system capable of producing useful nowcast and forecast information for the coastal region. A quasi-operational system based on the coupling of the POM ocean model to the Eta-32 mesoscale atmospheric model has been in operation since 1993. The forecast cycle generates coastal ocean forecasts out to 24 hours. Products include:

- Water level elevations,
- Surface currents
- Significant wave height and direction
- Surface wind analysis and forecasts
- For the coastal ocean, additional products include water temperatures, currents, and salinity at 200 meter depth and at the ocean's bottom

Example products for the Chesapeake Bay are shown on Figure 5-8a, and for the coastal environment on Figure 5-8b. Both show forecasted current speeds. While POM is used for the coastal ocean, the Model for Estuarine and Coastal Circulation Assessment (MECCA) has been used for the Bay. MECCA is a three-dimensional circulation model that uses sigma vertical coordinate (similar to POM), but employees square cells. It does not appear the two models are coupled. Note that Figure 5-8b illustrates that the near shore boundary of the ocean circulation model does not extend to the boundary of the Chesapeake Bay.

5.2.6 Finite element model application to the Gulf of Maine (Lynch et al., 1995)

This is the only case study included in this paper that illustrates the application of a finite element model to a coastal circulation problem. The model applied is QUODDY, developed at Dartmouth College. The authors expound the advantages of the finite element model over "conventional modeling strategies", which are assumed to be finite difference techniques. Advantages listed include:

- Freedom to use unstructured, non-uniform computational grids of various sized elements, such as triangular elements. This allows high resolution of local topographic features, without having to sacrifice the extent of the spatial domain.

- Freedom to use different numbers of elements vertically, as needed, rather than a constant number as for the sigma coordinate system.

The model simulated the Gulf of Maine from Long Island north to the Laurentian Channel, and east to the 1000-meter isobath. Approximately 6800 horizontal nodes were in the mesh. The modeling study examined a number of processes including:

- Tidal rectification of the M2 tide averaged over a tidal cycle to see the residual tidal effects on circulation.

- The effects of stratification were evaluated and were shown to increase peak velocities.

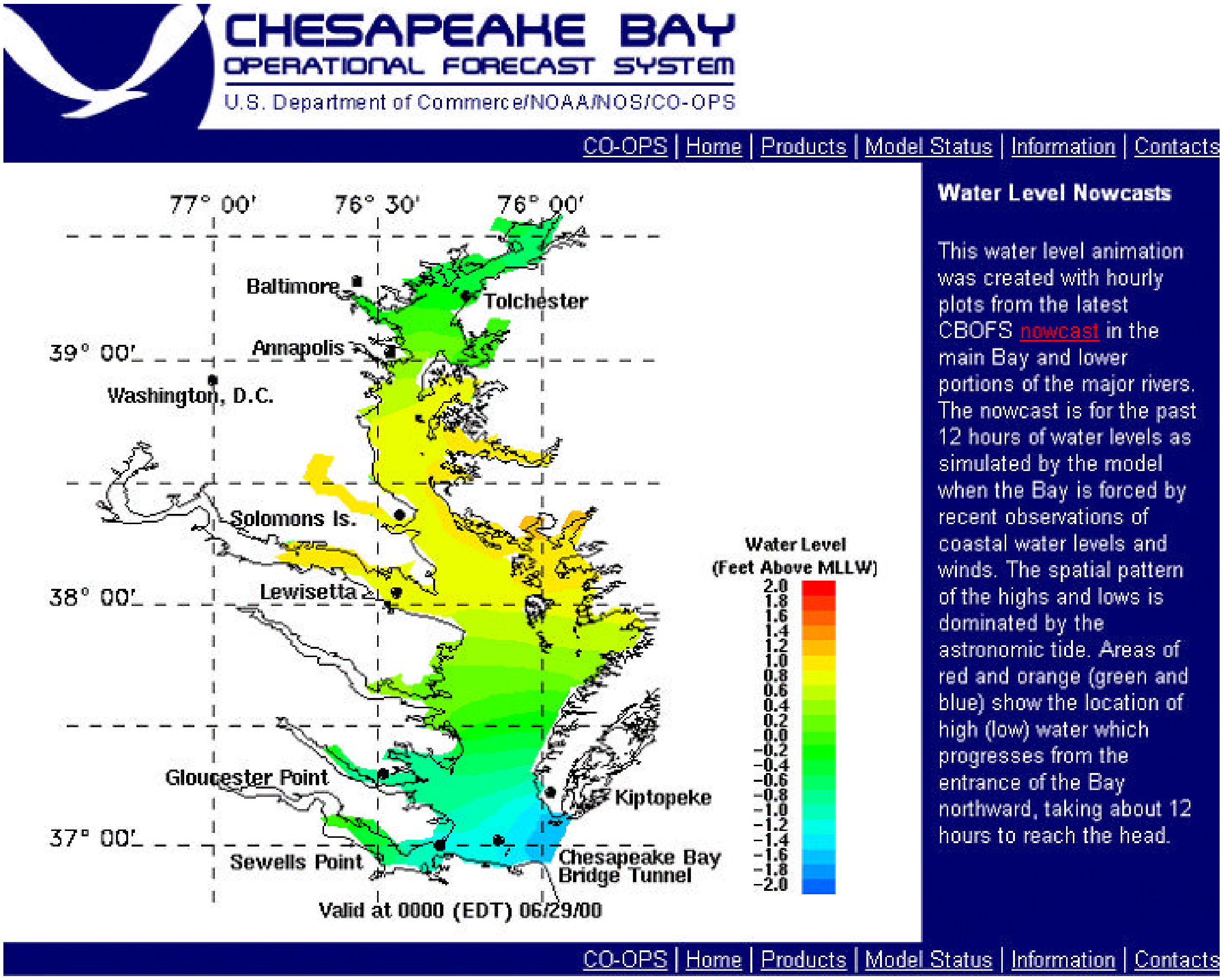

Figure 5-8a. Nowcast of water level information.

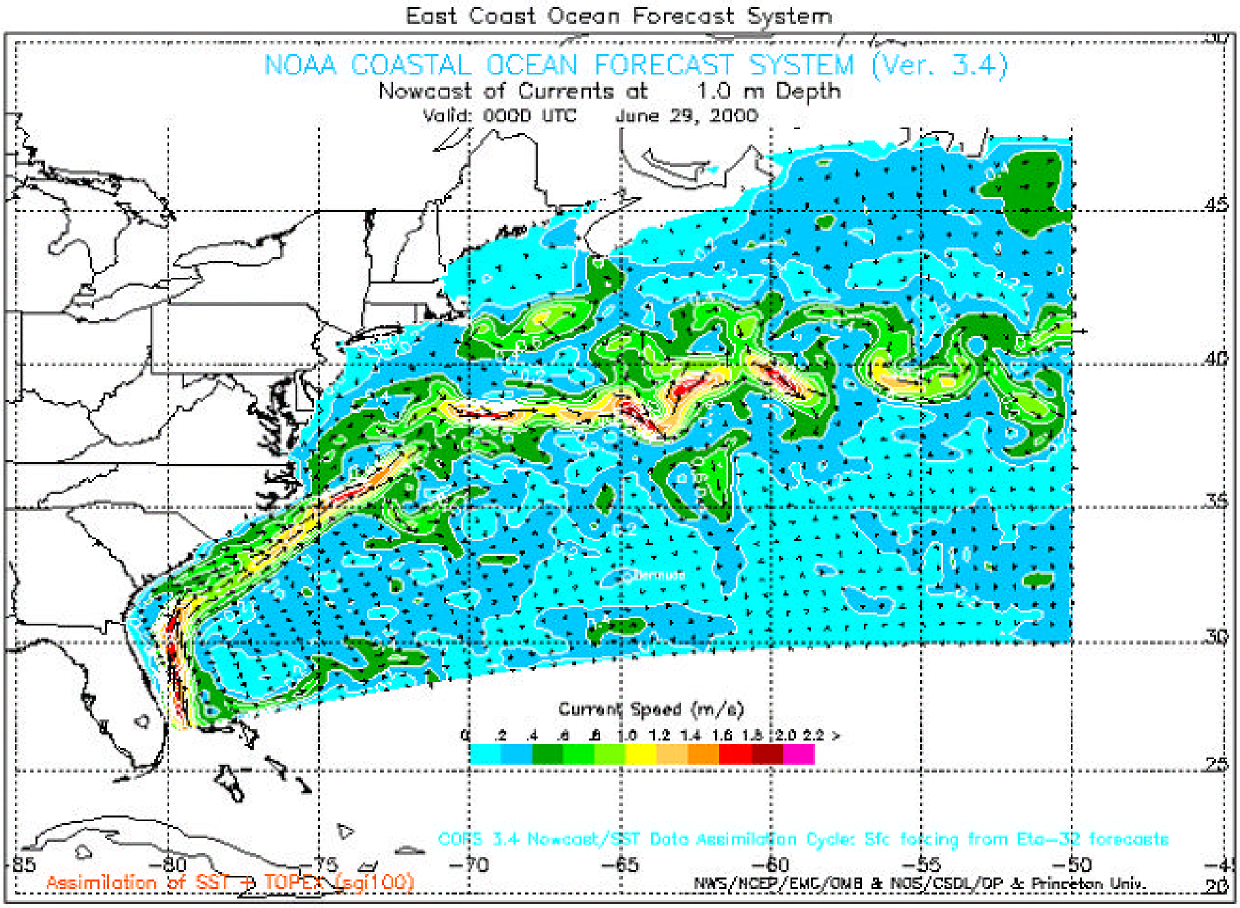

Figure 5-8b. Nowcast of currents of 1 meter depth.

- Seasonal composite circulation forced by climatological wind stresses and the M2 tides.

- Transport processes were studied by both the Lagrangian Particle Tracking techniques, and the advective-diffusion equations.

The study concluded that the finite element model provided a flexible and comprehensive tool to evaluate coastal circulation problems.

5.2.7 Naval Research in Ocean modeling (Harding et al. (1999)

The U.S. Navy is engaged in comprehensive research on the development and application of ocean models for their purposes. The Navy works with a variety of researchers who develop ocean models, including Princeton University (POM), University of Miami (MICOM), and Dartmouth college (QUODDY). The paper of Harding et al. (1999) provides an overview of the ongoing and planned work. The URLs given in that reference and in this paper provide a volume of additional information. This work is particularly relevant to the District because much of the present effort has focused on the Coastal Pacific Ocean, including the Southern California Bight.

The Navy, prior to 1991, used ocean models primarily to assist in anti-submarine warfare activities associated with the deep ocean. More recently the focus has shifted to coastal applications, such as mine warfare, amphibious warfare, and special operations. Consequently, models that can make nowcasts and forecasts in this environment are needed. The Navy is embracing the concept of embedded domains/grids to effectively generate the detailed resolution needed. Figure 5-9 illustrates the concept. Computer resources to execute this nested domain concept reside in central locations for the more intensive computational requirements, and locally for the less computational models that generate the local, higher resolution information.

The Naval research is intended to develop new models that can replace existing ones, as the need exists. For example, Harding et al. (1999) report that POM will be replaced within a year by the more recently developed Navy Coastal Ocean Model (NCOM), which is described in Martin (1998a, 1998b). Further in the future the next generation ocean model may be a version of the University of Miami's MICOM.

The Navy has implemented the North Pacific Ocean Nowcast/Forecast System (NPACNFS) for automated real-time ocean predictions for the North Pacific Ocean. (http://www7320.nrlssc.navy.mil/npacnfs_www/NPACNFS_info.html). The NPACNFS consists of a data assimilative model based on POM, a statistical three-dimensional ocean temperature/salinity analysis model, and a real-time data stream. The system is restarted everyday for previous nowcast fields. Forecasts of up to 72-hours are produced. The system runs on the NRL Ocean dynamics and Prediction Branch workstations. The POM appears to have been renamed for this application to PWC (http://www7300.nrlssc.navy.mil/html/mel-home.html). An application of the PWC on the URL shows surface water temperatures for the Southern California Bight, and the warm and cold core eddies (see Figure 5-10).

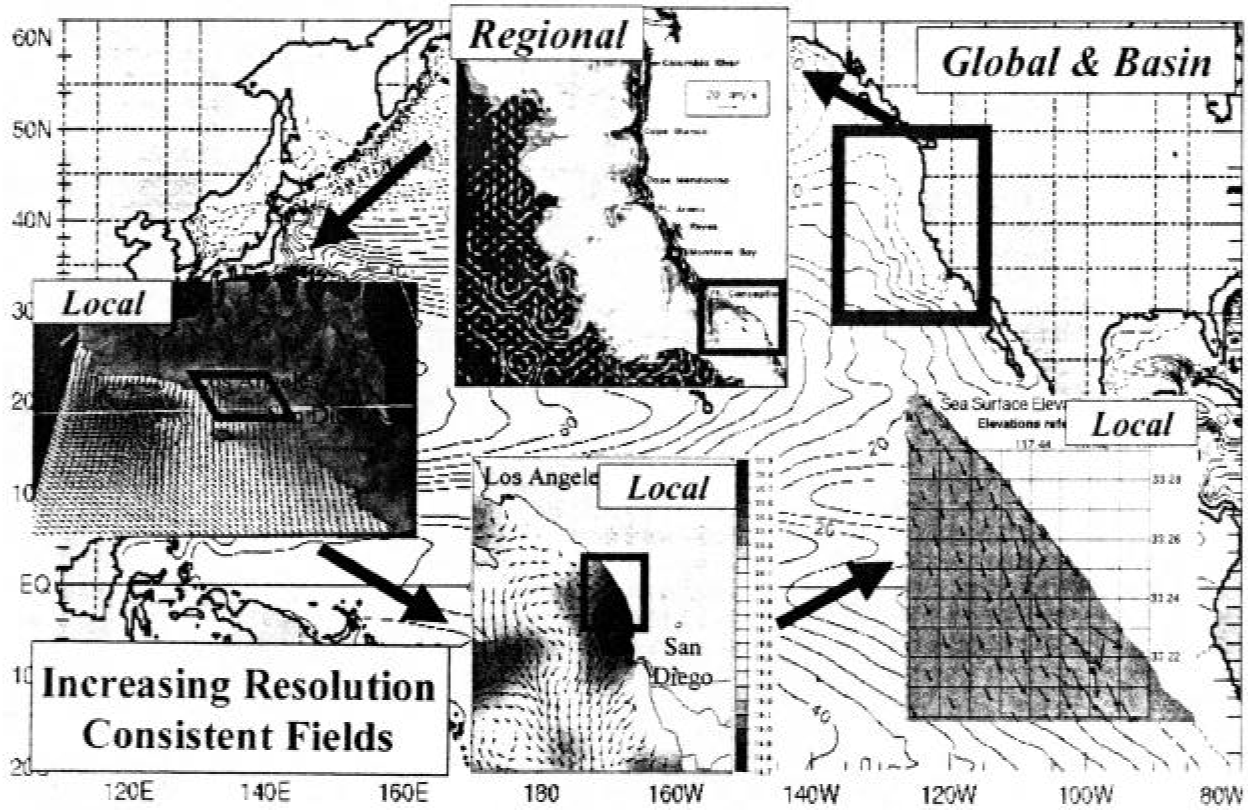

Figure 5-9. The NRL ocean forecast strategy envisions a cascading nesting of domains with ever-higher resolutions.

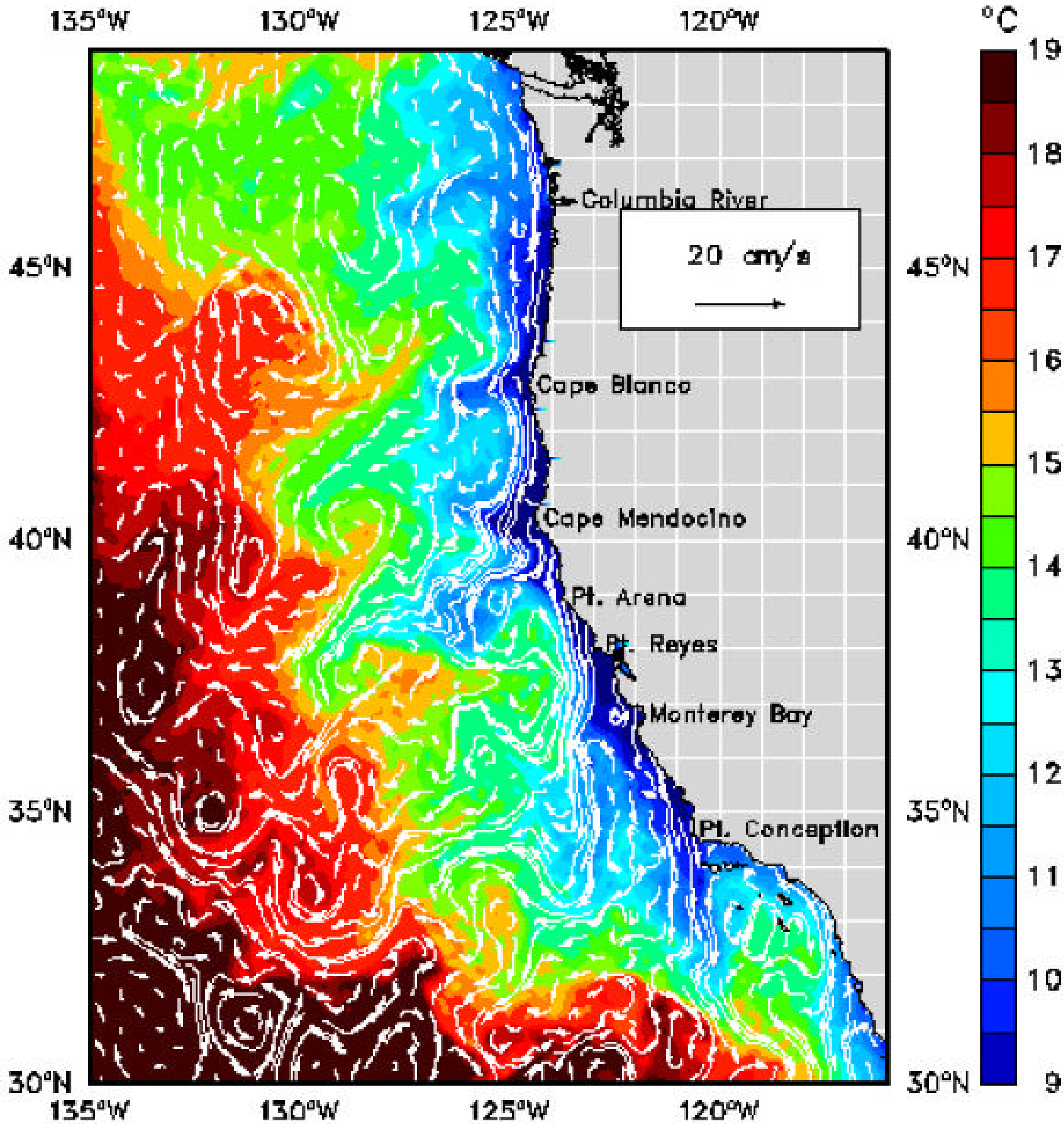

Figure 5-10. Princeton West Coast (PWC) model result for day 600, corresponding to August 31 of the second year of model simulation.

6.0 Review of Ocean Models and Modeling Systems

The review in this section is intended to introduce both three-dimensional far field and near field models. First the far field circulation models are presented, and are then followed by the near-field models (some of which have a simplified far field component). The recent book by Martin and McCutcheon (1999) provides a review of models including hydrodynamic and water quality models for estuaries. A number of those models are included here, as appropriate. A second review article by Abbott (1997) presents circulation and water quality models from the point of view of dimensionality (one-, two-, or three-dimensional) and functionality. Haidvogel and Beckmann (1999) also provide a review of ocean models.

6.1 Far Field Models

Table 6-1 provides an overview of numerical three-dimensional circulation models. This table is intended to provide general information, such as references, URLs, and whether the model is finite element or finite difference. Even with the extensive search performed for this review, it has become apparent that it is not possible to locate and discuss all ocean circulation models in this rapidly expanding field. See the URL http://stommel.tamu.edu/~ baum/ocean_models.html for brief discussions of a number of circulation models, many of which have been given different names depending on their applications. Most, but not all, of those models are included here.

Table 6-2 provides more detailed information on combined circulation and water quality modeling systems. The number of such models is significantly less than the number of ocean circulation models. Typically, these modeling systems have been developed by (or for use by) consulting organizations, and typically contain detailed documentation, user friendly features, and other pre- and post-processing capabilities. Appendix B provides descriptions of many of the combined circulation and water quality models.

The development of the first significant ocean models occurred over the decade of the 1960's at the Geophysical Fluid Dynamics Laboratory, operated by NOAA and now located at Princeton University. Bryant built an ocean model that was to be used with atmospheric models to study climate. Along with co-worker Cox, he developed a series of models, including two-dimensional, three-dimensional box model, and then a model of full circulation of the world's ocean. That model became known as MOM (Modular Ocean Model). This early model used a "rigid lid" assumption to eliminate high-speed external gravity waves and would allow a longer time step. The early models used a grid spacing in the horizontal of about two degrees, or about 150 km, and 12 vertical layers. The model took months of real time to simulate a few years. Then, even coarser grids were used (five degrees). However, using these coarse grids, it was not possible to model many important features of the world's oceans, such as fast moving and relatively narrow (more narrow than the grid spacing) current systems (for example, the Gulf Stream).

To achieve more resolution, attempts were made to run the ocean models on more resolved grids (20 km resolution) in the early 1970's. To achieve this within the limitations of the computer speeds available, domain size and the number of vertical layers were reduced. Two- and three-layer quasi-geostrophic models were widely used during that period.

Table 6-1 goes here

Table 6-2 goes here

By the mid-1980's, progress had been made in simulating more realistic aspects of ocean circulation, with much of the progress resulting from increasing computational power. Global MOM-type models could be run for centuries with three-degree (300 km) resolution. During this time a number of alternative model formulations were developed, such as finite difference techniques that used curvilinear coordinates (POM), or models that used coordinate surfaces of constant density (MICOM). The latter class of models (isopycnal) tend to reduce excessive artificial horizontal diffusion, a process important for dispersion modeling.

As computational power continued to increase, grid resolution dropped to ¼ degree for some applications during the late 1980's. Model output comparisons began, with a project called CME (Community Modeling Evaluation), discussed in a subsequent section.

In the early 1990's, more efforts were focused on retaining the free surface features in models without incurring the tremendous computational costs of doing so. Los Alamos National Laboratory was one of the developers of the new techniques (POP series models).

Models use even more resolved grids today (approaching 1/10 of a degree). Computational times for this resolution is about three days per simulated year of the world's oceans. Vector computers and massively parallel machines are needed that are continually faster and faster. Machines with speeds of teraflops are anticipated that will reduce computational times (or allow finer resolution grids). Consequently, ocean models need to be written to take advantage of such computer architecture. Such has been done on at least some models (MICOM and POP).

6.2 Near Field Mixing Models

Near field mixing models are widely used components of ocean outfall plume dispersion modeling systems, whether those systems are simple or complex. They can be used to predict the initial mixing characteristics of the plume (that is, during the first few minutes following release from the outfall), when the far field model is not applicable. See Appendix C for discussions of two of the most widely used systems.

6.3 Data Requirements for Circulation and Dispersion Models

The specification of data requirements for the models is not as straightforward as it may first appear. The amount of data depends on, among other factors, the spatial and temporal variability of the forcing functions that drive the model, as well as the degree of variability within the domain and on the boundaries of the domain simulated. Further, different modelers may choose to estimate missing data based on their understanding of the modeling problem, while others may insist missing data be quantified from more intensive monitoring.

Here an overview of model data requirements is presented. More details of data requirements for specific models can be obtained by consulting the users manuals for those models.

Table 6-3 summarizes input data requirements. The categories in the table are not intended to be mutually exclusive, but provide a convenient way of looking at the required data from several points of view. Historical data provide the data pool from which much of the data used for

Table 6-3 goes here

modeling will come. Should those data be inadequate to characterize, for example, the boundary conditions, then supplemental data will need to be collected, or generated in an alternative manner.

Initial and boundary condition data refer to the two major categories of data needed by models. The initial condition data describe the state of the system at the time the simulation begins. Boundary condition data describe the data required to prescribe what is happening on the domain boundaries over the entire simulation period. Such information can be hard to quantify over the entire boundaries, and can be sources of significant model errors during simulation.

Additionally, a portion of the historical data may be needed to calibrate and verify the model. The historical data should generally be scrutinized quite closely to determine if such data exist.

6.4 Ocean Circulation Benchmarking and Test Problems

Ocean circulation models can be compared against each other (typically the process is called benchmarking) to examine comparative model performance, or models can be compared against simpler problems that have known analytical solutions (test problem validation). While benchmarking in concept appears straightforward, and appears to be a way of establishing superiority of one model over the others, in reality this does not happen. It is often very difficult to set up and apply a series of models to a real-world problem in a completely unambiguous way. It is often difficult to explain exactly why model results differ from one another (For example, are model formulations different enough to cause the differences? Are the input data sets really comparable?)

Even with these problems, some systematic comparisons among ocean circulation models have been conducted over the past decade. Below, three such projects are described:

- CME (Community Modeling Effort). This study was initiated by the National Center for Atmospheric Research, and subsequently expanded as other groups joined. In CME, apparently only one model was used (MOM), so this was not benchmarking in the sense described above. Rather, starting from a baseline representation of the North Atlantic, the influence of forcing functions, grid resolution, and sub-grid parameterizations were evaluated.

- DYNAMO (Dynamics of North Atlantic Models). For this benchmarking study, three models were used (MOM, MICOM, and SPEM). A goal of the study was to examine the influence of alternative ways of handling the vertical coordinate. This was not completely achieved. The models were assessed for their ability to reproduce essential features in the North Atlantic Ocean circulation patterns.

DAMEE (Data Assimilation and Model Evaluation Experiment). Seven United States modeling groups were involved in developing nowcasting capability with basin-wide forecasting skill. The models used were geopotential (MOM and DieCAST), sigma-coordinate (SCRUM and POM), isopycnal (MICOM and NLOM), and finite element (SEOM). Freedom was given to each modeling group to set up certain aspects of each problem solved in the study.

Ocean circulation test problems have also been developed over the years by a number of researchers as they have developed and tested their models. Examples of references to such test problems include Blumberg et al. (1984), Muin and Spaulding (1996, 1997a), McCalpin (1995), and the ROMS website. These test problems are useful for not only to validate the code, but to examine how different grid types and resolutions influence the solutions, and to estimate computational resources for real applications. They also provide a way to compare different numerical models in a more unambiguous way than the benchmarking described above.

A summary of the test problem from the ROMS web site is provided in Appendix D.

6.5 Example Conceptual Application of Quasi-Analytical Models to District's Plume

In this section an approach to simulate the District's plume using quasi-analytical tools is presented. This level of analysis is more simplified than an approach that uses numerical models (illustrated in the next section). Advantages of the simpler approach include:

- Far less data requirements
- Numerical grids are not needed
- Model can be executed on PCs in a few seconds to minutes
- Alternatives can be expeditiously evaluated
- Approach is more easily understand to a wider audience

The term "quasi-analytical" refers to models that can be solved analytically (or exactly), rather than numerically (or approximately). Quasi-analytical solutions may contain integrals or infinite series that can be evaluated to a high degree of accuracy; thus the models solve the more simplified equations exactly. Further, numerical grids are not needed with such models, and so the overhead required to prepare and execute those models is much less.

The approach illustrated below consists of three major components:

1. A model component that predicts the initial dilution from the wastewater plume that occurs within the first few minutes to hours following discharge through the submerged outfall. Such a model can either be executed once over the period of time to be simulated or the model can be executed multiple times within the simulation period to predict evolving initial dilutions.

2. A particle tracking model component that tracks the centerline of the plume as the plume migrates in the far field over the days following discharge.

3. A fate and transport model component that predicts the concentrations of constituents of concern in the plume over a period of days following release. Such models typically consider advection by ocean currents, turbulent diffusive mixing, decay, and the effects of boundaries (such as the shoreline or seabed).

Recently developed quasi-analytical modeling techniques that appear to consider one or more of these three model components are: Roberts (1999); Frick et al (1997); and Hendricks and

Stolzenbach (1997). However such models can differ significantly from each other, in ways that include:

- The choice of the three modeling components
- The proprietary or not-proprietary nature of the models
- The user-friendly features (or lack of) of the models (e.g., does the model have a graphical user interface and develop graphical output?) that significantly affect their ease of use
- The amount of post-processing done to statistically interpret simulation results over long periods of time

Thus, quasi-analytical models can be quite different from each other both in what they can do, and in the user's ease in doing it.

For component #1 (initial dilution models) the most widely used choices over the past several years appear to be either Visual Plumes or CORMIX, both described in detail in Appendix C. CORMIX is a propriety model that can be purchased for approximately $500.00. The newest version has a graphical user interface, and is run on a Windows operating systems. Visual Plumes has completed beta testing and will be freely distributed by CEAMS (Center for Exposure Assessment Models). Visual Plumes consists of a number of plume models, similar to those used at Manala Bay. Also visual plumes can simulate a time series of initial dilutions, which is a very useful feature for the District's application.

The purpose of the initial dilution models is to predict concentrations, dilutions, and locations within the water column at the completion of this initial mixing period. Figure 6-1 illustrates the effluent plume after leaving the diffuser. Due to combination of upward momentum and positive buoyancy, the plume rises. It may eventually overshoot its trapping level, and eventually settle back to this level. At this time, the initial dilution process is complete.

As illustrated in Figure 6-2, the initial dilutions can constantly change over time, due to changing ambient velocity, density stratification, and effluent volumetric flow. Thus, if a continuous simulation of the fate of a plume (say continuous over several months) were to be made, these changing initial dilutions would need to be simulated to get a realistic three-dimensional picture of the fate of the plume over that period of time.

At the completion of the initial mixing process the concentration of constituents in the plume can be estimated by:

$$C_f(t) = C_a + \left[\frac{C_e(t) - C_a}{S_a(t)} \right] \tag{6-1}$$

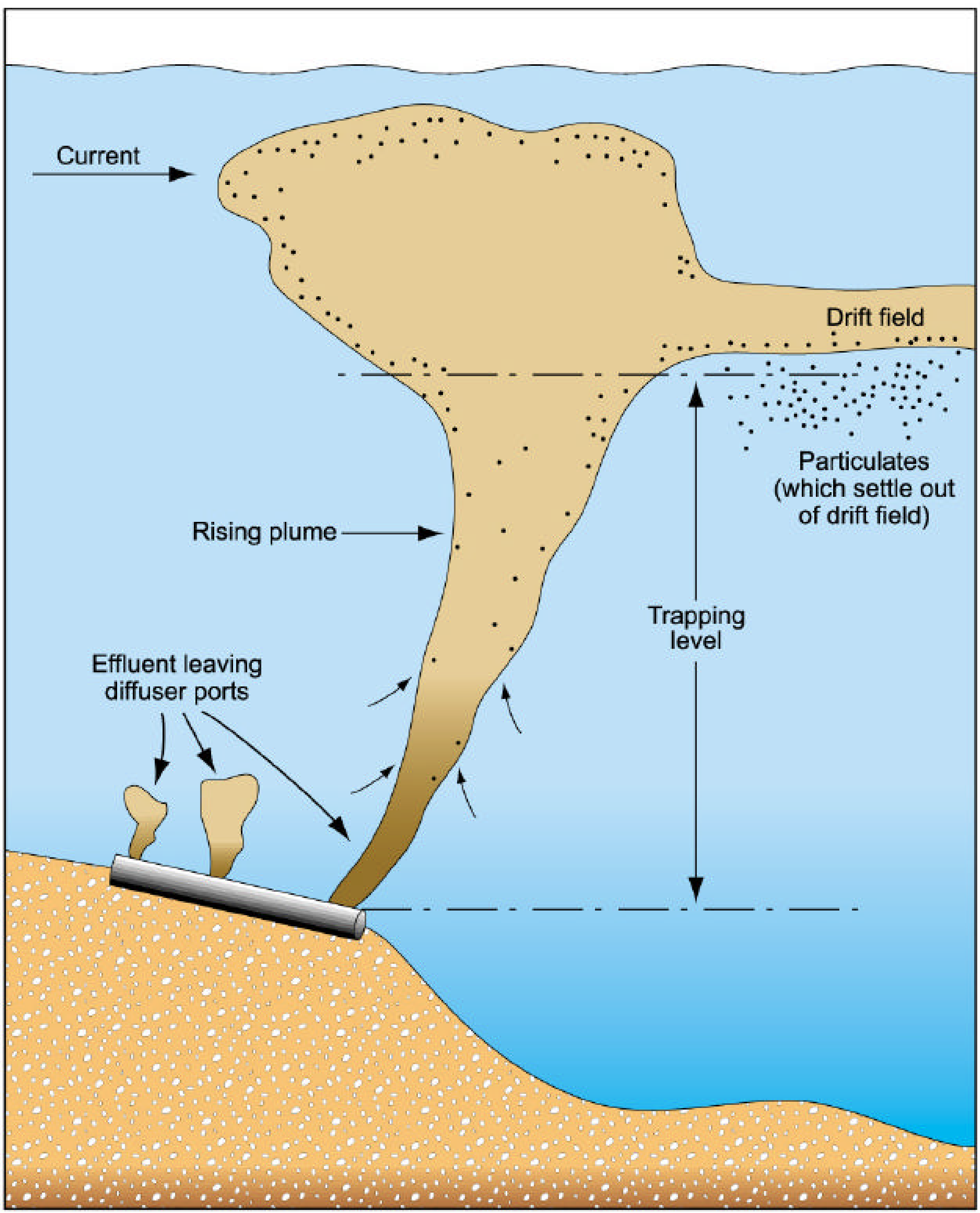

Figure 6-1. Initial waste field generated by marine outfall.

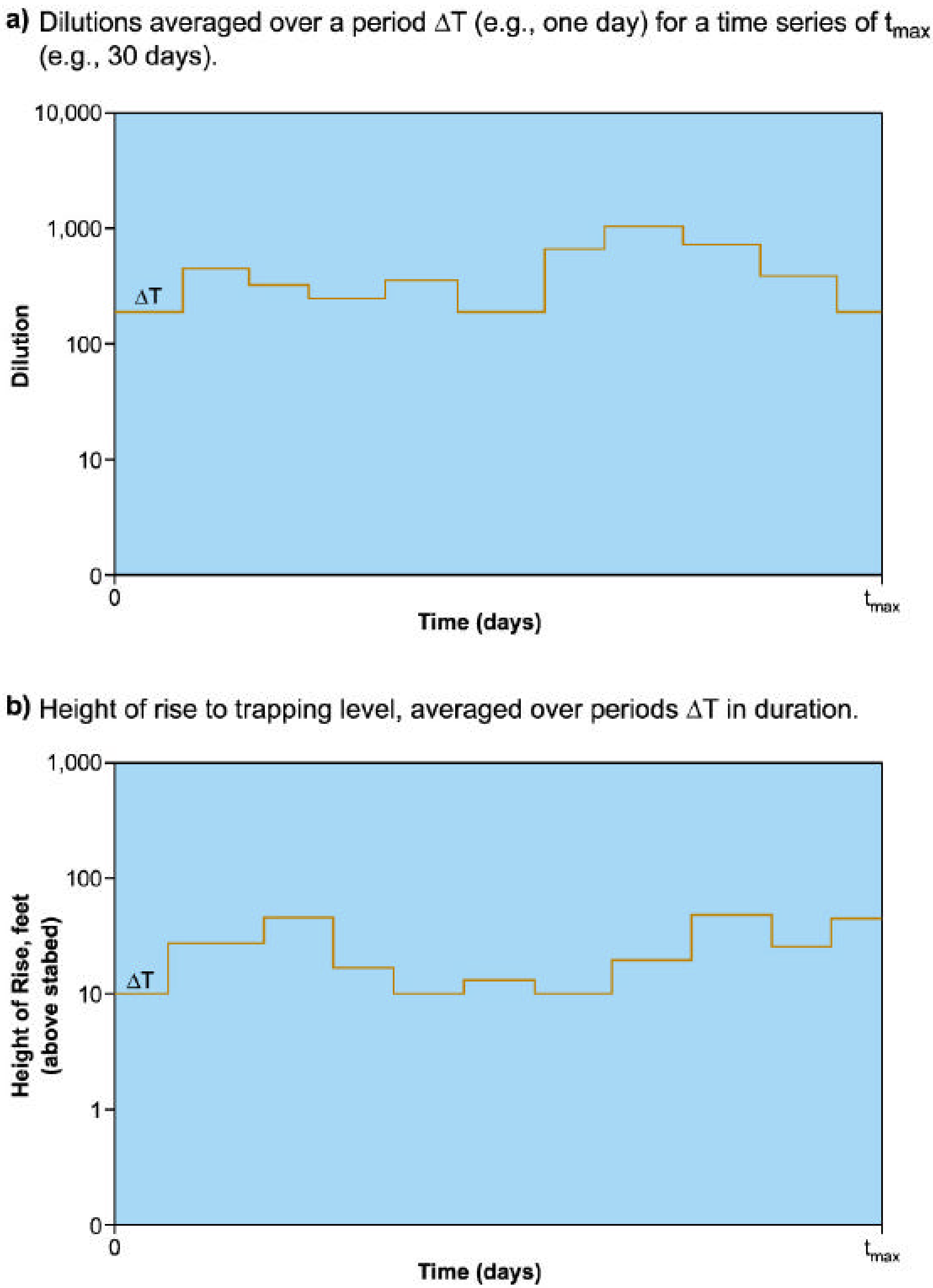

Figure 6-2. Typical time series of plume initial dilution parameters.

where

C_a	=	ambient concentration
C_e	=	effluent concentration
S_a	=	initial dilution
C_f	=	concentration following initial dilution

The above equation can predict the time variability in C_f, since normally C_e and S_a are known, or can be calculated over time. The concentration C_f is used in the far-field component (#3) of the overall model, as discussed subsequently. First, component #2 (particle tracking) is discussed.

While the particle tracking component is not actually needed to predict far-field concentrations, it is a very valuable component of the modeling methodology since it allow user to visualize where the plume is going (assuming appropriate graphics are available to display the results) as illustrated in Figure 6-3.

In the figure, two particle traces are shown. Particle trace #2 is assumed to occur on day 2, just after trace #1 (day 1). Each trace uses a zone of initial dilution (ZID) calculated for that day (daily average). The two ZIDs shown reflect the changes in the initial dilution that have occurred between the two days. Note that during day #2, both traces continue to evolve; but the source of trace #1 no longer contributes.

To simulate these traces, equations similar to the following are used:

$$x(t+\Delta t) = x(t) + u(t)\Delta t + f_x\sqrt{2\varepsilon_x \Delta t} \qquad (6\text{-}2a)$$

$$y(t+\Delta t) = y(t) + v(t)\Delta t + f_y\sqrt{2\varepsilon_y \Delta t} \qquad (6\text{-}2b)$$

$$z(t+\Delta t) = z(t) + w(t)\Delta t + f_z\sqrt{2\varepsilon_z \Delta t} \qquad (6\text{-}2c)$$

where

$x(t + \Delta t)$, $y(t + \Delta t)$, $z(t + \Delta t)$,	=	location of a particle at time $t + \Delta t$ after release
u, v, w	=	velocity components
$\varepsilon_x, \varepsilon_y, \varepsilon_z$	=	turbulent diffusion coefficients
f_x, f_y, f_z	=	normally distributed random variable that takes the value +1 or -1.

The particle's position is thus governed by advection and turbulent diffusion. The random variables have values of +1 or -1 to allow the particles to randomly move. Typically the last term in (6-2a) is negligible if x is in the direction of the predominant current. However, if v or w is small, then the turbulent correction term in (6-2b) and (6-2c) should not be ignored. Particularly in (6-2c), w may denote a small settling velocity or buoyant velocity (for emulsion droplets) and the diffusion term becomes extremely important.

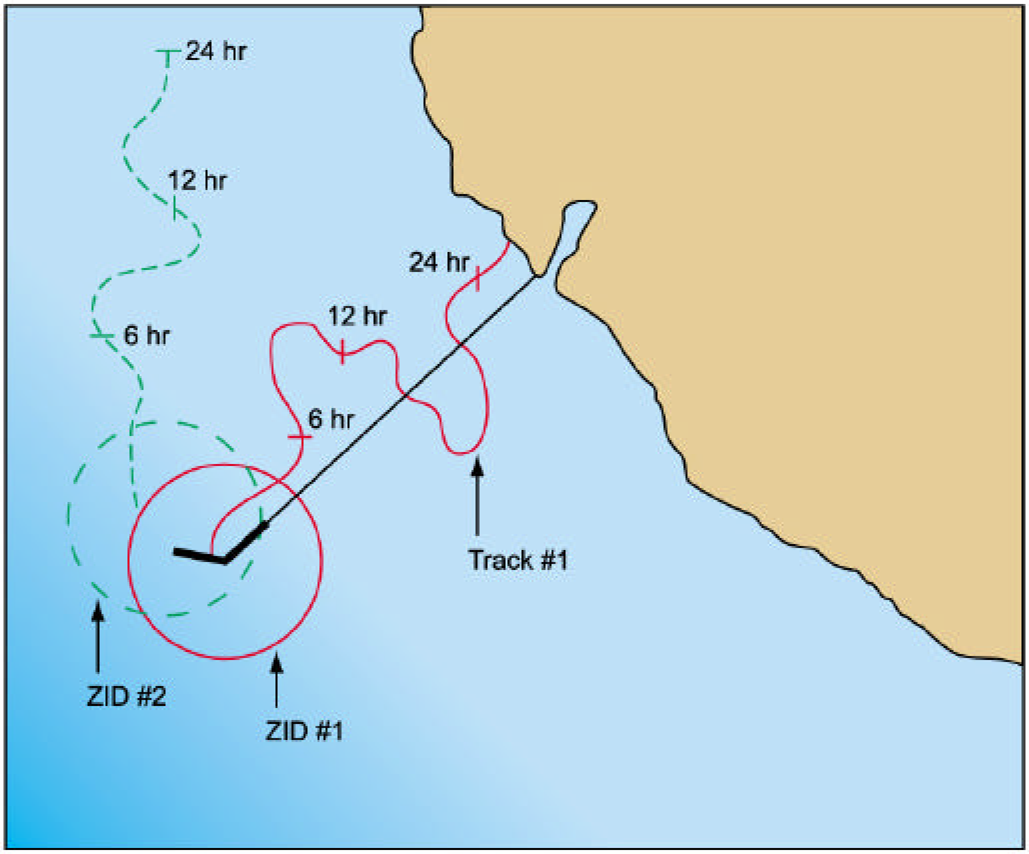

Figure 6-3. Illustration of two plume traces.

For the far-field models (component #3), many transport equations are available, only a few of which are shown below. One of the most widely used formulas (applied to 301(h) applications) predicts the centerline concentration of a decaying constituent on the plume centerline:

$$C(t) = C_a + \frac{C_f - C_a}{D_s} \exp(-kt) \qquad \text{(6-3a)}$$

where

- $C(t)$ = concentration on plume centerline at a time t after completion of initial dilution
- D_s = dilution attained subsequent to the initial dilution

D_s itself can be given by alternatives formulas. For coastal waters, the 4/3 law is typically used, and so:

$$D_s = \left[\operatorname{erf} \left(\frac{3/2}{\left(1 + \frac{8\varepsilon_0 t}{b^2}\right)^3 - 1} \right)^{\frac{1}{2}} \right]^{-1} \qquad \text{(6-3b)}$$

where

- b = initial width of plume
- ε_0 = turbulent diffusion coefficient corresponding to a plume width of b.

More recently this type of approach has been generalized to accommodate different turbulent mixing laws and to accommodate predications off the centerline:

$$C(x,y,t) = C_a + \frac{C_f - C_a}{2} \exp(-kt) \left\{ \operatorname{erf} \left(\frac{\frac{b}{2} + y}{\sqrt{\frac{4\varepsilon_0}{V} \int_0^x f(x)dx}} \right) + \operatorname{erf} \left(\frac{\frac{b}{2} - y}{\sqrt{\frac{4\varepsilon_0}{V} \int_0^x f(x)dx}} \right) \right\} \qquad \text{(6-4a)}$$

The function f(x) is related to the diffusion law used:

$$\varepsilon_y = A\sigma_y^n \qquad \text{(6-4b)}$$

For example:

$$f(x) = \begin{cases} 1, n = 0 \left(\text{constant } \varepsilon_y\right) \\ \left(\dfrac{8\varepsilon_0 t}{b^2} + 1\right)^2 \quad n = \dfrac{4}{3} \end{cases}$$

Thus equation (6-4a) is a more general than equation (6-3a).

Even more complex quasi-analytical models have been developed. Stacy (2000), described previously, accounted for vertical boundaries and vertical mixing. However, based on the limitations of data available, vertical mixing can often be neglected and the predicted maximum concentrations may increase a bit.

One of the big advance in plume modeling over the past five years is related to the software available to visualize results. Even quasi-analytical models of the type just described benefit greatly by showing model predictions in two- or three-dimensional depictions with the environmental setting as background.

If the quasi-analytical models were executed over a season of the year, for example, and the initial dilution allowed to vary over that time (say daily), then it is likely that the plume would have visited much of the three-dimensional volume of ocean water in the few kilometers that surround the outfall. By dividing the ocean water up into small cells with known (x, y, z) coordinates, each time the plume visited those locations, that information could be recorded. This allows statistical results of the plume, over the period simulated, to be generated. Example analyses could include:

- Distribution of concentrations (say sorted from low to high) at critical locations, so the frequency of exceedances can be estimated.
- Contours of concentrations at selected depths.
- Contours of plume travel times to show where the plume typically resides.

6.6 Example Conceptual Application of Numerical Model to District's Plume

In contrast to analytical models where no grids are required, and model predictions can be at any (x, y, z, t) location where the model is valid, numerical models make predictions at discrete locations. Those locations are predefined (before the model is executed) based on a selected grid. The spacing (Δx, Δy, Δz, Δt) can change spatially and temporally. For example, two adjacent points might be (x, y, z, t) and ($x + \Delta x$, y, z, t). Predictions are not made between x and ($x + \Delta x$), although an interpolation procedure can be used to generate such estimates (this is not typically done however).

Grids, of course, have boundaries. The interior of the grid is referred to as the domain, or the piece of space where predictions are made. Two plausible grid boundaries that might apply to the District's Outfall are shown in Figure 6-4. The interior of each grid contains the District's Outfall. The larger grid contains all the regional outfalls shown in Figure 6-4.

Why choose one grid over another? Some considerations are:

- If the plume from the District's discharge does not interact with the other plumes in any significant way, then a smaller grid that excludes those outfalls may be appropriate.

- On the other hand, if the chemical quality of the coastal ocean and beaches around the District's Outfall are thought to be impacted by external sources such as upcoast outfalls, then those sources can be simulated if contained within the grid.

- The smaller grid requires less data to define initial and boundary conditions. However, the smaller grid should not be so small that the boundary is influenced by the District's plume.

- The larger grid or domain would require much more data to quantify the internal sources and boundary and initial conditions, but could produce a cleaner picture of the importance of all sources.

Ocean modeling today is progressing to the point where global or regional models can be applied at coarser scales to predict the boundary conditions for the inner grids, as described in previous sections of this report. It is conceivable that someday both grids #1 and #2 could be used together.

Numerical models typically take orders of magnitude longer than the quasi-analytical models to execute. For example, analytical models to generate the two plume traces shown in Figure 6-1 would take only a few seconds on fast PCs that have PII or PIII chips. However, solving the same simple problem using a complex 3D numerical model might take hours, depending on how the problem was set up, the time step used, and the grid resolution.

The biggest differences between the quasi-analytical and numerical models previously discussed, however, are the processes that can be evaluated. Typically quasi-analytical models consider a smaller set of processes that can include:

- Advection (currents), typically in the horizontal plane only

- Turbulent diffusion (often in one or two directions, but rarely in three)

- Decay of pollutants, typically a first order process, and not time dependent

The numerical models can include not only the above processes but others as well. The above processes can be simulated in more detail (and hopefully more accurately) and can be extended to three-dimension, as appropriate. More general chemical reactions can be considered as well.

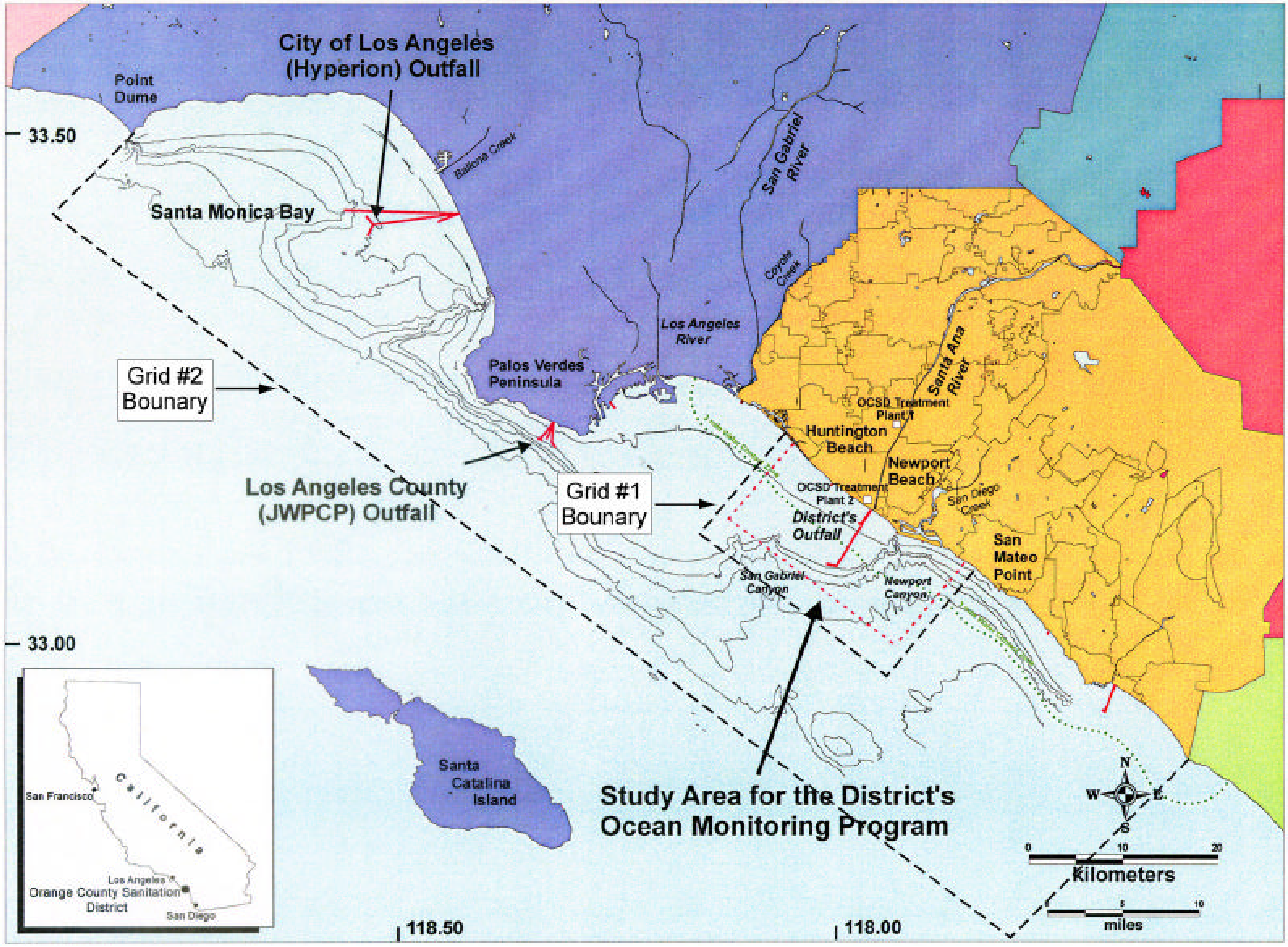

Figure 6-4. Illustratration of two alternative numerical grid boundaries that contain the District's Outfall.

Figure 6-5 illustrates the spatial and temporal scale of motions in the atmosphere and oceans. Note that different processes are relevant over different scales. For example, Rossby waves are applicable over scales of thousands of kilometers, and time scale of a few years. Such waves are important for El Nino events, but much less important for their influence on the District's plume. Thus such influences are not expected to be included in coastal model application that may last for a few days or weeks. However, for decadal simulations of oceans, such processes may be needed, depending on the model application.

In Figure 6-5, two boxes have been sketched in that show the typical temporal-spatial scales of concern for the two applications of global ocean modeling and coastal wastewater plume modeling. Note the following:

- The dominant processes considered in oceanic models may not be in coastal ocean models (and vise-versa).
- The scales of resolution needed for ocean wide models may be multiple kilometers, and is far too coarse to predict wastewater plume behavior.
- Ultimately, the grid resolution needed to simulate wastewater plume dispersion may be 1 mm(!). Very small eddies exist at this scale that ultimately could be simulated. Today, such resolution is order of 10^3 – 10^5 times finer than routinely used at the coastal scale, and 10^7 – 10^8 times finer than ocean model grids.

6.7 Accumulation and Fate of Chemicals in Surface Microlayer

The interface between the ocean and atmosphere is where momentum, energy, mass, and gases are exchanged that ultimately have a great impact on our climate and local phenomena. Such exchange processes have been exhaustively studied, particularly the surface energy balance, where radiation (e.g., sensible) heat fluxes are exchanged. More recently, the study of exchange processes has expanded as the fate of anthropogenic chemicals has become of interest.

Transfer occurs through the surface microlayer that separates the atmosphere from the ocean. Surface waves play an important role here by virtue of their ability to determine the roughness of the sea surface, and their ability to disrupt the surface microlayer. At sufficiently high wind speeds, for example, ocean spray and droplets may be entrained directly into the atmosphere, leading to very high (but temporary) exchanges.

The process of accumulation of small positively buoyant particles (e.g., emulsions) at the sea surface atmosphere interface is shown in Figure 6-6. Note that the positively buoyant particles tend to separate from the main body of the plume, and eventually reach the surface where they may accumulate and dissipate into a dissolved phase, volatilize, or undergo degradative processes (e.g., photolyze).

One way to evaluate this process is by simulating discrete particles, and tracking those particles. The particles may be randomly assigned buoyancy-induced velocities, for example. Once the particles reach the surface, they can be assumed to remain there, and such an assumption would be translated into model code consistent with the assumption.

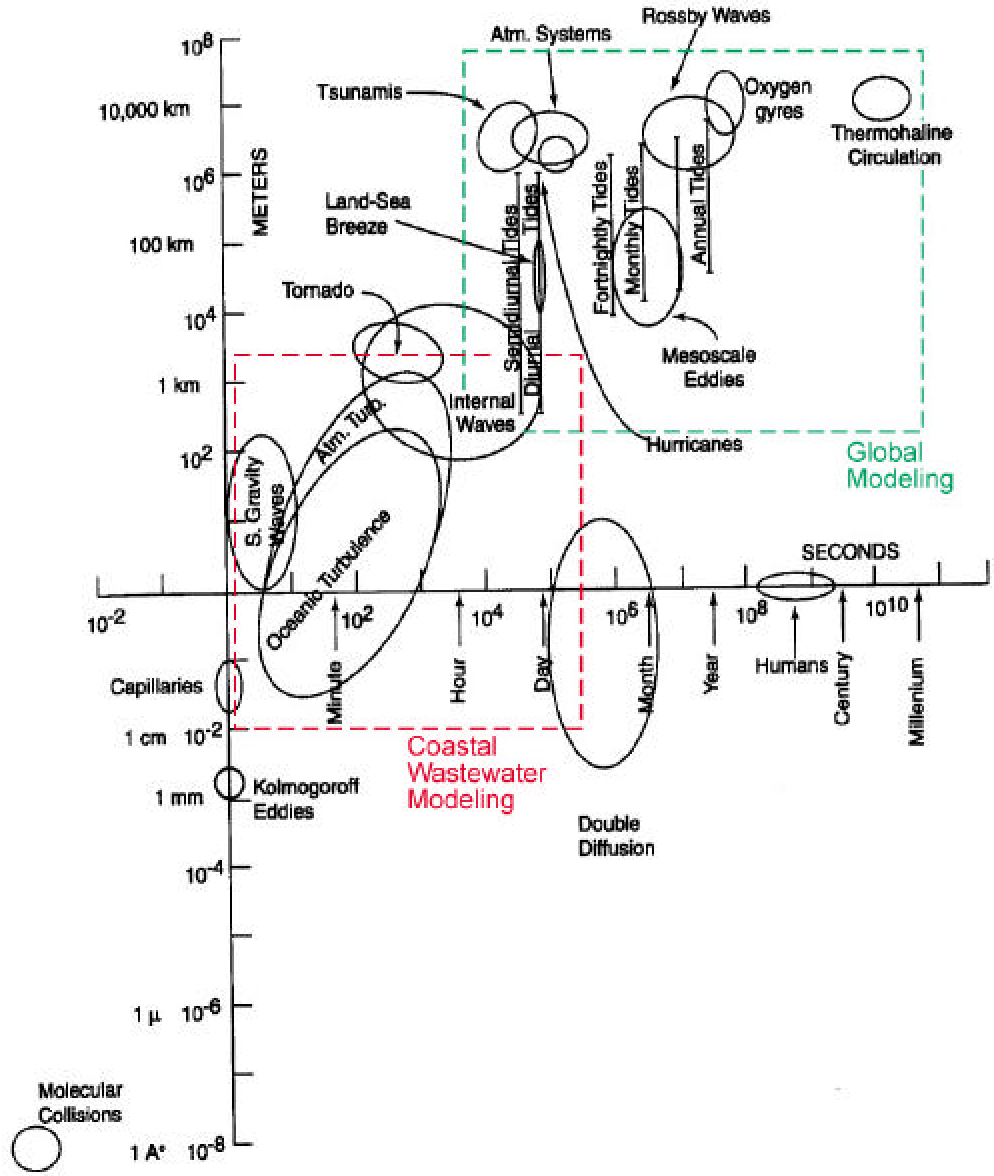

Figure 6-5. The range of spatial and temporal scales of motions in the atmosphere and the oceans. The motions span over a 10-decade range in both space and time (Kantha and Clayton, 2000).

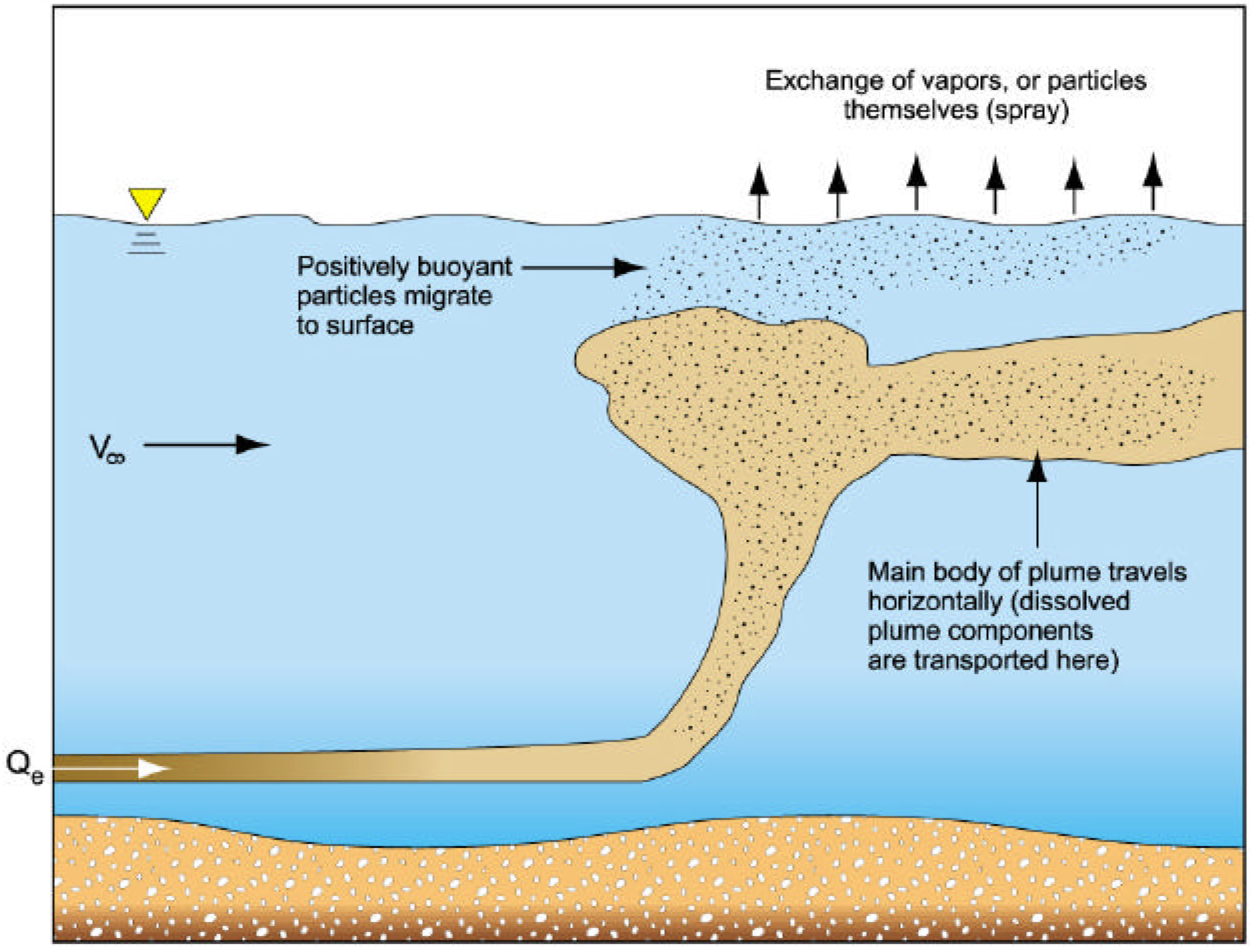

Figure 6-6. Conceptualization of fate of positively buoyant particles discharged from a submerged plume.

Once at the surface, algorithms to calculate the concentration at the interface and flux across the interface can be applied. Particle tracking to simulate plumes or (in this case) particles dissociated from plumes, are often though to be impractical due to the number of particles needed to be simulated. However, such an opinion is not universal and the method holds much promise for specialized applications. Otherwise if particle tracking methods are not used then the advection-dispersion equations/models that have been discussed in the bulk of this document would be used. Such a model would need to include:

- A vertical component of velocity that simulates the rising particles and particles dissolution of components. Either multiple particle sizes would be needed (e.g., large, medium, and small particles) or a continuous size distribution of particles.
- The surface boundary condition would need to be modified to account for turbulent transfer of constituents across the interface.

Below a brief discussion is provided of several methods that have been used in the past to accomplish the transfer. One of the earlier methods, and conceptually the simplest, is called two-film theory (see Figure 6-7). The concept is that the volatilization of components at the air-sea interface is controlled by a thin gas layer, and a thin liquid film. While this conceptual model appears to apply to more quiescent water bodies, in fact much of the early research (1970's) was conducted for ocean-atmosphere exchanges using such a model.

One interesting feature of the model is that the volatilization of many chemicals is limited by its resistance through either the liquid film or gas film. This is illustrated in Table 6-4. The top part of the table shows Henry's Law Constants (K_H) for seven chemicals. Note that they range from 3.7 atm $\cdot$ m^3 $\cdot$ $mole^{-1}$ for vinyl chloride to 2.0 $\cdot$ 10^{-7} for dieldrin. In the second part of the table, typical volatilization rates from the ocean's surface are calculated using two-film theory for a range of K_Hs. Note that for the high K_H values the volatilization rate approaches a constant of 20 cm/hr, and gets no higher. But for low K_H values the volatilization rate continues to drop. This says that volatilization is liquid-film limited for $K_H > 10^{-3}$; gas film limited for $K_H < 10^{-6}$, and is influenced by both films for intermediate K_H values. Since K_H values of many constituent are known, the volatilization behavior of those constituents can be readily evaluated.

Due to the complexity of the transfer process across the air-sea interface, the modeling approaches normally parameterize the unknowns into a bulk exchange coefficient. This exchange coefficient thus reflects our ignorance of the process, and requires us to make estimates. Obviously site-specific data over a range of environmental conditions is preferable, but not possible. Second, and more practical is to use a theoretical model, such as two-film theory or surface renewal theory, to provide this information, along with some more readily obtainable site-specific information such as wind speeds.

Since these transfer rates are obviously time variable (they are influenced by wind speeds, for example), quite a bit of data provided into a numerical model would be the preferred, detailed approach. Alternatively, simplified analyses could be performed to scope out the magnitude of the transfer to gain a feel for its importance.

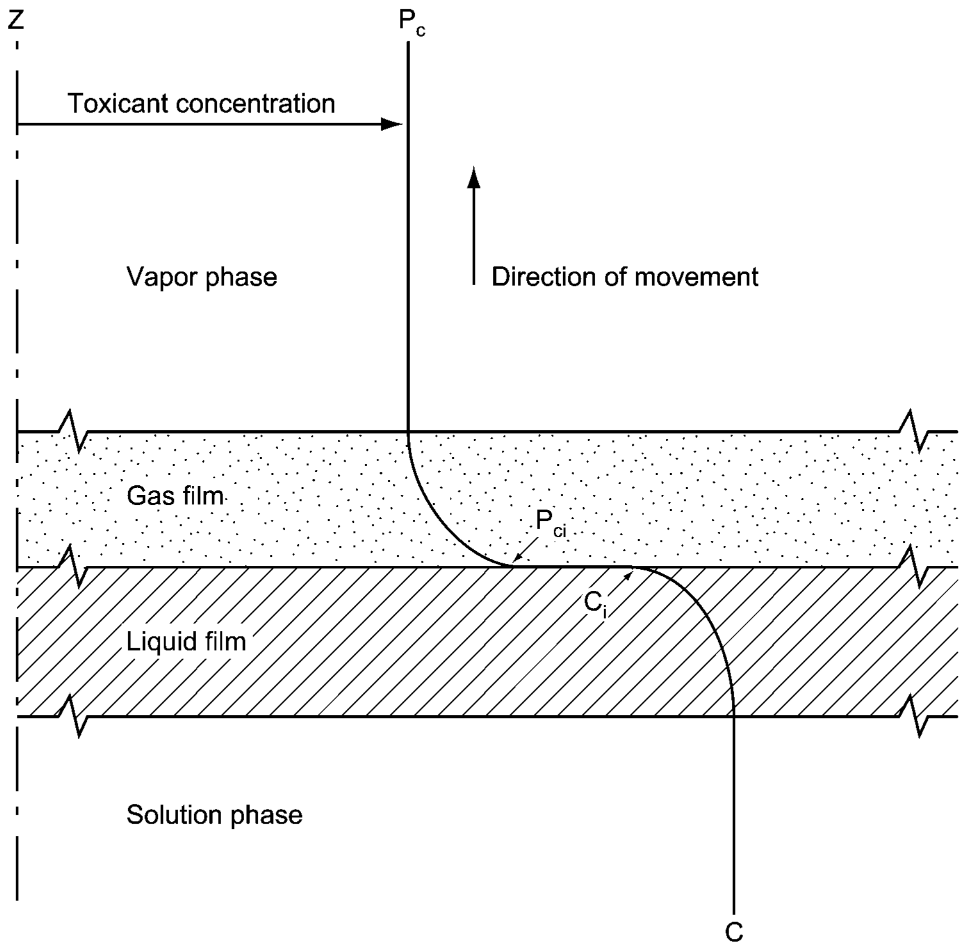

Figure 6-7. Schematic representation of volatilization from solution phase to liquid phase.

Table 6-4a
Henry's Law Constants for Selected Compounds

Compound	Henry's Law Constant (atm · m^3 /mole)
Vinyl Chloride	3.7
Carbon Tetrachloride	2×10^{-2}
Toluene	6.7×10^{-3}
Aroclor 1254	2.8×10^{-3}
Flourene	2.4×10^{-4}
DDT	3.9×10^{-5}
Dieldrin	2.0×10^{-7}

Table 6-4b
Typical Values of Pollutant Volatilization Rates in Ocean Waters

K_H (atm · m^3 /mole)	k_v (cm/hr)
10^{0}	20
10^{-1}	20
10^{-2}	19.7
10^{-3}	17.3
10^{-4}	7.7
10^{-5}	1.2
10^{-6}	0.1
10^{-7}	0.01

7.0 Presenting Results of Dispersion Models

7.1 Visualization

Visualization of dispersion model results based on state-of-the-art software is essential in conveying meaning to model predictions. An additional benefit of visualization is that problems associated with model predictions can more easily be spotted, and then corrected. One way to view the type of visualization of results most appropriate to a specific problem is to ask “How would I like to view the results?” That is, results can now be visualized in practically any imaginable way, so imagination is becoming the limiting factor, not the software. Thus state-of-the-art visualization software should be a standard component of ocean circulation and plume dispersion models.

A number of the previous URL’s showed examples of visualization techniques. A summary of several additional URLs is shown in Table 7-1. The visualizations include animations, and fly-by examples. The fly-by examples simulate an observer moving through space to view the surroundings.

Much of the visualization software utilizes either NetCDF, MATLAB, or AVS. NetCDF is a machine-independent binary format developed at National Center for Atmospheric Research, and is designed for large arrays of scientific data. MATLAB is a scientific platform that supports advanced graphics, some of which are discussed at http://crusty.er.usgs.gov/omviz/. AVS produces high quality visualization software that can be adapted for virtually any application. AVS software is widely used for three-dimensional model visualizations.

7.2 Skill Assessment

Skill assessment reflects the skill of the model in making predictions. It can also be called model verification. A discussion of this concept is presented in Martin and McCutcheon (1999), and is not repeated here. Only a few general comments will be made.

Great care should be taken in regard to assessing model skill. Many traditional indicators were developed years ago, and are still in use today. Some may have limited applicability. For example, consider the skill of a model in predicting far field dissolved oxygen using a formula that calculates relative error at some user-specified location. Background dissolved oxygen may be 6 mg/L, and the dissolved oxygen concentration at the assessment point may be 4 mg/L. If the model predicts 5 mg/L, the relative error is about 20 percent. Note that the relative error is somewhat insensitive to the model’s predictive capability, and is likely to be seen as “low”. Now repeat this exercise with a constituent that has zero background concentration. If the plume

Table 7-1 goes here

model circulates the plume a bit off the specified location, the relative error may be close to 100 percent. But the concentrations may be close to observed if the measurement location were to be moved slightly. Thus, whether the model has good predictive skill goes beyond simple formulas: the use of the model comes into consideration.

8.0 Overall Perspective on Ocean Circulation and Dispersion Modeling

In this section, perspectives are provided on the applicability and limitations of ocean circulation and plume dispersion models gained from the review reported in the previous sections. Simultaneously, suggestions are provided to assist the District as they proceed in the application of such model.

Perspective #1: Ocean circulation and dispersion models are embodied as equations that attempt to capture the important relevant circulation/dispersion processes, and are then solved approximately, and with limited information that describes the system's initial conditions and boundary forcing over the period of simulation. Take the above statement apart into pieces. First, some errors in solutions will exist due to the fact that our understanding of the processes that influence plume evolution is limited, but the knowledge is increasing over time. Second, the approximate equations themselves are solved only approximately by numerical methods (the discussion of these techniques leads to text explanations that are practically indecipherable to all but a few numerical modelers). The degree that the numerical techniques adequately solve the equations is most often difficult to determine. Then, the information that is fed into the model during the course of the solution is incomplete, and may be inaccurate as well. Thus even completely correct equations and solution techniques could all be worthless unless the appropriate forcing were input to the model.

Response #1: This perspective is intended to show the District that the state of the art still needs improvement, and in fact is improving. It is also intended to show that **every** prediction will have an error associated with it. Such a result is still acceptable if the error can be controlled. It is possible to control some of the above errors. A good numerical solution technique, applied correctly, can minimize the error between the exact solution to the approximate equations and a poor solution to the approximate equations. This can be done by performing sensitivity tests on the grid used to solve the problem, where progressively finer grids are used until the solution no longer changes (that is the solution is independent of the grid). Modelers may choose not to perform such tests for reasons such as limitations on time and money.

Other related tests that can be performed to help establish validity of model codes are to benchmark the models against standard test problems available in the literature. Again this is not always done, but eventually any ocean/dispersion model should have completed a variety of relevant validation tests. Examples of such tests were discussed previously in Section 6.4. (Note: the authors experience in benchmarking exercises has been mixed; often new questions arise that replace the original ones).

Model calibration and verification on the system to be modeled should be an ongoing part of the modeling activity. That is, continually verifying that the model responds correctly is important. For example, an entirely new set of conditions may occur for which the model may not have been verified. Storm conditions may be one such example that could stress the model's predictive capabilities and be important as well. Such opportunities should be used to test the model's capabilities whenever possible.

Perspective #2: No impressive case study results were found to convince the authors that plume model dispersion in the open ocean is really predictive. The reviewer would have liked to have seen hundreds of model success sources; only a few applications were found.

Response #2: It is interesting to note that at many sites of open ocean outfalls, the modeling approach of choice in the past has been simpler quasi-analytic models. Even at the Mamala Bay outfall, both analytical and numerical models were applied. Both models gave promising results, but both were not completely predictive, either. For example, the water temperature field was not predicted by the numerical model, but rather specified, because its complex temporal variations could not be resolved.

Perspective #3: The large surge in ocean modeling activity that is occurring, and will likely occur in the future, is not specifically being driven by ocean outfall plume modeling, but rather by other applications such as climate change issues or military applications. Consequently, the circulation models that are being developed may contain assumptions that limit their utility in the near coastal region to predict the fate of a buoyant plume. For example, these models may employ the hydrostatic assumption which is typically appropriate for large or mesoscale applications, but may limit the model's applicability in the vicinity of an ocean outfall. This is because the hydrostatic assumption assumes vertical accelerations are negligible in comparison to other terms in the vertical momentum equation. Such an assumption breaks down in the vicinity of the outfall discharge.

Today, some work has been done on coupling near-field models that can accommodate the vertical acceleration issue with the far field ocean circulation models. However, this is only a partially satisfactory solution, since near field models have limitations themselves (such as not accommodating spatially variable currents that may occur over depth).

Response #3: Modelers should always provide a list of the important assumptions that may influence an application of a model, how that assumption is thought to influence the solution, and if needed, how to overcome this limitation.

Perspective #4: There are only a few organizations that appear to have as a principal emphasis the fate of plumes from ocean outfalls or other near shore processes. Those organizations include Woods Hole Oceanographic Institute, and the Naval Research Laboratory (NRL). While no NRL applications on wastewater outfall plumes were found, nevertheless the NRL has been using the nested-grid concept to perform nowcasts/forecasts in the Southern California Bight, has developed and applied techniques to assimilate data into the models, and appears to have experience using both finite difference and finite element models (including NLOM, POM, PWC, POP, and MICOM models).

Response to #4: A more current and detailed state of the appropriate work that is being done by the WHOI and the NRL should be researched by directly contacting those organizations and perhaps visiting them. The NRL, particularly, seems to have experience in the Southern California Bight, have used nested models in the Southern California Bight, have used different platforms as needed to run the models, and are experimenting with finite element models as well as finite difference models. Overall, the number of organizations with direct experience in addressing the Districts desire to eventually perform prognostic modeling is small.

Perspective #5: Both finite difference and finite element models of ocean circulation and plume dispersion have been developed. However, the majority of models presently available are the finite difference models. Those modelers who have developed finite element models claim superiority in the flexibility of the grid: a very flexible, unstructured grid can be developed that can fit the most complicated bottom topography. Apparently the NRL, who has used primarily finite difference models is planning on evaluating and using finite element models as part of their coastal modeling work.

However, finite difference models now can handle more complex bathymetry and shoreline configurations using curvilinear coordinates systems, for example. Thus whether the advantages of the finite element approach will disappear remains uncertain. Even so, at least one issue remains with finite element models, and that is the conservation of mass (say contaminant mass). The finite element model never solves the mass conservation equations themselves, but rather a weighted residual version. Thus the question arises, is mass completely conserved in such models? This may not be an issue in ocean circulation applications, such as water temperature predictions, but could be important in the simulation of constituents, such as coliform organisms. Also, computational time for finite element models may be longer, due to high-order interpolation schemes.

Response #5: This potential problem can be evaluated by appropriate tests. Actually, such tests should be performed for both finite element and finite difference models on a problem similar to the type of problem the District wants to evaluate. One way to do this is to inject a known amount of conservative substance in the system, and monitor the mass that remains in the system over time. For a large enough grid, all the mass should remain in the system, so that the mass should not decrease over time for either type model. If it does, then the percent loss should be calculated, and determined if this is within acceptable tolerance.

Perspective #6: The National Oceanographic Partnership Program (NOPP) which has been in existence over the past few years offers funding opportunities in areas such as “pollution problems in the coastal ocean”. The NOPP encourages development of partnerships with state and local governmental agencies, with bid amounts less than $ 500,000/year over three years, or less.

Response #6: The District appears to be in a position to bid on such a project. A team could be assembled that includes, for example, SCRIPPS, UCLA, and others that could prepare a winning bid. More information is available at the URL http://core.cast.msstate.edu/NOPP00BAA.html.

Perspective #7: Alternative uses of dispersion models are in the diagnostic mode and in the prognostic (nowcast/forecast) mode. To date, the type of ocean outfall applications appear to be limited to diagnostic applications (that is, specifying the type of analysis to be simulated, such as a surfacing plume, and predicting its fate). On a larger scale, however, the fate of plumes such as the fate of the low salinity Chesapeake Bay water on the Atlantic Ocean salinity has been predicted (by NRL).

Response #7: It appears that the initial applications of numerical models to the District's outfall should be in a diagnostic mode. From these applications, the feasibility of the prognostic mode can be more easily evaluated.

Perspective #8: Appropriate measures of model success or failure will likely require additional data collection activities by the District, and then the development of appropriate quantitative error indices to determine the predictive capabilities of the model. Even these quantitative indices have some measure of subjectivity, however. For example, suppose the model predictions are completely incorrect in terms of plume location by about one kilometer, but predict the time series correctly. Are the model's predictions correct or incorrect?

Perspective #9: The linkage of near and far field models has been done for both analytical and numerical models. However, an issue of concern is whether mass is conserved by this linkage process. There are reasons for concern that mass may not be conserved.

Response #9: The linkages used should be evaluated carefully for mass conservation. The far field models can be tested to see if the mass in the plume (for conservative substances) is the same as the mass released into it.

Perspective #10: Which is the harder problem: predicting global ocean circulation, or the real-time position and constituent concentrations in a coastal plume? While there may be arguments for both problems, the question is intended to reinforce the notion that the latter problem offers formidable challenges, and should not be viewed as having been solved. The plume problem also has a number of aspects that are not as much of an issue in large scale ocean modeling. One aspect that has not been emphasized is that the numerical algorithms that solve the problem can be more stressed (or in other words, put to the test more rigorously) than for ocean circulation problems. This is because of the nearly infinite spatial concentration gradients that may exist near the boundary of plumes. It is very difficult to simulate these gradients correctly, and often even the best numerical schemes smear the front so that predictions in this region (which may be important since this denotes the first arrival of the plume to a new location) are not reliable.

Perspective #11: One reasonable analogy to the challenge of ocean circulation modeling and outfall plume modeling is that of weather forecasting. Models for weather forecasting(on a continental scale) have been developed and are available for public examination via their web sites. They attempt to provide short-term forecasts (for example for 24 hours up to one week). Historically, much more effort has been devoted to weather forecasting than to ocean modeling, so that field has advanced further. The analogy that is most relevant is that weather predictions can be made more reliably on a mesoscale than on a local one. For example, the movement of frontal systems can generally be predicted, but specific locations and intensities of thunderstorms and tornados can not be. Thus the important local predictions are difficult to make due to the limited understanding of all relevant processes, and due to the lack of local data of sufficient spatial resolution. These are the same issues that face ocean circulation and plume dispersion models. Experience tells us that sometimes the local weather is predicted very well; other times predictions are completely inaccurate.

Perspective #12: Some of the best visualization tools available today are developed by AVS (Advanced Visualization Systems), and are appropriate for analyzing large quantities of data in addition to visualizing model output.

Response #12: If the District has not already done so, it is suggested they begin to develop a three-dimensional visualization system to examine the data they have been collecting over the years. This is not only helpful in providing better interpretation of that data, but also to help better understand data gaps and limitations, and could assist in helping to design modifications to their sampling program. Concurrently, the data collected over the years should be evaluated for use in modeling analysis.

Perspective #13: One decision that District will make is whether to set up and run the ocean modeling system themselves (some of the tools described in this report can be purchased, or gotten without cost), or to rely on the expertise of experts.

Response #13: The preferable path is to allow knowledgeable experts to set up and maintain the modeling system, with oversight by District. Such systems are never as easy to use as we may initially think.

Perspective #14: Little emphasis has been given to the limitations of using the circulation models in the near field, or of linking near field models with far field models (although some linking has been done, as described earlier). Concerns that should be addressed are the potential for errors in mass balances of constituents simulated, and the implications of the simplications in the near field models on simulating the initial fate of the effluent through a deep water column where near field model assumptions are likely to be violated routinely. These issues appear to be under-examined in the literature.

Response #14: More work can be done in this area relatively easily. One, a more detailed focus on the work reported in the literature can be done. The best ways of linking the models should be understood and used. Two, the District’s near field data can be examined over all seasons (actually, time series of information should be examined) to see how often conditions exist that violate the assumptions of existing near field models, the implications of this, and how to address the problem.

Perspective #15: A number of the dispersion models have sediment transport and sediment bed models. For some outfalls, sediment accumulation (and associated contaminant accumulation) can be an issue. Our perspective is that the sediment accumulation models are generally very simplified, and may not be very predictive.

Response #15: If sediment and toxicant accumulation is a concern to the District, a more detailed review of those components of the circulation/water quality models may be desirable.

Perspective #16: Ocean circulation and plume dispersion models need to be written in a manner to take advantage of the fastest available (and envisioned) computer architecture, especially if nowcasting/forecasting is to be accomplished.

Perspective #17: Artificial horizontal numerical diffusion can be introduced in circulation models, and needs to be controlled to an acceptable manner.

Response #17: Isopycnal models may offer the best approach for doing this. An evaluation of the importance of this process is suggested.

Perspective #18: Ocean models that are resolved to 1/10 degree have a grid spacing of about 10 km. Since the domain of concern to the District is also about 10 km, such a grid spacing is inadequate in providing the boundary condition resolutions needed for the dispersion modeling of the plume. Assuming a 100 m resolution is needed on the inner-most domain, this would correspond to about a 1/1000 degree grid resolution. This seems to be about two orders of magnitude beyond the present state of the modeling.

Further, the temporal scale of the plume dispersion modeling is minutes to days, which is quite different from the years to centuries time scale of ocean models. Thus not only is the spatial scale orders of magnitude finer for dispersion models, but so is the temperal scale. This may make the attainment of nowcast models difficult in the near term.

Response #18: The issues of required grid and temporal resolution for plume dispersion modeling vs. the achievable resolutions should be investigated to understand how, if at all, this presents a problem in achieving nowcasts/forecasts.

Perspective #19: Based on previous modeling experience with a variety of models and clients, it is usually the case that new model users overestimate what a model can do, and underestimate the effort required to do it. Because this has been such a universal experience, Figure 8-1 was developed a number of years ago as part of modeling workshop presentations, primarily to new users of the models. It shows that initial expectations are high, but that trouble lurks ahead that may arise from misconceptions, lack of performance or other reasons. Finally, the success (or lack of) may ultimately rest on the persistence or resolve to continue model development or application until the envisioned outcome is attained.

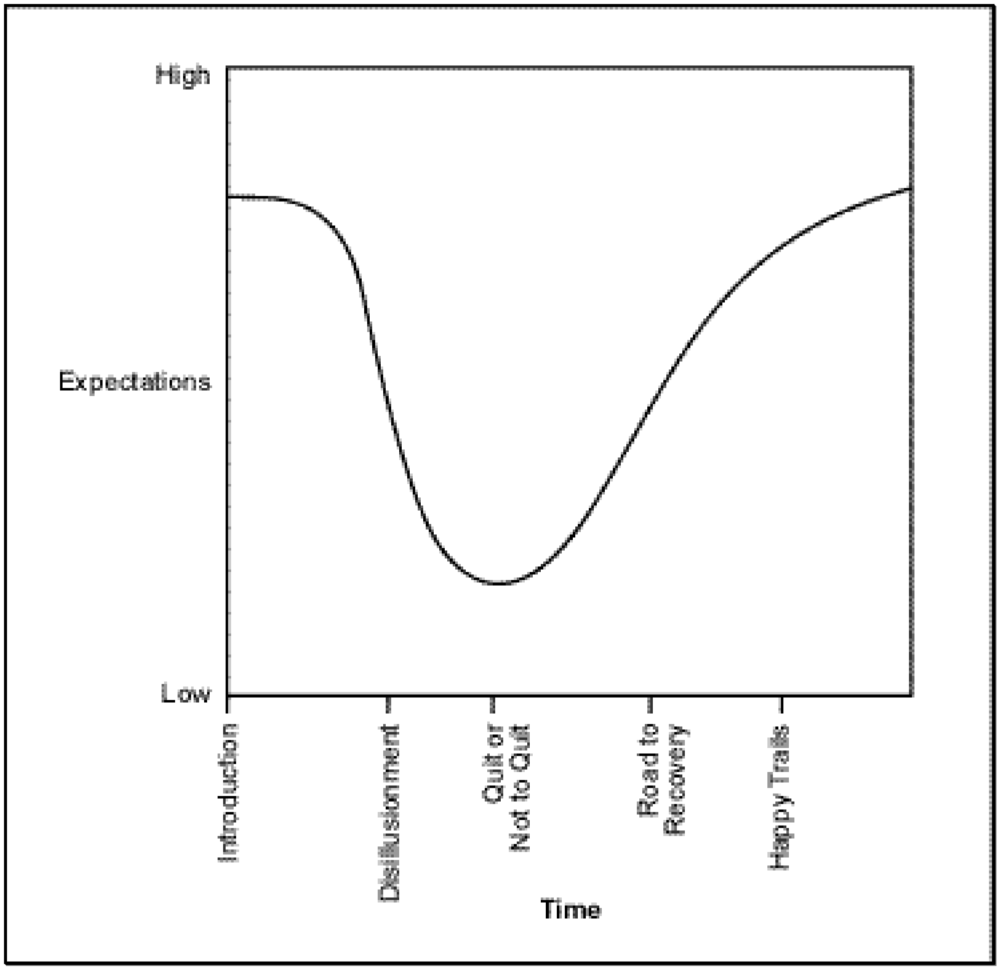

Figure 8-1.   User expectations of software.

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Appendix A
Regional Setting of Orange County Sanitation District's Discharge

Within a larger regional context, the District's discharge is into San Pedro Bay, which is a part of the larger Southern California Bight (Figure A-1). The Southern California Bight has been, and continues to be, studied extensively. Reasons for this include the complexity of the currents within the bight, as well as the need to understand the current system because of numerous wastewater discharges that occur there. The mesoscale circulation of the bight is partially governed by the California Current that flows equatorially past Point Conception most of the year. South of Point Conception, the equatorial flow is further offshore, and weakens further to the south. A component of the California Current turns shoreward and then moves poleward in a large eddy known as the Southern California Countercurrent. The countercurrent has a seasonal variation in that the maximum poleward component occurs in late summer and also in winter; the minimum poleward flow occurs in the fall. The poleward flow is strongest at 50 to 100 meters depth, and is therefore referred to as an undercurrent. Near the outfall location, currents are predominantly upcoast and downcoast, as Figure A-2 shows. At the depth of 72 meters, the countercurrent is flowing predominantly upcoast. At a depth of 14 meters, the downcoast component is more significant than at the 72 meters depth, but the upcoast component is still dominant. Vertical velocity shear is likely to exist in the water column that, when present, would influence plume behavior.

Example profiles of water temperature, salinity, and density in the vicinity of the outfall are shown in Figure A-3 for each of the four seasons of the year. Note that the salinity does not vary significantly over depth except for the January 1993 example, when the surface salinity was sharply lower, perhaps due to large storm-induced freshwater discharges from the Santa Ana River. Water temperature typically exhibits vertical gradients, with the appearance of a thermocline during the summer, when the surface temperatures are warmest, and the bottom temperatures are colder than during winter.

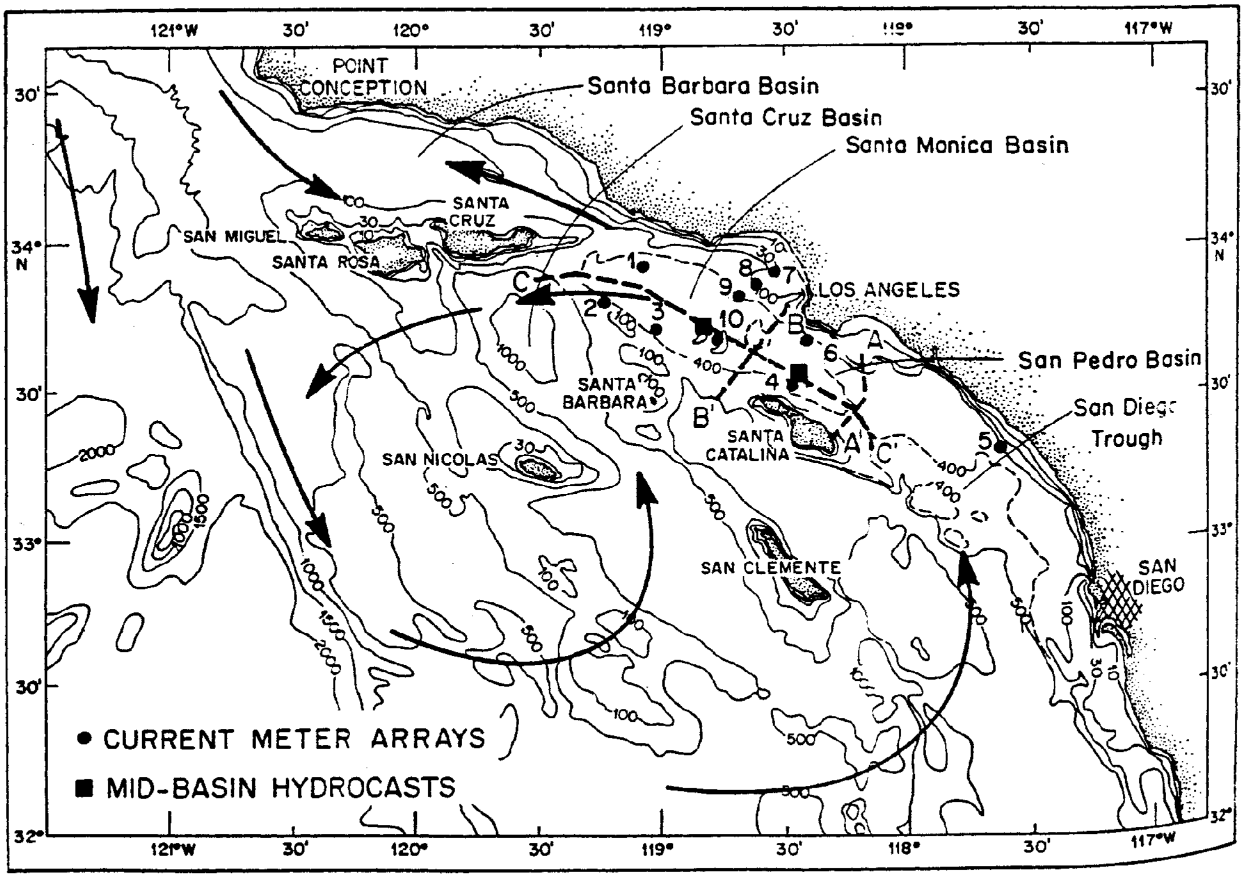

Figure A-1. Bottom topography and schematic mean circulation pattern in the Southern California Bight. Depth contours are in fathoms.

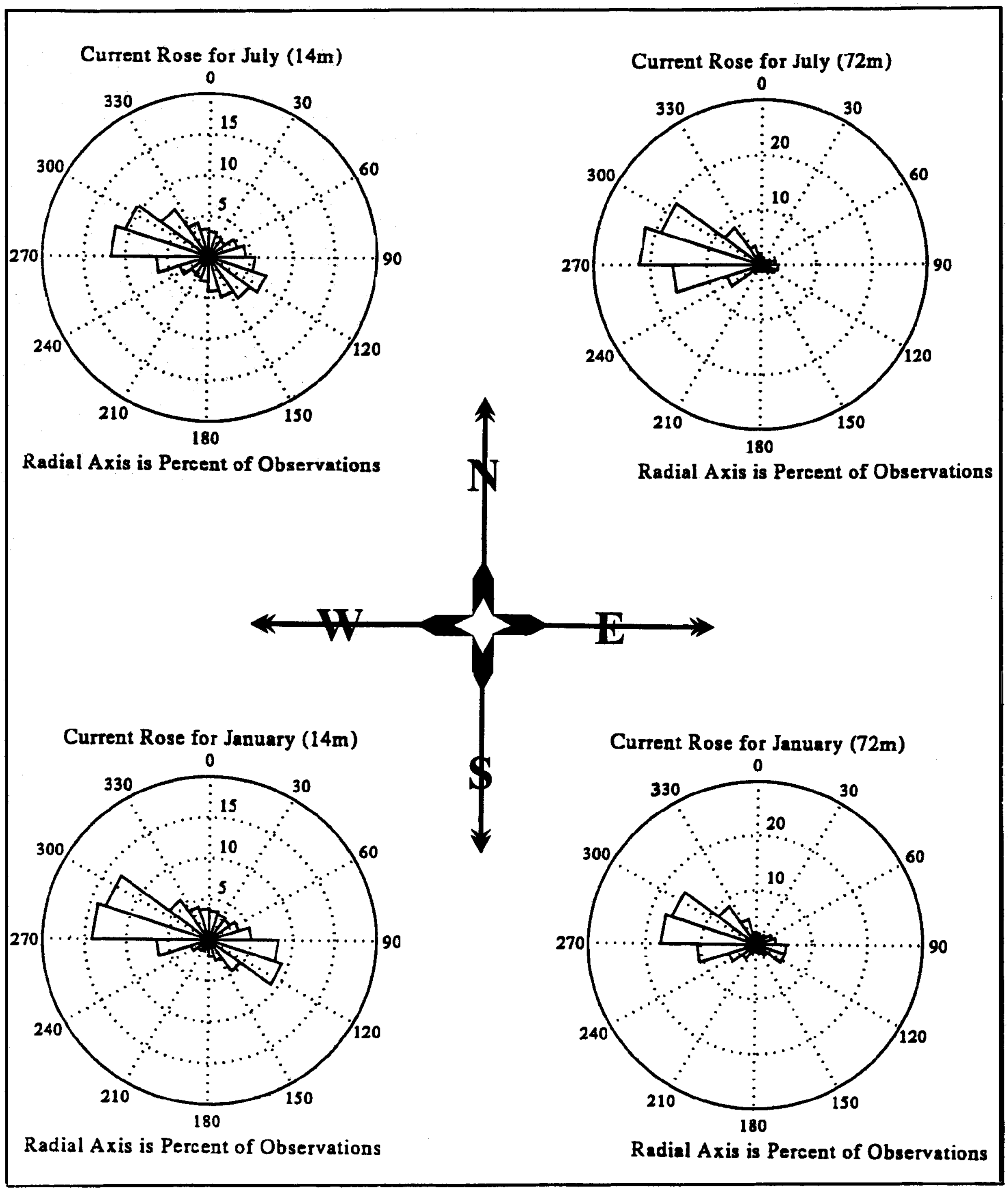

Figure A-2. Current direction (percent of observations shown by current rose) in July and January for combined data from July 1986 – 1988 and 1993 – 1994, near-surface (14 m) and near-bottom (72 m) depths.

Note: North, south, east, and west (N, S, E, and W) designations predominance of currents in upcoast and downcoast directions indicated by current rose.

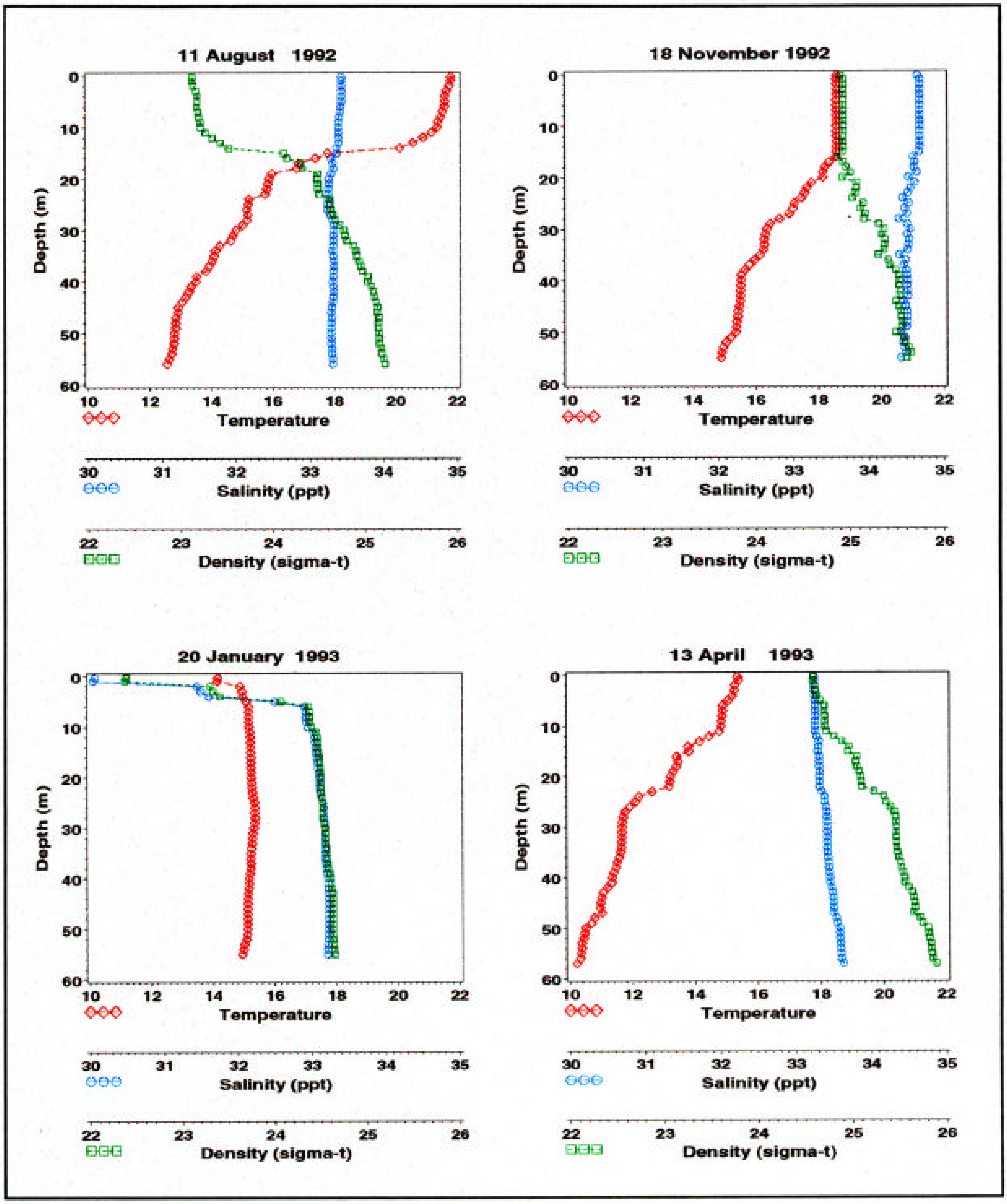

Figure A-3. Seasonal patterns of vertical stratification of temperature (°C; red), salinity (ppt; cyan), and density (sigma-t; green) at reference stations for typical summer (August 1992), fall (November 1992), winter (January 1993), and spring (April 1993) months.

During 1998-99, the average volumetric discharge through the outfall was 239 million gallons per day (MGD). Peak flow rates have been as high as 550 MGD, such as during the winter of 1996. As the population served by the sanitation district has increased over the past 25 years (see Figure A-4) so has the volumetric discharge rate. The year-to-year fluctuations also reflect whether a year was dry or wet, so the trend, while upward, is not monotonic. It is anticipated that by the year 2020 the average daily discharge will be 352 MGD. Peak storm water discharges may be as high as 775 MGD, which far exceeds the 480 MGD design rated capacity of the 120-inch outfall. At times in the future, then, wastewater will likely be infrequently discharged through the 78-inch outfall as well as through the 120-inch outfall during times of heavy rainfall.

As Figure A-4 further shows, the mass loading of constituents such as biological oxygen demand, total suspended solids, and copper have all decreased over time, reflecting the decreased effluent concentrations for these constituents. For example, effluent copper loads have decreased from 600 pounds/day in the 1970s to about 75 pounds/day in 1998-99.

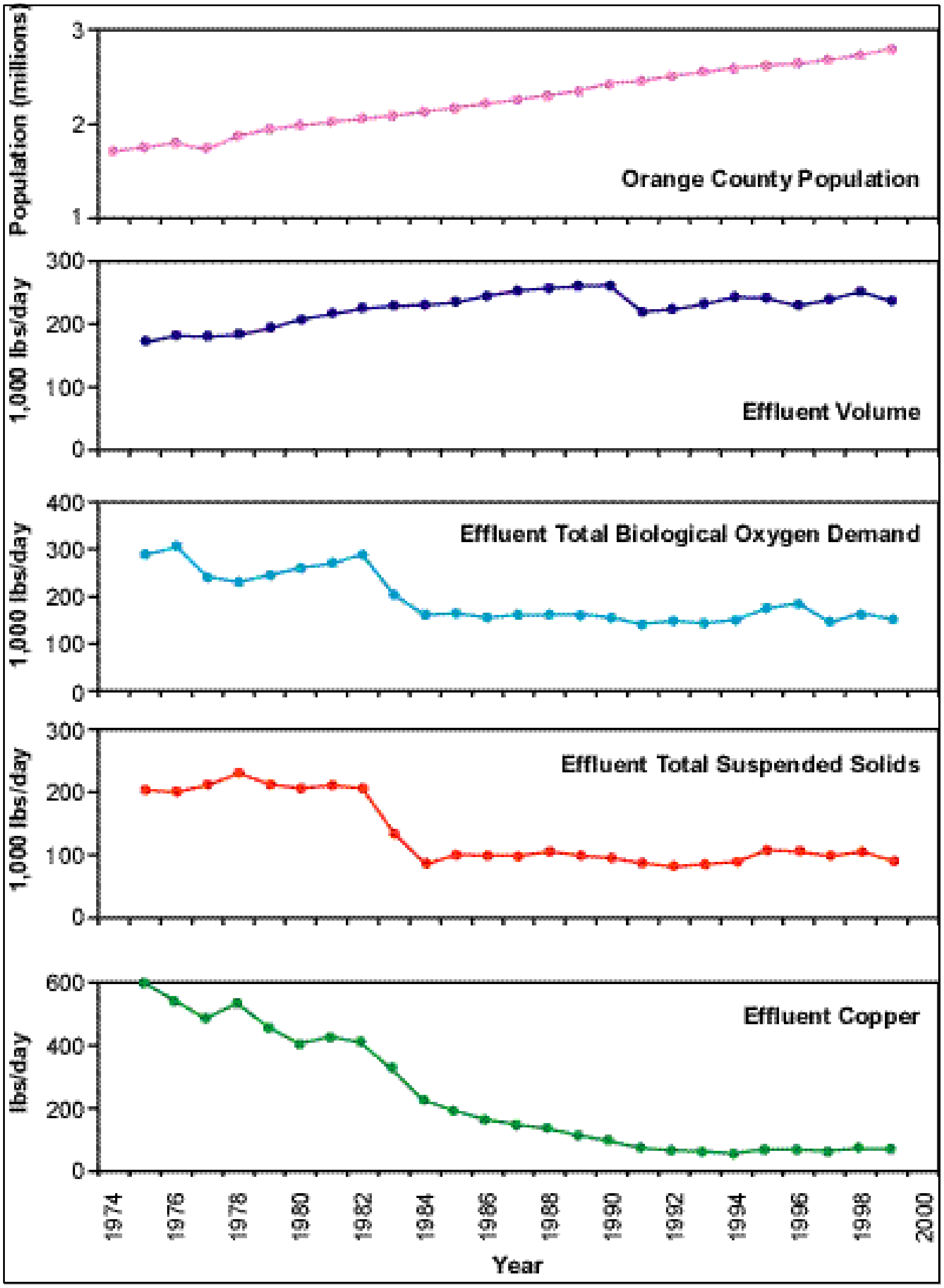

Figure A-4. Example of trends in the districts' effluent discharges to the San Pedro Shelf Region, 1974-1999. MGD = millions of gallons per day; lbs/day = pounds per day.

Appendix B
Descriptions of Selected Combined Far Field Circulation and Water Quality Modeling Systems

In this appendix an overview of most combined modeling systems is provided. In some cases more details are provided than in others. This reflects the detail of the available literature reviewed.

B.1 HydroQual's ECOM/RCA

ECOM is an outgrowth of the Princeton Ocean Model (POM) that is used in a proprietary mode by HydroQual. A version of ECOM called ECOM-si incorporates an implicit scheme developed by Vincenzo Casulli for solving the gravity wave so that the need for separate barotropic and baroclinic time steps is eliminated. The modeling framework is shown in Figure B-1.

ECOM incorporates a turbulence closure model to parameterize vertical mixing processes. The model uses a coordinate system such that the number of grid points in the vertical is independent of depth. The prognostic variables are water levels, temperature, salinity, turbulence kinetic energy, turbulence macroscale and the three components of velocity. The momentum equations are non-linear and incorporate a variable Coriolis parameter. Other computer variables include density, vertical eddy viscosity and vertical eddy diffusivity.

RCA is a generalized framework for modeling contaminant transport and fate in natural water bodies. It is based on a compartment modeling approach and driven by advective and dispersive transport fields provided by its companion hydrodynamic modeling program ECOM. RCA can be applied in a 1-D, 2-D or 3-D mode and is designed to permit easy substitution of user-written kinetic subroutines into the program structure. RCA has been used in water quality investigations of pathogenic organisms (indicator organisms and specific pathogens), biochemical oxygen demand and dissolved oxygen dynamics, nutrients and eutrophiction, wetland processes, including periphyton and emergent vegetation, and organic chemical and heavy metal contamination.

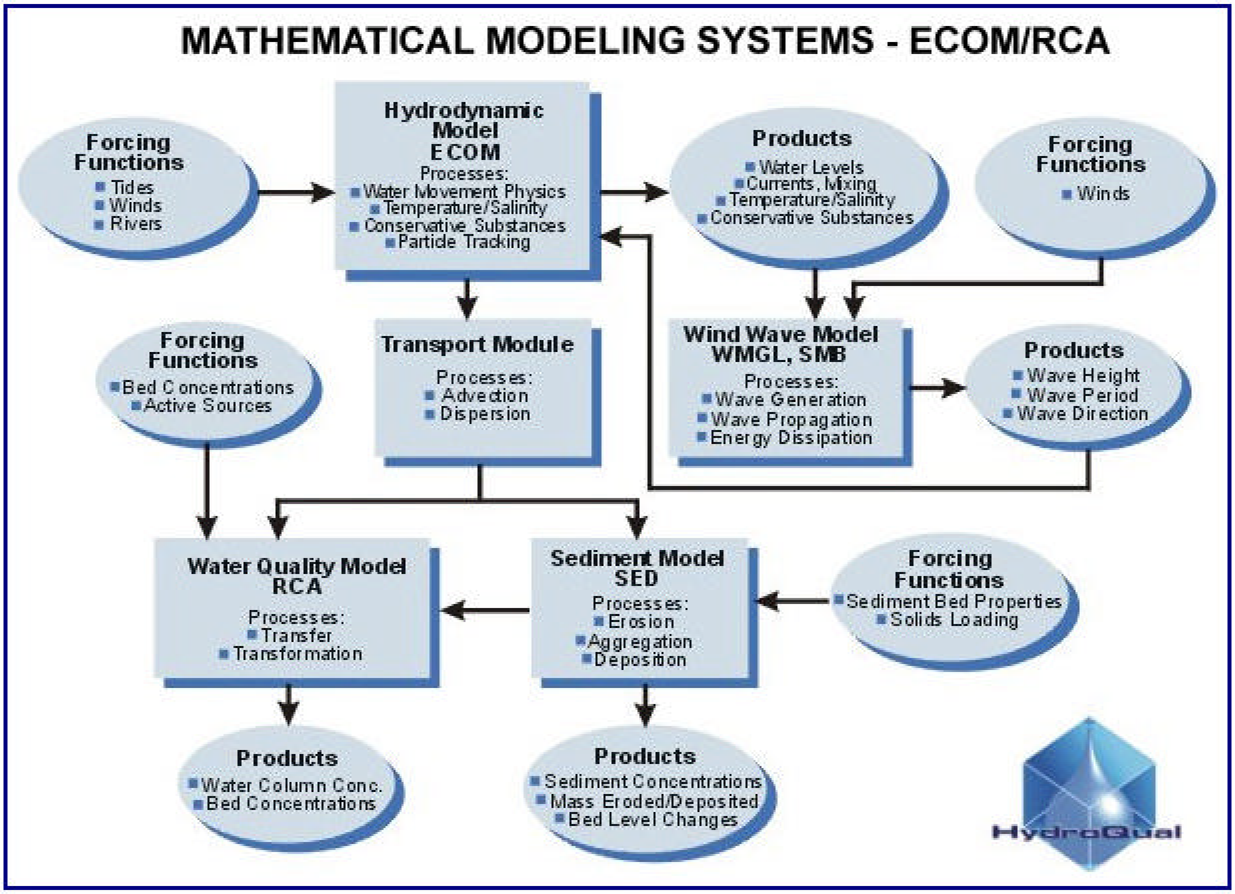

Figure B-1. Mathematical modeling systems.

ECOMSED is the sediment transport model used and simulates cohesive and noncohesive sediment transport. It is comprised of coupled hydrodynamic, wave and sediment transport models, in either two- or three-dimensions. ECOMSED uses in-situ field measurements to describe resuspension and deposition processes, including he effects of flocculation of cohesive sediments, and the effect of salinity on flocculation. For many studies involving the fate and transport of chemicals in the aquatic environment, ECOMSED computations are conducted to support one or more chemical models.

B.2 MIKE3

MIKE3 is a mathematical modeling system designed for applications in areas such as:

- Oceanography
- Coastal regions
- Estuaries and lakes

The system is fully three-dimensional solving the momentum equation and continuity equations in the three Cartesian directions. MIKE3 simulates unsteady flow taking into account density variations, bathymetry and external forcing such as meteorology, tidal elevations, currents, and other hydrographic conditions. MIKE3 can be applied to:

- Oceanographic studies
- Costal circulation studies
- Water pollution studies
- Environmental impact assessment studies
- Heat and salt recirculation studies
- Sedimentation studies

MIKE3 is composed of three fundamental modules: The hydrodynamic module, the turbulence module and the advection-dispersion module. Various features such as free surface description, laminar flow description and density variations are optionally invoked within the three fundamental modules.

A number of application modules have been implemented and can be invoked optionally These are advection-dispersion of conservative or linearly decaying substances, a water quality module describing BOD-DO relations, nutrients and hygienic problems, eutrophication module simulating algae growth and primary production, and a mud transport module simulating transport along with erosion and deposition of cohesive material. A Lagrangian based particle module can also be invoked for simulating tracers, sediment transport, or the spreading and decay of E-coli bacteria.

The modeling system is based on the conservation of mass and momentum in three dimensions of a Newtonian fluid. The flow is decomposed into mean quantities and turbulent fluctuations. The closure problem is solved through the Boussinesq eddy viscosity concept relating the Reynold stresses to the mean velocity field. To handle density variations, the equations for conservation of salinity and temperature are included. An equation of state constitutes the relation between the density and the variations in salinity and temperature and mud concentrations.

In the hydrodynamic module, the prognostic variables are the velocity components in the three directions and the fluid pressure. The model equations are discretised in an implicit, finite difference scheme on a staggered grid and solved non-iteratively by use of the alternating direction implicit technique. A phase and amplification analysis neglecting effects of viscosity, convective terms, rotation, and density variations has been performed. Under these circumstances, the finite difference scheme is unconditionally stable.

The transport of scalar quantities, such as salinity and temperature, is solved in the advection-dispersion module using an explicitly, finite difference technique based on quadratic upstream interpolation in three dimensions. The finite difference scheme, which is accurate to fourth order, has attractive properties concerning numerical dispersion, stability and mass conservation.

The decomposition of the prognostic variables into a mean quantity and a turbulent fluctuation leads to additional stress terms in the governing equations to account for the non-resolved processes both in time and space. By the adoption of the eddy viscosity concept these effects are expressed through the eddy viscosity, which is optionally determined by one of the following five closure models: a constant eddy viscosity, the Smagorinsky sub-grid (zero-equation) model, the *k*- (one equation) model, the standard k-ε (two equation) model and, finally a combination of the Smagorinsky model for the horizontal direction and k-ε model for the vertical direction. The turbulence models are all solved in an explicit manner except for the one-dimensional (vertical) k-ε model, which is solved by an implicit scheme.

There are several types of equations of state for the density of seawater. In MIKE3, the definition given by UNESCO has been adopted relating local density to salinity, temperature and pressure.

Traditionally, the finite difference technique is used in the field of hydraulics, and thus it is also used in (almost) all existing models developed at the Danish Hydraulic Institute. The grid that has been adopted is the Arakawa C staggered grid.

The adopted staggered grid allows for the spatial discretization of the differential equations. The mass equation is space centered in every node, whereas the momentum equations are space centered in the corresponding velocity 'nodes.' The time derivatives imply the definition of certain time levels, also, leading to either explicit or implicit schemes. In general, all prognostic variables in implicit schemes are defined at the same time level and then an iterative technique is applied to invert the matrix to advance the solution one-time step.

This inversion may be performed on the entire matrix in one step, which, due to the size of the matrix, is costly. Alternatively, the inversion may be split into three operations according to the three directions. In each operation, only the prognostic variables directly associated with the directions are considered as prognostic, whereas the other direction variables are locked. This technique is known as the Alternating Directions Implicitly (ADI) algorithm.

In almost all of the modeling systems developed at the Danish Hydraulic Institute, the ADI-technique has been adopted to inverse the matrices. Usually, iterative methods are required for the inversion of the matrices due to the non-linear terms in the momentum equations. However, applying two special techniques allows for a non-iterative ADI algorithm to be adopted. The first of these two techniques is called the fractional-step technique. Basically, the fractional-step technique is a time staggering of the prognostic variables. This technique has been described in detail by Leendertse (1967).

The second special technique is called ‘side-feeding’ and is basically a semi-linearization of the non-linear terms. Details on this side-feeding technique are given by Abbott (1979).

The primitive equations will mathematically form an ill-posed problem whenever the fluid pressure and the velocities constitute the prognostic variables due to a weak coupling between the pressure and velocity. The system is said to be stiff as both slow and fast processes are present, which inherently cause difficulties in the numerical algorithm. The fast processes are eliminated by replacing the time derivative of the density in the mass conservation equation with the pressure term in the equation of state, whereby a compressibility of the fluid is introduced. The fast processes are then subsequently eliminated through an artificial compressibility. This approach is known as the artificial compressibility approach and was first proposed by Chorin 1967.

The MIKE3 model also simulates the following:

- Water quality
- Eutrophication
- Mud transport
- Particles
- Metals in water column and sediments

B.3 Delft3D

The hydrodynamic module is a multi-dimensional hydrodynamic simulation program that calculates non-steady flows and transport phenomena resulting from tidal and meteorological forcing on a curvilinear, boundary-fitted grid. In 3D simulations, the hydrodynamic module applies the sigma coordinate transformation in the vertical, which results in a smooth representation of the bottom topography. It also results in computing efficiency because of the constant number of vertical layers over the whole computational domain.

The hydrodynamic module is based on the full Navier-Stokes equations with the shallow water approximation applied. The equations are solved with a highly accurate unconditionally stable solution procedure. The supported features are:

- Three co-ordinate systems, i.e. rectilinear, curvilinear and spherical in the horizontal directions and a sigma co-ordinate transformation in the vertical;

- Simulation of drying and flooding of intertidal flats (moving boundaries);

- Coriolis force and (optionally) tide generating forces;
- Density gradients due to a non-uniform temperature and salinity concentration distribution;
- Inclusion of density (pressure) gradients terms in the momentum equation (density driven flows);
- Turbulence model to account for the vertical turbulent viscosity and diffusivity based on the eddy viscosity concept;
- Selection from four turbulence closure models: k-epsilon, k-L, algebraic, and constant coefficient;
- Shear stresses exerted by the turbulent flow on the bottom based on a quadratic Chézy or Manning's formula;
- Wind stresses on the water surface modeled by a quadratic friction law;
- Simulation of the thermal discharge, effluent discharge and the intake of cooling water at any location and any depth in the computational field (advection-diffusion module).
- Automatic conversion of the 2D bottom-stress coefficient into a 3D coefficient;
- Horizontal turbulent exchange coefficients composed of a 3D turbulence model and a 2D sub-grid turbulence model;
- The effect of the heat flux through the free surface;
- On-line analysis of model parameters in terms of Fourier amplitudes and phases enabling the generation of co-tidal maps;
- Space varying wind and barometric pressure, including the hydrostatic pressure correction at open boundaries (optional);
- Drogue tracks (optional);
- On-line visualization of model parameters enabling the production of animations (in preparation).

The transport of substances is commonly represented by the so-called advection-diffusion equation. The water quality module is based on this equation and it offers different computation methods to solve it numerically (in one, two or three dimensions) on an arbitrary irregular shaped grid or a grid of rectangles, triangles or curvi-linear computational elements. In order to model waste loads and water quality processes the advection-diffusion equation is extended with an extensive water quality library of source/sink terms. The model is capable of describing any combination of constituents and is not limited with respect to the number and complexity of the water quality processes.

The water quality processes may be described by arbitrary linear or non-linear functions of the selected state variables and model parameters. For many water quality problems, these process formulations have been standardized in the form of a library, which interfaces with the water quality module. The library contains over 50 water quality processes routines covering 140 standard substances. A graphical user interface within the WAQ module enables the user to select substances and associated water quality processes.

Water quality processes are incorporated in the advection diffusion equation by adding an additional source in the mass balance. Examples of water quality processes are:

- Exchange of substances with the atmosphere (oxygen, volatile organic substances, temperature);
- Adsorption and desorption of toxicants and ortho-phosphorous;
- Deposition of particles and adsorbed substances to the bed;
- Resuspension of particles and adsorbed substances from the bed;
- The mortality of bacteria;
- Biochemical reactions like the decay of BOD and nitrification;
- Growth of algae (primary production);
- Predation (e.g. zooplankton on phytoplankton).

Special attention is paid to the treatment of the interaction with the bottom:

- All suspended sediment is modeled as cohesive sediment that can be transported with the water flow just like a dissolved substance;
- All particulate inorganic matter can be represented by three size fractions or components;
- All particulate organic matter is represented by separate components, namely detrital carbon, other organic carbon, diatoms, non-diatom algae (Green), adsorbed phosphorus and organic carbon from loads;
- The bottom sediment is modeled via two separate layers. Each layer is considered homogeneous (well mixed). The different layers can have different compositions. The density of a layer is variable depending on the sediment layer composition, which is also variable. The porosity within a given layer is constant (user defined);

- A third (deeper) layer exists (but is not explicitly modeled) which can supply sediment for upward sediment transport 'digging';
- Sedimentation and resuspension are modeled using the Krone-Partheniades approach (see the description of the sediment transport module Delft3D-SED.

The sediment transport module, Delft3D-SED, can be applied to model the transport of cohesive and non-cohesive sediments, i.e. to study the spreading of dredged materials, to study sedimentation/erosion patterns, to carry out water quality and ecology studies where sediment is the dominant factor.

For sedimentation the following assumptions apply:

- Sedimentation takes place when the bottom shear stress drops below a critical value;
- There is no correlation between the sediment components (i.e. each of the particulate fractions can settle independently);
- Sedimentation always results in an increase of sediment in the uppermost sediment layer;
- The total shear stress is the linear sum of the shear stresses caused by water velocity and wind effects. Effects of shipping and fisheries can also be included.

The effects of 'hindered settling' (i.e. decrease in sedimentation velocity at very high suspended solids concentration) can be included.

For resuspension the assumptions are:

- The bottom sediments are homogenous within a layer. Therefore, the composition of the resuspending sediment is the same as that of the bottom sediment;
- The resuspension flux is limited based on the available amount of sediment in a sediment layer for he variable layer option. The resuspension is unlimited if the fixed layer option is used;
- As long as mass is available in the upper sediment layer, resuspension takes place from that layer only;
- Resuspension flux is zero if the water depth becomes too small.

Burial is the process in which sediment is transferred downward to an underlying layer. The sediment layer is assumed to be homogeneous, therefore the composition of the sediment being buried is the same as that of the (overlying) sediment layer.

Digging is the process in which sediment is transferred upward from an underlying layer. The sediment layers are homogeneous, therefore the composition of the sediment being transported upwards is the same as that of the (underlying) sediment layer. A third and deeper layer allows for an unlimited 'digging' flux to the second layer. The quality of this third layer must be defined by the user and is not modeled.

For non-cohesive sediment (sand) the transport rate is calculated according to the transport formulae of Engelund-Hansen and Ackers-White. These (semi-) empirical relation describes the total transport (bed load and suspended load) in the situation of local equilibrium.

The implementation recognizes two options: unlimited supply of sand via the boundaries and the presence of absence of bedrock.

To apply the sediment transport module the following limitations must be observed:

- In the sedimentation process, there is no correlation between the cohesive and non-cohesive components, i.e. between sand and silt; each is treated independently;

- The effect of short waves must be taken into account through the hydrodynamic module or through a localized wave effect estimation (that is, the waves are considered to be in equilibrium with local circumstances);

- The sedimentation model should only be used for short-or medium-term (days, weeks, months) modeling of erosion and sedimentation process as the changes on bottom topography and its effects on the flow are neglected. For long-term processes (years), whereby the flow changes induced by changing bottom topography is significant, the separate morphological and sediment module (Delft3D-MOR) should be used. This module has advanced on-line coupling capabilities with the hydrodynamic flow and wave modules.

The particule tracking module is a 3-dimensional near-field water quality model. It estimates a dynamic concentration distribution by following the tracks of thousands of particles in time. The model can describe concentration contours of instantaneous or continuous releases of salt, oil, temperature or other conservative or simple decaying substances. This section gives a brief introduction to the computer module and its applications.

The particle transport model simulates transport processes and simple chemical reactions of substances. The present release also allows for red tide modeling. The module allows the simulation of detailed shapes of patches of wasted material.

The physical components in the system are:

- The water system: a lake, estuary, harbor or river, possibly with open boundaries to other water systems. Tidal variations are included;

- Outfalls due to human activities;

- Chemical substances like rhodamine dyes, salt, oil or a demand of oxygen due to fast chemical reactions;

- Physical quantities like temperature and density;
- Wind fields;
- Stratification of the water column in two layers;
- Red Tides, nutrients and sun light;
- Settling velocities.

In terms of physical processes or phenomena the particle tracking model can represent:

- The dynamics of patches close to an outfall location;
- Simple first-order decay processes like the decay of several fractions of oil;
- Vertical dispersion for well-mixed systems;
- Limited vertical dispersion due to stratification. Stratification may occur near outfall locations due to a waste of heat or a waste of salt;
- Horizontal dispersion due to turbulence. According to turbulence theory this dispersion increases in time;
- Horizontal dispersion that decreases in time due to buoyancy-driven currents near an outfall of heat or salt;
- The effects of time-varying wind fields on the patches;
- The effects of bottom-friction on the patches;
- The existence of a plume at the outfall (rather than a point-source) by starting the simulation from a circular plume with an estimated or field-measured radius.
- The transport and growth of red rides, steered by nutrients and light;
- Settling of particles;
- Floating of oil at the water surface, and dispersion of oil induced by wind waves (depending on wind speed and oil characteristics). Evaporation of floating oil is modeled as well.
- The model may be started from a known initial distribution of material, e.g. a remote sensing image of an oil spill.

The particle transport model can simulate up to 400,000 particles with a maximum of 8 substances. This requires about 64 Mbyte internal (hard core) computer memory. A computer simulation requires for most applications less one-hour, and takes most often less 200 Mbyte of disk space

The far-field water quality module models algae using an approach based on Monod kinetics and are routinely included in the process library. Ecological module contains the more sophisticated algae model II (Los, 1991) that is based on an optimization technique.

In the chemical module, the water is coupled to the chemical equilibrium model. The chemical equilibrium module calculates the distribution of elements over a pre-specified set of chemical species. The model is based on two principles: the conservation of mass and the minimization of the Gibbs free energy.

B.4 TELMAC-3D

TELEMAC-3D is a computation model to be used for situations where variations in the vertical dimension are important (and therefore a depth-integrated flow model is not adequate).

TELMAC-3D simulates the following processes:

- Tidal motions
- Vertical and horizontal velocity variation
- Salinity, temperature, suspended matter concentration
- Turbulent viscosity
- Coriolis force, wind stress, bed friction
- Density variation

Typical TELEMAC-3D applications include:

- Marine modeling
- Estuarine flows (salinity variation)
- Cooling water flows
- River modeling, beds, training structures

TELEMAC-3D features and benefits:

- Unstructured finite element grid of triangles
- Hydrostatic approximation yields efficient results

- Turbulence model by k-epsilon or mixing length (with stratification effects)
- Use of state of the art post processor for graphics and animations
- Developed under Quality Assurance procedures

PLUME-RW is a well-established model developed by HR Wallingford for studies of pollutant dispersion in estuaries and coastal waters. Either dissolved pollutants, such as bacteria from sewage discharge, suspended pollutants, such as sediment released by dredging operations, or spilled oil can be simulated The model has been validated against field data at many sites, and applied in projects throughout the world.

PLUME-RW simulates the following processes:

- Transport by prevailing currents
- Turbulent dispersion
- Bacterial decay
- Dispersion of positively-, neutrally-, and negatively-buoyant pollutants
- Deposition and re-suspension of particulates at the sea bed
- Weathering and stranding of spilled oil

Typical applications of PLUME-RW:

- Optimization of outfall location and waste treatment levels
- Planning of dredging operations
- Oil spill contingency planning

Features and benefits of PLUME-RW include:

- Flexible code, with many applications
- Two-and three-dimensional modules
- Multiple pollutant capability
- Unrestricted output grid resolution
- Proven in many validation simulations

Flow in a coastal region consists of large-scale tidal motion, wind-driven currents and small-scale turbulent eddies. In order to model the dispersal of suspended mud in such a region, the effects of these flows on suspended mud plumes must be simulated. A random walk dispersal model represents turbulent mean velocities computed by the three-dimensional free surface flow model.

In SEDPLUME-3D, the release of suspended mud in coastal waters is represented as a regular or intermittent discharge of discrete particles. Particles are released throughout a model run to simulate continuous mud disturbance or for part of the run to simulate mud disturbance over an interval during the tidal cycle, for instance to represent the resuspension of fine sediment during dredging operations. At specified sites a number of particles are released in each model time-step and, in order to simulate the release of suspended mud, the total mud released at each site during a given time interval is divided equally between the released particles. Particles can be released either at the precise coordinates of the specified sites, or distributed randomly, centered on the specified release sites. The particles can be released at the surface or evenly distributed through the water column. This allows the representation of the initial spreading of plumes of material released by for example, a dredger. The available water quality model simulates bacteria, dissolved oxygen, adsorption/desorption of heavy metals or radioactive elements.

B.5 WQMAP System

WQMAP (Water Quality Mapping and Analysis Program) is an integrated system for modeling the circulation and water quality of estuarine and coastal waters. The system allows the user to generate boundary conforming grid systems to represent the study area, to perform simulations with a suite of circulation and water quality models, and to display the model predictions in the form of time series plots, vector and contour plots, and color animation. WQMAP operates on a Pentium personal computer, features a Window's based user interface, and is controlled by pull down menus and point and click operations. The software is designed for making new applications to any geographic area simple and fast (Spaulding and Howlett, 1995). Selected key features of the software are summarized below.

Given its geographic information system (GIS) base WQMAP may be set up for any number of regions in the world. The user can rapidly switch from one location to another by simply "pointing" the system to the appropriate data set. The number of locations and associated supporting data is limited only by the amount of available disk storage space. This location functionality allows WQMAP to be completely re-locatable and is the core of the system architecture. The geographic location, defined by a base map and a series of GIS layers of vector or raster data, can be at any resolution and at any location in the world and provides the reference for all model applications. GIS maps and layers may be prepared by digitizing from paper charts, by importing from existing GIS databases, or the user may simply make a map from WQMAP's global database for any region in the world. The simplest implementation of a location is a map that represents land and water features (polygons) that define the waterland interface for the grid generator. More complex coastal features such as marshes and intertidal zones may also be introduced.

The embedded GIS allows the user to input, store, manipulate, analyze, and display geographically referenced information. The GIS is fast, user-friendly, interactive, and simple to operate. The GIS is often used to provide input data to the models. It is also helpful in the presentation and interpretation of model predictions. Additional information can be linked to the GIS including charts, graphs, tables, tutorials, bibliographies, photographs, video, text, or other software (e.g. spreadsheets, word processors).

Although the spatial analysis tools of traditional GIS are powerful it is difficult to employ them when large amounts of time varying data are used. This results in slow and generally poor quality animations. WQMAP addresses this problem by providing a stand-alone application with simplified interactive GIS functionality and highly optimized viewer for animation of temporally and spatially varying model results. It also has the option to export model results efficiently to external GIS applications for further analysis.

WQMAP includes three basic components: a boundary fitted coordinate grid generation module, a three dimensional hydrodynamics model, and three separate water quality or pollutant transport and fate models. These components are accessed through the user interface. Supporting data is accessed through the location specific data sets, the GIS, or input through the menu windows. All models are configured for operation on a boundary conforming grid system. They can also be operated on a rectangular grid or any orthogonal curvilinear grid, as these are special cases of the boundary conforming grid. Each model is briefly described below.

Boundary Fitted Grid Generation Module – The boundary fitted grid generation module and associated interface is an interactive tool that can be used to quickly and efficiently generate non-orthogonal boundary conforming grids for the hydrodynamic and water quality models. The basic foundation of the approach is to construct grids such that all domain boundaries are coincident with coordinate lines. This is accomplished using a set of coupled quasilinear elliptic transformation equations to map an arbitrarily shaped, multi-connected horizontal region in physical space to a rectangular mesh in the transformed boundary conforming space (Thompson et al, 1977; ASA, 1997). Even though the transformed set of governing equations are specified on straight lines and the coordinate spacing is uniform in the transformed space. Orthogonal and conformal curvilinear grids, as well as simple stretched rectangular grids, are special cases of the generalized boundary conforming grid system.

Key boundary points are specified interactively by the user on a base map of the study area. The structure of the computational grid is defined in the physical domain by pointing and clicking with the mouse and form driven input. After the key grid nodes (grid corners) along the domain boundaries are specified the model interpolates the remaining boundary nodal locations at user defined spacing. It then numerically solves the coupled, elliptic coordinate transformation equations to determine the interior grid points within the model domain. Editing tools are available to add, delete, and move nodes. These tools can be used to adjust interior grid points to follow key bathymetric features such as channels. An interrogation function is also available which allows the user to determine the physical (latitude and longitude) and computational location of any point in the field. The selection of the key grid nodes is used to define the intersection between the two boundary conforming coordinate lines. Alternate selection approaches can be used to either represent the coast as one coordinate line or through a series of steps with altering coordinate lines. The flexibility afforded by this strategy gives the user an excellent ability to represent topographically complex areas, including those with multiple branching rivers, islands, and varying size coves, bays, and sounds.

Use of boundary conforming grids eliminates the “staircase” grid problem encountered in square/rectangular grids, allows highly variable grid aspect ratios to account for different length scales (e.g. narrow riverine versus broad bay-sound systems) and allows the model boundaries to conform to the physical boundaries of he domain. Since the gird system is not limited by an orthgonality constraint, grid design and construction are much simpler and more flexible than for models that use orthogonal curvilinear grids. Grid generation and updating are fast and efficient. The grid generation system can also be used to generate simpler grids (square, rectangular, orthogonal boundary conforming) to interface with other model systems.

The module also has a tool that generates the depth for each boundary conforming grid. Input to the program includes digital data providing the depths at selected locations in the study area and the coordinates of the boundary conforming grid system. The module averages all depth measurements within a given grid and provides the mean depth for that grid as output. The user can interrogate, edit, or smooth the depths in each grid through the interface.

Hydrodynamic Model – The hydrodynamic model solves the three dimensional, conservation of water mass, momentum, salt and energy equations on a spherical, non-orthogonal, and boundary conforming grid system and is applicable for estuarine and coastal areas (Muin, 1993; Muin and Spaulding, 1996, 1997a,b). Solutions are also predicted for the two dimensional, vertically averaged circulation. The eddy viscosities can be specified by the user of based on a one-equation turbulent kinetic energy (TKE) model. Output of the TKE model can be used in conjunction with a prescribed mixing length to determine the vertical eddy viscosities. A sigma stretching system is used to map the free surface and bottom to resolve bathymetric variations. The model employs a split mode solution methodology (Madala and Piaseck, 1977). In the exterior (vertically averaged) mode, the Helmholtz equations, given in terms of the sea surface elevation, is solve by a semi-implicit algorithm to ease the time step restrictions normally imposed by gravity wave propagation. In the interior (vertical structure) mode the flow is predicted by an explicit finite difference method, except that the vertical diffusion term is treated implicitly. The time step generally remains the same for both exterior and interior modes. Computations are performed on a space staggered grid system in the horizontal and a non-staggered system in the vertical. Time is discretized using a three-level scheme. Muin and Spaulding (1996, 1997a) provide a detailed description of the governing equations, numerical solution methodology, and in depth testing against analytic solutions for two and three dimensional flow problems. Additional applications are described in Swanson and Mendelsohn (1993, 1996) and Mendelsohn et al (1995).

The WQMAP system allows the user to present the results of any simulations performed. The user opens the scenario file of interest and then selects the type of output desired. As an example for the hydrodynamics model the user selects the variable (currents, temperature, surface elevation, salinity) and the vertical level (sigma layer) and then animates the results (color contours or vectors) over the model simulation period. The animation control allows forward, step forward, and rewind options. The animations can also be overlaid on the bathymetric data to allow the user to visualize the relationship between the predicted values (currents, salinity, and temperature) and the depth. The user can also select a section view window (vertical transect along user selected line) that allows the variable of interest to be visualized along the section line at the same time as the plan view is animated. An environmental data window is also available to display time series of environmental forcing data such as tide height, solar radiation, and air temperature.

Pollutant Transport Models – There are three separate models within the QMAP pollutant transport model system. The first is a single constituent transport model, which includes first order reaction terms. This model is suitable for a single constituent contaminant that settles, decays, or grows. The second is a multi-constituent transport and fate model with a reaction matrix that can be specified by the user. This can be used to custom design a multi-component water quality model system. The third is a multi-constituent eutrophication model (e.g. nitrogen, phosphorous, dissolved oxygen), which incorporates EPA WASP5 kinetic rate equations (Ambrose et al, 1994). The user can set the parameters of the rate equations via the user interface or select default values. The suite of models allows the system to be efficiently used for a wide range of pollutant transport and fate studies, extending from simple single parameter systems to complex, multi-constituent problems with interacting components.

In each model either the two or three dimensional advective diffusion equation is solved on a boundary conforming grid for each constituent of interest. The model employs the same grid system and obtains the face centered, contra-variant velocity vector components from the hydrodynamic model. This procedure eliminates the need for aggregation or spatial interpolation of the flows from the hydrodynamic model and assures mass conservation. Its drawback, compared to aggregation, is an increase in computational time for a given simulation.

The transport model is solved using a simple explicit finite difference technique on the boundary conforming grid (ASA, 1997). The vertical diffusion however is represented implicitly to ease the tie step restriction caused by the normally small vertical length scale that characterizes many coastal applications. The model includes five options to solve the advective transport: 2nd order Lax-Wendroff, 1st and 2nd order upstream differencing, MIE 2nd order upstream and 2nd order QUICKEST (Thompson, 1984). These can be selected through the user interface to address the particular problem of interest. The horizontal diffusion term is solved by a centered in space, explicitly technique. The solution to the advective diffusion equation has been validated by comparison to one and two-dimensional analytic solutions for a constant plane and line source loads in a uniform flow field and for a constant step function at the upstream boundary. The model has also been tested for salinity intrusion in a channel (Muin, 1993).

The river and open boundary conditions for the pollutant transport and fate model are entered via pointing and clicking on a boundary grid (or series of grids) and specifying the value in a grid attribute file. The loading information is stored in a GIS object file. The load information is specified through the object attribute utility, which can link with a spread sheet or ASCII file. This approach allows an efficient technique to input a variety of alternative loads, typical of model calibration and validation or alternative assessment.

The output module of the pollutant transport model allows the user to animate model predictions and display time series using the same strategies as for the hydrodynamic model. Simultaneous plan and section views (along a user specified section line) can be animated in color.

All model simulations within WQMAP are organized on a scenario basis. The scenario is specified through the user interface (model parameters, terms in governing equations, bathymetric data set, grid system, output file specifications, hydrodynamic data set, contaminant loading, river input, and boundary conditions). Once the simulation is complete the results are stored in a scenario output file. Both the input and output files are stored and can be visualized. This approach creates a record of each simulation including both the input parameters and data files employed in the simulation and the associated output. Scenario files can be archived or deleted depending on the need.

The basic WQMAP system has been extended to include real time data monitoring and data assimilation procedures (Spaulding and Opishinski, 1995; Opishinski and Spaulding, 1995, 1996; Spaulding et al, 1998). The data module in this extended system provides access to the real time monitoring module. The real time monitoring module allows the user to directly interface with the instruments and the associated communication system. The user, via the base communication system, can retrieve data, set the instruments sampling and storage intervals, turn sensors on and off, and alter the operation of the communication system. The user can also add, update, and delete observation stations from the system. A status board is also provided to allow the user to view (e.g. last value, most recent time series) the output from each sensor in the system and the operations status of the power supply. The user can also link directly to a data processing module that allows standard times series analysis (e.g. filtering (high, low and band pass with selectable filter type and characteristics), harmonic composition and decompositon, and spectral analysis) and plotting of the resulting data. This analysis can be done either on data archived in the system or the most recently collected information. Output from this module can be linked directly to the environmental models either as direct input (e.g. boundary conditions, surface forcing) or via data assimilation (i.e. nudging). Data can be distributed via radio telemetry, satellite, cell telephone or the Internet. The system can also be configured with an automated FTP.

B.6 Ocean Models at Rutgers University

Rutgers University has developed a series of ocean models including both finite difference and finite element. They are presently working with UCLA to enhance their ROMS model.

This S-Coordinate Primitive Equation Model (SPEM) solves the hydrostatic primitive equations under the assumption of a rigid lid at the surface. In the vertical, a generalized bottom following coordinate allows effective incorporation of steep and/or tall bathymetry, without undue loss of resolution at the sea surface. In the horizontal, an orthogonal curvilinear coordinate on an Arakawa C grid is used. Second-order finite differences are used throughout; an earlier version, employing a Chebyshev Galerkin formulation in the vertical (Haidvogel et al., 1991), is also available.

The SCRUM model, which solves the hydrostatic primitive equations with a free sea surface, is an outgrowth of the s-coordinate model originated by Song and Haidvogel (1994). Many of its algorithmic features - e.g., vertical and horizontal coordinates, finite difference treatments, mixing options, etc. - are compatible with SPEM. However, split-explicit time differencing is required for efficient handling of the free surface in SCRUM. A version of SCRUM optimized for execution on the CM-class (SIMD) parallel computers is also available.

The Spectral Element Ocean Model (SEOM) solves the hydrostatic, and alternatively the non-hydrostatic, primitive equations using a mixed spectral / finite element solution procedure. Potential advantages of the spectral element method include flexible incorporation of complex geometry and spatially dependent resolution, rapid convergence, and attractive performance on parallel computer systems. A 2D version of SEOM, which solves the shallow water equations, has been extensively tested on applications ranging from global tides to the abyssal circulation of the Eastern Mediterranean. The 3D SEOM is undergoing initial testing for later release.

The Regional Ocean Model System (ROMS) is a free-surface, hydrostatic, primitive equation ocean model that uses stretched, terrain following coordinates in the vertical and orthogonal curvilinear coordinates in the horizontal. Initially, it was based on the S-coordinate Rutgers University Model (SCRUM) described by Song and Haidvogel (1994). ROMS was completely rewritten to improve both its numerics and efficiency in single and multi-threaded computer architectures. It also was expanded to include a variety of new features including high-order advection schemes; accurate pressure gradient algorithms; several subgrid-scale parameterizations; atmospheric, oceanic, and benthic boundary layers; biological modules; radiation boundary conditions; and data assimilation.

For computational economy, the hydrostatic primitive equations for momentum are solved using a split-explicit time-stepping scheme which requires a special treatment and coupling between barotropic (fast) and baroclinic (slow) modes. A finite number of barotropic time steps, within each baroclinic step, are carried out to evolve the free-surface and vertically integrated momentum equations. In order to avoid the errors associated with the aliasing of frequencies resolved by the barotropic steps but unresolved by the baroclinic step, the barotropic fields are time averaged before they replace those values obtained with a longer baroclinic step. A cosine-shape time filter, centered at the new time level, is used for the averaging of the barotropic fields. In addition, the separated time stepping is constrained to maintain exactly both volume conservation and constancy preservation properties which are needed for the tracer equations (Shchepetkin and McWilliams, 2000). Currently, all 2D and 3D equations are time discretized using a third-order accurate predictor (Leap-Frog) and corrector (Adams-Molton) time-stepping algorithm which is very robust and stable. The enhanced stability of the scheme allows larger time steps, by a factor of about four, which more than offsets the increased cost of the predictor-corrector algorithm.

In the vertical, the primitive equations are discretized over variable topography using a stretched terrain-following coordinates (Song and Haidvogel, 1994). The stretched coordinates allow increased resolution in areas of interest, like thermocline and bottom boundary layers. The default stencil uses centered, second-order finite differences on a staggered vertical grid. Options for higher order stencil are available via a conservative, parabolic spline reconstruction of vertical derivatives (Shchepetkin and McWilliams, 2000). This class of model exhibits stronger sensitivity to topography which results in pressure gradient errors. These errors arise due to splitting of the pressure gradient term into an along-sigma component and a hydrostatic correction (for details, see Haidvogel and Beckmann, 1999). The numerical algorithm in ROMS is designed to reduce such errors and follows Song and Wright (1998) and Shchepetkin and McWilliams (2000).

In the horizontal, the primitive equations are evaluated using boundary fitted, orthogonal curvilinear coordinates on a staggered Arakawa C-grid. The general formulation of curvilinear coordinates includes both Cartesian (constant metrics) and spherical (variable metrics) coordinates. Coastal boundaries can also be specified as a finite-discretized grid via land/sea masking. As in the vertical, the horizontal stencil utilize a centered, second-order finite differences. However, the code is designed to make the implementation of higher order stencils easily.

ROMS has various options for advection schemes: second- and forth-order centered differences; and third-order, upstream biased. The later scheme is the model default and it has a velocity-dependent hyper-diffusion dissipation as the dominant truncation error (Shchepetkin and McWilliams, 1998). These schemes are stable for the predictor-corrector methodology of the model. In addition, there is an option for conservative parabolic splines representation of vertical advection which has dispersion properties similar to an eight-order accurate conventional scheme (Shchepetkin and McWilliams, 2000).

There are several subgrid-scale parameterizations in ROMS. The horizontal mixing of momentum and tracers can be along vertical levels, geopotential (constant depth) surfaces, or isopycnic (constant density) surfaces. The mixing operator can be harmonic (3-point stencil) or biharmonic (5-point stencil). See Haidvogel and Beckmann (1999) for an overview of all these operators.

The vertical mixing parameterization in ROMS can be either by local or nonlocal closure schemes. The local closure scheme is based on the level 2.5, turbulent kinetic energy equations by Mellor and Yamada (1982). The nonlocal closure scheme is based on the K-profile, boundary layer formulation by Large et al. (1994). The K-profile scheme has been expanded to include both surface and bottom oceanic boundary layers. In addition, there is a wave/current bed boundary layer scheme that provides the bottom stress and sediment transport (Styles and Glenn, 1999) which become important in coastal applications.

Currently, the air-sea interaction boundary layer in ROMS is based on the bulk parameterization of Fairall et al. (1996). It was adapted from the COARE (Coupled Ocean-Atmosphere Response Experiment) algorithm for the computation of surface fluxes of momentum, sensible heat, and latent heat. This boundary layer is used for one- or two-way coupling with atmospheric models.

The data assimilation in ROMS is via a multivariate, intermittent Optimal Interpolation (OI) scheme (Gandin, 1963; Bretherton et al., 1976; Lorenc, 1978) in which observations and model data are melded together taking into account errors in the observations and prediction. This data assimilation scheme is very efficient and inexpensive, but it is sub-optimal. In addition, there is also an implementation of the reduced-state Kalman filter algorithm described by Fukumori and

Malanotte-Rizzoli (1995). Progress has been made to incorporate Lermusiaux and Robinson (1999) data assimilation scheme via Error Subspace Statistical Estimation (ESSE).

ROMS is a modern code and uses C-preprocessing to activate the various physical and numerical options. The code can be run in either serial or parallel computers. The code uses a coarse-grained parallelization paradigm which partitions the computational 3D grid into tiles. Each tile is then operated on by different parallel threads. Originally, the code was designed for shared-memory computer architectures and the parallel, compiler dependent, directives (OpenMP Standard) are placed only in the main computational routine of the code. An MPI version of the code is currently being developed and in the future both shared- and distributed-memory paradigms will coexist together in a single code.

ROMS has extensive pre- and post-processing software for data preparation, analysis, plotting, and visualization. The entire input and output data structure of the model is via NetCDF which facilitates the interchange of data between computers, user community, and other independent analysis software.

B.7 Description of the EFDC Model

The Environmental Fluid Dynamics Code or EFDC (Hamrick, 1992a) comprises an advanced three-dimensional surface water modeling system for hydrodynamic and reactive transport simulations of rivers, lakes, reservoirs, wetland systems, estuaries, and the coastal ocean. The modeling system was originally developed at the Virginia Institute of Marine Science as part of a long-term research program to develop operational models for resource management applications in Virginia’s estuarine and coastal waters (Hamrick, 1992b). The EFDC model is public domain, with current users including universities, governmental agencies, and engineering consultants. Tetra Tech, Inc., currently maintains EFDC and continues its development with primary support from the U.S. Environmental Protection Agency. The model is currently being reviewed for EPA endorsement and subsequent distribution. The following sub-sections describe the model’s capabilities and previous applications and its theoretical and computational formulations.

The EFDC model has three primary functional components: hydrodynamics, water quality-eutrophication, and sediment-toxic contaminant transport and fate, fully coupled and integrated into a single software system. The full integration of the three components is unique among currently available models and eliminates the need for complex interfacing of multiple models to address both hydrodynamic and biogeochemical processes. The hydrodynamic model component is based on the three-dimensional shallow water equations and includes dynamically coupled salinity and temperature transport. The basic physical process simulation capabilities of the EFDC hydrodynamic component are similar to those of the Blumberg-Mellor or POM model (Blumberg et al., 1987), the U.S. Army Corps of Engineers’ CH3D-WES model (Johnson et al., 1993), and the TRIM model (Casulli et al., 1992). Notable extensions to the EFDC hydrodynamic model include representation of hydraulic structures for controlled flow systems, vegetation resistance for wetland systems (Hamrick et al., 1996), and high frequency surface wave radiation stress forcing for nearshore coastal simulations (Hamrick et al., 1995).

The EFDC model’s water quality or nutrient cycling simulation capability is based on a 20 state variable water column eutrophication model coupled with a 26 state variable sediment biogeochemical processes model (Park et al., 1995). The nutrient cycling or eutrophication model is based on a recoding of reaction kinetics of the U.S. ACOE's CE-QUAL-IC or Chesapeake Bay water quality model (Cerco et al., 1993). The sediment processes model is also based on a recoding of the CE-QUAL-IC sediment processes model developed by DiToro and Fitzpatrick (DiToro et al., 1993). A simplified version of the eutrophication model, functionally equivalent to the U.S. EPA's WASP5 model (Ambrose et al., 1993), having 9 water column state variables and 22 sediment processes, can be optionally utilized.

The EFDC model's sediment-toxic contaminant transport component allows the simulation of multiple-sized classes of cohesive and noncohesive sediments and an arbitrary number of sorptive heavy metals and organic contaminants. The sediment transport formulation includes: concentration and shear dependent settling of cohesive sediment, concentration dependent settling of noncohesive sediment, bed stress and bed composition dependent resuspension of cohesive and noncohesive sediment, and a multi-layer consolidating sediment bed composed of mixed sediment classes and pore water. The sediment transport capabilities and formulations are consistent with peer models including the U.S. ACOE's CH3D-SED (Spasojevic et al., 1997) and the SEDZL model (Ziegler et al., 1995). Total contaminant concentration is simulated in the water column and bed with dissolved and particulate fractions determined by equilibrium partitioning. Water column-bed exchange of dissolved and particulate contaminants includes deposition and associated surface water entrainment, resuspension and associated pore water entrainment, pore water expulsion due to consolidation, and diffusion between the surface water and pore water phases. The contaminant transport capabilities and formulations are consistent with peer models including the U.S. ACOE's CE-QUAL-IC/TOXI (Spasojevic et al., 1997) and the TOXI module of the WASP5 model (Ambrose et al., 1993).

The EFDC model has been applied to over 40 water bodies for more than 50 environmental and engineering studies. Representative hydrodynamic model applications include: discharge dilution, shoreline modification, and shellfish larvae transport studies in the James and York Rivers, Virginia (Hamrick 1992b, 1994a,; Hamrick et al., 1995; Shen et al., 1999), salinity intrusion studies in the Indian River Lagoon and Sebastian River, Florida (Tetra Tech 1994; Sucsy et al., 1998), large-scale wetland simulation in the Everglades (Hamrick 1994b), and thermal simulation of Lake Okeechobee, Florida (Hamrick 1996), Nan Wan Bay, Taiwan (Systech Engineering 1997), and the Potomac River (Tetra Tech 1999a). Water quality-eutrophication model applications include the Peconic Bays, New York (Tetra Tech 1998a), and the Christina River Basin in Delaware and Pennsylvania (Tetra Tech 1999b). The EFDC model has been applied for coastal and estuarine sediment transport simulation at Vero Beach, Florida (Zarillo et al., 1995), and Morro Bay, California (Tetra Tech 1999c), and sediment-contaminant transport simulation in the Blackstone River, Massachusetts (Tetra Tech 1999d), and Elliott Bay and the Duwamish River, Washington (King County 1999).

The EFDC model solves the vertically hydrostatic momentum and continuity equations for turbulent flow in a coordinate system that is curvilinear and orthogonal in the horizontal and stretched or topography-free surface in the vertical direction.

The transport of dynamically active constituents such as salinity, temperature, and suspended sediment is coupled with the momentum equations through an equation of state and the hydrostatic condition.

The solution of the hydrodynamic and mass transport equations requires specification of the vertical turbulent viscosity and diffusivity, horizontal and vertical boundary conditions, and the source and sink terms. To provide the vertical turbulent viscosity and diffusivity, the second moment turbulence closure model (Mellor et al., 1982; Galperin et al., 1988) is used. The model relates the vertical turbulent viscosity and diffusivity to the turbulent intensity, a turbulent length scale and a Richardson number.

The numerical solution of the EFDC model equations uses a finite volume-finite difference spatial discretization with a MAC or C grid staggering of the discrete variables. The velocity components are located on the faces of the primary or continuity control volume with the depth, buoyancy, and concentration of transported constituents located at the centroid. The excess pressure is defined on the top face of the continuity control volume. Horizontally staggered control volumes are defined for the horizontal momentum equations with advective momentum fluxes located on the faces and shear stresses located on the top faces. An additional set of control volumes, staggered vertically are used for the transport equations for the turbulence parameters. Finite volume spatial integration over the four sets of control volumes combined with finite difference approximations of horizontal depth, excess pressure, and bottom elevation gradients results in centered, second order accurate spatial discretizations. The Coriolis and curvature accelerations in the momentum equations are discretized using a second order accurate, energy conserving scheme (Arakawa et al., 1977).

The temporal integration of the momentum and continuity equations uses a second order accurate, semi-implicit, three-time-level, leap frog trapezoidal scheme, with the period insertion of a two-time-level trapezoidal step to suppress the computational mode generated by the three-time-level scheme. An external-internal mode splitting scheme is also utilized to partially decouple the external or barotropic mode solution, which is implicit in the horizontal, from the internal, baroclinic or shear mode solution, which is implicit in the vertical.

B.8 Miami Isopycnic Model (MICOM)

Isopycnal surfaces may seem the most natural vertical coordinate system for ocean modeling, since water mass transports in the ocean occur approximately along isopycnal surfaces. Isopycnic models are designed to facilitate the representation of such transports because there occurs no spurious diapycnal mixing due to the numerical representation of advection. In addition, diapyncnal mixing can be added in a controlled form. A recent overview on the philosophy of isopycnal modeling is given by Bleck (1998).

The utilization of an ispycnic coordinate leads naturally to an adaptive vertical grid, which conveniently resolves regions of vertical density gradients (thermocline, surface fronts). This differs from other ocean models in that the vertical grid is time-dependent and can in principle adjust to the dynamic situation of the ocean.

The model description can be found in Bleck *et al.* (1992) and Bleck and Chassignet (1994); a user's manual and the latest references can be obtained from the MICOM web page.

The ispycnal concept has some inherent limitations. The most obvious is the fact that the use of a single potential density both for layer definition and for baroclinic pressure gradient is dynamically inconsistent. This is a fundamental problem which cannot be cured by an increase in resolution. Therefore, only one of the thermodynamic variables *?* or *S* is usually computed. This however, leads to a systematic deviation from the thermal wind relation. It appears that the problem might be reduced to some extent through choice of a different reference pressure (2000 dbar instead of the surface) although such choice may create other problems in the upper ocean. Also, isopycnal coordinate models require special advective treatments in the limit of vanishing layer thickness, and repeated evaluation of the nonlinear equation of state. This may represent a significant computational overhead depending on which algorithmic approaches are used. Thermobaricity is now included in MICOM (Sun *et al*., 1999).

The model is only available with a split explicit free sea surface scheme. The solution of the barotropic component is shifted in time. It is treated by a forward-backward scheme using the latest update of the continuity equation and the last pressure field.

Horizontally, MICOM is discretized on the Arakawa "C" grid, with curvilinear coordinates like SPEM/SCRUM. Arbitrary topography can be included.

MICOM makes use of the time splitting concept; *i.e*., each individual term of the tendency equations is used to produce an update of the prognostic variable before the next term is evaluated. The computational mode introduced by the leap-frog time-stepping scheme is reduced by an Asselin time filter (see Bleck and Smith, 1990).

Advantages and disadvantages of this model concept are closely related. High resolution in areas of sharp density gradients (both vertically and horizontally) is a highly desirable feature; however, by necessity, vertical shear in homogeneous or near-homogeneous fluid is resolved poorly. This might be important in areas where velocity shear exists in weakly stratified fluid (like in the upper mixed layer).

Also, the diapycnal transports induced by nonlinearities in the equation of state (cabbeling and themobaricity) are new additions to the code and have not been tested extensively. In the past, attempts have been made to alleviate this by using a different reference level for the density coordinate. The thermodynamic problems mentioned above have been reduced significantly (Sun *et al*., 1999).

Future developments include a hybrid version of MICOM, which will provide, in contrast to the purely ispycnic version, vertical resolution in the mixed layer and on the shelf. The capability of assigning several coordinate surfaces to the oceanic mixed layer will not only allow for vertical shear near the surface but also make it possible to replace the presently used Kraus-Turner slab mixed layer model and with a more sophisticated turbulent closure scheme.

Another ispycnic ocean model is OPYC (Oberhuber, 1993a, 1993b). Differences from MICOM include the use of the “B” grid, and, more importantly, the variation of potential densitities in all layers.

Appendix C
Descriptions of Near Field Mixing Models

C.1 CORMIX

The Cornell Mixing Zone Expert System (CORMIX) is a software system for the analysis, prediction, and design of aqueous toxic or conventional pollutant discharges into diverse water bodies. It was developed under several cooperative funding agreements between U.S. EPA and Cornell University during the period 1985-1995. It is a recommended analysis tool in key guidance documents on the permitting of industrial, municipal, thermal, and other point source discharges to receiving waters. Although the system's major emphasis is on predicting the geometry and dilution characteristics of the initial mixing zone so that compliance with water quality regulatory constraints may be judged, the system also predicts the behavior of the discharge plume at larger distances.

The highly user-interactive CORMIX system is implemented on IBM-DOS windows compatible microcomputers, utilizes a rule-based systems approach to data input and processing, and consists of three subsystems. These are: (a) CORMIX1 for the analysis of submerged single port discharges, (b) CORMIX2 for the analysis of submerged multiport diffuser discharges and (c)CORMIX3 for the analysis of buoyant surface discharges. Without specialized training in hydrodynamics, users can make detailed predictions of mixing zone conditions, check compliance with regulations and readily investigate the performance of alternative outfall designs. The basic CORMIX methodology relies on the assumption of steady ambient conditions. However, recent versions also contain special routines for the application to highly unsteady environments, such as tidal reversal conditions, in which transient recirculation and pollutant build-up effects can occur.

In addition, several post-processing options are available. These are CORJET (the Cornell Buoyant Jet Integral Model) for the detailed analysis of the near-field behavior of buoyant jets, FFLOCATR (the Far-Field Plume Locator) for the far-field delineation of discharge plumes in non-uniform river or estuary environments, and CMXGRAPH, a graphics package for plume plotting.

Several factors provided the original impetus for system development including: (a) the considerable complexity of mixing processes in the aquatic environment, resulting from the great diversity of discharge and site conditions and requiring advanced knowledge in a specialized field of hydrodynamics; (b) the failure of previously existing models (e.g. the U.S. EPA plume models (4) originally developed for municipal discharges in deep coastal waters) to adequately predict often routine discharge situations, especially for more shallow inland sites; (c) the issuance in 1985 by the U.S. EPA of additional guidelines (1) for the permitting of toxic aqueous discharges, placing yet another burden on both applicants and regulators in delineating special zones for the initial mixing of these substances; and (d) the availability of new computer methods, so-called expert systems, for making accessible to the user, within a simple personal computing environment, the expert's knowledge and experience in dealing with complex engineering problems.

Four separate publications describe the scientific basis for the CORMIX system and demonstrate comparison and validation with field and laboratory data. The results of these works are summarized in the peer-reviewed literature. The CORMIX systems approach and its performance relative to the earlier U.S. EPA plume models in the context of estuarine applications is also described in EPA's technical guidance manual for performing waste load allocations in estuaries (3).

EPA's established policy is to make the CORMIX system freely available to all potential users through its modeling software distribution facility at the U.S. EPA Center for Environmental Assessment Modeling (CEAM) in Athens, Georgia. Some of the CORMIX subsystems have been available to the industrial and regulatory user communities since December 1989 when distribution of CORMIX1 was commenced by Cornell University for the purpose of identifying subtle programming errors through application to actual mixing zone analysis problems by a controlled users group. After this testing was deemed complete, CEAM commenced the distribution of CORMIX1 in November 1990. A similar approach was used to introduce CORMIX2 which began CEAM distribution in October 1991. In 1992, CORMIX1, CORMIX2, and CORMIX3 were integrated a single program and distributed by USEPA-CEAM as CORMIX Version 2.1 as of 1993. More recently Windows based versions have been released by the Oregon Graduate Institute.

C.2 PLUMES for Windows (Visual Plumes)

PLUMES for Windows, is a Windows-based enhancement of the DOS-based PLUMES (Baumgartner, Frick, and Roberts, 1994, third edition) mixing zone modeling system, which it is intended to supersede. Based on continuity, it might be called the fourth edition, suggesting the acronym P4. For brevity and clarity, PLUMES for Windows will be called PLUMES4, or simply P4. Many of PLUMES capabilities have been modified and expanded in P4. It simulates similar types of plume behavior including single and merging submerged plumes in arbitrarily stratified ambient flow plus surface floating plumes. The outputs include but are not limited to, plume travel, dilution, rise, and diameter, both in the initial dilution and far-field regions. Some of the new features include: graphics, time-series input files, a sensitivity analysis capability, non-volatile unit conversion, a conservative tidal background-pollutant build-up capability, a multi-component pathogen decay model, and surface discharge. Some additional models are provided, including the DKHW (windows version of UDKHDEN 3-dimensional submerged diffuser model) and the PDS (Davis, 1999) surface discharge model. The Windows version of the UM model (WUM) is now a three-dimensional flow model, somewhat simplified in parallel currents. RSB has evolved into the NRFIELD and FRFIELD models. The Brooks equations are retained from PLUMES and may be used to simulate far-field behavior.

The most obvious difference between the two modeling systems is in appearance. The Windows interface offers many more user-friendly features. Numerous other changes are not as apparent. For example, the decay-rate time constants for the first-order decay algorithm for pathogens optionally can be based on a pathogen decay model developed by Mancini (1978). This model predicts coliform mortality based on temperature, salinity, and solar insolation, and is invoked by simply picking the solar insolation unit (langleys/hr) off the decay rate units list. As other examples, P4 offers a one-dimensional background pollutant build-up capability. Like PLUMES, P4 allows the user to run many cases, however, multiple cases are easier to set up and to compare. Determining model sensitivity to various input parameters is easily accomplished. The ability of P4 to run different models such as UM and UDKHDEN side by side and compare the results in graphical form, makes it a powerful platform for model comparison. It is intended that P4 will be expanded and additional models added as they are developed and become available.

Perhaps no other capability sets P4 apart from PLUMES more than its ability to link in time-series files. This capability provides a way to simulate outfall performance over a long period of time and, thereby, over many environmental scenarios. Most effluent and ambient variables, such as effluent discharge rate and current direction, can be read from files containing values that change with time over different time intervals. Thus, a 24-hour diurnal flow file, cycled repeatedly, might be combined with a current-meter data set thousands of records long. This is the heart of the pollutant-buildup capability, the ability in one-dimensional tidal rivers or estuaries to estimate background pollution from the source in question. The time-series file linking capability is served by "summary" graphics, i.e., graphics panels that focus on overall performance indicators, like mixing zone dilutions or concentrations. The use of time-series files does imply the preparation of the necessary data in ASCII form, as described herein.

The development philosophy of P4 is to help the user achieve long-term conceptual clarity and operational efficiency. Thus, after completing the tutorials and becoming familiar with the help system, the user will hopefully attain a degree of mastery of the subject, while enjoying the ability to experiment and perform mixing zone analyses with relatively little effort.

Another enhancement over earlier models is the ease in selecting units. On both diffuser and ambient tabs, the user can click on the line above the input headers to change units from a pop-up list of up to five choices. Unless otherwise specified, the data in the affected columns are automatically updated to reflect the change. In addition, some of the columns are multi-use columns. For example, the salinity column can be changed to a density column by simply selecting a density unit from the list of unit options. Additional features allow for note keeping, model configuration, and for a display of peripheral modeling parameters. The special settings tab provides a choice of output variables and access to other controls, parameters, and options. Finally, the database files are compatible with Paradox and other database applications, in which the archetypal files were set up. However, if they are manipulated outside of P4, you should be aware that each closed db file is headed by several rows of data that represent units and other information. If these are changed inadvertently there generally will not be loss of data, however, P4 may infer the wrong units and manual corrections or further manipulation in P4 may be necessary to recover from such corruption.

Resident Models

There are four updated models within the present P4 platform: WUM, DKHW (an updated windows version of UDKHDEN), PDSWin (a windows version of PDS), and NRFIELD/FRFIELD (replacing RSB, but not available in the beta version of P4). WUM is an acronym for the Windows version of Updated Merge, a Lagrangian model that features the projected-area-entrainment (PAE) hypothesis (Winiarski and Frick, 1976; Frick, 1984). This established hypothesis (Rawn, Bowerman, and Brooks, 1960) is a statement of forced entrainment, the rate at which mass is incorporated into the plume in the presence of a current. In this model, it is assumed that the plume is in steady state, implying in the Lagrangian formulation that successive elements follow the same trajectory (Baumgartner et al., 1994). The plume envelope remains invariant while elements moving through it change their shape and position with time. However, conditions can change as long as they do so over time scales which are long compared to the time in which a discharged element reaches the end of the initial dilution phase, usually at maximum rise. UM has been enhanced in P4. For example, the PAE forced entrainment hypothesis has been generalized to include the third-dimensional entrainment term. Thus, single-port plumes are simulated as truly three-dimensional entities. The sideways entrainment of merged plumes is distributed over all plumes. Dilution from diffusers oriented parallel to the current is estimated by limiting the effective spacing to correspond to a cross-diffuser flow angle of 20 degree. Also, the variable-time step algorithm has been improved. In addition to being controlled by the amount of entrainment, the time step is now also sensitive to the amount of trajectory curvature. In some cases, this sensitivity to curvature actually reduces the number of time steps needed to produce a simulation because the sensitivity to entrainment can be reduced.

DKHW is a fully 3-dimensional multiple port submerged diffuser model that allows arbitrary diffuser and discharge angles relative to the ambient current. It is an updated version of UDKHG (UDKHDEN) discussed in *Fundamentals of Environmental Discharge Modeling* (Davis, 1999). It uses the Eulerian integral method to solve the equations of motion for plume trajectory, size, concentration and temperature. In the Eulerian method, integration is with distance whereas in the Lagrangian formulation, integration is with time. It makes detailed calculations in both the zone of flow establishment and fully developed zone and considers gradual merging of neighboring plumes. Because of more detailed calculations, it runs more slowly than UM. Within P4, DKHW runs from a DOS SHELL so you will see a DOS window come up when it is run. Depending on your operating system, you may need to close the DOS window once DKHW is finished. Wait until the minimized DOS window displaying “DKHW” says finished, then close the window. DKHW is presently limited to positively buoyant plumes.

PDSWIN is a version of the PDS surface discharge program, which has been modified to be compatible with P4. It is discussed in detail in *Fundamentals of Environmental Discharge Modeling* (Davis, 1999). This 3-dimensional surface discharge program provides simulations for temperature and dilution over a wide range of discharge conditions. It was used to develop the nomograms in (Shirazi and Davis, 1972). PDS solves the equations of motion using Eulerian integral methods for the surface discharge of a buoyant fluid into a moving ambient body of water and includes the effects of surface heat transfer. The plume is assumed to remain at the surface with buoyancy causing it to rise and spread in all directions. The initial discharge momentum causes the plume to penetrate the ambient with the ambient current causing the plume to bend in the direction of flow. Discharge is assumed to be from a rectangular conduit into a large body of water. The program calculates plume trajectory, average and centerline dilution, plume width and depth and centerline excess temperature. It also calculates the areas within selected isotherms. These can be found by viewing the PDS.OUT file in the default directory using any convenient text editor after each run. The user must monitor boundaries. Calculations beyond the point where the plume hits a boundary are questionable. Plume attachment at the near shore can be simulated using the image method in which the discharge flow and width are doubled and only one half of the resulting plume is considered. In P4, PDSWIN runs from a DOS SHELL. As with DKHW, you may see a DOS window pop up that you will have to close when PDSWIN is finished. Also be aware that some of the variables on the diffuser tab, such as port depth, spacing, and contraction coefficient are ignored in PDSWIN runs.

NRFIELD (RSB), as its entry on the Model menu suggests, is the successor to the PLUMES RSB model. NRFIELD is an empirical model for multiport diffusers based on the experimental studies on multiport diffusers in stratified currents described in Roberts, Snyder, and Baumgartner (1989, a, b, c) and subsequent experimental works. P4 will run NRFIELD if at least four ports are indicated, as the model is based on experiments with T-risers each have two ports. An important assumption is that the diffuser may be represented by a line source. This assumption can have important consequences for small mixing zones, in which the plumes may not have merged.

The FRFIELD model estimates the long-term distribution of pollutants in the vicinity of the outfall. This two-dimensional “visitation-frequency” model is not operational, except in the context of the one-dimensional pollutant-buildup of background concentration capability for tidally-influenced rivers.

Compared to the PLUMES version, the Brooks far-field algorithm has been considerably improved. In addition to having better control over output variables, the algorithm, through the P4 time-series capability can now simulate time-dependent behavior. Thus, diel and other cycles can now be simulated. This is very important for estimating the effect of highly variable mechanisms such as bacterial decay, which depends greatly on the intensity of ultra-violet radiation.

All models have strengths and weaknesses, which is one reason that P4 is a platform for several overlapping models. Clearly, WUM is more rigorous with individual plumes than with parallel merged plumes. A user might choose to run DKHW or NRFIELD instead. In the future, JETLAG, CORJET, and other models may be available. Unfortunately, the multiplicity of models can lead to the inconsistent implementation of regulation. It is the desire of the authors to see that in future editions of P4 a built-in methodology is developed for selecting from the models in a consistent way, based on comparisons with established standard data sets and rules of engagement. Individual developers would then be able to continue to improve their models in the effort to broaden the usage of their models in subsequent revisions of the selection process. In any case, the common platform does help to identify the important areas of difference between the models.

Appendix D
Ocean Circulation Test Problems from ROMS Web Site

Rossby Equational Soliton

This test problem considers the propagation of a *Rossby soliton* on an equatorial beta-plane, for which an asymptotic solution exists to the inviscid, nonlinear shallow water equations. In principle, the soliton should propagate westwards at fixed phase speed, without change of shape. Since the uniform propagation and shape preservation of the soliton are achieved through a delicate balance between linear wave dynamics and nonlinearity, this is a good context in which to look for erroneous wave dispersion and/or numerical damping.

Coastally Trapped Waves in a Circular Basin

Lamb describes a class of waves on an *f*-plane in a circular basin with a flat bottom. These waves differ from Kelvin waves in that they are dispersive and have a non-zero off-shore velocity component. A test problem based on these waves has been developed by Curchitser. This test problem is meant to determine the effects of the numerical implementation of curved coastlines on the propagation of coastally trapped waves.

Gravitational Adjustment of a Density Front

The uniform advection of a passive scalar, initially distributed in some specified shape, is a traditional test of behavior for advection algorithms (see Rood, 1987). A related, but more demanding, problem involves the gravitational adjustment of a two-density-layer system, initially separated by a vertical wall (Wang, 1984). At time zero, the vertical wall dividing the two immiscible fluids is removed; thereafter, the fluid layers adjust at the internal gravity wave phase speed to form a stably stratified, two-layer system. During and after the adjustment, sharp density fronts divide the two layers both horizontally and vertically. Density fronts of this type are often observed in estuaries; Geyer and Farmer (1989) discuss this in the context of Fraser estuary.

This problem would presumably be best handled with an isopycnal model, which automatically respects the layered structure of the solution. The large majority of ocean circulation models, http://www.marine.rutgers.edu/po/tests/wbc/index.html however, use non-isopycnal coordinates, and therefore must carefully consider how to deal with sharp density fronts. As discussed in Haidvogel and Beckmann (1999), low-order schemes are typically either diffusive or dispersive in nature. In the former instance, positive-definiteness of tracer fields can be preserved, but often at the expense of excessive smoothing of sharp transitions. The first-order upwind scheme is the traditional example of this trade-off. Dispersive schemes (of which centered differencing is an example) are much less diffusive; however, they are not guaranteed to be either monotonic or positive definite. (That is, they can produce artificial tracer extrema and "wiggles".) In order to maintain smoothness, large values of explicit diffusivity are therefore often necessary.

Effects of Grid Orientation on Western Boundary Currents

This test problem investigates the accuracy of different numerical realizations of the linear homogeneous wind-driven flow in a square basin with sinusoidal wind forcing. The dependence of the solution on increasingly fine grid spacing is quantified for different horizontal grid arrangements ("B" and "C", as well as unstructured grids), for rotated grids relative to the model domain, and for both free-slip (no stress) and no-slip boundary conditions. Of particular interest are the consequences of grid orientations which lie at an angle to the western boundary (and hence necessitate a ``staircase" (representation of the boundary).

Convergence is tested for three different horizontal resolutions (50, 25 and 12.5 km; all on the order of the boundary layer width), for three different orientations of the numerical grid relative to the zonal direction (0º, 17º and 45º) and for two different lateral boundary conditions (free-slip and no-slip). (Note that the boundary condition enters the problem only via lateral viscous terms.) The rotated basin results illustrate the effect of step-like representation of a curved coastline in ocean models that use masking to represent irregular lateral boundaries.

Wind-driven Residual Currents over a Coastal Canyon: Constant Density Case

This is the first of two test problems exploring residual (time-mean) currents driven by oscillatory winds over a continental shelf/slope in the presence of an across-shelf canyon. These experiments have been run with a variety of models as described in Haidvogel and Beckmann (1999).

The tests have been configured to offer a wide range of challenges to the models. For example, the topography is both tall (20m to 4000m) and steep (maximum slope=30%). Also, except where specified, the continuum problems have been posed in the inviscid limit; models are to be run with as little viscosity/diffusivity as is practical. Processes which appear to be present in these test problems include form-stress-driven mean circulations, flow separation and recirculation, and undercurrents.