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Modeling as a Scientific Tool in NRDA for Oil and Chemical Spills.

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Abstract

In natural resource damage assessments, as well as in analyses of response alternatives, modeling is a useful and effective scientific tool in assessing injury and risk. Often field data documenting spill impacts are incomplete, such that injuries are underestimated or impossible to assess. In order to quantify impacts using field observations, comprehensive sampling of affected biota is needed in both exposed and unaffected areas. Because marine organisms are so patchy in their distribution, large numbers of stations and samples within stations are needed to accurately map abundance. Such extensive sampling of all (or even selected) species affected is often not feasible, given the rapidity at which the evidence disappears (by scavenging of killed organisms and by migration of animals into the impacted area). What is feasible and cost-effective, is to estimate impacts using existing scientific knowledge of the fates and toxicity of oil components, along with as much site-specific data as is available or feasible to collect. Oil and chemical fates and effects models integrate this information into a form that may be calibrated to and/or verified with field data, such that injuries are quantified with a combined field-based and modeling approach.

Introduction

The goal of Natural Resource Damage Assessment (NRDA) is to restore injured natural resources and associated lost services. The quantification of injuries includes consideration of any primary restoration performed to speed recovery. Compensation to the public is for the interim losses from the time natural resources are injured until they return to baseline (in the form of compensatory restoration, scaled to the magnitude of the interim losses; National Oceanic and Atmospheric Administration [NOAA], 1996a,b). However, for oil spills into aquatic environments where typically the majority of the injuries occur in time scales of days to weeks over large geographic areas, quantitative field data sufficient to assess injuries are rarely available. In order to fully characterize the impact by field sampling, visual observations (wildlife) and sampling (water, sediment, biota) are needed at frequent time intervals over the first few weeks after the release (and especially in the first 24-48 h), and with enough spatial coverage to characterize the extent of contamination and exposure. In addition, comprehensive sampling of each of the species affected is needed in the exposed and unaffected areas. Because wildlife and aquatic organisms are so patchy in their distributions, large numbers of observations and samples are needed to map abundance accurately. Natural variability requires even more sampling to detect sublethal and long-term effects. Such extensive sampling of all (or even selected) species affected is typically not possible, given the rapidity at which the evidence disappears (by scavenging of killed organisms and by migration of animals into the impacted area) and the logistical difficulties in mobilizing field teams on short notice (especially in remote areas). Thus, in practice, comprehensive sampling of all injuries is either not feasible or too costly to be justifiable by the expected impact of the spill.

In spite of these obstacles, in many cases, injury quantification is based primarily on collected field data. A more practical and realistic approach is to combine field sampling with modeling of oil fates and effects. With such an approach, injuries are estimated using existing knowledge of: the physical and chemical properties of oils, their transport in the environment, distributions and behavior of organisms that affect exposure, effects levels given exposure, and population and ecosystem responses to perturbation. The model must quantify the fate of the oil both on and beneath the water surface in order accurately estimate transport and exposure to wildlife (birds, marine mammals and sea turtles) and aquatic organisms.

The objective of this paper is to evaluate the efficacy and accuracy of using modeling as a scientific tool to quantify injury resulting from an oil spill in a NRDA context. There is reluctance by some parties to use modeling in an NRDA injury assessment role. Modeling is often dismissed as a “black box”, based on “oversimplifications” or “synthetic” evidence of injury, or just “abstract” and “theoretical”, whereas field-based studies have been described as the only way to obtain “real” information on injury.

However, modeling can and should involve scientifically-based quantitative analyses of the best available information, both from field data, as possible, and the scientific literature. The issue is not whether to use modeling for quantification of injuries and scaling of restoration, as modeling of some form must be used to be quantitative. Rather the choices involve the appropriateness of the model design and implementation, the assumptions and data used as input, as well as the degree of accuracy needed in order to reach a fair settlement that is truly compensatory and, thus, satisfactory to all parties. The modeling should and can be based on science, and also be cost-effective in both the assessment and restoration implications.

Modeling is Part of Scientific Practice

What is a Model?

A model is a description of processes, stated quantitatively, based on available scientific information. A model is used to calculate the resulting implications of process descriptions and data inputs. It is tested, modified, calibrated and validated using laboratory and field observations.

Computer models of natural systems simulate the real world through sets of mathematical equations developed from laboratory and field studies. For example, studies have determined the effect of wind speed on the movement of oil on water surfaces. This relationship, combined with wind speed and direction data plus current data, can be used to predict oil movement. Sophisticated computer models combine large numbers of these relationships or equations to enable a comprehensive understanding of environmental events. This technology is used to examine the likely results of hypothetical events, to compare various response activities, or to fill gaps in field data in quantifying impacts from a real spill.

Is it Science?

Yes, modeling is in fact science. The scientific method involves development of hypotheses, testing, modification of understanding, retesting and validation. A model is simply a formalized quantitative statement of the scientific analysis. There are uncertainties in all areas of science: in field data, laboratory data and modeling. The most powerful and quantitative assessments integrate field evidence, laboratory data, and model algorithms describing physical, chemical and biological processes to determine the most likely account of the circumstances and injuries resulting from a spill.

Qualitative models

In general, interpretation and analysis of data involves developing a conceptual model of the relationships and mechanisms that account for observations. There are many examples of the formalized use of conceptual models in scientific and regulatory practice. For example, in the US Environmental Protection Agency (USEPA) Guidelines for Ecological Risk Assessments, a Conceptual Site Model is developed to identify pathways and exposure, and to design field data collection. The NRDA regulations follow similar guidance for injury assessment (NOAA, 1996a). Indeed, in all scientific studies and specifically in pollution impacts evaluations, the first step is to develop a conceptual model of:

- important species distributions and dynamics, as well as connections between species, habitats and the environment;
- processes that determine fates and effects;
- pathways and potential exposure of biota; and
- likely effects on individuals, populations and ecosystems.

Quantitative models

After developing a qualitative model, the next step is to develop quantitative relationships and appropriate equations to describe the processes, observations and implications. The scientist identifies gaps in existing information and develops data requirements for input to the model, which might be filled by field studies, laboratory analyses, and or further analysis of literature and other information.

Quantitative models may be empirical/statistical, i.e., where equation(s) are fit to observational data; or mechanistic, i.e., based on physical, chemical and biological mechanisms, principles and research. An empirical approach is used to infer injuries based on experience in other spills. The limitation of this approach is that data are needed from similar environments and circumstances to the spill of concern, with respect to oil volume, oil type, weather, habitats affected, etc. The problem is that “one never sees the same spill twice” (Jacqueline Michel, Research Planning Inc., personal communication). The empirical approach requires large data sets on both the present and past spills, making this approach logistically infeasible (and not cost-effective) except for a few habitats that have been previously well-studied, such as saltmarshes and mangrove swamps.

Quantitative mechanistic models allow the scientist to predict results outside the range of experience, presuming there is sufficient understanding of the mechanisms and relationships between important processes. The mechanistic model is developed by combining scientific principles and natural laws, knowledge of similar systems to the resources of interest, experimental data and observations, and spill experience to develop a quantitative understanding, allowing a best estimate of injuries to be made.

Historically, mechanistic models were limited by ability to solve the system of equations, as computers were (first) not available or (later) too limited in memory to handle complex equations and data storage requirements. Before computers, calculus was used, requiring only a few equations in standard form be included in the model. In rare exceptions, scientists solved complex models iteratively by incrementing changes in “state variables” over multiple time steps (using a slide rule, a time consuming a tedious process; Riley, 1946, 1949). Later, as computers became available, the power and memory of the computer limited the complexity and resolution (temporal and spatial accuracy) of models. For example, when the Type A NRDA models were developed in the 1980s and early 1990s (French et al. 1996), there were limits to the complexity and size of model grids defining shoreline, habitats, water depth and environmental data. Presently, computers are powerful enough that the limitations on models are more related to data or scientific understanding than computational power. As our scientific understanding is rapidly improving, so are the models that utilize this information.

Limitations and Reliability of Field Data Collections

Uncertainty in Injury Quantification Based on Field Data

Observational efforts and sampling are difficult to plan and execute after an oil spill because it is often unclear if, when, where injury occurred. Difficulties with the sampling logistics essentially relate to the fact that (1) the spatial coverage cannot be comprehensive over the area of exposure plus reference area(s); and (2) the temporal coverage cannot be frequent enough to fully define an empirical curve of injury and recovery. This results in sample data for limited spatial and time windows (i.e., a series of snapshots). In addition, acute exposure usually occurs sooner than one can respond, such that sampling occurs after the majority of the exposure has past. Also, synoptic sampling typically requires a large effort, and so can be expensive.

In addition, there are problems of interpretation. Causality may not be clear: how much exposure is due to the spill versus to background contamination? Suitable reference sites are difficult to find and monitor. There are also large uncertainties due to natural variability, sampling and measurement errors. Thus, it is difficult to statistically measure a difference related to spill contamination. Our experience with the *Exxon Valdez* oil spill is a case in point – even with an unprecedented large field effort, the uncertainties make demonstration of injury difficult and controversial.

What is a “Real” Injury?

Is it the case that the only “real” injury is one that is measurable in the field? What if suitable reference sites are not available? How can measured concentrations and biological changes be discriminated from background? What if the sampling effort missed the time and/or spatial window where injury was apparent? What if natural variability is higher than impact signal, does that infer there was no injury? What if level of effort (or funding) is insufficient to detect differences? What if injuries don’t become apparent until a longer time after exposure than field sampling addresses? If a tree falls in the forest and no one is there to see it go down, didn’t it really fall, even if the tree decayed before someone got out in the forest to observe it?

Field studies may result in a finding of no or little injury because of these difficulties, when there is in fact a significant injury, given the high degree of uncertainty in the data collections. Thus, the most likely result of an assessment based on field data alone is an underestimate of injuries caused by a spill.

Limitations and Reliability of Laboratory Studies

Examples of the use of laboratory studies to evaluate mechanisms abound in science. It is well understood that data from laboratory experiments do not replicate actual field conditions. However, the experimental setup allows control of variability and ease of sampling. If appropriately designed, laboratory studies can provide needed data injury quantification, as well as for development of mechanistic model algorithms, improving the overall modeling of fate and effects of spills.

Limitations and Reliability of Modeling

A scientifically reliable model requires a good scientific basis, as well as accurate model coding and testing. Ideally, a model should be calibrated and verified with observational data from spills. Calibration involves adjustment of model inputs and refinement of assumptions to fit observational data. Calibrated models have good predictive power for the same spill or similar situations. Validation/verification involves comparing model results to independently-collected data. A validated model has more predictive capability for other spills and situations where similar mechanisms and processes occur than a model that has only been calibrated.

One has often heard the modeling mantra: garbage in, garbage out. The converse is also true; reliable results may be obtained if model inputs are based on reliable data. Thus, the accuracy of the model results depends not only on model algorithms, but on the accuracy of the scientific and field-based inputs. Therefore, one cannot make a simple judgment as to whether a model is good or bad. One must consider the accuracy of the data inputs for the specific application, as well as the basic model equations and assumptions.

There are also a number of model inputs that derive from modeling experience. For example, the parameters that quantify the scale of turbulence are often highly uncertain because of the complexity of the physical environment and natural variability, and require the modeler’s judgment and interpretation of results to determine appropriate values (French-McCay et al., 2007; Payne et al., 2007). The results of injury quantification studies are sensitive to these parameters, necessitating a sensitivity or stochastic analysis be performed to quantify uncertainty (see also Galt, 1998). In such an analysis, the modeler varies the most uncertain data inputs. The resulting NRDA claim and settlement should consider the range of potential injuries resulting from this uncertainty, as well as most likely result.

Use of Modeling for Environmental Assessments and Policy

Once a model is calibrated and verified, the consequences of various scenarios can be explored. Integrated model systems are used to quantify environmental impacts of real events (as in the NRDA context), of hypothetical spills (ecological risk assessment) and of response management strategies (contingency planning). Modeling allows quantification of answers so that objective decision-making may occur. It also may be used as an education tool to illustrate the derivation of an estimated impact and the net environmental benefits of actions or, alternatively, of no action.

For many years, results of environmental models and assessment analyses have influenced environmental regulation and policies at local, national and international levels. There are numerous examples of such uses of models in scientific practice and policy. For example, climate change policies are now based on modeling of implications of greenhouse gas emissions; fisheries quotas are based on fish population modeling; discharge permits are based on fate and transport modeling; and regulatory standards are based on modeling of toxic endpoint thresholds.

Role of Modeling in NRDA

Key components of a NRDA are (1) the establishment of pathway(s) between the release and exposed resources and (2) documentation that resource injuries are caused by the released contaminants. These relationships are complicated by other sources of contamination and stress, which may have additive or synergistic effects. Modeling technology is directly applicable to pathways and injury analysis in that models link source of contamination with effects, offer complete spatial and temporal coverage, can be calibrated using available field-collected data, and can in some cases forecast future injury. The advantages of using a (scientifically reliable) model include that it:

- completes the mass balance and provides a comprehensive analysis of injuries;
- can differentiate background from spilled contamination;
- provides an objective measure that falls out of what is known and scientific understanding, which is unbiased, especially if parties can agree on data inputs and assumptions; and if sensitivity analysis is performed to determine uncertainty and the most likely result.

In addition, if similar modeling is used on the injury and restoration side of the equation, this results in a fair scale of restoration, compensable to the injury. Thus, modeling of injury should be performed in concert with and using the same assumptions as the scaling of restoration.

NRDA Models in Regulation and Practice

Applied Science Associates (ASA) developed the oil (and chemical) spill model system for the US Department of the Interior (USDOI), which became the basis of the Comprehensive Environmental Response, Compensation and Liability Act of 1980 (CERCLA) NRDA regulations for Type A (simplified, requiring minimal field work) assessments, i.e., the Natural Resource Damage Assessment Model for Coastal and Marine Environments (NRDAM/CME; French et al., 1996). ASA further developed the model as SIMAP (Spill Impact Model Application Package; French McCay, 2003, 2004) for use in both marine and freshwaters; and for impact and ecological risk assessments, cost-benefit analyses, spill response planning, as well as natural resource damage assessment (Figure 1).

The three-dimensional physical fates model in SIMAP estimates distribution (as mass and concentrations) of whole oil and oil components on the water surface, on shorelines, in the water column, and in sediments. Simulated processes include: spreading (gravitational and by shearing), evaporation of volatiles from surface oil, transport on the surface and in the water column, randomized dispersion, emulsification, entrainment of oil as droplets into the water (natural and facilitated by dispersant), dissolution of soluble components, volatilization of dissolved hydrocarbons from the surface water, adherence of oil droplets to suspended sediments, adsorption of soluble and semi-soluble aromatics to suspended sediments, sedimentation, stranding on shorelines, and degradation. The algorithms and assumptions of the 3-d fates model are described in French McCay (2004).

The biological effects model (French et al., 1996; French McCay, 2003, 2004) estimates short term (acute) exposure of biota of various behavior types to floating oil and subsurface contamination (in water and subtidal sediments), resulting percent mortality, and sublethal effects on production (growth). For each wildlife behavior group, the model assumes that a portion of the animals in the area swept by surface oil over a threshold thickness die, based on probability of encounter with the oil on the water surface multiplied by the probability of mortality once oiled. Toxicity to aquatic biota in the water and subtidal sediments is estimated from dissolved aromatic concentrations and exposure duration, using laboratory-based bioassay data for oil hydrocarbon mixtures (French McCay, 2002). For each species group of fish, invertebrates and wildlife, percent loss is multiplied by density at the time of the spill to quantify injury.

Detailed descriptions of the algorithms and assumptions in the model are in published papers (French McCay 2002, 2003, 2004). The model has been validated with more than 20 case histories, including the *Exxon Valdez* and other large spills (French and Rines, 1997; French McCay, 2003, 2004; French McCay and Rowe, 2004), as well as test spills (French et al., 1997). The model has been applied to numerous injury assessments (e.g., French McCay et al., 2003c) 2003c), as well as environmental assessments and cost-benefit analyses (e.g., French McCay et al., 2004, 2005a,b,c)

Recommended Approach: Modeling with Strategic Measurements

Based on experience with the *North Cape* (French-McCay, 2003) and other spills, the most practical and realistic approach to estimating injuries resulting from a spill is to combine field sampling with modeling. The field sampling can then focus on measurable injury categories and provision of data for model calibration. For analysis of injuries to birds and other wildlife, as well as shoreline habitats, important field data that may be used as model input include environmental data (winds, currents, etc.), geographical information (shoreline, habitat mapping, bathymetry), oil properties (density, viscosity, potential to emulsify), details of cleanup activities, and spatial distributional data for the affected biota. Data used to calibrate the model include overflight maps and other mapping of the movements of floating oil, information on shoreline contamination (timing and degree of oiling), and collections of oiled birds and other wildlife.

The modeling should be performed as a two-step process: (1) first a reliable oil fate model simulation is developed and calibrated with available information; (2) then, biological effects modeling is used to estimate exposure to oil and resulting injuries. The biological modeling estimates may be compared to those estimated by field methods for verification, as data are available.

The following procedure is recommended to estimate short-term (acute) oil impacts to aquatic organisms in the water column and subtidal sediments.

1. Determine if significant concentrations of dissolved aromatics would be expected to occur in the water. If the spill volume is small, is released over a long time period (at a slow rate), is released at the water surface, and the temperature is warm

(accelerating evaporation), the dissolved aromatic contamination in the water is likely to be very low and not acutely toxic. However, the highest concentrations would be expected for subsurface releases under turbulent conditions, i.e. where whole-oil entrainment is high and predominantly in small droplet sizes. Preliminary fates modeling may be used to evaluate if dissolved aromatic contamination should be significant and where the contamination would be expected.

2. Sample the source oil, the water column, and the sediments and measure polynuclear aromatic hydrocarbons (PAHs; all, individually) in these samples. Benzene, toluene, ethybenzene and xylenes (BTEX) and substituted benzenes should also be measured (individually) if their content in the source oil is significant (e.g., for gasoline, jet fuels). Water and sediment samples should be taken at representative locations, as well as reference sites, as early as possible after the spill. This should include the first 24-48 h after the release.
3. Evaluate the chemical sample results to determine contamination resulting from the spill (as opposed to background contamination).
4. Use fates modeling to complete the picture of the fate of the soluble and semi-soluble aromatics in the oil, accounting for the entire mass balance in space and time. The field-collected concentration data, combined with overflight and shoreline oiling observations, are used to calibrate the model simulation to best fit the observations.
5. Calculate the toxicity of the oil for the particular spill conditions using the measurement data on percent composition of individual aromatics and an additive toxicity model (see French McCay, 2002).
6. Compare the acute (e.g., Lethal Concentration to 50% of exposed organisms, LC50) and No Observable Effects Level (NOEL) concentrations to the modeled concentrations resulting from the spill to determine if there was any potential for effects.
7. To estimate mortality of aquatic organisms, the time and temperature dependence of toxicity needs to be addressed. The biological effects model in SIMAP evaluates exposure concentrations to organisms over time by simulating the movements of organisms relative to the dissolved aromatic plume. Acute effects such as mortality are estimated using exposure time- and temperature-corrected LC50s.

Note that the procedure may be performed stepwise, since many oil spills do not significantly impact aquatic organisms and preliminary analysis is capable of identifying these conditions.

Finally, restoration scaling should use similar metrics and data as for injury quantification. Restoration scaling is a modeling exercise: ecological and/or human services gained by the restoration are integrated over time and the size of the restoration project is such to provide the same magnitude of services as that lost (i.e., scale of the injuries). Examples of restoration scaling using modeling, and metrics employed during injury quantification, are in French et al. (2003a,b) and French McCay and Rowe (2003).

Conclusions

In conclusion, models are powerful and cost-effective tools for injury quantification. It is typically not possible or cost-effective to evaluate all spill impacts using field data exclusively. Spill impacts may be accurately quantified using modeling combined with as much site-specific data as can feasibly be collected (focused on important injury categories) for documentation of specific injuries and calibration of model results. Needed information to improve the accuracy of oil fates and effects modeling and combined approaches to determine spill injuries includes: more accurate environmental data (i.e., winds and currents); more accurate field observations of pre-spill abundance (in advance of oil or in nearby areas during the spill); error estimation on abundance and observations of oiled biota; and explicit reporting of the details of field observations and subsequent calculations.

This paper addressed the scientific merits of modeling. The point of the discussion is that modeling is scientific analysis formalized to be quantitative and use best available information to develop the most defensible results possible. The model should and can be based on science, and be cost-effective in both the assessment and restoration implications.

Biography

Deborah French-McCay received her bachelor's degree in Zoology from Rutgers in 1974 and her Ph.D. in Biological Oceanography from the University of Rhode Island in 1984. She is a Principal at Applied Science Associates (Narragansett, RI, USA), where she specializes in quantitative assessments and modeling of aquatic ecosystems and populations, oil and chemical transport and fates, toxicity, exposure and the bioaccumulation of pollutants by biota, along with the effects of this contamination. These models have been used for impact, risk, and natural resource damage assessments, as well as for studies of the biological systems.

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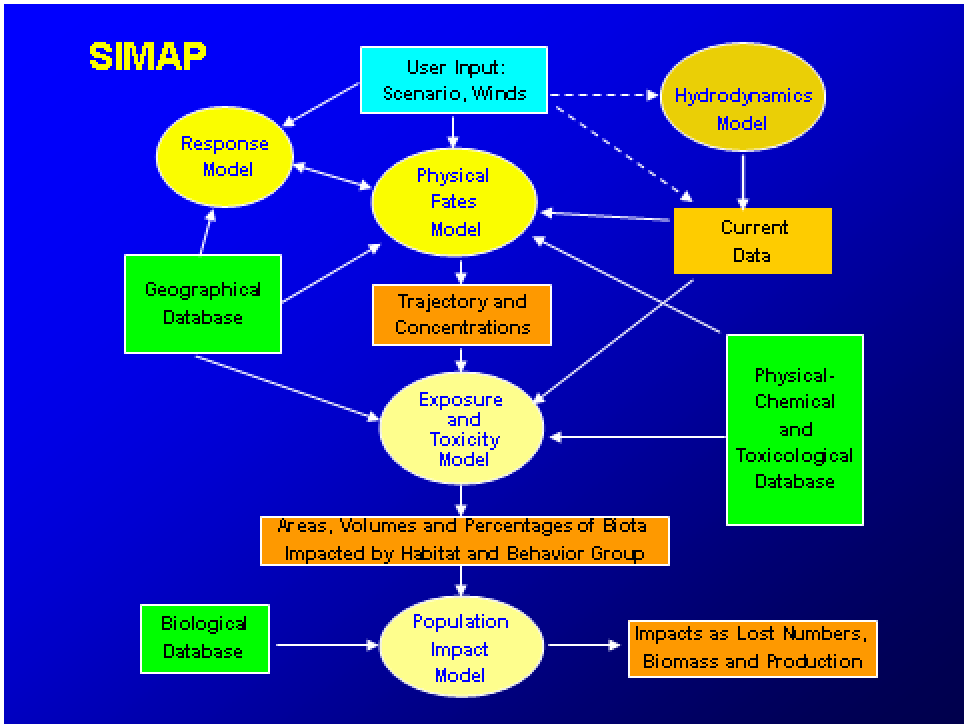

Figure 1. Diagram of SIMAP often used for NRDA modeling.