Modelling of dispersant application to oil spills in shallow coastal waters

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Abstract

Application of dispersants in shallow water remains an issue of debate within the spill response community. An experimental oil spill to evaluate potential environmental impacts and benefits of applying dispersants to spills in shallow water has therefore been under consideration. One site being considered was Matagorda Bay, on the Texas coast. Coupled three-dimensional oil spill and hydrodynamic models were used to assist in the design of such an experiment. The purpose of the modeling work was to map hydrocarbon concentration contours in the water column and on the seafloor as a function of time following dispersant application. These results could assist in determining the potential environmental impact of the experiment, as well as guiding the water column sampling activities during the experiment itself.

Eight potential experimental oil spill scenarios, each of 10 bbl in volume, were evaluated: 4 release points, each under two alternate wind conditions. All scenarios included application of chemical dispersants to the slick shortly after release. Slick lifetimes were under 5 h. Due to the shallow depths, some fraction (2–7%) of the released hydrocarbons became associated with bottom sediments. The algorithms used for the oil droplet—sediment interactions are theoretical, and have not been verified or tested against experimental data, so the mass balances computed here must be considered tentative.

Currents computed by the hydrodynamic model are consistent with previous observations: the circulation is largely tidally driven, especially near the ship channel entrance. In the center of the bay, the circulation appears relatively weak. The use of water column drifters with surface markers during the experiment would augment model results in assisting activities to monitor concentrations. These simulations suggest that the eventual behavior of an oil droplet cloud in the middle of the bay will be relatively insensitive to release point or time in the tidal cycle.

A limited analysis was run to evaluate model sensitivity to the oil-sediment sorption coefficient. Increasing this coefficient by a factor of 10 results in an approximately linear increase in the fraction of oil in the sediments. Sensitivity of estimated time-to-zero-volume for the 0.1-ppm concentration contour demonstrated that the model prediction of 3.5 days was associated with an uncertainty of ±12 h for a release of 10 barrels. This time estimate is also a function of the oil-sediment interaction rate, since more oil in the sediments means less oil in the water column.

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1. Introduction

This paper describes a numerical modeling effort to understand the probable distribution of hydrocarbons in a shallow coastal bay following a hypothetical release of oil to which chemical dispersant is applied. Four potential release sites were evaluated in Matagorda Bay, Texas (Fig. 1). Two basic scenarios were simulated for each site, with winds from the northeast and the southeast, the dominant wind directions for the proposed autumn date. The releases assumed an Arabian medium crude oil from which approximately 15% is “topped”,

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or pre-evaporated. The composition of this topped crude is shown in Table 1.

All scenarios are of magnitude 10 barrels (1.41 metric tons) released over 5 min, at a thickness of approximately 1 mm. Dispersant application begins almost immediately after release of the oil, and any oil which is under-dosed during the initial application is sprayed with additional dispersant shortly thereafter (i.e. the treatment is 100% efficient; dispersant quantity is not a limiting factor).

### Table 1

<table>
<thead>
<tr>
<th>Oil Component</th>
<th>Conc. (%)</th>
</tr>
</thead>
<tbody>
<tr>
<td>C9-saturates (n-/iso-/cyclo)</td>
<td>3.36</td>
</tr>
<tr>
<td>C3-Benzene</td>
<td>1.89</td>
</tr>
<tr>
<td>C10-saturates (n-/iso-/cyclo)</td>
<td>4.94</td>
</tr>
<tr>
<td>C4 and C4 Benzenes</td>
<td>0.17</td>
</tr>
<tr>
<td>C11-C12 (total sat + aro)</td>
<td>8.12</td>
</tr>
<tr>
<td>Phenols (C0-C4 alkylated)</td>
<td>0.01</td>
</tr>
<tr>
<td>Naphthalenes 1 (C0-C1-alkylated)</td>
<td>0.44</td>
</tr>
<tr>
<td>C13-C14 (total sat + aro)</td>
<td>7.79</td>
</tr>
<tr>
<td>Naphthalenes 2 (C2-C3-alkylated)</td>
<td>0.53</td>
</tr>
<tr>
<td>C15-C16 (total sat + aro)</td>
<td>4.12</td>
</tr>
<tr>
<td>PAH 1 (Medium soluble polyaromatic hydrocarbons (3 rings-non-alkylated; &lt;4 rings)</td>
<td>0.18</td>
</tr>
<tr>
<td>C17-C18 (total sat + aro)</td>
<td>4.06</td>
</tr>
<tr>
<td>C19-C20 (total sat + aro)</td>
<td>3.12</td>
</tr>
<tr>
<td>Unresolved Chromatographic Materials (UCM: C10 to C36)</td>
<td>0.09</td>
</tr>
<tr>
<td>C21-C25 (total sat + aro)</td>
<td>7.71</td>
</tr>
<tr>
<td>PAH 2 (Low soluble polyaromatic hydrocarbons (3 rings-alkylated; 4-5+ rings)</td>
<td>0.33</td>
</tr>
<tr>
<td>C25+ (total)</td>
<td>53.14</td>
</tr>
<tr>
<td>Total</td>
<td>100.00</td>
</tr>
</tbody>
</table>

### 2. Environmental data

Depths used in the simulations (Fig. 2) are taken from a chart of the bay. Historical winds were used to identify dominant wind directions for the proposed release month of October. Results indicated that wind directions are primarily from the southeast and northeast. Average wind speed is about 7 m/s for the three October months sampled. It was therefore decided to use constant winds...
at 7 m/s from the southeast and the northeast to simulate the evolution of individual releases from each site.

Current measurements reported by the Conrad Blucher Institute, Texas A&M University at specific locations in the bay were obtained from two Internet web sites: http://hyper20.twdb.state.t.us/data/bays—estuaries/studies/mat88sites, and http://hyper20.twdb.state.t.us/data/bays—estuaries/studies/mat93sites. These data show that the tidal signal is diurnal, with a maximum flow of about 1 m/s into Matagorda Bay through the shipping channel. A spatial time series recorded with radar was downloaded from: http://dnr.cbi.tamucc.edu/~hfradar/HFRMata.html. These data suggest a strong tidal signal, with little apparent wind effect at low wind speeds.

3. Hydrodynamic model

Based on this and other available information, a three-dimensional finite element, hydrostatic pressure model with a one-equation (k-equation) turbulence closure scheme (Utnes and Brørs, 1993) was applied to compute time-variable current fields to support the oil spill simulations.

A grid mesh with 5224 horizontal nodes was generated. The lateral boundary was fitted to the 0.5 m depth contour of the bathymetry data shown in Fig. 2. Depths were interpolated to the nodes of the grid mesh. The model was run with a resolution of 14 layers (15 nodes) in the vertical. The thickness of the layers was reduced towards the surface and bottom to 2% of the local depth, which averaged about 5 m. A horizontal eddy viscosity of 2 m²/s and a bottom roughness of 0.002 m were used. Surface winds of 7 m/s SE and NE were applied at the air-water interface. The tide was simulated by prescribing a sinusoidal variation in water elevation at the open boundaries to the south of Matagorda Bay, with amplitude $a = 0.6$ m and period of $T = 24$ h. For each wind direction, current fields for two complete tidal cycles were archived, following a 120 h “spin-up” time.

Snapshots of the mid-depth velocity field as used by the oil spill model OSCAR2000 are shown at maximum flood and ebb velocities in Figs. 3a and b, respectively. The latter show that the velocities in the proposed study area are relatively low, such that hydrocarbon in the water column will tend to be retained locally. High velocities are generally limited to the ship channel entrance.

4. Oil spill model

The oil spill contingency and response model OSCAR2000 was used to simulate the behavior and fate of alternative experimental oil releases in Matagorda Bay. OSCAR is a 3-dimensional model system that represents oil as a complex mixture of multiple components or pseudo-components (e.g. Table 1).

OSCAR2000 is specifically designed to support oil spill contingency and response decision-making. Environmental consequences are important components
of such decisions. The model therefore addresses potential effects in the water column with verisimilitude at least equal to that achieved on the water surface and along shorelines. The model quantifies the evolution of oil on the water surface, along shorelines, and dispersed and dissolved oil concentrations in the water column, allowing relatively realistic analyses of dissolution, transformations through degradation, and toxicology. Key components of the system are databased oil weathering model, a three-dimensional oil trajectory and chemical fates model, and an oil spill combat model. The system also includes tools for exposure assessment within GIS polygons (delineating, for example, sensitive environmental resource areas).

Both surface and sub-surface calculations by OSCAR have been verified in considerable detail (Reed et al., 1996, 2000). OSCAR2000 differs from its predecessors (Reed et al., 1995a,b,c, 1998, 1999a,b; Aamo et al., 1997) in that the user can specify a relatively large number (30 in the present version) of individual components, pseudo-components, or metabolites to represent the oil and its degradation products. Each component is associated with an array of parameters that govern process rates: solubility, vapor pressure, transformation (first-step degradation) rates, density, adsorption-desorption partition coefficient, and toxicological parameters.

5. Spreading rates for spilled oil

Spreading rates for all spills simulated with dispersant application were similar, with variations resulting from variations in alignment of winds and currents. Fig. 4a is
typical, showing the change in oiled surface area with time for the release from site 3, winds from the southeast. Fig. 4b, from site 3 with the wind from the northeast, is the most atypical. Releases from site 3 reflect the most variability because site 3 experiences the highest tidal velocities, and therefore the most near-surface velocity shear. In all cases most of the oil disappears from the water surface within 4–5 h, with over 90% of the slick dispersed in less than 2 h.

6. Mass balances

Mass balances for all scenarios are relatively similar. That the droplet plume remains out in the middle of the bay results in little sedimentation. Less than 8% of the total mass appears in the sediments after 24 h in these simulations. Fig. 5 shows a typical evolution of the mass balance, using default sediment sorption coefficients. After 96 h, the total sedimented mass is nearer 20% of that released (Fig. 6).

7. Sediment concentration fields after 24 h

Sediment concentration distributions are presented (Figs. 7 and 8) here as representative summaries of the trajectories of dispersed oil in the water column. The shallow waters result in a clearly definable signal in the sediments, from the modeling point of view. In practice, these low sediment concentrations will likely be lost in the background typical of previously polluted shallow areas. It is interesting to note that the net subsurface flow is almost directly against the wind, due to the enclosed nature of the basin.
8. Total hydrocarbon concentrations: volumetric time series

Figs. 9 and 10 give time series for volumes of water exceeding total hydrocarbon concentrations (THC) of 10, 50, 100, 1000, and 10,000 ppb (or 0.01, 0.05, 0.1, 1, and 10 ppm).

The volume-exceedence graph for site 1, NE winds (Fig. 9) are typical for these simulations. When the simulations are continued for 96 h (Fig. 10), it is seen that the 0.01 ppm contour continues to increase for about 2.5 days, whereas the higher concentrations start to decline earlier.

The high initial concentrations seen in these scenarios are due to the thick oil conditions when the dispersant was applied. This is somewhat of an artifact of the experimental release scenario being modeled, as the dispersant application is assumed to occur prior to release, while the oil is still retained in a boom on the sea surface.

9. Total hydrocarbon concentrations: spatial time series

Fig. 11a–d depict the evolution of the total hydrocarbon concentration field (water accommodated fraction plus droplets) for Site 1, wind from the Northeast.

Vertical section A–B is shown in the inset of Fig. 11a,b. The release site is depicted by a white square containing an x. The wind drives the surface oil towards the Southwest. The oil is treated with dispersant almost immediately upon release, and dispersion into the water column begins. Subsurface currents drive the water column concentrations toward the northwest. The “oldest” portion of the concentration field, at end A of the vertical section, displays the deepest penetration and the broadest horizontal spread, due to a longer mixing time. The most recently dispersed hydrocarbons, at end B of the section, lie directly under the remaining surface oil, and are limited to the top 1–2 m of the water column. The source
for this “plume” is the surface oil, moving at about 25 cm/s towards the southwest.

10. Sensitivity analyses

Due to the shallow depths, a fraction (<10%) of the released hydrocarbons becomes associated with bottom sediments after 24 h. The algorithms used for the oil droplet–sediment interactions are theoretical parameterizations, and have not been verified or tested against experimental data, so the mass balances computed must be considered tentative. The algorithms assume that oil–sediment interactions will occur primarily in the nepheloid layer near the seafloor, as turbulent mixing carries droplets into that region. For oil droplets that mix into this layer, a whole-oil adhesion coefficient is used to estimate the fraction of the oil that remains in the sediments.

The benthic nepheloid layer is assumed here to include the bottom 0.5 m of the water column under low wind conditions, and to have suspended particulate concentrations a factor of 10 higher than the upper water column (e.g. Kullenberg, 1982). The cohesion of oil droplets to suspended particulate matter is modeled as:

$$F_c = K_c C_{ss} F_{oil}$$

where $F_c$ is the fraction of oil droplets cohered to suspended particulate matter and retained in the nepheloid layer; $K_c$ is the cohesion partition coefficient; $C_{ss}$ is the concentration of suspended particulate matter; and $F_{oil}$ is the fraction of oil droplets which remains free in the water column.

Assuming values of $C_{ss}$ at 100 mg/l in the benthic
nepheloid layer, and $K_c$ at 2000 results in a retention of about 17% during each droplet excursion into this bottom layer. Data reported by Page et al. (2000) and results from several laboratory and field studies (Lessard and DeMarco (2000) indicate that chemically dispersed oil has much less affinity for adhesion to sediments than untreated oil. Oil droplets produced when dispersants are used have a hydrophilic surfactant “coating” that reduces their tendency to adhere to suspended sediment. Sedimentation of chemically dispersed oil may therefore be less likely than mechanically dispersed oil. However, it is not known how long this condition persists, since the surfactant layer is also highly water-soluble. The simulations reported above are based on the assumption that chemically dispersed oil has a reduced sorption coefficient of 200, or one tenth of that for non-chemically treated oil.

The oil–sediment interaction algorithm applied here is incomplete in that it does not account for droplet–particle interactions in the water column outside the benthic boundary layer. Such interactions will be more important in higher wind wave conditions, which will result in layer suspended sediment loads higher in the water column.

To address the uncertainty associated with the sedimentation of oil in the model, extra scenarios were run, with wind from the southeast. In these scenarios, the sorption coefficient for chemically dispersed oil was increased by a factor of 10 to produce a sort of “worst case” simulation set for sediment accumulation. Sediment concentration fields and associated mass balances after 24 h are reported for releases from Site 1 and 4 in Figs. 12 and Fig. 13. In these simulations the total mass of oil in the sediments increases by 5–10 times, to 30–40% of the total after 24 h. Associated maximum concentrations are in the range 10–20 ppm.

Finally, it should be noted that OSCAR2000 is a particle-based model, in which random walk procedures play a role in developing the concentration fields. Two simulations of a single scenario (release from site 4, 10 barrels, southeast wind) were run to demonstrate potential variability between different realizations of the same event or scenario. Fig. 14 displays the variation in volume exceeding given concentration thresholds. Although the variation between subsequent realizations of the scenario is small, the time-to-zero-volume may be quite different from one run to the next, since the curves become nearly horizontal at the right-hand tail of the time series. Thus the 0.1-ppm threshold varies only by about 0.0005 km$^3$ after 3 days (Fig. 14), but the time-to-zero-volume varies from a little over 3 to almost 4 days between the two scenarios.

Fig. 15 demonstrates that the model estimate for time versus maximum THC value is relatively robust from one realization to the next, even for quite small releases.

11. Conclusions

Eight potential experimental oil spill scenarios, each of 10 bbl in volume, were evaluated: 4 release points, each under two alternate wind conditions. All scenarios included application of chemical dispersants to the slick shortly after release. Slick lifetimes were under 5 h. Due to the shallow depths, some fraction (2–7%) of the released hydrocarbons became associated with bottom sediments. The algorithms used for the oil droplet–sediment interactions are theoretical, and have not been verified or tested against experimental data, so the mass balances computed here must be considered tentative.

Currents computed by the hydrodynamic model are consistent with previous observations: the circulation is
Fig. 14. Comparison of volumes exceeding different concentration thresholds as a function of time (10 barrel release from site 4, southeast wind). The estimated time-to-zero-volume for low concentrations is sensitive to small variations in the concentration field. Thus the model is only able to estimate the time-to-zero-volume for the 0.1-ppm contour as between 3 and 4 days.

Fig. 15. Variability of the maximum THC value among 4 different realizations of a 1-barrel release.

largely tidally driven, especially near the ship channel entrance. In the center of the bay, the circulation appears relatively weak. The use of water column drifters with surface markers during the experiment would augment model results in assisting activities to monitor concentrations. These simulations suggest that the eventual behavior of an oil droplet cloud in the middle of the bay will be relatively insensitive to release point or time in the tidal cycle.

A limited analysis was run to evaluate model sensitivity to the oil–sediment sorption coefficient. Increasing this coefficient by a factor of 10 results in an approximately linear increase in the fraction of oil in the sediments. Sensitivity of estimated time-to-zero-volume for the 0.1-ppm concentration contour demonstrated that the model prediction of 3.5 days was associated with an uncertainty of ±12 h for a release of 10 barrels. This time estimate is also a function of the oil–sediment interaction rate, since more oil in the sediments means less oil in the water column.

The model computations appear numerically well behaved and robust, but the oil–sediment interaction algorithms require good observational data for calibration and verification. The model offers great value in evaluating the environmental tradeoffs of dispersant use in shallow waters. It allows analyses of multiple scenarios (e.g. release points, wind directions, oil volumes) once the basic system hydrodynamics and bathemetry have been established. This provides spill response planners with insight on a variety of considerations that address sensitive resources found in water column, sediment and shoreline habitats.
References


