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Improving environmental assessments by integrating Species Sensitivity Distributions into environmental modeling: Examples with two hypothetical oil spills

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ABSTRACT

A three dimensional (3D) trajectory model was used to simulate oil mass balance and environmental concentrations of two 795,000 L hypothetical oil spills modeled under physical and chemical dispersion scenarios. Species Sensitivity Distributions (SSD) for Total Hydrocarbon Concentrations (THCs) were developed, and Hazard Concentrations (HC) used as levels of concern. Potential consequences to entrained water column organisms were characterized by comparing model outputs with SSDs, and obtaining the proportion of species affected (PSA) and areas with oil concentrations exceeding HC5s (Area_ \geq_{HC5}). Under the physically-dispersed oil scenario \leq 77% of the oil remains on the water surface and strands on shorelines, while with the chemically-dispersed oil scenario \leq 67% of the oil is entrained in the water column. For every 10% increase in chemical dispersion effectiveness, the average PSA and Area_ \geq_{HC5} increases (range: 0.01–0.06 and 0.50–2.9 km², respectively), while shoreline oiling decreases (\leq 2919 L/km). Integrating SSDs into modeling may improve understanding of scales of potential impacts to water column organisms, while providing net environmental benefit comparison of oil spill response options.

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1. Introduction

Modeling is an essential component of environmental assessments, as it can help guide and scale the mobilization of resources, prioritize protection or mitigation strategies, and inform management decisions (e.g., Castanedo et al., 2006). Oil spill trajectory and effects models, for example, can be used to quantitatively predict the behavior and movement of oil in the environment by using algorithms describing fate processes, while providing information on the relative spatial and temporal extent of potential ecological consequences. These models have proven useful in pre-planning emergency response (MacFadyen et al., 2011; Mearns et al., 2001, 2003), as well as in natural resource damage assessment (French-McCay, 2003; French McCay et al., 2004). Within the context of oil spills, modeling can facilitate analyses of impact to biological resources by considering a set of oil recovery actions and response strategies (e.g., Reed et al., 1999), including the use of chemical dispersants.

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With the exception of the Deepwater Horizon oil spill, where an unprecedented volume of dispersants was used, dispersants have rarely been used in response to oil spills. In the US and prior to the Deepwater Horizon oil spill, chemical dispersants were used in the Gulf of Mexico in eight occasions between 1990 and 2005 (Gugg et al., 1999; Henry, 2005; Stoermer et al., 2001) and in two occasions in 2009 (NOAA, 2014). Dispersants were also used during the 1984 Puerto Rican vessel incident off San Francisco Bay (Zawadzki et al., 1987). The use of dispersants has also been approved but never used during other oil spills in the US (17 total; e.g., 2004 MV Selendang Ayu and 2006 MV Cougar Ace oil spills, Alaska), and were minimally used during the 1989 Exxon Valdez oil spill due to limited availability of dispersant products and adequate application equipment, among other reasons (NOAA, 2014). Notable examples of dispersant use outside the US include the 1996 Sea Empress oil spill in Wales (Lunel et al., 1997), the 1996 Braer tanker spill in Scotland (Lunel, 1995), the 2006 Solar 1 tanker oil spill in the Phillipines (Yender and Stanzel, 2010), the 2007 container ship MSC Napoli incident in the UK (Law, 2008), and the 2009 Montara wellhead platform incident in Western Australia (Tan, 2011).





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One important premise on the use of chemical dispersants is that by reducing the surface tension of oil, dispersants reduce the amount of floating oil on the water surface reducing exposure risks to wildlife and sensitive shoreline habitats, and increasing microbial degradation (NRC, 1989, 2005). However, chemical dispersion of oil at the water surface enhances the rate of partitioning of oil into the top few meters of the water column, particularly of the lighter oil fractions (e.g., benzene, toluene, ethylbenzene, xylenes, etc.), resulting in higher oil concentrations compared to oil physically dispersed by currents, wind and waves (NRC, 1989, 2005). As a result, organisms entrained in water masses containing chemically dispersed oil are exposed to potentially toxic oil concentrations, though exposures may generally be of short duration because of the rapid dilution and water column mixing occurring in open waters. In addition, the use of dispersants increase the concentration of small oil droplets (generally <70 um in diameters), which are not only readily biodegradable but also remain entrained in the water column because of their slow rising velocities (Cormack and Nichols, 1977; NRC, 2005). Yet, the relative contribution of oil droplets to the overall toxicity to entrained water column organisms is largely unknown partially because little empirical information exists on the link between oil droplet size and concentration, and toxicological effects (reviewed in Bejarano et al., 2014b).

Characterizing in situ impacts to entrained water column organisms is challenging, resulting in reliance of laboratory toxicity tests with a small number of species to infer potential impacts to a broader number of species. Comparisons of relative sensitivities across species and derivation of levels of concern can be achieved via cumulative distributions of existing physically or chemically dispersed oil toxicity data (e.g., median lethal, LC50 and effects concentrations, EC50), commonly known as Species Sensitivity Distributions (SSDs) (Posthuma et al., 2002). This type of approach has been used in oil spill research and assessments (Barron et al., 2013; Bejarano et al., 2013; de Hoop et al., 2011), but have not previously been incorporated into oil trajectory models. Consequently, the primary objective of this study is to demonstrate how SSDs can be used to improve model-based assessments of oil spill impacts under different chemical dispersant use scenarios. For the purpose of these analyses, hypothetical spill scenarios were developed for two areas: off San Francisco Bay, and off Charleston Harbor, South Carolina, and modeled oil concentrations in the water column compared to SSDs.

2. Methods

2.1. Oil mass balance and environmental concentrations

One of the tools used to model the fate, surface and subsurface transport, and three dimensional trajectories of spilled oil is the General NOAA Oil Modeling Environment (GNOME) (NOAA/ERD, 2013). While a number of related models are also available (e.g., SIMAP, French-McCay, 2004), the selection of GNOME was driven by its availability in the public domain. GNOME predicts the

trajectory and spreading of oil, and generates trajectory outputs based on site-specific parameters, wind-driven currents and horizontal and vertical mixing (i.e., wind, local hydrodynamics, water column turbulence), while accounting for best guess (trajectories created assuming that all model inputs are correct) and minimum regret (trajectories created accounting for possible forecast errors in model inputs) forecast solutions (Beegle-Krause, 2001; Simecek-Beatty et al., 2002). Because GNOME incorporates oilspecific fate and behavior information (e.g., evaporation, dispersion, sedimentation) from an oil weathering model (Automated Data Inquiry for Oil Spills, ADIOS2) (Lehr et al., 2002), oil trajectories can be used to quantitatively describe the distribution of oil across several components (i.e., air, surface water and water column, shorelines), including estimates of average oil concentrations (Total Hydrocarbon Concentration, THC; hereafter) in the water column. Consequently, GNOME models environmental concentrations of physically or chemically dispersed oil in the water column, allowing for quantitative estimates of the potential footprint of oil impacts.

Oil trajectories for two hypothetical spills involving the release of 795,000 L (5000 barrels) of oil (major spill volume) were developed using GNOME with site-specific input parameters. For the purpose of demonstrating the flexibility of this approach, two oils with different chemical and physical characteristics (intermediate fuel oil [IFO] and Qua Iboe oil) were used in simulations. Only one oil type was used at each spill location: the Gulf of the Farallones (an area offshore San Francisco Bay), and an area offshore Charleston Harbor, South Carolina. Each of these hypothetical spills was modeled under two scenarios: a scenario involving natural (physical) dispersion of oil, and a scenario involving the use of chemical dispersants. The latter was further modeled assuming a 35% dispersant operational effectiveness, which is the upper level of dispersant effectiveness reported under field conditions (5-30%; NRC, 2005), and assuming a 80% dispersant effectiveness, which is considered to be an extreme case scenario under field conditions. Here, dispersant effectiveness is defined, from an operational perspective (not laboratory), as the amount of oil that is dispersed into the water column relative to the amount of oil that is dispersed by physical processes alone (wind, currents, waves). Modeled conditions, and oil and dispersant characteristics (e.g., oil type, physicochemical characteristics, dispersant effectiveness) are summarized in Table 1. For each of these scenarios, GNOME was used to produce outputs containing information on oil trajectory, oil mass balance, oil concentrations in the water column (from the water surface to the pycnocline), and oil loadings on shorelines over space and time (120 h). Because of model uncertainty, oil concentrations in the water column were bounded by upper and lower limits defined as $5 \times$ and $0.2 \times$ of the mean value, respectively. GNOME generates oil concentrations by grid summarized as mean and maximum THC concentrations. Grid sizes ranged from 0.25 to 1.0 square kilometers (km²) in the case of Gulf of the Farallones scenario, and from 0.25 km^2 near the source to $3-5 \text{ km}^2$, 10-15 km down coast in the case of the Charleston Harbor scenario.

Table 1

Model inputs of two hypothetical oil spills, each involving the release of 795,000 L of oil (major spill volume). In all cases, models scenarios were run under physical dispersion only (no dispersants), and chemical dispersion with dispersant effectiveness of 35% (operational case) or 80% (extreme case).

Characteristics	Off San Francisco Bay, CA	Off Charleston Harbor, SC
Location	37°51′N, 122°46′W 25 km WNW Golden Gate (39 m isobath)	32°41.6'N, 79°45.72'W 11.4 km SE Charleston Harbor entrance (10 m isobath)
Oil type	IFO 380 (API 18.3)	Qua Iboe (API 35.8)
Wind velocity (knots)	10 West	15 South
Water column mixing depth/pycnocline depth (m)	10	5
Breaking wave height (m)	1	1

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Fig. 1. GNOME outputs for the hypothetical 795,000 L oil spill off San Francisco Bay at 0, 24, 48 and 96 h post-release (left to right) for the physically (top) and chemicallydispersed oil scenarios (35% dispersant effectiveness only; operational case) (bottom). Panels on right show estimated average and maximum oil concentrations in the top 5 m of the water column as a function of time post-release for grid cells that contain oil. In all cases, the symbol "+" shows the location of the spill site.



Fig. 2. GNOME outputs for the hypothetical 795,000 L oil spill off Charleston Harbor at 0, 24, 48 and 96 h post-release (left to right) for the physically (top) and chemicallydispersed oil scenarios (35% dispersant effectiveness only; operational case) (bottom). Panels on right show estimated average and maximum oil concentrations in the top 5 m of the water column as a function of time post-release for grid cells that contain oil. In all cases, the symbol "+" shows the location of the spill site.

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Fig. 3. GNOME's estimated oil mass balance of physically (left) and chemically (middle, right) dispersed oil from hypothetical spills of 795,000 L of oil off San Francisco Bay (top) and off Charleston Harbor (bottom). The chemically-dispersed oil scenario includes dispersant effectiveness set at 35% (operational case) or 80% (extreme case).



Fig. 4. Density distribution of average and maximum GNOME's estimated oil concentrations (mg THC/L) entrained in the top 5 m of the water column for the hypothetical spills off San Francisco Bay (left) and off Charleston Harbor (right). The chemically-dispersed oil scenarios include dispersant effectiveness set at 35% (operational case) or 80% (extreme case). Red dots represent median values, while embedded black lines display the first and third quartile values of a standard box-plot. The length of the density plots represents the minimum and maximum values, while the widths represent their frequency distributions. (For interpretation of the references to colour in this figure legend, the reader is referred to the web version of this article.)

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Fig. 5. Species Sensitivity Distributions (SSD) from varying exposure durations, and estimated HC values. Symbols represent the geometric mean of empirical values by individual species, while solid and dashed lines represent the mean and the 95% CI of the SSD. Note that HC5 and HC1 concentrations decrease with time (increased toxicity).

2.2. Toxicity data and Species Sensitivity Distributions

For the scenarios at hand, acute toxicity data were compiled and used to develop Species Sensitivity Distributions (SSD). SSDs are cumulative distributions of acute toxicity data that allow for comparisons of the relative sensitivities of aquatic species to the same chemical (e.g., petroleum hydrocarbons) (Posthuma et al., 2002), where each point on the SSD represents the geometric mean of acute toxicity values for individual species. Data used in the development of SSDs were queried from a recently developed toxicity database (Bejarano et al., 2014a), and included toxicity data (median lethal concentration, LC50; effective median concentration, EC50) reported on the basis of THC (milligrams per liter [mg/L]) from tests performed with oil physically (e.g., water accommodated fraction, WAF) and chemically (e.g., chemically enhanced water accommodated fractions, CEWAF) dispersed. Combination of CEWAF and WAF data for the development of SSDs was deemed appropriate as recent analyses (Bejarano et al., 2014b) and previous data compilations (NRC, 1989, 2005) have shown no scientific evidence that the toxicity of CEWAF (dispersed with current generation dispersants) is substantially greater than that of WAF. Toxicity data from medium and light oils, and from CEWAF prepared using Corexit 9500 or Corexit 9527 under recommended dispersant to oil ratios (DOR 1: >10, v:v) were included. Toxicity data for heavy fuels (e.g., IFO 380) are lacking in the database, and therefore, data from medium and light oils were used as surrogates.

Time-varying SSDs were developed using all available acute toxicity data from tests performed under <24, 24, 48 and 96 h exposure durations. For the purpose of these analyses, it was assumed that the 1st and 5th percentiles of the SSD represent concentrations protective of 99% and 95% of the species in the SSD curve (i.e., Hazard Concentrations 1 and 5, HC1 and HC5). SSDs and their associated HC values were derived by fitting the data to a log-normal distribution function, and re-sampling this function 2000 times to derive central tendencies and 95% confidence intervals (95% CI) (Bejarano and Farr, 2013).

2.3. Characterization of potential ecological risks

Model outputs from GNOME, specifically estimated maximum oil concentrations within the few top meters (5 m) of the water column and area of potential impacts (km²), were used to demonstrate the use of SSDs in characterizing potential adverse toxicological consequences. Maximum oil concentrations from GNOME were used as a precautionary approach biased towards overprotection of aquatic species. For the purpose of the analyses presented here, it is assumed that all aquatic species entrained and transported with the water mass containing physically or chemically dispersed oil are at potential risk of adverse effects. Within the context of these analyses, physically-dispersed oil scenarios are defined as those where oil is dispersed and entrained in the water column by natural physical processes (e.g., currents, wind, waves in open waters); while chemically-dispersed oil scenarios are defined as those where oil is treated with chemical dispersants at the water surface to enhance its dissolution and partitioning into the water column.

Two approaches were used to characterize effects to entrained water-column organisms: a time-varying (varying concentrations with time) and a time-static (static concentrations with time) approach. The time-varying approach compared estimated maximum oil concentrations at each time post-release (e.g., 1–120 h) with time-varying SSDs from the closest exposure duration (e.g., time post-release <24 h vs. <24 h-SSD). This approach may be considered more environmentally realistic as concentrations under field conditions are expected to decrease over time, due to water column mixing, dilution and biodegradation. With the time-static approach, comparisons were made of the estimated maximum oil concentrations at each time post-release with the SSD from the longest exposure duration (i.e., time post-release <24 h vs. 96 h-SSD). This approach may be preferred when there are concerns about particularly sensitive aquatic species, but it is biased towards overprotection of aquatic species. Both approaches allowed the estimation of the proportion of species affected (PSA; a.k.a. Potentially Affected Fraction, PAF) (Posthuma et al., 2002) as a function of time post-release, and area (km²) with maximum oil concentrations exceeding HC5 values (Area_{>HC5}) (e.g., time-varying approach: area at 20 h post-release vs. HC5 from 24 h-SSD; timestatic approach: and area at 20 h post-release vs. HC5 from 96 h-SSD).

3. Results

3.1. Oil mass balance and environmental concentrations

A total of six GNOME models were developed to illustrate how site specific conditions, oil types, as well as the use of chemical

dispersants, influence oil fate (see Supplementary Content Information of oil spill scenario animations). Representative examples of GNOME trajectory outputs (snap shots), along with estimates of average and maximum oil concentrations in the top 5 m of the water column as a function of time, are shown in Figs. 1 and 2. Oil mass balance from GNOME are compartmentalized into oil floating at the water surface, entrained in the top few meters of the water column, evaporated into the atmosphere, and stranded on shorelines (Fig. 3).

For the hypothetical spill off San Francisco, and under the physically-dispersed oil scenario, 63% of the total oil volume is estimated to remain on the water surface and strand on shorelines. Under this scenario, 5% of the oil is entrained in the water column, while the remaining volume volatilizes into the atmosphere (32%). By comparison, and assuming 35% and 80% dispersant effective-ness, 42% and 13% of the total oil volume, respectively, would remain on the water surface and strand on shorelines, while 31% and 65%, respectively, would be entrained in the water column (mostly offshore). The remaining oil volume would volatilize into the atmosphere (27% and 22%, respectively).

For the hypothetical spill off Charleston Harbor, and under the physically-dispersed oil scenario, 56% of the total oil volume would remain on the water surface and strand on shorelines. Under this scenario, 5% of the oil is entrained in the water column, while the remaining volume volatilizes (39%). By comparison, and assuming 35% and 80% dispersant effectiveness, 36% and 11% of the total oil volume, respectively, would remain on the water and strand on shorelines, while 32% and 67%, respectively, would be entrained in the water column (mostly offshore). The remaining oil volume would volatilize into the atmosphere (32% and 22%, respectively).

These hypothetical spill simulations show that the use of chemical dispersants, and particularly increased dispersant effectiveness, can reduce the amount of oil on the water surface ultimately stranding on shorelines, while increasing the partitioning of oil into the water column. For the San Francisco spill and under the physically-dispersed scenario, average estimated oil concentrations in the upper 5 m of the water column over 120 h (Fig. 4) are 0.15 ± 0.11 mg THC/L. Under the assumption of 35% or 80% dispersant effectiveness, average oil concentrations are 1.5 and 3.2 times higher $(0.49 \pm 0.30 \text{ mg THC/L} \text{ and } 0.89 \pm 0.62 \text{ mg THC/L})$ over the same period, respectively, than concentrations under the physical dispersion scenario. Maximum oil concentrations are 4-6 times higher than the average concentrations over the same period. Similarly, for the Charleston Harbor spill and under the physicallydispersed oil scenario average estimated oil concentrations in the upper 5 m of water column over 120 h are 0.04 ± 0.05 mg THC/L. Under the assumption of 35% or 80% dispersant effectiveness, oil concentrations are 8 and 17 times higher $(0.22 \pm 0.35 \text{ mg THC/L})$ and 0.94 ± 0.77 mg THC/L), respectively, than concentrations under the physical dispersion scenario. Maximum oil concentrations are 3 times higher than average concentrations.

While it is clear that each scenario produces different oil concentrations in the water column, these concentrations decrease in space and time, and therefore analyses discussed further, take into account this variability. Because of model uncertainty, assessments of potential ecological consequences to entrained water column organisms use a precautionary approach biased towards overprotection of aquatic species by assuming maximum oil concentrations in the water column.

3.2. Toxicity data and Species Sensitivity Distributions

Most of the acute toxicity data (LC50 and EC50) currently available were from tests performed with early life stages of several aquatic species. Time-varying SSDs were developed from toxicity data collected from <24, 24, 48 and 96 h exposure duration tests (Fig. 5). While there were less species-specific toxicity data for exposures <24 h (5 species total), estimated HC1 and HC5 values (mg THC/L) decrease over time, with <24 h HC values being 7 times larger (lower toxicity) than HC values for 96 h exposures. Based on these time-varying SSDs, HC1 and HC5 values can be estimated as a function of exposure duration (h) with the following equations: HC1 = $4.43 * \text{Exp}^{(-0.03*h)}$ (Adj. $R^2 = 0.65$); HC5 = $5.67 * \text{Exp}^{(-0.03*h)}$ (Adj. $R^2 = 0.71$). Both the concentrations associated with PSA on the SSDs, and estimated HC5 values, are used to characterize potential effects to aquatic species entrained and transported with the water mass containing physically or chemically-dispersed oil.

3.3. Characterization of potential ecological risks

GNOME's estimated maximum oil concentrations in the top 5 m of the water column as a function of time post-release and area with estimated oil concentrations were used to characterize potential risks to entrained water column organisms. Assessments were based relative to both time-varying SSDs and time-static SSDs (i.e., 96 h-SSD; conservative approach). The former may be considered more environmentally realistic as environmental concentrations are expected to decrease with time, while the latter may be preferred when there are concerns about particularly sensitive aquatic species, but it is overprotective. In both instances, PSA was estimated by comparing oil concentrations in the top 5 m of the water column with equivalent concentrations on the SSD, and by estimating the total area (km^2) exceeding HC5 values (Area \geq HC5).

Under the physically-dispersed oil scenario for the hypothetical spill off San Francisco Bay, most concentrations in the top 5 m of the water column, with the time-varying approach (declining concentrations with time), are below the assumed protective concentration (HC1 and HC5), with maximum PSA and Area $_{\geq HC5}$ of 0.05 (77 h post-release) and 0.22 km² (73 h post-release), respectively. In contrast, the time-static approach (static concentrations with time) produced estimated values that are at least 5 times higher (maximum PSA = 0.19 [36 h post-release]; maximum Area > HC5 of 1.79 km² [8 h post-release]). Both PSA and Area > HC5 are higher with the use of chemical dispersants. Assuming 35% dispersant effectiveness (operational case), the time-varying approach (Fig. 6) produced average PSA and Area $_{>HC5}$ of 0.13 ± 0.08 and 8.68 ± 5.60 km², respectively, with the greatest potential for adverse effects occurring between 75 and 77 h post-release, when the maximum PSA and Area_{\geq HC5} are 0.35 and 18 km², respectively. In contrast, the time-static approach had values that are on average 5 times higher, with most pronounced differences occurring <24 h post-release (average PSA = 0.30 ± 0.15 and average Area_{$\geq HC5$} = 13.73 ± 3.76 km²). Under this approach, the greatest potential for impact to a larger number of species would be 16 h post-release (maximum PSA = 0.61), but the greatest areal extent would occur 66 h post-release (maximum Area $_{\geq HC5}$ = 19.49 km²). Assuming 80% dispersant effectiveness (extreme case), the time-varying approach produced average PSA and Area_{\geq HC5} of 0.38 ± 0.13 and 19.01 ± 10.3 km², respectively. In contrast, the time-static approach had values that are on average 2 times higher, with most pronounced differences $PSA = 0.49 \pm 0.14;$ ≼24 h post-release (average average Area_{\geq HC5} = 24.31 ± 7.9 km²). Under both approaches, the greatest potential for impact to a larger number of species would be ≤ 24 h post-release (maximum PSA), but the greatest areal extent would occur 112 h post-release (maximum Area > HC5).

Under the physically-dispersed oil scenario for the Charleston Harbor spill, all concentrations in the top 5 m of the water column, using the time-varying approach (declining concentrations with time), are below the assumed protective concentrations (HC1 and HC5). In contrast, the time-static approach (static concentrations with time) produced estimated values that are at least 5 times

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Off San Francisco Bay

Fig. 6. Contour plot, based on 1 h running averages, of the estimated peak of proportion of species affected (PSA) as a function of area above the HC5 (km²; Area_{\geq HC5}) and time post-release (h) for the hypothetical spill off San Francisco Bay under the chemically-dispersed oil scenarios: 35% dispersant effectiveness (top) and an extreme 80% dispersant effectiveness (bottom). The PSA was derived based on modeled maximum environmental concentrations in the top 5 m of the water column, and comparisons made relative to time-variable and time-static SSDs. Plots also display maximum estimated PSA and maximum Area_{\geq HC5}.

higher (maximum PSA = 0.09 [8 h post-release]; maximum Area $_{\geq HC5}$ of 0.34 km² [21 h post-release]). Assuming 35% dispersant effectiveness (operational case), the time-varying approach (Fig. 7) produced average PSA and Area $_{\geq HC5}$ of 0.002 ± 0.01 and $17.71 \pm 11 \text{ km}^2$, respectively. Under this approach, the greatest potential for impact to a larger number of species would occur 4 h post-release (maximum PSA = 0.54), but the greatest areal extent would occur 38 h post-release (maximum Area_{≥HC5} = 24 km²). In contrast, the time-static approach had values that are on average 5 times higher, with most pronounced differences occurring within the ≤ 24 h post-release (average PSA and Area $_{\geq HC5}$ are PSA 0.06 \pm 0.12 and 25.34 \pm 7.10 km², respectively). Assuming 80% dispersant effectiveness (extreme case), the time-varying approach produced average PSA and Area $_{\geq HC5}$ 0.11 ± 0.08 and $35.28 \pm 19.71 \text{ km}^2$, respectively. In contrast, the time-static approach had values that are between 2 and 5 times higher, with most pronounced differences occurring \leqslant 24 h post-release (average PSA = 0.27 ± 0.20 ; average Area_{>HC5} = $42.56 \pm 15.49 \text{ km}^2$). Under both approaches, the greatest potential for impact to a larger number of species would occur ≤10 h post-release (maximum PSA), but the greatest areal extent would occur 115 h post-release (maximum Area \geq HC5).

While it is clear that there are differences between the timevarying (declining concentrations with time) and time-static (static concentrations with time) approaches in terms of PSA, Area_{\geq HC5} and timing of potential effects, the greatest differences are scenario driven (Fig. 8). For both hypothetical spills, the PSA and Area_{>HC5} of the physically-dispersed oil scenario are considerable smaller than those of the chemically-dispersed oil scenarios. Both average PSA and Area_{>HC5} increase linearly as a function of dispersant effectiveness such that for every 10% increase in dispersant effectiveness, average PSA increases between 0.01 and 0.06, while Area_{>HC5} increases between 0.50 and 2.9 km². More pronounced changes across scenarios are noted in PSA for the spill off San Francisco, and in Area_{>HC5} for the spill off Charleston Harbor.

While thus far discussions have focused on potential impacts to aquatic species entrained and transported with the water mass (top 5 m of the water column) containing physically or chemically-dispersed oil, it is important to recognize that one of the assumed benefits of chemical dispersant use deals with the reduction of oil impacts on shoreline habitats. For the hypothetical spills off San Francisco Bay and off Charleston Harbor, a total of 19.6 km and 98.2 km of shoreline, respectively, were assessed for stranded oil under each scenario (Fig. 9).

The physically-dispersed oil scenario off San Francisco Bay resulted in shorelines with an average oiling of $29,061 \pm 45,936$ L oil/km and 485,499 L of total stranded oil. By contrast, the use of dispersants under the 35% and 80% dispersant effectiveness assumptions reduced the estimated shoreline oiling by 33% (19,426 ± 30,645 L oil/km) and 81% (5604 ± 8168 L oil/km), respectively. Under the 35% and 80% dispersant effectiveness assumptions, the total volume of oil stranded on shorelines are 323,295 L and 93,279 L, respectively.

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Off Charleston Harbor

Fig. 7. Contour plot, based on 1 h running averages, of the estimated peak of proportion of species affected (PSA) as a function of area above the HC5 (km^2 ; Area_{\geq HC5}) and time post-release (h) for the hypothetical spill off Charleston Harbor under the chemically-dispersed oil scenarios: 35% dispersant effectiveness (top) and an extreme 80% dispersant effectiveness (bottom). The PSA was derived based on modeled maximum environmental concentrations in the top 5 m of the water column, and comparisons made relative to time-variable and time-static SSDs. Plots also display maximum estimated PSA and maximum Area_{\geq HC5}.

Similarly, the physically-dispersed oil scenario off Charleston Harbor resulted in shorelines with an average oiling of 3621 ± 5703 L/km and 441,247 L of total stranded oil. By contrast, the use of dispersants under the 35% and 80% dispersant effectiveness assumptions, respectively reduced the estimated shoreline oiling by 53% (1728 ± 2783 L oil/km) and 79% (756 ± 1217 L oil/km), respectively. Under the 35% and 80% dispersant effectiveness assumptions, the total volume of oil stranded on shorelines are 207,753 L and 90,892 L, respectively.

Approximately, for every 10% increase in dispersant effectiveness, average estimated shoreline oiling for the spills off San Francisco Bay and off Charleston Bay were reduced by 2919 L/km and 1405 L oil/km, respectively, equivalent to 49,125 L and 42,963 L of total oil stranded on shorelines, respectively. A reduced oiling of shoreline habitats with offshore use of chemical dispersants may translate into lower impacts from oil to shorelines, and shoreline and nearshore biological communities, as well as reduced impacts from potentially invasive and physically disruptive oil cleanup activities.

4. Discussion

GNOME has been used in trajectory simulations (e.g., Marta-Almeida et al., 2013; Yang et al., 2013), ecological risk assessments with focus on the use on dispersant use (Mearns et al., 2001, 2003), and decision support during real oil spills (MacFadyen et al., 2011). Here, GNOME was used as a platform to demonstrate the practical integration of trajectory modeling with SSDs to facilitate the guantification of potential adverse effects to entrained water column organisms. Modeled oil concentrations and assessments of potential effects based on maximum oil concentrations in the top 5 m of the water column are assumed to be conservative relative to assessments following sea trials testing and actual oil spills. Because the goal of these analyses was to demonstrate the use of SSDs in oil trajectory modeling, the starting spill volume (795,000 L) is higher than those from field trials (379-1,895 L range) (e.g., Cormack and Nichols, 1977; Lunel, 1994; McAuliffe et al., 1980, 1981; Strom-Kristiansen et al., 1997). As a result, high oil concentrations within the first 24 h (up to 15.88 mg/L) exceed concentrations measured in the top 1-2 m of the water column immediately following chemical dispersion of oil (generally ≤1 mg/L) (Cormack and Nichols, 1977; Lunel, 1994; McAuliffe et al., 1980, 1981; Strom-Kristiansen et al., 1997; reviewed in Bejarano et al., 2014b). Comparable concentrations to the maximum modeled concentrations reported here are typically achieved within the first 30 min of dispersant application (Cormack and Nichols, 1977; Lunel, 1994; McAuliffe et al., 1981; Strom-Kristiansen et al., 1997). As an example, oil concentrations at 1 m depth following surface dispersant use during the Deepwater Horizon oil spill were up to 2 mg/L approximately 30 min of dispersant use (Bejarano et al., 2013), though this oil was substantially weathered before dispersants were applied.

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Fig. 8. Density distribution of the estimated proportion of species affected (PSA; top) and area above the HC5 (km^2 ; Area $_{\geq HC5}$; bottom) for the hypothetical spills off San Francisco Bay (left) and off Charleston Harbor (right) relative to time-variable and time-static SSDs. The chemically-dispersed scenario includes dispersant effectiveness set at 35% (operational case) or 80% (extreme case). Red dots represent median values, while embedded black lines display the first and third quartile values of a standard box-plot. The length of the density plots represent minimum and maximum values, while the width represent their frequency distributions. (For interpretation of the references to colour in this figure legend, the reader is referred to the web version of this article.)



Fig. 9. Density distribution of GNOME's estimated shoreline oiling (L oil/km) from the hypothetical spills off San Francisco Bay (left) and off Charleston Harbor (right). The chemically-dispersed oil scenario includes dispersant effectiveness set at 35% (operational case) or 80% (extreme case). Red dots represent median values, while embedded black lines display the first and third quartile values of a standard box-plot. The length of the density plots represents the minimum and maximum values, while the widths represent their frequency distribution. (For interpretation of the references to colour in this figure legend, the reader is referred to the web version of this article.)

Regardless of the artificially high oil concentrations in the water column of the two hypothetical spills, as demonstrated here, SSDs can provide additional information to environmental assessments of dispersant use. Ecological risk assessments that support evaluations of spill response actions, including the use of dispersants, have commonly relied on a consensus or best professional judgment approach to derive concentrations of concern to characterize potential impacts to water column organisms (Aurand, 1995; Mearns et al., 2001, 2003). Under the consensus approach, a 24 h exposure to 1 mg/L of oil would be a medium to high level of concern for sensitive life stages, while 2 mg/L would be a medium level of concern for adult crustaceans (e.g., Mearns et al., 2001). With the alternate approach presented here, developed primarily with data from early life stages, the 24 h SSD-based HC1 and HC5 values for a wide range of species would be 2.12 mg/L and 2.64 mg/L, respectively. Interestingly, both the consensus and the SSD-based levels of concern concentrations are within factors of 2–3. However, one advantage of the alternate approach presented here is that it is based entirely on quantitative data, increasing the certainty of environmental assessments.

Furthermore, because of uncertainties in species sensitivities, SSDs developed here are conservative as toxicity data included results from tests using a high dispersant to oil ratios ($1:\ge 10$). While a 1:10 ratio is required for toxicity testing under the National Contingency Plan Subpart J (USEPA, 2006), the standard ratio needed to achieve effective oil dispersion under field conditions is at least 1:20 (based on manufacturer's recommendations) (e.g., Lessard and DeMarco, 2000). Consequently, toxicity data derived

from aqueous media preparation using a 1:10 ratio would result in higher oil concentrations in the exposure media (e.g., smaller HC values), and hence greater toxicity, compared to tests performed with media prepared using a lower ratio (e.g., 1:20). Conversely, SSDs developed based on 1:20 dispersant to oil ratios would likely have larger HC values, which in turn would result in smaller PSAs and Area \ge_{HC5} s than those reported here.

Although SSDs-based PSA have been used in environmental assessments in the past (e.g., Carriger and Rand, 2008; Klepper et al., 1998; Posthuma and De Zwart, 2006; Posthuma et al., 2002) they have not been used to improve or support assessments based on oil trajectory modeling. As shown here, modeled environmental concentrations of oil as a function of time can be compared to concentrations associated with toxicity summarized in the form of SSDs such that PSA can be estimated. This is an improvement over comparisons relative to static thresholds as it facilitates a greater understanding of the potential scale of adverse effects to water column organisms under different scenarios. Moreover, estimates of the areal extent with oil concentrations exceeding specific levels of concern (e.g., Area $_{\geq HC5}$) are also valuable in that these provide a measure of spatial scale of potential impacts.

SSD incorporation into trajectory modeling is also useful in characterizing potential impacts to species of concern. Analysis of toxicity data using early life stages of red abalone (Haliotis rufescens) (Singer et al., 1996, 1998) as a surrogate for the endangered white and back abalone (Haliotis sorenseni and Haliotis cracherodii) showed that the placement of this species was towards the upper end of a SSD derived from spiked exposures with larvae (Bejarano et al., 2014b). Based on GNOME outputs, none of the maximum oil concentrations from the hypothetical spill off San Francisco Bay reached concentrations associated with toxicity effects to this species (22 mg THC/L). As a reference this species falls within a PSA of 0.6 and \geqslant 0.8 based on the ${\leqslant}24\,h$ SSD and 24–96 h SSDs, respectively. Similarly, while the area of the Gulf of the Farallones through which the hypothetical dispersed oil travels over several days is over 800 km², the maximum estimated Area_{$\geq HC5$} under worst case exposure conditions was 19.49 km². This Area > HC5 likely represents a small fraction of the distribution of abalone larvae within the water column. Consequently, integration of SSD information into GNOME and similar oil trajectory models may help provide a more quantitative representation (spatial/temporal scaling) of potential adverse effects to water column organisms. However, future refinements are needed to incorporate SSDs of toxic fractions (namely polycyclic aromatic hydrocarbons, PAH) into trajectory modeling, as PAHs are the fractions in oil that drive acute toxic responses (Carls et al., 2008; Couillard et al., 2009; French-McCay, 2002; Pelletier et al., 1997). However, comparable model development has been hindered by the lack of availability of detailed analytical chemistry for PAHs in the scientific literature related to oil toxicity testing (reviewed in Bejarano et al., 2014b).

In the current analyses, comparisons were made between potential impacts to entrained water column organisms versus impacts to shoreline habitats based on several dispersant use scenarios. This is the crux of the tradeoff decision process. Similar assessments are routinely undertaken in analyses of Net Environmental Benefits (NEBA) of different oil recovery actions (e.g., in-situ burning, use of chemical dispersants, mechanical oil recovery) in response to oil spills. NEBA assessments generally indicate shifting risks from the use of dispersants between wildlife/shoreline habitats and aquatic organisms (Mearns et al., 2001). As shown here, the use of chemical dispersants and their increased effectiveness results in greater PSA and Area_{>HC5} compared to physicallydispersed oil scenarios, but also resulting in a considerable reduction of oil volume (L oil/km and L of total stranded oil) in shoreline habitats. However, similar analysis including levels of concern specifically developed for shoreline oiling need to be considered

to truly quantify the magnitude of shifting risks from shoreline habitats (physical dispersion) to water column impacts (chemical dispersion). While it is clear that modeled oil concentrations under the chemically-dispersed scenarios have a greater potential to cause impacts to entrained water column organisms, continued dilution in open water, and increased biodegradation potential reduces exposure to elevated oil concentrations. This is one of the premises supporting the use of dispersants in offshore waters (NRC, 1989, 2005).

While quantitative analyses shown here demonstrate the potential use of SSDs in oil trajectory modeling, these exercises are not intended to replace, but rather to augment knowledge from field quantification of potential impacts arising from oil spills and the use of dispersants. Future efforts will focus on exploring the use of SSDs in modeling undertaken to support natural resource damage assessment and related activities.

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Appendix A. Supplementary data

Trajectory modeling movies from GNOME for each scenario (6 movies). Supplementary data associated with this article can be found, in the online version, at http://dx.doi.org/10.1016/j.marpolbul.2015.01.022.

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