APPENDIX B – SPILL MODELING

Purpose

This technical appendix describes the methods used to simulate the fate and transport of oil in the Buzzards Bay system following the B120 oil spill on April 27, 2003. These methods rely on a hydrodynamic model known as the Generalized Environmental Modeling System for Surface waters (GEMSS). GEMSS is an integrated system of three-dimensional hydrodynamic and transport models married to familiar graphic display tools and GIS. For oil spill modeling, GEMMS is supplemented with COSIM (the Chemical / Oil Spill Impact Module). This module is specifically designed to simulate oil spills based on the unique physical and chemical properties governing oil fate and transport.

The text below describes the 5 discrete steps within the simulation process;

- Characterization of environmental conditions during and following the release;
- Chemical characterization of the oil;
- Release scenario construction;
- Grid construction and current estimation; and
- Fate and transport modeling.

Environmental characterization

COSIM requires data describing the winds, tides, temperatures, suspended solid concentrations, and shoreline substrates that characterized the system during and after the release.

Winds

The National Climatic Data Center (NCDC) and the National Data Buoy Center (NDBC), two agencies within the National Oceanic and Atmospheric Administration (NOAA), have several stations near Buzzards Bay which measure wind data. The closest NCDC wind stations and NDBC stations were examined to determine which locations would provide the most appropriate data (Figure B-1). Three stations, BUZM3, Falmouth Otis Air Force Base, and New Bedford Municipal Airport were selected.

BUZM3 is a NDBC station that continuously measures wind, meteorological, and wave data at a height of 24.8 m above mean sea level. The station is located in the open water at the mouth of Buzzards Bay.

Falmouth Otis Air Force Base, located in Falmouth, Massachusetts, continuously records standard meteorological measurements including wind at a height of 39.9 m above sea level.

New Bedford Municipal Airport (New Bedford) is a NCDC station located in New Bedford, Massachusetts. This station continuously monitors standard meteorological measurements including wind at a height of 24.4 m above sea level.

Figure B-1 Locations of wind data stations

Analyses were conducted to determine which wind file most accurately characterized the winds that prevailed during and after the spill. Wind files generated by each station as well as a several spatially averaged wind files were tested during this analysis. By comparing known slick locations and shoreline oiling, it was determined that the interpolated spatially averaged wind files were best suited for fate and transport modeling.

Prior to final utilization in COSIM these data were

- converted from Local Standard Time (LST) to Daylight Standard Time (DST),
- winds described as having a "variable" direction were given a speed of zero to reflect no-net wind influence,
- wind speeds and directions that were blank in the database were given the values of the previous time step, and
- the data, which were measured form anemometers at elevations ranging from 75 ft to 131 ft, were adjusted to reflected surface conditions using standard conversion methods.

<u>Tides</u>

Tidal propagation is estimated by model. The tidal model we employed was calibrated using a comprehensive set of tide and current harmonics (Signell 1987) and tidal measurements from the NOAA Woods Hole, MA and Montauk, NY stations (www.co-ops.nos.noaa.gov).

<u>Air Temperature / Water Temperature</u>

Based on measured values at Buoy BUZM3, average air temperatures and water temperatures were calculated for the three days following the spill.

Total Suspended Solids

TSS values for Buzzards Bay were unavailable. Therefore, 18 water samples were collected from six sites throughout Buzzards Bay in June 2004 (Figure B-2). Samples were collected at depths of 1, 6, and 12 feet at each of the six sites.

Shoreline substrates

Shoreline substrate data were derived from NOAA's Environmental Sensitivity Index (ESI) atlas (NOAA 1997). COSIM estimates oil adhesion to the shoreline based on 10 primary codes (Table B-1). Because shorelines with more than one classification are classified from the land seaward only the shoreline type closest to the water was utilized

Table B-1. ESI Codes

ESI Code	Substrate
1	Exposed Boulders and Man Made Structures
2	Wave Cut Platform
3	Fine to Medium Grained Sand
4	Course Grained Sand
5	Mixed Sand and Gravel
6	Gravel and Riprap
7	Exposed Tidal Flat
8	Sheltered Boulders, Riprap and man made structures
9	Sheltered Tidal Flats and Low Vegetated Banks
10	March and Swamp

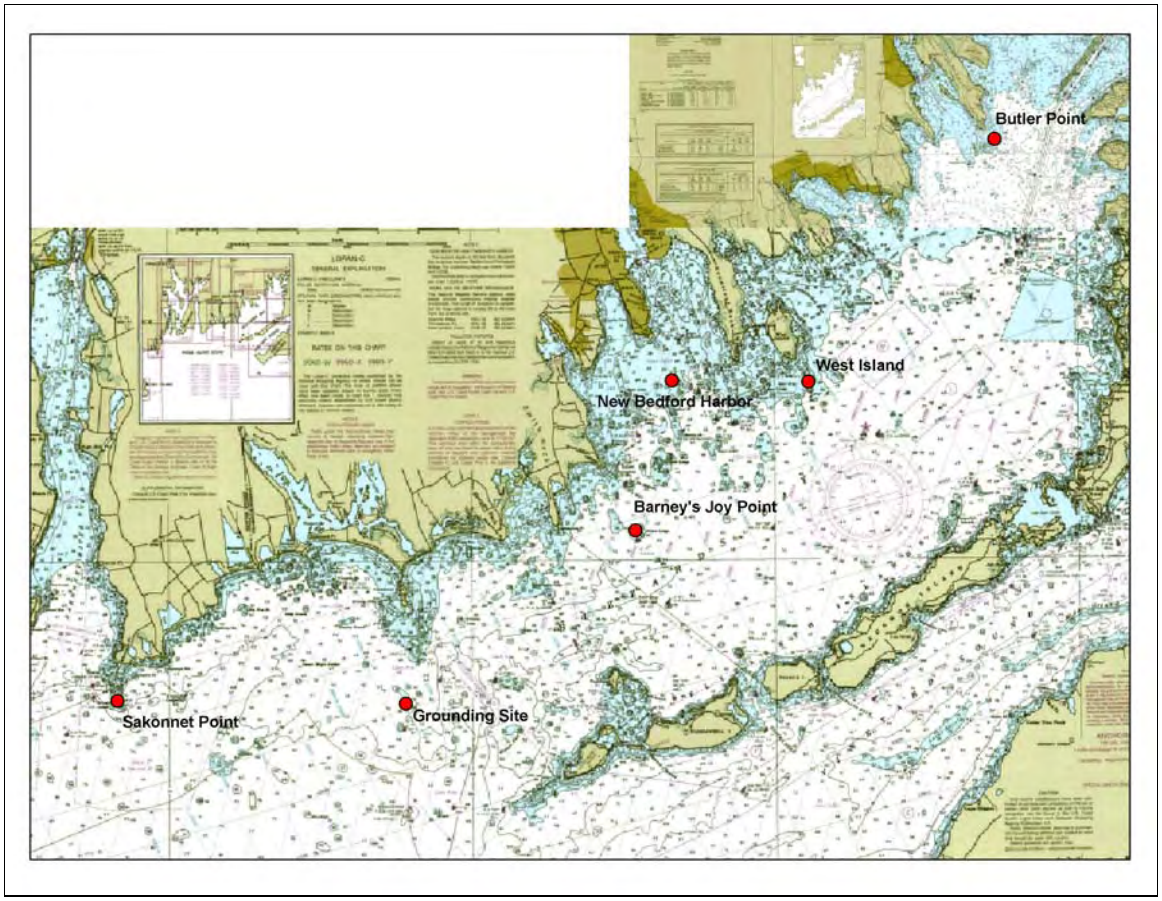

Figure B-2. June 2004 TSS Sampling Locations

Chemical characterization of the oil

A sample of the source/neat oil from the B-120 was collected on April 29, 2003 and analyzed for hydrocarbon concentrations. Detailed analysis was performed on aromatic and aliphatic content. Physical and chemical properties of the aromatic constituents including melting point, boiling point, molecular weight, vapor pressure, solubility, and density were determined.

Using B120 cargo measurements taken by ITS/Caleb Brett, Independent Maritime Consulting Ltd. determined that the B-120 cargo had an API gravity of 9.2. An API gravity of 9.2 corresponds to a density of 1.0057 kg/L at 60°F. Using the slope of the regression of Bunker C Fuel oil density varying with temperature (Section 2.2.1) the density of the B120 oil at 7.3 °C (the temperature of Buzzards Bay at the time of the spill) is 1011.8 kg/ m^3.

Release Scenario

A spill time line was constructed by reviewing ship's logs, USCG overflight data, Bouchard records, and first hand observations. D. Hall (Minton, Treharne, and Davies USA Inc.) used this timeline, meteorological data, and his knowledge of oil transport to construct a likely spill release scenario.

We have simulated the following scenario. The barge grounded in shallow waters near Buoys G1 and R2 (N41° 25.843' W71° 2.263') at about 15:30. Over the next hour, 60 percent of the oil leaked at a relatively constant rate as the barge moved from the impact site to an area where it was sheltered by the Elizabeth Islands (N41 27.83 W70 58.200). A further 30 percent of the total spill volume likely left the barge between 16:30 and 17:30 as the barge traveled to buoy “BB” (N41 31.37 W70 49.80). The final 10 percent of the total spill volume likely left between 17:30 and 20:11 as the barge made its way to Lima Anchorage (Figure B-3). There have been many estimates of the total volume of oil spilled. The model was run for 98,000 gallons and 50,000 gallons to reflect the range of possibilities under discussion.

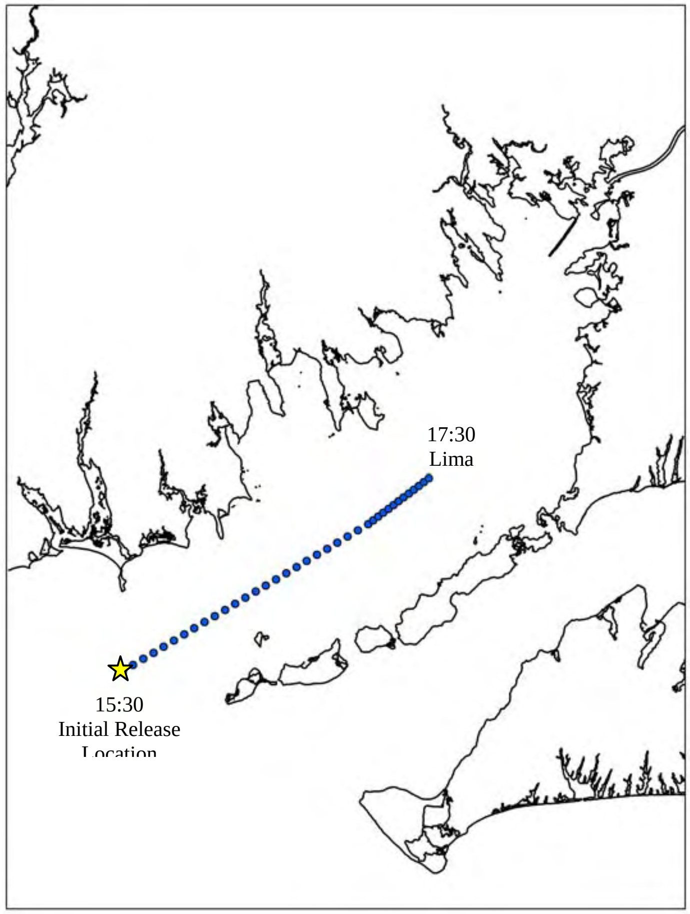

Figure B-3. Locations of modeled spill releases.

Grid Construction and Current Estimation
Applied Science Associates (ASA) provided an existing hydrodynamic grid (Figure B-4) and a data set describing current vectors for use in COSIM. The high-resolution grids and current vector data cover approximately 99 percent of the oil slick as the USCG delineated it on the evening of April 27, 2003.

According to ASA (2004):

> *The hydrodynamic model's governing equations and validation are described in detail in Spaulding (1984), Muin (1993), Muin and Spaulding (1997a, b), Spaulding et al. (1999a), and Sankaranarayanan and Spaulding (2003). The boundary-fitted grid is a mesh of quadrilateral cells of varying size and included angles, which is capable of handling variable geometry and flow regimes. The boundary fitted coordinate system uses general curvilinear coordinates to map the model grid to the shoreline of the water body being studied. It also allows enormous versatility in grid sizing so that many of the smaller features may be resolved, along with the larger, without being penalized by an excessive grid size (number of cells)."*

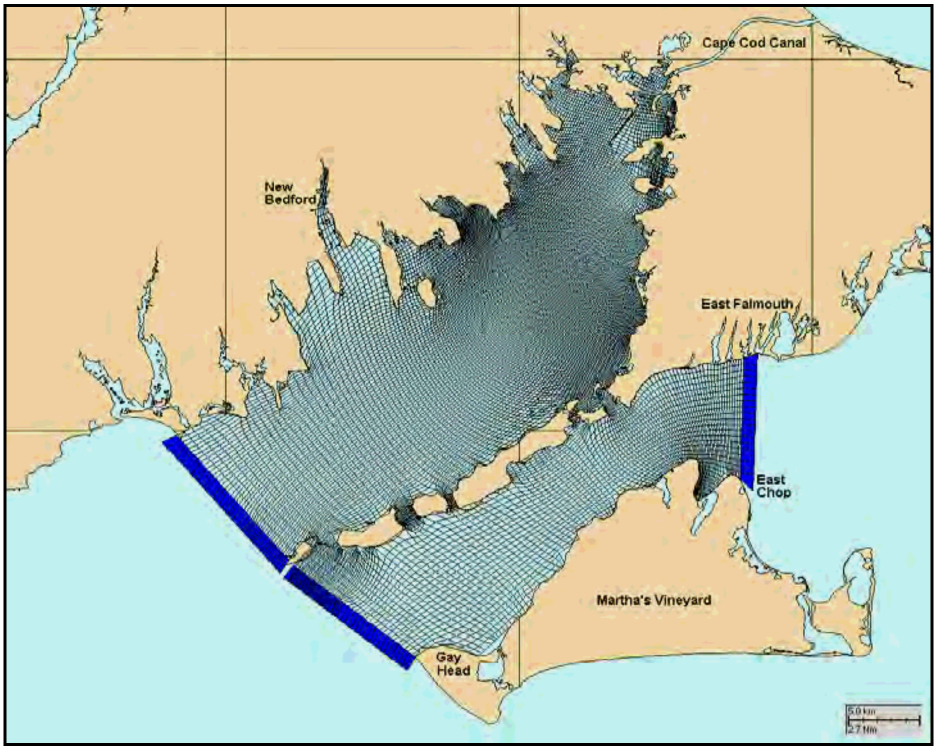

Figure B-4. Buzzards Bay oil spill model grid

COSIM Fate and Transport Modeling

When integrated with GEMSS' hydrodynamic module (GEMSS-HDM), COSIM calculates the mass balance of oil over time and space. The transport and fate of the modeled oil is completely described by the following processes:

- advection-motion caused by winds, currents and external forces;
- dispersion and spreading -motion along the surface or radiating into the water column caused by a lack of cohesion;
- sinking;
- evaporation- transfer of the surface slick from the liquid phase into the atmosphere;
- volatilization-transfer out of the water column into a gaseous state;
- photo-oxidation (mass broken down by sunlight);
- biodegradation-mass broken down by biological reactions;
- removal by on-water cleanup operations (skimmers, booms);
- removal of shoreline deposition;
- shoreline deposition;
- entrainment and resurfacing-transfer of the surface slick or dissolved mass into droplets within the water column;
- emulsification-similar to entrainment but oil droplets are larger;
- partitioning to suspended solids-mass adsorbed onto particulates; and
- dissolution-mass dissolved into the water column.

However, for this COSIM analysis, sinking was not a factor due to the density differences between the oil and the marine water. Also, removal of shoreline deposition and on-water cleanup operations were not included in the modeling.

Surface Particles

Surface particles are released traveling outwards from the spill location during the spill release time period. Since the oil was released from the B120 as a moving source, the particle release rate was timed to coincide with the estimated locations of the barge and the amount released during various stages of its travel. The movement of these particles on the surface of the water is based upon grid specific advection and dispersion. The mass associated with each particle can be lost due to sinking, lost to the atmosphere via evaporation, volatilization, or photo-oxidation, or lost to the system via biodegradation, removal during on water clean up operations, or shoreline adhesion.

Sinking is a function of the oil's density relative to the density of the water into which it was released. In this case, the density of the B120 oil at 7.3°C (the temperature of Buzzards Bay at the time of the spill) is 1011.8 kg/m^3. The density of seawater at this temperature is 1.027 kg/m^3. These physical parameters dictate that the bulk of the oil will remain on the surface of the water after initial release. Modeling approaches for the remaining physical processes are described in Table B-2.

Entrained and Emulsified Particles

Entrained oil mass particles are derived based on the chemistry and physical processes effecting the surface particles described in the previous paragraph. COSIM's entrainment algorithm is based on NOAA's Natural Resource Damage Assessment Model (French et al. 1996). However, spatial variability and sub-surface advection of entrained oil particles are accounted for by constantly obtaining spatial and temporally varying hydrodynamics currents from GEMSS-HDM.

Dissolved Particles

Dissolution is a function of the chemical and physical forces effecting both surface and entrained particles. One dissolved particle of variable mass is released per time step during all time steps in which dissolution is believed to occur. The model keeps track of both the total dissolved mass per particle as well as the mass of the each individual fraction comprising the dissolved oil. Neighboring particles may fuse into a single particle using particle regrouping algorithms. This manages the distribution of the oil mass while maintaining the total number of dissolved particles within a user-defined value. The movement of these particles, in three dimensions, is based upon both advection and dispersion. Advection is driven by the combined action of tides, winds and density forcing (Kolluru 2000), while diffusion is based on a 3-D random walk method (Bear and Verruijt 1987).

Estimating Oil Fates

COSIM integrates incident-specific oil chemistry to increase the reliability of modeled phase partitioning. COSIM utilizes an advanced mass balance to estimate the transfer of the oil mass between the various phases and media. For Buzzards Bay, COSIM divided the oil mass into 11 “cuts” of similar chemical structure ranging from monoaromatics to heavy insoluble residuals. This enables the model to simulate weathering processes as it tracks dissolved concentrations. Additionally, grouping chemical constituents of similar structure allows cut-specific particulate sorption. This allows the model to accurately reflect the tendency of organics to sorb to solids which varies over the spectrum of organics comprising the oil.

The region of concern is spatially divided into grid cells where dissolved aromatic and aliphatic compound concentrations within the water column are averaged. The oil spill model farfield grid size is selected based on hydrodynamic circulation. This approach avoids spurious dilution effects. Each farfield grid cell near the shoreline is subdivided into 20 sub-cells to accurately model the shoreline processes (e.g. deposition and removal).

Table B-2: COSIM processes and algorithms

Process	Algorithm and Description
Advection	Drift rate: Constant drift factor - Wind forcing is a constant fraction of wind speed. Varying with wind speed: drift factor decreases with increasing wind speed. (Youssef & Spaulding, 1993) Drift angle: Constant drift angle - Oil is moved at a constant angle to wind direction Function of wind speed: (Youssef & Spaulding, 1993; Samuels, 1982) Blowout: Lee and Cheung (1990) modified using blowout relations described in Fanneløp, and Karl Sjoen (1980) uses higher order advection scheme that includes both velocity magnitude and rate of change of velocity magnitude during integration.
Dispersion	Random walk dispersion: (Bear and Verruijt, 1987) Different methods used for estimation of horizontal and vertical dispersion coefficients.
Spreading	Mackay thick slick or thin slick: (Mackay et al., 1980; Kolluru and Mandelson, 1995)
Evaporation off surface slick and shoreline	Evaporative Exposure: Analytical approach developed by Stiver and Mackay (1984) and modified by Kolluru and Mandelson (1995) Distillation cuts: Pseudo-component approach using discrete fractions or cuts based on boiling points or carbon number (Payne et al., 1984). The COSIM model currently handles 24 cuts
Entrainment and resurfacing	Mackay’s breaking/non-breaking wave: Entrainment of oil due to breaking and non-breaking waves. Large droplets coalesce and return rapidly to water surface. Small droplets below a critical size remain in water column (Mackay et al. 1980) Breaking wave/droplets: Entrainment as a function of oil droplet size, breaking wave energy and oil properties (Delvigne and Sweeney, 1988)

Table B-2: COSIM processes and algorithms (continued)

Process	Algorithm and Description
Dissolution	User defined rate: Exponential decay process with user controlled rate Mass transfer approach: Using mass transfer coefficient and oil solubility for each oil fraction (Mackay and Leinonen, 1977)
Emulsification	Mackay's wind speed approach: Exponential rise based on laboratory data; varies with wind speed; works well for heavy crude oils (Mackay and Zagorski, 1982) Instantaneous rise; lag time: Recent field experiments show that there is a lag before a drastic increase in oil viscosity (Bobra, 1991)
Photo-Oxidation	First order decay: Photo-oxidation rates computed from absorption of light energy by the water column (WASP5, 1993; Chapra, 1997)
Biodegradation	First order decay: User specified bio degradation rate (WASP5, 1993)
Partitioning from water Column	Equilibrium partitioning kinetics: function of cut's mass weighted Log K_{OW} (Thomann and Mueller, 1987)
Sinking and sedimentation out of the water column	Sinking of oil using constant sedimentation rate: Rate of change of volume of oil lost to sedimentation is proportional to the sediment concentration and water salinity (Kolpack et al. 1977)
Cleanup operations	Case specific: Includes skimmers, dispersant applicators, booms, burning and offload platforms
Volatilization from the water column into gaseous state	Mass transfer rate: Using Ficks law of diffusion (Lymann et al. 1990; Ruiz and Terry, 2001)
Shoreline deposition and Removal	Simplification of COZOIL model: (Reed et al., 1989) Shoreline deposition occurs when an oil parcel intersects shore surface and ceases when the holding capacity for the shore surface is reached. Shoreline oil is removed exponentially with time. Removed oil is put back into the water column only when there is a rising tide (sufficiently high to wet the oiled surface) and offshore winds (Read and Gundlach, 1989; Read et al., 1989; Kolluru et al., 1994)

References

Bear, J., A. Verruijt. 1987. Modeling Ground Water Flow and Pollution with Computer Programs for Sample Cases. Kluwer Academic Publishers.

Bobra, M. A. 1991. Water-in-Oil Emulsification: A Physicochemical Study, Proceedings of the International Oil Spill Conference, American Petroleum Institute, Washington, D. C., pp. 483-488.

Chapra, S. C. 1997. Surface Water-Quality Modeling, McGraw-Hill Series in Water Resources and Environmental Engineering. McGraw-Hill.

Delvigne, G.A.L, C.E. Sweeney. 1988. Natural Dispersion of Oil, Oil and Chemical Pollution, Vol. 4. pp. 281-310.

Fanneløp, T. K., K. Sjoen, 1980. Hydrodynamics of Underwater Blowouts, Norwegian Maritime Research, No. 4, 1980.

French, D. P., M. Reed, K. Jayko, S. Feng, H. Rines, S. Pavignano, T. Isaji, D. Gifford, J. McCrue, and T. Opishinski. 1996. The CERCLA Type A Natural Resource Damage Assessment Model For Coastal and Marine Environments (NRDAM/CME). Technical Documentation Vol. I – V. Final Report submitted to the office of Environmental Policy and Compliance. U.S. Dept. of the Interior. Washington, DC. April, 1996. Contract No. 14-0001-91-C-11.

French-McCay, D., M. Ward, S. Sankaranarayanan, and P. Hall. 2004. Technical Approach and Interim Report: Hydrodynamic Modeling of Buzzards Bay and Rhode Island Sound for Oil Spill Modeling of the April 2003 Bouchard 120 Oil Spill.

Hall, P., S. Sankaranarayanan, C. Galagan and K. Knee. 2004. Buzzards Bay Disposal Site Analysis. ASA Report 03-089. Prepared for The Maguire Group for submission to Massachusetts Coastal Zone Management Agency. April 2004.

Kolluru, V. S., D. Mandelson. 1995. A Simplified Approach to Compute Constants Used in Mackay's Evaporation Model. Proceedings of the 18th Arctic and Marine Oil Spill Program (AMOP) Technical Seminar. Edmonton, Alberta.

Kolluru, V.S., M. L. Spaulding, E. Anderson. 1994. A Three Dimensional Subsurface Oil Dispersion Model using a Particle Based Approach. In Proceedings of the 17th Arctic and Marine Oil Spill Program (AMOP) Technical Seminar, Vancouver, British Columbia, Canada. pp. 867-894.

Kolpack, R. L., N.B. Plutchak, R.W. Stearns. 1977. Fate of Oil in a Water Environment - Phase II, a Dynamic Model of the Mass Balance for Released Oil. University of Southern California. Prepared for American Petroleum Institute, API Publication 4313, Washington, D.C.

Lee, H. W., V. Cheung. 1990. Generalized Lagrangian Model for Buoyant Jets in Current. Journal of Environmental Engineering 116(6):1085-1106.

Lymann J. W., W. F. Reehl, D. H. Rosenblatt. 1990. Handbook of Chemical Property Estimation Methods (Environmental Behavior of Organic Compounds), Chapter 15: Volatilzation from water written by Richard G. Thom.

Mackay, D., P. J. Leinonen. 1977. Mathematical Model of the Behavior of Oil Spills On Water with Natural and Chemical Dispersion. Prepared for Fisheries and Environment Canada, Economic and Technical Review Report EPS-3-EC-77-19.

Mackay, D., W. Zagorski. 1982. Water-in-Oil Emulsions, Environment Canada. Manuscript Report EE-34, Ottawa, Canada.

Mackay, D., S. Paterson, K. Trudel. 1980. A Mathematical Model of Oil Spill Behavior, Department of Chemical and Applied Chemistry, University of Toronto, Canada.

Muin, M. 1993. A Three-Dimensional Boundary Fitted Circulation Model in Spherical Coordinates. Ph. D. Dissertation, Department of Ocean Engineering, University of Rhode Island, Kingston, RI.

Muin, M., M. L. Spaulding. 1997a. Three-dimensional boundary fitted circulation model. J. Hydraulic Eng. 123(1):2-12.

Muin, M., M. L. Spaulding. 1997b. Application of three dimensional boundary fitted circulation model to Providence River. J. Hydraulic Eng. 123(1):13-20.

Payne, J. R., B.E. Kirstein, G.D. McNabb, J. L. Lambach, R. Redding, R.E. Jordon, W. Horn, C. Oliveira, G. S. Smith, D. M. Baxter and R. Geagel. 1984. Multivariate Analysis of Petroleum Weathering in the Marine Envrionment—SubArctic. Vol. I and II. In: Environmental Assessment of the Alaskan. Continental Shelf. Final Report to Principal Investigators. U. S. Dept. of Commerce, NOAA/OCSEAP. Final Report 21 and 22.

Read, M., E. Gundlach, T. Kana. 1989. A coastal zone oil spill model: development and sensitivity studies. Oil and Chemical Pollution 5:419-449.

Read, M., E. Gundlach. 1989. Hindcast of the Amoco Cadiz event with a coastal zone oil spill model. Oil and Chemical Pollution 5:451-576.

Ruiz, C. E., T. Gerald. 2001. RECOVERY version 2.0, a mathematical model to predict the temporal response of surface water to contaminated sediments. ERDC/EL TR-01-3. U. S. Army Engineer Research and Development Center, Vicksburg, MS.

Samuels, W. B., N. E. Huang, D. E. Amstutz. 1982. An Oil Spill Trajectory Analysis Model with a Variable Wind Deflection Angle. Ocean Engineering 9:347-360.

Sankaranarayanan, S., M. L. Spaulding. 2003. A study of the effects of grid non-orthogonality on the solution of shallow water equations in boundary-fitted coordinate systems. Journal of Computational Physics 184(1):299-320.

Signell, R. P. 1987. Tide- and Wind-Forced currents in Buzzards Bay, Massachusetts, WHOI Tech. Rpt., WH-87-15, Woods Hole Oceanographic Institution, Woods Hole, MA.

Spaulding, M. L. 1984. A vertically averaged circulation model using boundary-fitted coordinates. J. Phys. Oceanography 14:973.

Spaulding, M., D. Mendelsohn, J.C. Swanson. 1999. WQMAP: An integrated three-dimensional hydrodynamic and water quality model system for estuarine and coastal applications. Mar. Tech. Soc. J. 33(3):38-54.

Thomann, R. V., J. A. Mueller. 1987. Principles of Surface Water Quality Modeling and Control. Harper & Row, NY.

WASP5. 1993. The Water Quality Analysis Simulation Program, WASP5: Part A: Model Documentation; Part B: The WASP5 Model Input Dataset. EPA, Athens, GA.

Youssef, M., M. L. Spaulding. 1993. Drift Current Under the Action of Wind and Waves. Proceedings of the 16th Arctic and Marine Oil Spill Program Technical Seminar, Calgary, Alberta, Canada, pp. 587-615.