Chapter 1 Operational oil spill modeling: from science to engineering applications in the presence of uncertainty

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Abstract Quantifying uncertainties in real-time operational oil spill forecasts remains an outstanding problem, but one that should be solvable with present science and technology. Uncertainties arise from the salient characteristics of oil spill models, hydrodynamic models, and wind forecast systems, which are affected by choices of modeling parameters. Presented and discussed are: (1) a systems-level approach for producing a range of oil spill forecasts, (2) a methodology for integrating probability estimates within oil spill models, and (3) a multi-model system for updating forecasts. These technologies provide the next steps for the efficient operational modeling required for real-time mitigation and crisis management for oil spills at sea. ¹

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1.1 Introduction

Modeling of oil spills on the water's surface has reached an important milestone. We believe the next major advance for improving operational oil spill forecasts is by addressing the accumulation of uncertainty in the wind, wave, and current models. In this chapter, we propose modeling approaches for real-time evaluation of uncertainty in oil spill trajectory models and explore the underlying sources and analyses methods for uncertainty. Our objective is to stimulate development of quantitative model evaluation methods that can be readily used to improve management and response of oil spills. Herein we develop two major options in advancing oil spill modeling with uncertainty: in $\S1.6$ a systems-level approach is proposed for evaluating real-time uncertainty at each level of modeling, and in $\S1.9$ a probability-based approach for oil spill modeling that could be used either as part of a systems-level approach or on its own if the uncertainty in wind, wave, and hydrodynamics can be *a priori* quantified.

Operational modeling of marine oil spill trajectories serves two key purposes: (i) forecast the likely spill path for immediate mitigation and capture operations [16, 23], *e.g.* deployment of booms, skimmer boats, and dispersants; and (ii) hindcast the likely impacted coastal shorelines, bays, and estuaries that might be affected by escaping oil and hence require further monitoring (*e.g.* [26]). We are focused on issues associated with operational modeling for the first purpose, where time constraints require immediate application of available models that can be quickly run immediately after a spill is reported.

Predictive oil spill models are inextricably linked to predictive numerical models of atmospheric and oceanic dynamics [14]. In many places, operational numerical models can provide the short-term (usually around the next 72 - 96 hours) forecasts for ocean currents, wave conditions, and wind fields as input to oil spill fate and transport models. These operational models integrate the conservation laws for mass and momentum forward in time to provide physics-based (in contrast to statisticsbased) predictions of ocean and atmosphere dynamics. Due to the nonlinear nature of the governing equations, there is a continuous need for acquisition of real-time ocean data to validate, update, and adjust the model to better match reality. The complex dynamics and limited predictability of coastal oceans has motivated development of Coastal Observing Systems (COS), which are being implemented in many regions (e.g. [30, 40, 44, 51]). COS typically monitor physical, chemical and biological ocean properties by combining remote monitoring (HF-Radar, satellite imagery) and *in situ* devices (floats, drifters, gliders, moorings, etc). This process, from the acquisition of real data to the dissemination of ocean currents for diagnostic or prognostic purposes, requires the combined efforts of basic and applied research in several engineering fields as well as computer sciences, along with coordination and support from government mission agencies. The goals for all such systems are essentially the same: fast, accurate and user-friendly tools with visual interfaces capable of providing the information needed for making timely and well-founded decisions regarding coastal protection, security and implementation of rapid, effective contingency plans [7, 11].

Oil spills in coastal waters require rapid deployment of mitigation personnel and equipment to the right places at the right time to maximize recovery and minimize environmental damage. For spills sufficiently far offshore in good weather, distance equates to time and emergency managers have the (relative) luxury of tracking actual spill motion via aircraft, boats, and satellite. However, as weather turns foul or a spill occurs close to shore (where response time is short), models provide a key source of information for equipment deployment decisions. The value of model-produced data for emergency managers depends on its timeliness and the reliability of the predictions – both *actual* and *perceived*. Unfortunately, there is little guidance available for practical evaluation of how well (or poorly) any particular model will predict spill transport or how cumulative effects of uncertainty should be evaluated. This hole in our knowledge is the motivating focus of our work.

This chapter presents an overview of a generic oil spill forecast system ($\S1.2$), followed by a discussion of salient characteristics of oil spill models ($\S1.3$), sources of uncertainty ($\S1.4$), model parameters affecting uncertainty ($\S1.5$), a proposed systems-level approach for producing a range of oil spill forecasts ($\S1.6$), a multimodel system for updating forecasts ($\S1.7$), discussion of uncertainty evaluation methods ($\S1.8$), and methods for integrating probability estimates within oil spill models ($\S1.9$).

1.2 Oil spill forecast systems

Predicting the fate and transport of an oil spill requires a system of models, including forecast models for wind, water currents, waves, oil advection/dispersion, and the weathering processes that alter oil properties [24]. A monolithic model that predicts all driving/response processes is simply impractical to build and maintain, so operational models generally use forecast models for wind, waves, and currents originally designed for other purposes. An efficient operational system requires automated linking of models (*i.e.* output from one model is input to another), along with integration of real-world observational data (e.g. [27, 47]). For rapid use in emergency operations, an oil spill forecast system also benefits from a user interface displaying the model predictions as a geo-referenced visualization that can be readily interpreted by oil spill response personnel. These components can be generally structured as in Fig. 1.1 with three different computational modules, (i) geophysical forcing, (ii) oil transport and chemistry, and (iii) visualization; which are linked to COS data and known (or estimated) information about the oil spill source [46]. Note that the spill forecast system illustrated in Fig. 1.1 has a unidirectional flow of data: there are no feedbacks from the oil spill model to the geophysical forcing models. However, we know that surface oil can affect wave development and the transfer of wind energy into the water, which in turn affects local surface currents and near-surface turbulence. Given the uncertainties in present modeling systems, it is likely that such feedback effects are of minor consequence, but this remains an

area where (to our knowledge) there have been no clear quantitative evaluations of these phenomena or applications within operational models.



Fig. 1.1 General structure of an oil spill forecast system. Geophysical models typically require data from a coastal observation system (COS). River inflow forecasts can be considered part of typical COS data. Individual components are discussed in text.

Oil spill data – An oil spill model requires data for the spill location, event time, spilled volume, oil type, fraction of oil at the water surface, and information on the ocean conditions that can affect the near-field behavior. Most oil spill transport models are designed to advect and disperse oil at (or near) the water surface at relatively coarse grid scales, so the near-field spill behavior must be either modeled separately (particularly for deep-water spills, [31, 56]) or estimated based on previous experience with similar spills.

Geophysical forcing models – Developing an integrated geophysical forecast system is a non-trivial effort. Ideally, such a system should be in place and continuously running so that nowcast and forecast winds, waves, tides, river inflows, and currents are always available. Such a modeling system should be integrated with COS data so that each successive forecast uses the latest available observations and the latest forecast data. Where predictive numerical models have not been developed and tested, it is possible to use COS measurements and climatology data to build a forecast model based on statistics [2]; however, until such models are more comprehensively tested, they are best used in response planning and management rather than for an actual event response.

Oil spill models – An oil spill model represents the physical and chemical processes governing advection, dispersion, and weathering of the spill. Oil advection is driven by water currents, wind, and waves [45]. The dispersion of the oil depends on wave conditions, turbulence in the ocean surface layer, and advective processes

smaller than the grid scale of the hydrodynamic model. Chemical processes lead to degradation and transformation of the spill (*e.g.* spreading, emulsification, dissolution, evaporation [57]), which can reduce the surface oil volume and change the oil response to physical forcing. For example, emulsified oil "tarballs" take on the density of the surrounding water and will sink below the water surface if advected into a region of warmer (less dense) water. Near-surface submerged tarballs can be affected by currents diverging from the surface currents, resulting in different transport paths.

Visualization and analyses – The output from an oil spill model is the time evolution of the expected location, composition, and extent of spilled oil. Ideally, an integrated operational system would include visualization of a probability envelope for the future spill positions, much as is done in the hurricane/typhoon forecasting community. However, present oil spill visualizations are generally based on producing either a snapshot map of representative oil spill particle trajectories (*i.e.* a "spaghetti" diagram), or a movie of an evolving point cloud of particles. As Geographical Information Systems (GIS) become more powerful and usable over mobile platforms (*e.g.* smart phones, tablets), oil spill visualization systems should employ GIS standard formats for output data to allow web-based access for emergency response personnel. Standardization within a GIS also allows spill trajectories to be linked to existing Environmental Sensitivity Indexes that classify sensitive coastal areas by their degree of exposure and vulnerability [20].

1.3 Oil spill models

Oil spill models typically represent the spill as a collection of mass-less particles moving passively with the water and without any particle-particle interaction. These Lagrangian particles are advected based on modeled fields of the wind, waves, and currents in a deterministic fashion: as the simplest example, given a position vector of a single particle at time step n as \mathbf{x}^n , the position at succeeding time step n + 1 is given by

$$\mathbf{x}^{n+1} = \mathbf{x}^n + \Delta t \left(\mathbf{U}_{\text{wind}} + \mathbf{U}_{\text{wave}} + \mathbf{U}_{\text{current}} \right)$$
(1.1)

where Δt is the particle transport time step and the U vectors are the modeled effects of wind, waves and currents on the particle. Note these are not the wind, wave, and current velocities themselves, but their modeled net effects with the underlying assumption of linear superposition. More complex algorithms are often used in place of the simple explicit Euler scheme above, *e.g.* the Runge-Kutta 4th-order (RK4) [6]. The U fields are typically based on coarse spatial and temporal scales relative to the finer-scale motions that physically spread oil across wider areas, so some form of dispersion (or diffusion) sub-model is required or the particle cloud will remain unrealistically compacted. For models including chemical evolution, the oil weathering can affect the spill's interactions with wind, waves, currents, and dispersion, which further change the spill response over time.

Oil spill models are available with several degrees of complexity for both physics and chemistry. The simplest physics represent only movement of surface particles driven by the 2-dimensional (2D) water surface velocity, wind drag, and waves. Such models typically use statistics-based dispersion parameterizations (e.g. white noise, Markov chains). More advanced physics models include 3D currents and transport [53], along with more physics-based dispersion models (e.g. mechanical spreading, particle breakup [43], Langmuir circulations [50]). Although 3D models should theoretically be preferred, representing the vertical distribution of oil in the near-surface water column remains a challenge: the vertical grid resolution in most hydrodynamic models is relatively coarse and we lack the comprehensive data on vertical oil dispersion under wave-breaking conditions that are necessary for coarse-grid model parameterization. Indeed, it remains an open question as to whether 3D models are necessary for operational modeling or if forecast uncertainties will dominate the 3D effects. Oil spill models with simpler physics are suitable where confidence in the underlying geophysical forcing models is low, e.g. where a coarse hydrodynamic model grid makes impossible to resolve the important velocity strain-rates required by a physics-based dispersion model.

The simplest oil spill chemistry model is no model at all, which is appropriate where uncertainty in the geophysical forcing dominates the results over short time periods (for which weathering is less important). More advanced models include effects of the type of oil along with processes such as dissolution, emulsification and/or evaporation [11]. It should be noted that 3D transport and chemical evolution for a deepwater blowout remains a scientific challenge due to the complex physics of an oil/gas plume and transformations of the gas phase during ascent [13].

1.4 Sources of uncertainty

From a science point of view, we seek to understand and minimize sources of error and uncertainty in any modeling system. However, for emergency management we need rapid answers to some practical questions: *How good is this prediction and can we rely on it for deploying response equipment?* Before trying to quantify uncertainty, it is useful to review the fundamental sources.

The major contributors to uncertainty in any modeling system fall into four categories:

- i) structure of the model,
- ii) empirical parameters,
- iii) initial conditions,
- iv) boundary conditions.

Structural uncertainty – Choices made in governing equations (e.g. use of hydrostatic instead of non-hydrostatic equations for a hydrodynamic model) and choices

made in developing a discrete version of the equations (*e.g.* grid scale, time step, numerical solution method) contribute to an underlying structural uncertainty, which imposes limitations on how well the model can represent the actual physics. This structural uncertainty exists for both geophysical and oil spill models.

Empirical parameter uncertainty – Any oil spill modeling system has dozens, if not hundreds, of parameters; e.g. coefficients for sub-models of turbulence, wind/wave drag, and oil spreading. Parameters are typically selected based on combinations of laboratory studies, prior field studies, theory, and modeling experience. Unfortunately, one can never be sure of having the exactly "correct" set of parameters - even if we simply define "correct" as the set of parameters for a given model structure that provides a prediction within some desired accuracy. To add further complexity, parameters are often used to compensate for model structural errors and thus cannot always be taken from experiments or theory without considering the model formulation. For example the turbulent eddy diffusion coefficient in a hydrodynamic model is typically a function of the local shear stress; at different grid scales the resolved shear will have different values and hence needs different eddy diffusion coefficients to match real-world physics. Furthermore, if the hydrodynamic eddy diffusion coefficient is overestimated then a corresponding underestimate of oil spill diffusion might be necessary for a highly-accurate prediction. We generally do not know whether a particular parameter is over -or under- estimated, so it is impossible to specifically set compensating parameters; as a result, there are multiple layers of interaction between parameter uncertainties.

Initial condition uncertainty - The output from an oil spill forecast system is subject to initial condition (IC) uncertainty for both the oil spill event and the geophysical forcing models. The IC uncertainty for the oil spill includes the initial volume [55] and the near-field forces that give shape to the initial slick. In some cases the chemical composition of the oil might also be uncertain at the time of the spill [37]. In contrast to this irreducible oil spill IC uncertainty, the geophysical forcing IC uncertainty can be readily addressed by having geophysical models that are continuously (or periodically) running. When a hydrodynamic model is started at some time t = 0, the initial velocity field over the entire model domain is typically zero because we do not have sufficient data for anything more complex. There is some spin-up time that it takes a model to "forget" that it started with the wrong velocities [21]. Hydrodynamic spin-up time can vary from days to several weeks, depending on the scales of the system. Testing for spin-up time is relatively straightforward by starting the model from successively older time points. When starting at an older time does not change the prediction for today, the model results are effectively independent of the starting conditions and the geophysical IC uncertainty is essentially zero. The key point is that operational oil spill models *must* start from a hydrodynamic model that is already running and past its spin-up time; for any significant domain, a hydrodynamic model cannot be expected to reach spin-up in time for an accurate forecast if the model is only started after a spill is reported.

Boundary condition uncertainty – Boundary condition (BC) uncertainty also includes both oil spill and geophysical forcing components. At the oil spill itself, any ongoing leakage and its subgrid (near-field) oil distributions are typically uncertain. Where the oil hits a land boundary, the processes by which the oil adheres or remobilizes are poorly understood, again resulting in highly uncertain BC. In geophysical modeling, the 3D currents and water surface elevations at the computational domain's edges are never known exactly, but modelers have developed sophisticated methods to reduce the effects of these uncertainties (*e.g.* [59]). Nevertheless, it is necessary that the hydrodynamic model's artificial boundaries should be as far as possible from the location of an oil spill to minimize BC effects.

Wind plays a major role in BC uncertainty. The spatial and temporal fluctuations of the wind field are never precisely known (even in hindcast), and the modeling of wind-driven waves, turbulence, and currents is strongly affected by empirical parameter choices and model structures. Added to these effects is the inherent uncertainty in the overall wind forecast speed and direction. It can be argued that the BC uncertainty associated with how energy from the wind affects waves, currents, and the oil spill is the dominant form of uncertainty for any spill.

In a more general sense, the uncertainties above can be divided into "epistemic" and "aleatoric" classes [32]. For our purposes, the former can be thought of as uncertainty developed in modeling system through lack of either adequate models or data (*i.e.*, things we either know or should know); whereas the latter can be thought of as uncertainty associated with the chaotic behavior of highly nonlinear systems, which is deterministically unknowable (*i.e.* things we can only "know" stochastically) [38]. This classification concept can be used to focus model development efforts on reducing epistemic uncertainties, whereas system operational efforts can be focused on evaluating effects of irreducible aleatoric uncertainties. For example, part of the uncertainty in near-surface ocean currents in a coarse-grid hydrodynamic model is epistemic uncertainty, which can be reduced by using finer grid -a choice made during model development. In contrast, the effects of aleatoric uncertainty associated with forecast wind conditions can only be evaluated for a particular event (e.g. by Monte-Carlo simulation using a range of possible forecasts), but cannot be precisely known *a priori*. However as a practical matter, once a modeling system has been put into operation - that is, the science has been executed to minimize epistemic uncertainty as much as practical for available resources – then any uncertainty in the system, whether aleatoric or epistemic, is essentially irreducible. Thus, we need practical methods for evaluating uncertainty during both model building (to focus our efforts in uncertainty reduction) and model operation (to understand effects of remaining uncertainty).

1.5 Model design and parameters affecting uncertainty

The generic forecast system of Fig. 1.1 includes models with a wide variety of parameters and settings that affect uncertainty. Many parameters are specific to particular model designs; but the following provides an overview of some of the more common parameters.

Oil spill model time step – The time step used for the Lagrangian integration of oil spill movement is a control on the relationships between space, time, and the partitioning of transport between advection and a stochastic model of diffusion. Coastal ocean studies have typically used 30 minute time steps consistent with their spatial resolution and water velocities, *e.g.* [22, 39]. For higher-resolution models close to shore, smaller time steps are typically necessary for velocity fields that are more highly variable in time and space.

Numerical scheme – Oil spill transport models can be coded with different options for transport. The simplest Lagrangian models are 1st-order forward Euler transport, which use time n velocity contributions at a particle position to compute the particle displacement, as in eq. (1.1) above. However, such simple models are recognized as having limited accuracy [5]. The Runge-Kutta 4th-order (RK4) is a popular high-order method as it takes into account the changing velocity field over a particle path. Although the RK4 itself is computationally efficient, its overall performance depends on the speed of the interpolation scheme from the hydrodynamic model grid to an arbitrary particle location. For an unstructured (triangular or generalized polyhedron) hydrodynamic grid, this interpolation can be computationally expensive.

Wind forcing – The direct force of the wind on an oil spill is arguably negligible; however, few operational hydrodynamic models are designed with the fineresolution vertical grid scales and algorithms that can accurately reproduce the surface and near-surface water velocities. Thus, the hydrodynamic model surface water velocity field is *not* the velocity field that an oil spill will actually see. Because the surface and near-surface velocities are strongly affected by the local speed and direction of the wind, oil spill models typically include a "wind drag" parameter that provides a correction to the hydrodynamically-modeled water surface velocities for particle transport.

Wave forcing – The transport cause by waves is typically added through a Stokes drift term that requires empirical parameterization. Selection of the parameter depends on the type of wave model.

Diffusivity – Diffusivity parameterization controls the overall spread of particles produced by an oil spill model; *i.e.* this is not *diffusion* of oil molecules into solution with water, but the *dispersion* or spreading of the oil on or near the water surface. This diffusivity is not generally a direct representation of the dispersion physics

acting on an oil slick, but instead a stochastic parameterization of turbulence and the unresolved spatial structure of the modeled water velocities. Thus, the appropriate oil spill diffusivity is difficult to directly link to physically-based eddy diffusion coefficients (*e.g.* [34]) or turbulence models used in hydrodynamic simulations. Diffusivity for an oil spill is often modeled as parameterized white noise.

Hydrodynamic model grid – Grid spacing affects the spatial and temporal velocity gradients that can be represented in the hydrodynamic model. Most models are limited by a CFL condition such that $u\Delta t/\Delta x < C_{limit}$, where *u* is the water velocity, Δt is the model time step, Δx is the local model grid scale in the same direction as *u*, and C_{limit} is the CFL limit that is typically O(1), with the exact value depending on the numerical algorithm. Thus, the model grid spacing also controls the model time step. For coarser model grids, both spatial and temporal gradients will be less accurate than with finer grids [9], so the wind forcing and diffusivity parameters will need to be different (typically higher). In particular, for large-scale oceanographic models the effects of submesocale instabilities are poorly modeled and must be parameterized [17].

The challenge facing any oil spill forecast system is that the parameterization of these different aspects are interdependent. Obtaining a "best" value of any given parameter is impossible without considering the system modeled, the types of models applied, and choices in the model setup (*e.g.* grid spacing). From the standpoint of uncertainty evaluation, determining the best value is less important than estimating a range of reasonable parameters for a given system. In §1.8 we discuss some of the ways that hindcast modeling and drifter data can be used to improve our understanding of these parameters.

1.6 Systems for real-time forecast uncertainty

Emergency responders need estimates of spill forecast accuracy and likely outcomes, such as when and where a spill might make landfall. Ideally, forecasts should contain a range of results, such as the earliest time landfall is expected or the widest range of beaches that could be affected. A single model forecast cannot provide the necessary range of data for effectively deploying emergency response equipment. Obtaining systematic estimates of real-time forecast uncertainty requires an operational system that evaluates the key uncertainty sources outlined in $\S1.4$, above. Some uncertainties can be minimized in model construction, but the remaining uncertainties need to be evaluated and reported to emergency managers with visualization tools that are easy to use and understand. Although some progress has been made (*e.g.* [18, 39, 41], presently there are no operational systems that can evaluate the accumulation of uncertainty from the wind forecast through hydrodynamic, wave, and oil spill modeling. Fortunately, the tools and technology to build such a system are now available.



Fig. 1.2 Top-level structure for multi-model operational forecast system. Multiple wind forecasts are used to drive sets of hydrodynamic models using different wave model parameters and different hydrodynamic parameters. Highlighted section is expanded in Fig. 1.3.

Perhaps the simplest way to evaluate forecast uncertainty is a brute-force multimodel approach that takes the real-time forecast system of Fig. 1.1 and creates multiple model instances in a hierarchical series of solutions (Figs. 1.2, 1.3). A multimodel operational system provides a range of forecast oil spills that can be used to develop probability maps instead of a prediction cloud. Some number, N_{wind} , of wind forecasts are created based on a primary wind forecast and likely perturbations. For each wind forecast a set of independent hydrodynamic models is run. These models use some N_{wave} different wave model coefficients and some N_{hydro} different hydrodynamic model conditions (*e.g.* different wind drag coefficients, tidal forecasts, or turbulence parameters). For each hydrodynamic model, a set of independent oil spill models is run with N_{IC} different oil spill initial conditions and N_{oil} different oil spill models and a total of $N_{wind}N_{wave}N_{hydro}N_{IC}N_{oil}$ oil spill models.

Three perturbations at each system level could be used to represent the expected parameters along with high and low sets that bound the expected values. Note that



Fig. 1.3 Second-level structure for multi-model forecast system. Each hydrodynamic model drives multiple oil spill models with different IC and different oil spill model parameters, providing multiple forecasts that can be used for probability map visualizations. This figure is expanded detail of highlighted portion of Fig. 1.2.

full Monte-Carlo methods (random selection of the parameters and conditions over a statistically valid set at each model level) would produce an impractically-large set of simulations. Selection of high and low conditions/parameters requires thorough understanding of uncertainty contributions, which can be readily handled by hindcast analyses during development of an operational system (§1.8). A system with three condition sets at each level (*i.e.* Figs. 1.2, 1.3) would require 27 hydrodynamic model runs and 243 oil spill model runs, which could be accomplished with modest investment in a set of standard workstation computers. A relatively small number of perturbations in each step of the modeling provides a wide range of model results for statistical processing.

Implementing an operational system with this large number of simulations might appear to be computationally impractical. However, the continuing advance of lowcost multiprocessor workstations and GPU computing changes the question from "can we do this?" to "given our budget, how big can N_x be for each component?" Compared to hydrodynamic models, oil spill models run very quickly and take relatively little memory, so running a large number of such models is eminently practical. Hydrodynamic models present a greater challenge, but can be implemented using separate logical processors of a single workstation for separate models (where

 N_{hydro} is small) or with multiple networked workstations (where N_{hydro} is large). The number of hydrodynamic models can be reduced if the uncertainty contributions in the wave model and hydrodynamic model parameters can be minimized; indeed, if these can be neglected the only uncertainty driving hydrodynamics will be wind forecast, so that $N_{hydro} = N_{wave} = 1$, and the number of hydrodynamic models is simply N_{wind} and the total number of oil spill models is $N_{wind}N_{IC}N_{oil}$. A key point is that multiple hydrodynamic model are only needed after a spill has occurred; that is only a single hydrodynamic model is necessary to minimize *initial condition uncertainty* of spin-up (§1.4). Thus, if new forecast data is available every 3 hours and a 72 hour forecast is desired, computational power must be continuously available to run a single hydrodynamic simulation at least $24 \times$ faster than real time. Additional computational resources are only needed when a spill occurs and the full multi-model forecast system is invoked.

The proposed operational forecast system described above is effectively *static*; that is, it provides the data for a single animation of a probability field for an oil spill location based on data available at the initiation of the modeling. However, during an emergency there will be new COS data and updated wind forecasts available on a regular basis, which requires a *dynamic* modeling system; *i.e.* the operational system should automatically obtain new data/forecasts, integrate the new data into the models, and re-run all the models to produce a new set of forecasts and visualizations. Techniques for handling these issues are discussed in §1.7, below. To make such a system practical, computational power needs to be made available such that an entire multi-model forecast sequence, from wind to hydrodynamics to oil spill model, can be completed before the next COS data and wind forecasts become available.

A further difficulty in providing operational forecasts is the fact that any Lagrangian particle simulation has a limited time-horizon for reliability. Because the Lagrangian particles are inherently integrative of error, their divergence from the real-world will increase with time. The most effective operational system will integrate data sources for estimating the real-world position of the oils spill (*e.g.* through satellite tracking, [54]) that can be used to periodically reset the oil spill particles to a new "known" position.

Clearly, creating and automating a multi-model operational system with forecast uncertainty presents a number of challenges, including (i) generation of perturbed wind forecasts, (ii) selecting parameter sets for wave, hydrodynamics, and oil spill models, (iii) selecting sets of reasonable initial conditions for the oil spill, (iv) analyzing and visualizing the combined forecast data, (v) automated updating of models as new data and forecasts are received, and (vi) creating a system that integrates models and data so that the user provides the location, estimated size, and oil type that is spilled and obtains an animation of the time-evolution of a probability map for the oil spill. To address some of these challenges, authors Sayol and Orfila have developed new techniques for probability simulations within oil spill models and probability mapping visualization (\S 1.9), while simultaneously authors Hou and Hodges have developed the HyosPy system of model integration (\S 1.7).

1.7 Multi-model integration and updating predictions

The Hydrodynamic and oil spill Python (HyosPy) code has been developed as a testbed for integrating hydrodynamics and oil spill models in a flexible manner [18, 19]. Presently, HyosPy is designed to integrate COS data, wind forecasts, and multiple hydrodynamic models linked to independent oil spill models, as illustrated in Fig. 1.4. The results are visualized in Google Earth/Maps applications. HyosPy uses the Python scripting language, which provides a flexible "wrapper" to integrate existing models, servers, connections to online data services, and visualization tools. The present version of HyosPy is being tested for coastal embayments of Texas (USA) with automatic tidal data downloads from the Texas Coastal Ocean Observation Network (TCOON) [49] and wind forecast data from a Texas A&M University server. The hydrodynamic model used is SELFE [42], which has been under review by the Texas Water Development Board (TWDB) and General Land Office (TGLO) as a replacement for the TxBlend model, which is presently the operational oil spill model used inside barrier islands along the Texas coastline [52]. The oil spill model for HyosPy is the NOAA PyGnome model, which is a new Linux/Python version of the GNOME operational oil spill model used by emergency response agencies across the USA [4, 33].



Fig. 1.4 HyosPy structure for automatic updating of forecasts and visualizations. Here each forecast wind/tidal condition drives a single hydrodynamics and oil spill model, with each model based on the latest available data and forecasts. Visualizations include both the latest forecasts and prior forecasts.

HyosPy was run as a real-time demonstration on Feb 4, 2014 using COS and forecast data downloaded from the internet as it became available and an imaginary oil spill near a beach in Corpus Christi Bay (Texas, USA). As shown in Figs. 1.5 and 1.6, HyosPy produced tracks 3 hours apart, where each track is based on combination of the latest available hindcast and forecast data with new instances of both the hydrodynamic model and the oil spill model. The oil spill diffusivity coefficient



Fig. 1.5 HyposPy visualization of forecast tracks for an imaginary oil spill in Corpus Christi Bay (Texas, USA). Upper frame is the initial forecast track available within minutes of the spill. The middle frame is the forecast tracks available at 0900 using new wind forecast data. Note the 0000-0600 forecasts are almost indistinguishable in their prediction of the 48 hour position. Lower frame shows predictions in the afternoon initially move away from and then back toward the beach. Continued in Fig. 1.6. Visualization using Google Earth with additional annotations (in yellow) for clarity.



Fig. 1.6 HyposPy visualization of forecast tracks, continued from Fig. 1.5. Forecast tracks in the second day (0000 to 1200) are moving consistently closer to the beach. Visualization using Google Earth

in these models is low, so the Lagrangian particle stay close together in each track, which provides clearer visualization of how the model operates.

Key innovations of HyosPy are (i) automated re-running of the hydrodynamic model as new data becomes available, and (ii) using successive forecasts in the visualization to provide insight into how the model predictions are changing as new data is added. Because HyosPy is a wrapper around models rather than a model itself, it can be readily modified to include multiple perturbed forecasts, hydrodynamic models, and oil spill models along each of the linear paths of Fig. 1.4; that is, we can implement Figs. 1.2 and 1.3 by creating multiple model instances within the existing system. As an operational approach, HyosPy could be set up with a single continuously-running hydrodynamic model using the latest wind/tidal forecast data. When a spill occurs, additional computer resources can be added to allow multiple hydrodynamics models and oil spill models to be run using perturbed forecast data. Recent tests have shown that HyosPy can be operated as a web service with a continuously-running hydrodynamic model [18, 19]. For a real (or imaginary) oil spill, the user enters the oil spill location, time, oil type, and quantity into boxes on a web site and HyosPy produces, then automatically updates, a series of predicted spill tracks. HyosPy handles the data manipulation, reformatting, and initiation calls between models without user guidance, which makes the complex multi-model processing entirely invisible.

HyosPy development was motivated by a need for integrative tools that are extensible and flexible so that new models and new data sources can be readily implemented. HyosPy is formulated with two module levels: high-level modules controls the overall logic and the Application Program Interface (API), whereas lower-level modules process specific tasks, *e.g.* converting data from particular hydrodynamics

model to a common NetCDF format for oil spill models. Adding new models or data is straightforward as the input/output for each module is designed without downward/upward restrictions. Using the Google Maps/Earth visualization tools provide portability, with results displayable over the web on any Java-enabled browser for all supported terminal platforms (e.g., laptop, tablet, and smart phone) and operating systems (Windows, Mac OSX, Linux, and Android) [18].

1.8 Evaluation of uncertainty

Evaluating uncertainty with hindcast models and field-deployed drifter experiments [35] can provide insight into setting up both the "best" parameters and upper and lower bounds for a multi-model operational system (*e.g.* as in §1.6). For an oil spill model, a typical IC uncertainty is in the oil spill shape. Typical BC problems include the appropriate effect of wind drag on the oil and effective diffusivity of the oil. Quantification methodologies for these issues are discussed and demonstrated below. These methodologies were designed to provide rapid multiple oil spill model predictions, which can be used to develop probability contours for emergency responders [39]. The present discussion is for a 2D oil spill confined to the water surface, however there are no theoretical impediments for extension to 3D.

Geometric uncertainty – A critical decision in the design of any operational oil spill forecast system is in the choice of the model grids – both for the hydrodynamic model and the oil spill model. For the hydrodynamic model, geometrical uncertainty is affected by interaction of the numerical algorithm accuracy, the hydrodynamic model time step, and the grid cell spacing. Further complexity is added by the choice of unstructured, curvilinear, or Cartesian grids. The advantages and disadvantages of different grid methods for hydrodynamics are subjects of ongoing debate; however, from the oil spill modeling perspective the important issue is that finer model grids provide a more accurate resolution of the spatio-temporal evolution of the surface currents, and hence reduce the uncertainty in oil spill modeling associated with hydrodynamics. Unfortunately, decreasing the grid length scale by 50% in each horizontal direction requires an increase of the number of horizontal grid cells of $4 \times$ and a reduction in the model time step by 50%, which leads to an 8× increase in computational requirements for only a factor of two improvement in grid resolution. Thus, operational models are a compromise between what is desirable and what is achievable with the computational resources at hand. As discussed in $\S1.6$, for a practical system the hydrodynamic model should be able to produce a set of velocities fields for the desired forecast interval (e.g. 72 hours) in substantially less than the time between new updated forecasts. This need inherently limits the practical grid resolution of the hydrodynamic model.

As further issue in geometrical uncertainty, Lagrangian particle transport oil spill models are faster (and easier to code) for structured model grids (either Cartesian or curvilinear) because Lagrangian particle models generally operate with each particle defined by vector position $\mathbf{s} = a\hat{i} + b\hat{j} + c\hat{k}$ in a 3D space (or 2D for surface models). To move a particles through space/time, the velocity at the particle's present location must be interpolated from the velocity field on the hydrodynamic model grid. If a structured hydrodynamic grid is used, identifying the neighbor velocities is trivial; however, for an unstructured grid the identification problem can be computationally expensive. Nevertheless, unstructured hydrodynamic grid is a a Lagrangian particle and unstructured hydrodynamic grid is to "rasterize" the velocity fields; *i.e.* interpolate the velocities to a structured grid before computing the Lagrangian particle motion. This adds a second layer of interpolation (hydrodynamics to raster, raster to Lagrangian particle) and hence another source of uncertainty

Geometrical uncertainty cannot be easily evaluated during run-time of an operational forecast system. Instead, the effects of geometrical uncertainty should be analyzed during development of the system through model-model comparisons and drifter analyses using hindcasts. For model-model comparisons, a hydrodynamic model can be run with the smallest practical grid and time step over a number of hindcast periods to provide a set of reference cases. These reference cases can be considered the best possible simulations for the available model. Statistical analyses can be used to evaluate the difference between the reference cases and simulations at the coarser grid scales and larger time steps that are practical for an operational system. There remains an open question as to the best approach to incorporate such data into an effective parameterization of uncertainty. The most obvious possibility is to use the local velocity variance to scale a random perturbation in the velocities used for the oil spill Lagrangian transport.

Wind drag coefficient - Modeled surface oil spills are directly affected by wind; that is they will move with velocity vectors slightly different than the modeled water currents at the surface. In hydrodynamics, the wind causes shear stress at the surface that creates 3D turbulence and transfers momentum down from the surface into the wind-mixed layer. Hydrodynamic models focus on getting the net downward transfer of energy and momentum, and the modeled "surface" velocity actually represents the spatially-averaged velocity in the surface grid cell whose thickness is typically O(1) - O(10) m, depending on the model scale. In contrast, the wind effect on surface oil (or a floating object) does not have a significant downward transfer of momentum and must be directly included in the floating oil particle transport computation. The effect of wind drag on the oil velocity (Uwind) is typically represented using a drag coefficient (γ) and the wind velocity (V_{wind}) such that $U_{wind} = \gamma V_{wind}$. Because the drag is generally small, γ is often reported as a percentage of the wind speed. Using winds measured at 10 m above the water surface, γ in the range [0, 3.5%] have been recommended [3, 29]. More recently, [22] argued for γ values up to 6.0%.

The sensitivity of an oil spill model to the selection of γ can be evaluated by model-model hindcast comparisons and the "best" γ for a particular combination of hydrodynamic and oil spill models can be selected by comparison to drifter experiments. As an example, a surface drifter was deployed during a cruise around

the Balearic Sea in October, 2012. An operational ROMS model is available for the same time period. Using the oil spill model of [39], an initially circular spill is transported as shown in Fig. 1.7



Fig. 1.7 Simulation of an initially circular oil spill advected for 72 hours with modeled ocean currents and a $\gamma = 0.5\%$ of wind velocity (provided by the atmospheric numerical model at 10m above the sea level). Black is initial spill location and the red is final distribution. Blue line is the real drifter trajectory for the same period.

The sensitivity of the results to the γ can be evaluated by running hindcast simulation similar to Fig. 1.7 for a range of values. Fig. 1.8 shows the Root Mean Square Error (RMSE) of the cloud of particles relative to the drifter position at the end of 72 hours for simulations with $0 \le \gamma \le 4\%$.

$$\text{RMSE} = \sqrt{\frac{1}{N_p} \sum_{n=1}^{N_p} d_n^2},$$

where N_p is the number of particles deployed, and d_n is the spherical distance (the arc-length over the Earth surface) between the virtual particle n and the real drifter after 72 hours, defined as the haversine formula:

$$d_n = \mathbf{R}_{\mathrm{T}} \alpha = \mathbf{R}_{\mathrm{T}} 2 \arcsin\left(\sqrt{\sin^2\left(\frac{\Delta_{\phi}}{2}\right) + \cos(\phi_n)\cos(\phi_d)\sin^2\left(\frac{\Delta_{\lambda}}{2}\right)}\right)$$

where R_T is the average Earth radius (6371 km) and α is an angle; for a particle and a drifter with positions (λ_n, ϕ_n) and (λ_d, ϕ_d) , the Δ terms are $\Delta_{\phi} = \phi_d - \phi_n$ and $\Delta_{\lambda} = \lambda_d - \lambda_n$.

For the modeled conditions, it is clear that $\gamma = 0.5\%$ should be preferred, and that both decreasing or increasing the drag will increase the error. Note that the γ derived

herein is merely illustrative for the particular model and conditions, and should not be taken as a recommended value for other models or conditions.



Fig. 1.8 RMSE (units in km) obtained for several wind drag values computed for the same initial cloud and period of study in relation to a real drifter.

The "best" drag coefficient for an oil spill model is a subject of ongoing research, and arguably depends on interactions between the modeled hydrodynamics and the oil spill. That is, our operational goal is to predict the probable movement of an oil spill, and the best γ is the the one that compensates for the difference between the modeled transport of near-surface currents ($U_{current}$) and the real transport. If the hydrodynamic model poorly predicts the near-surface current effects, then the best γ will be different than what would be used with a hydrodynamic model that has better predictions. Thus γ will inherently be uncertain and a multi-model operational system (§1.6) should include oil spill models with at least three γ values (low, high, best) to cover a range of possible results. In particular, using a $\gamma = 0$ as a lower bound provides the expected transport for subsurface oil, and can be useful for oil spill models that are otherwise confined to modeling 2D surface transport (*e.g.* GNOME, [58]).

Diffusivity – The physical diffusion of oil into water is a very slow process, and is generally not represented in an oil spill model. Indeed, by definition the Lagrangian particles used in oil spill models are unitary and cannot diffuse. Instead, the "diffusivity" (or dispersion) model for Lagrangian particles is designed to represent the transport processes and turbulence effects that are not resolved in either the hydrodynamic model or the oil spill model itself [10]. A stochastic approach to diffusivity is to modify eq. 1.1 to include a diffusion term for each particle as

$$\mathbf{x}^{n+1} = \mathbf{x}^n + \Delta t \left(\mathbf{U}_{\text{wind}} + \mathbf{U}_{\text{wave}} + \mathbf{U}_{\text{current}} \right) + \delta \mathbf{x}_{\text{diff}}$$
(1.2)

where $\delta \mathbf{x}_{\text{diff}}$ represents a vector random walk added to the deterministic particle motion from the U terms. A diffusion rate (D) resulting in a normal distribution

over time Δt will have a variance $\sigma^2 = 2D\Delta t$, such that the standard deviation (σ) is an expected length scale for diffusive transport [8]. A random walk distance vector can be modeled using the ratio of the variance of the diffusivity to the variance of a random number generator, e.g. [25, 36], as:

$$\delta \mathbf{x}_{\text{diff}} = \mathbf{R} \sqrt{\frac{2D\Delta t}{\sigma^2}} \tag{1.3}$$

where **R** is a uniform random number vector in the range [-1,1] with a vanishing mean and a variance of $\sigma^2 = 1/3$. Note that Δt here is the time step of the oil spill model, which is not necessarily the same as the time step of the hydrodynamic model. The effects of varying diffusivity can be illustrated as shown in Fig. 1.9. Determining the appropriate diffusion coefficient for an oil spill model is a challenge as it depends directly on how well the hydrodynamic model captures the structure of velocity field, which may vary in both time and space. If we assume spatial variability in diffusion is a primary concern, the approach of [39] allows development of a spatial map of estimated diffusivity based on multi-year simulations of particle transport.



Fig. 1.9 Simulation of a circular oil spill advected for 72 hours with $\gamma = 0.5\%$ with no diffusivity (left), with $D = 100 \text{ m}^2/\text{s}$ (center) and with $D = 100 \text{ m}^2/\text{s}$. Black circle indicates the initial location of particles whereas the red dots the final distribution. The drifter trajectory is depicted with the blue line where the blue cross is the starting position and the blue circle the final one.

Oil spill shape – Although aerial or satellite imagery can sometimes be used to obtain a visual approximation of an oil spill's initial shape, there will generally be some uncertainty in the shape and/or extent of coverage for the early stages of spill. There is an open question as to how uncertainties in the initial shape and size of an oil spill affect the forecast. Unfortunately, the overall effect of the initial shape is also likely influenced by the selected diffusivity, with higher diffusivities being less affected by the initial shape. A simple test for the influence of the shape and diffusivity can be carried out with representative initial shapes. If a and b are defined as the major and minor semi-axis of an initial elliptical distribution of oil particles, insight can be provided with study cases: (i) a = b a circle, (ii) a = 2b a prolate

ellipse, and (iii) a = b/2 an oblate ellipse. For each shape, a set of diffusivities over the range 0 to 100 m²/s has been run using the same simulation setup as in Fig. 1.9. The RSME results are provided in Table 1.1, with typical particle clouds after 72 hours of simulation shown in Fig. 1.10. These results indicate that the model tested is relatively insensitive to the initial shape, and a circular spill is a reasonable initial condition when more detailed data is not available.



Fig. 1.10 Trajectories of virtual particles deployed inside a circle (left), ellipse oriented N-S (middle) and ellipse oriented W-E (right). Simulations are performed for 72 hours with $\gamma = 0.5\%$ and with $D = 10 \text{ m}^2/\text{s}$. Black cloud indicates the initial location of particles and the red dots the final distribution. The drifter trajectory is depicted with the blue line.

RMSE [km]	$D = 0 m^2/s$	$D = 1 m^2/s$	$D = 10 m^2/s$	$D = 100 m^2/s$
a=b	7.44	7.57	8.25	12.7
a=2b	6.89	7.03	8.04	12.48
a=b/2	8.09	8.15	8.71	13.07

Table 1.1 Root Mean Square Error (in km) for circular and elliptical initial distributions of oil spill particles for simulations similar to Fig. 1.10.

1.9 Integrating probability within an oil spill model

A disadvantage of the multi-model approach ($\S1.6$) is the need for systemic, realtime uncertainty modeling through all models of the forecasting system. This problem might be reduced by making use of a computationally inexpensive oil spill model to rapidly create real-time simulation ensembles that can be visualized as probability maps. In the simplest incarnation, such an approach is complementary to the multi-model system, *i.e.* simply replacing the multiple oil spill models and initial condition perturbations in Fig. 1.3 with a single ensemble model. However, there is

also the potential for an alternative approach that entirely replaces the multi-model system. Our principal concern is in the range of possible future positions of the oil spill and the probabilities associated with this range. If the uncertainties in wind, wave, and hydrodynamic models (driving forces) can be quantified in terms of their effects on stochastic diffusivity (particle response) [29], then the multi-model system could be replaced with single instances of best estimate wind, wave, and hydrodynamic models accompanied by an ensemble uncertainty approach. This approach requires all the uncertainties in the wind, wave, and currents to be re-parameterized in terms of diffusivity. Methodologies and metrics for translating the chain of uncertainties from driving force models to particle models remain relatively unexplored, but are likely to require extensive hindcast analyses that are customized to the driving models and the regional/local conditions [39].

An ensemble approach requires setting perturbation values for the parameters and initial conditions for the oil spill model. These can be set as part of a Monte Carlo approach over the expected range. Lagrangian particle from all simulations are then combined into a single data set that can be analyzed for any particular time point using the following steps:

- (i) Define a bounding box covering all the particles at a given forecast time.
- (ii) Subdivide the bounding box in a grid.
- (iii) Compute the probability density based on particle counts in the grid cells.
- (iv) Accumulate probability starting from high values and working downwards so that the integrated probability over the area is 100%.
- (v) Construct and visualize probability contours.



Fig. 1.11 The simulation from Fig. 1.7 using a probability approach for the particle distribution instead of the particle cloud. Color in left and center panels represents probability of finding a Lagrangian particle in each subgrid cell of the bounding box. Right panel compares the particle cloud (red) to 50%, 70% and 90% contours of accumulated probability.

A demonstration of the probability approach is illustrated in Fig. 1.11. The grid size within the bounding box is chosen to ensure statistically significant grid cells over majority of the forecast spill area, which will depend on the number of simulated particles and their effective diffusion. The probability density can be computed by any number of kernels, (*e.g.* Chapter 9 of [28]), but a simple Gaussian kernel is arguably appropriate for an oil spill [1, 39]. Accumulating probability contours from

high to low values allows development of probability distributions with multiple local maxima and disconnected contours. The probability approach, whether adopted within a multi-model forecast system or simply within the oil spill model itself, provides the end user with a better understanding of the results of an oil spill simulation than does the traditional point cloud or particle tracks.

1.10 Conclusions

This chapter has presented a discussion of the major challenges and opportunities involved in creating oil spill forecasting systems that account for uncertainty. Forecast uncertainty is added with each modeling step and parameterization, from the initial wind forecast to the oil spill diffusivity. There is a need for emergency responders to have a real-time understanding of the uncertainty of the forecast for today's spill, which might not be well predicted by hindcast studies at different times or locations. A systematic approach to including uncertainty at all levels in real-time forecasts has been proposed ($\S1.6$), but there are significant engineering challenges to putting these ideas into operation at any particular location. Probably the most daunting challenge for many operational agencies will be bureaucratic rather than scientific or engineering: for a viable multi-model uncertainty forecast system, a research team needs direct access to an operational coastal hydrodynamic model to run multiple simulations with different wind forecasts. However, if the uncertainty associated with wind, wave, and hydrodynamic forecasts can be parameterized into a range of diffusivities for an oil spill model, then an approximation of the multimodel uncertainty can be directly integrated into an ensemble approach to the oil spill modeling ($\S1.9$). The key point is that uncertainty in wind forecasts and the surface water's response to the wind are the critical drivers of uncertainty [27, 48], and therefore must be included in any uncertainty evaluation system - either directly through a multi-model approach, or indirectly through hindcast analyses and parameterization of particle diffusivity for a forecast oil spill model.

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