Trajectory Modelling in Support of the Nexen Energy ULC Flemish Pass Exploration Drilling Project (2018-2028) Relief Well Modelling

Appendix A: SIMAP and OILMAPDeep Model Descriptions

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Summary

This Appendix A is provided as a reference to RPS Technical Report: Trajectory Modelling in Support of the Nexen Energy ULC Flemish Pass Exploration Drilling Project (2018-2028) Relief Well Modelling. Appendix A provides a detailed description of the SIMAP model and the fates processes and algorithms that were used, as well as a description of the theory and implementation of the OILMAP Deep model.

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1 SIMAP Model Description

The analysis was performed using the model system developed by Applied Science Associates (ASA) called SIMAP (Spill Impact Model Analysis Package). SIMAP originated from the oil fates and biological effects submodels in the Natural Resource Damage Assessment Models for Coastal and Marine Environments (NRDAM/CME) and Great Lakes Environments (NRDAM/GLE), which ASA developed in the early 1990s for the U.S. Department of the Interior for use in "type A" Natural Resource Damage Assessment (NRDA) regulations under the Comprehensive Environmental Response, Compensation and Liability Act of 1980 (CERCLA). The most recent version of the type A models, the NRDAM/CME (Version 2.4, April 1996) was published as part of the CERCLA type A NRDA Final Rule (Federal Register, May 7, 1996, Vol. 61, No. 89, p. 20559-20614). The technical documentation for the NRDAM/CME is in French et al. (1996 a-c). This technical development involved several in-depth peer reviews, as described in the Final Rule.

While the NRDAM/CME and NRDAM/GLE were developed for simplified natural resource damage assessments of small spills in the United States, SIMAP is designed to evaluate fates and effects of both real and hypothetical spills in marine, estuarine and freshwater environments worldwide. Additions and modifications to prepare SIMAP were made to increase model resolution, allow modification and site-specificity of input data, allow incorporation of temporally varying current data, evaluate subsurface releases and movements of subsurface oil, track multiple chemical components of the oil, enable stochastic modelling, and facilitate analysis of results.

Below are brief descriptions of the fates and effects models presented in SIMAP. Detailed descriptions of the algorithms and assumptions in the model are in published papers (French McCay, 2002; 2003; 2004; 2009). 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 designed to verify the model (French et al., 1997).

1.1 Physical Fates Model

The three-dimensional physical fates model 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. Oil fate processes included are oil spreading (gravitational and by shearing), evaporation, transport, randomized dispersion, emulsification, entrainment (natural and facilitated by dispersant), dissolution, volatilization of dissolved hydrocarbons from the surface water, adherence of oil droplets to suspended sediments, adsorption of soluble and sparingly-soluble aromatics to suspended sediments, sedimentation, and degradation.

Oil is a mixture of hydrocarbons of varying physical, chemical, and toxicological characteristics. In the model, oil is represented by component categories, and the fate of each component is tracked separately. The "pseudo-component" approach (Payne et al., 1984; 1987; French et al., 1996a; Jones, 1997; Lehr et al., 2000) is used, where chemicals in the oil mixture are grouped by physical-chemical properties, and the resulting component category behaves as if it were a single chemical with characteristics typical of the chemical group.

The most toxic components of oil to aquatic organisms are low molecular weight aromatic compounds (monoaromatic and polycyclic aromatic hydrocarbons, MAHs and PAHs), which are both volatile and soluble in water. Their acute toxic effects are caused by non-polar narcosis, where toxicity is related to the octanol-water partition coefficient (K_{ow}), a measure of hydrophobicity. The more hydrophobic the compound, the more toxic it is likely to be. However, as K_{ow} increases, the compound also becomes less soluble in water, and so there is less exposure to aquatic organisms. The toxicity of compounds having $\log(K_{ow})$ values greater than about 5.6 is limited by their very low solubility in water, and consequent low bioavailability to aquatic biota (French McCay, 2002, Di Toro et al., 2000). Thus, the potential for acute effects is the result of a balance between bioavailability (exposure), toxicity once exposed, and duration of exposure. French McCay (2002) contains a full description of the oil toxicity model in SIMAP, and French McCay (2002) describes the implementation of the toxicity model in SIMAP.

Because of these considerations, the SIMAP fates model focuses on tracking the lower molecular weight aromatic components divided into chemical groups based on volatility, solubility, and hydrophobicity. In the model, the oil is treated as comprising eight components (defined in Table 1). Six of the components (i.e., all but the two non-volatile residual components representing non-volatile aromatics and aliphatics) evaporate at rates specific to the pseudo-component. Solubility is strongly correlated with volatility, and the solubility of aromatics is higher than aliphatics of the same volatility. The MAHs are the most soluble, the 2-ring PAHs are less soluble, and the 3-ring PAHs slightly soluble (Mackay et al., 1992). Both the solubility and toxicity of the non-aromatic hydrocarbons are much less than for the aromatics, and dissolution (and water concentrations) of non-aromatics is safely ignored. Thus, dissolved concentrations are calculated only for each of the three soluble aromatic pseudo-components.

Table 1. Definition of four distillation cuts and the eight pseudo-components in the model (Monoaromatic Hydrocarbons, MAHs; Benzene + Toluene + Ethylbenzene + Xylene, BTEX; Polycyclic Aromatic Hydrocarbons, PAHs).

Characteristic	Volatile and Highly Soluble	Semi-volatile and Soluble	Low Volatility and Slightly Soluble	Residual (non-volatile and very low solubility)
Distillation cut	1	2	3	4
Boiling Point (°C)	< 180	180 - 265	265 - 380	>380
Molecular Weight	50 - 125	125 - 168	152 - 215	> 215
$\mathrm{Log}(K_{ow})$	2.1-3.7	3.7-4.4	3.9-5.6	>5.6
Aliphatic pseudo-components: Number of Carbons	volatile aliphatics: C4 – C10	semi-volatile aliphatics: C10 – C15	low-volatility aliphatics: C15 – C20	non-volatile aliphatics: > C20
Aromatic pseudo-component name: included compounds	MAHs: BTEX, MAHs to C3-benzenes	2 ring PAHs: C4-benzenes, naphthalene, C1-, C2-naphthalenes	3 ring PAHs: C3-, C4-naphthalenes, 3-4 ring PAHs with $\log(K_{ow}) < 5.6$	$\geq$4 ring aromatics: PAHs with $\log(K_{ow}) > 5.6$ (very low solubility)

This number of components provides sufficient accuracy for the evaporation and dissolution calculations, particularly given the time frame (minutes) over which dissolution occurs from small droplets and the rapid resurfacing of large droplets (see discussion above). The alternative of treating oil as a single compound with empirically-derived rates (e.g., Mackay et al., 1980; Stiver and Mackay, 1984) does not provide sufficient accuracy for environmental effects analyses because the effects to water column organisms are caused by MAHs and PAHs, which have specific properties that differ from the other volatile and soluble compounds. The model has been validated both in predicting dissolved concentrations and resulting toxic effects, supporting the adequacy of the use of this number of pseudo-components (French McCay, 2003).

The lower molecular weight aromatics dissolve from the whole oil and are partitioned in the water column and sediments according to equilibrium partitioning theory (French et al., 1996a; French McCay, 2004). The residual fractions in the model are composed of non-volatile and insoluble compounds that remain in the “whole oil” that spreads, is transported on the water surface, strands on shorelines, and disperses into the water column as oil droplets or remains on the surface as tar balls. This is the fraction that composes black oil, mousse, and sheen.

1.2 Oil Fate Model Processes

The schematic in Figure 1 depicts oil fates processes simulated in open water conditions, while the schematic in Figure 2 depicts oil fates processes that are simulated at and near the shoreline. Because oil contains many chemicals with varying physical-chemical properties, and the environment is spatially and temporally variable, the oil rapidly separates into different phases or parts of the environment:

- Surface oil
- Emulsified oil (mousse) and tar balls
- Oil droplets suspended in the water column
- Oil adhering to suspended particulate matter in the water
- Dissolved lower molecular weight components (MAHs, PAHs, and other soluble components) in the water column
- Oil on and in the sediments
- Dissolved lower molecular weight components (MAHs, PAHs, and other soluble components) in the sediment pore water
- Oil on and in the shoreline sediments and surfaces

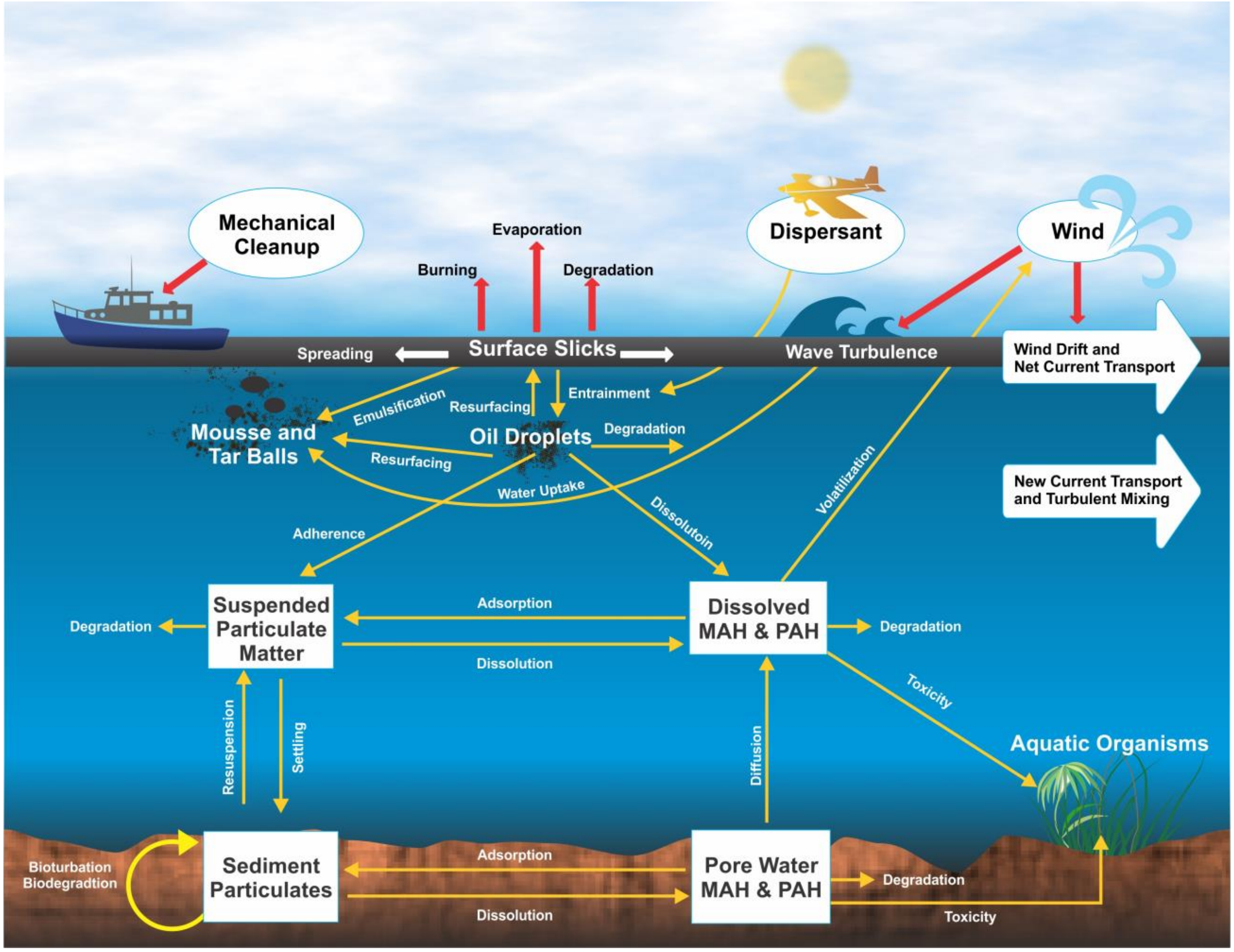

Figure 1. Simulated oil fates processes in open water.

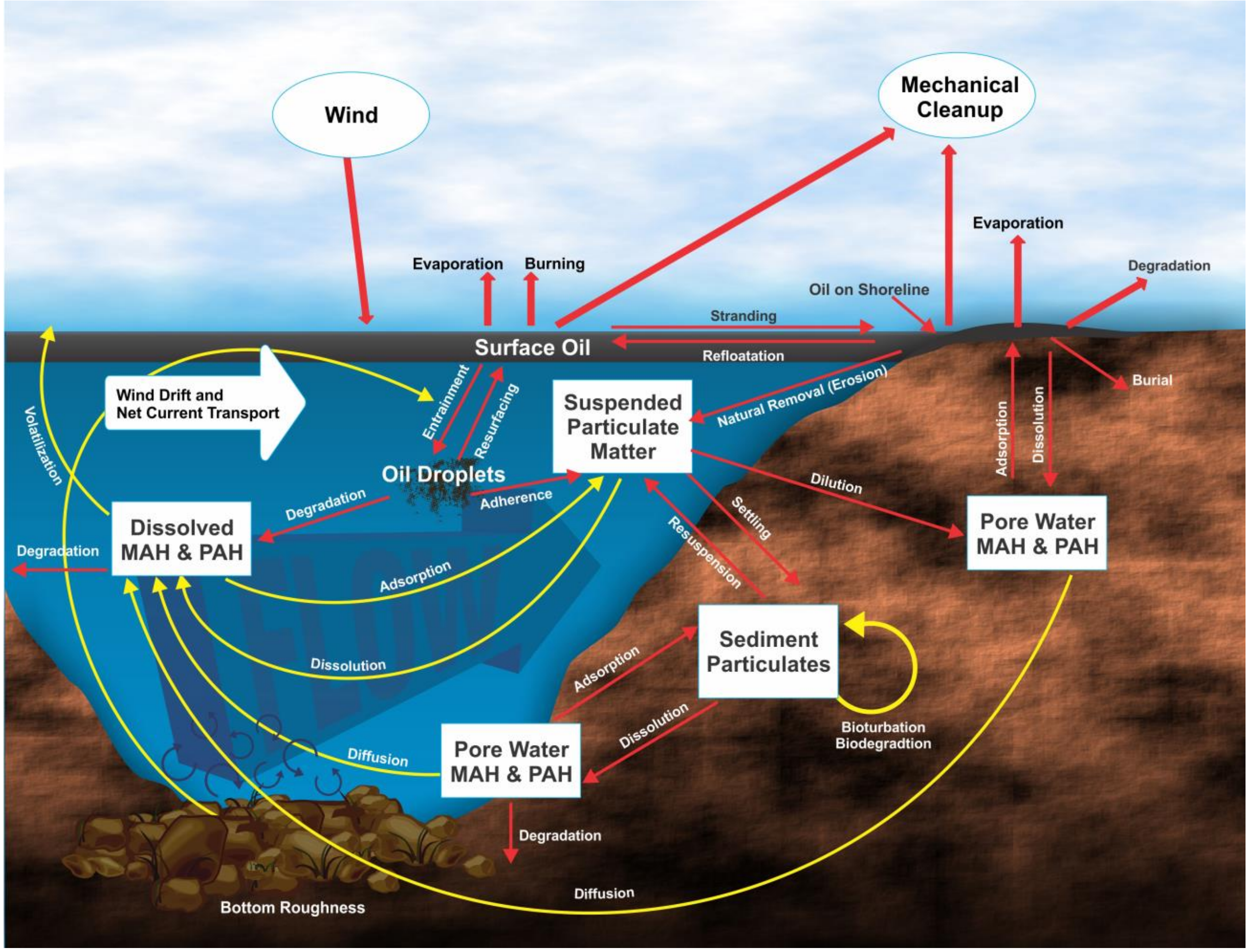

Figure 2. Simulated oil fates processes at the shoreline.

The schematics in Figure 1 and Figure 2 represent oil fates processes that are simulated in the model:

- Spreading is the thinning and broadening of surface slicks caused by gravitational forces and surface tension. This occurs rapidly after oil is spilled on the water surface. The rate of spreading is faster if oil viscosity is lower. Viscosity decreases as temperature increases. Viscosity increases as oil emulsifies.
- Transport is the process where oil is carried by currents.
- Turbulent dispersion: Typically, there are also “sub-scale” currents (not included in the current data), better known as turbulence that move oil and mix it both in three dimensions. The process by which turbulence mixes and spreads oil components on the water surface and in the water is called turbulent dispersion.
- Evaporation is the process where volatile components of the oil diffuse from the oil and enter the gaseous phase (atmosphere). Evaporation from surface and shoreline oil increases as the oil

surface area, temperature, and wind speed increase. As lighter components evaporate off, the remaining "weathered" oil becomes more viscous.

- Emulsification is the process where water is mixed into the oil, such that the oil makes a matrix with embedded water droplets. The resulting mixture is commonly called mousse. It is technically referred to as a water-in-oil emulsion. The rate of emulsification increases with increasing wind speed and turbulence on the surface of the water. Viscosity increases as oil emulsifies.
- Entrainment is the process where waves break over surface oil and carry it as droplets into the water column. At higher wind speeds, or where currents and bottom roughness induce turbulence, wave heights may reach a threshold where they break. In open waters, waves break beginning at about 12 knots of wind speed and wave breaking increases as wind speed becomes higher. Thus, entrainment becomes increasingly important (higher rate of mass transfer to the water) the higher the wind speed. As turbulence from whatever source increases, the oil droplet sizes become smaller. Application of chemical dispersant increases the entrainment rate of oil and decreases droplet size at a given level of turbulence. Entrainment rate is slower, and droplet size is larger, as oil viscosity increases (by emulsification and evaporation loss of lighter volatile components). The droplet size determines how fast and whether the oil resurfaces.
- Resurfacing of entrained oil rapidly occurs for larger oil droplets. Smaller droplets resurface when the wave turbulence decreases. The smallest droplets do not resurface, as typical turbulence levels in the water keep them in suspension indefinitely. Local winds at the water surface can also prevent oil from surfacing. Resurfaced oil typically forms sheens. In open water where currents are relatively slow, surface slicks are usually blown down wind faster than the underlying water, resurfacing droplets come up behind the leading edge of the oil, effectively spreading the slicks in the down-wind direction.
- Dissolution is the process where water-soluble components diffuse out of the oil into the water. Dissolution rate increases the higher the surface area of the oil relative to its volume. As the surface area to volume ratio is higher for smaller spherical droplets, the smaller the droplets the higher the dissolution rate. The higher the wave turbulence, the smaller the droplets of entrained oil. Dissolution from entrained small droplets is much faster than from surface slicks in the shape of flat plates. The soluble components are also volatile, and evaporation from surface slicks is faster than dissolution into the underlying water. Thus, the processes of evaporation and dissolution are competitive, with evaporation the dominant process for surface oil.
- Volatilization of dissolved components from the water to the atmosphere occurs as they are mixed and diffuse to the water surface boundary and enter the gas phase. Volatilization rate increase with increasing air and water temperature.
- Adsorption of dissolved components to particulate matter in the water occurs because the soluble components are only sparingly so. These compounds (MAHs and PAHs) preferentially adsorb to particulates when the latter are present. The higher the concentration of suspended

particulates, the more adsorption. Also, the higher the molecular weight of the compound, the less soluble, and the more the compound adsorbs to particulate matter.

- Adherence is the process where oil droplets combine with particles in the water. If the particles are suspended sediments, the combined oil/suspended sediment agglomerate is heavier than the oil itself and the water. If turbulence subsides sufficiently, the oil-sediment agglomerates will settle.
- Sedimentation (settling) is the process where oil-sediment agglomerates and particles with adsorbed sparingly-soluble components (MAHs and PAHs) settle to the bottom sediments. Adherence and sedimentation can be an important pathway of oil in near shore areas when waves are strong and subsequently subside. Generally, oil-sediment agglomerates transfer more PAH to the bottom than sediments with PAHs that were adsorbed from the dissolved phase in the water column.
- Resuspension of settled oil-sediment particles and particles with adsorbed sparingly-soluble components (MAHs and PAHs) may occur if current speeds and turbulence exceed threshold values where cohesive forces can be overcome.
- Diffusion is the process where dissolved compounds move from higher to lower concentration areas by random motion of molecules and micro-scale turbulence. Dissolved components in bottom and shoreline sediments can diffuse out to the water where concentrations are relatively low. Bioturbation, groundwater discharge and hyporheic flow of water through stream-bed sediments can greatly increase the rate of diffusion from sediments (see below).
- Dilution occurs when water of lower concentration is mixed into water with higher concentration by turbulence, currents, or shoreline groundwater.
- Bioturbation is the process where animals in the sediments mix the surface sediment layer while burrowing, feeding, or passing water over their gills. In open-water soft-bottom environments, bioturbation effectively mixes the surface sediment layer about 10 cm thick (in non-polluted areas).
- Degradation is the process where oil components are changed either chemically or biologically (biodegradation) to another compound. It includes breakdown to simpler organic carbon compounds by bacteria and other organisms, photo-oxidation by solar energy, and other chemical reactions. Higher temperature and higher light intensity (particularly ultraviolet wavelengths) increase the rate of degradation.
- Floating oil may strand on shorelines and refloat as water levels rise, allowing the oil to move further down current (downstream).

For a spill on the water surface, the gravitational spreading occurs very rapidly (within hours) to a minimum thickness. Thus, the area exposed to evaporation is high relative to the oil volume. Evaporation proceeds faster than dissolution. Thus, most of the volatiles and semi-volatiles evaporate, with a smaller fraction dissolving into the water. Degradation (photo-oxidation and biodegradation) also occurs at a relatively slow rate compared to these processes.

Evaporation is more rapid as the wind speed increases. However, above about 12 knots (6 m/s) of wind speed and in open water, white caps begin to form, and the breaking waves entrain oil as droplets into the water column. Higher wind speeds (and turbulence) increase entrainment and results in smaller droplet sizes. From Stoke's Law, larger droplets resurface faster and form surface slicks. Thus, a dynamic balance evolves between entrainment and resurfacing. As high-wind events occur, the entrainment rate increases. When the winds subside to less than 12 knots, the larger oil droplets resurface and remain floating. Similar dynamics occur in turbulent streams.

The smallest oil droplets remain entrained in the water column for an indefinite period. Larger oil droplets rise to the surface at varying rates. While the droplets are under water, dissolution of the light and soluble components occurs. Dissolution rate is a function of the surface area available. Thus, most dissolution occurs from droplets, as opposed to from surface slicks, since droplets have a higher surface area to volume ratio, and they are not in contact with the atmosphere (and so the soluble components do not preferentially evaporate as they do from surface oil).

If oil is released or driven underwater, it forms droplets of varying sizes. More turbulent conditions result in smaller droplet sizes. From Stoke's Law, larger droplets rise faster, and surface if the water is shallow. Resurfaced oil behaves as surface oil after gravitational spreading has occurred. The surface oil may be re-entrained. The smallest droplets in most cases remain in the water permanently. As a result of the higher surface area per volume of small droplets, the dissolution rate is much higher from subsurface oil than from floating oil on the water surface.

Because of these interactions, the majority of dissolved constituents (which are of concern because of potential effects on aquatic organisms) are from droplets entrained in the water. For a given spill volume and oil type/composition, with increasing turbulence either at the water surface and/or at the stream bed: there is an increasing amount of oil entrained; the oil is increasingly broken up into smaller droplets; there is more likelihood of the oil remaining entrained rather than resurfacing; and the dissolved concentrations will be higher. Entrainment and dissolved concentrations increase with (1) higher wind speed, (2) increased turbulence from other sources of turbulence (waves on a beach, rapids, and waterfalls in rivers, etc.), (3) subsurface releases (especially under higher pressure and turbulence), and (4) application of chemical dispersants. Chemical dispersants both increase the amount of oil entrained and decrease the oil droplet size. Thus, chemical dispersants increase the dissolution rate of soluble components.

These processes that increase the rate of supply of dissolved constituents are balanced by loss terms in the model: (1) transport (dilution), (2) volatilization from the dissolved phase to the atmosphere, (3) adsorption to suspended particulate material (SPM) and sedimentation, and (4) degradation (photo-oxidation or biologically mediated). Also, other processes slow the entrainment rate: (1) emulsification increases viscosity and slows or eliminates entrainment; (2) adsorption of oil droplets to SPM and settling removes oil from the water; (3) stranding on shorelines removes oil from the water; and (4) mechanical cleanup and burning removes mass from the water surface and shorelines. Thus, the modelpredicted concentrations are the resulting balance of all these processes and the best estimates based on our quantitative understanding of the individual processes.

The algorithms used to model these processes are described in French McCay (2004). Lagrangian elements (spillets) are used to simulate the movements of oil components in three dimensions over time. Surface floating oil, subsurface droplets, and dissolved components are tracked in separate spillets. Transport is the sum of advective velocities by currents input to the model, surface wind drift, vertical movement according to buoyancy, and randomized turbulent diffusive velocities in three dimensions. The vertical diffusion coefficient is computed as a function of wind speed in the surface wave-mixed layer. The horizontal and deeper water vertical diffusion coefficients are model inputs.

The oil (whole and as pseudo-components) separates into different phases or parts of the environment, i.e., surface slicks; emulsified oil (mousse) and tar balls; oil droplets suspended in the water column; dissolved lower molecular weight components (MAHs and PAHs) in the water column; oil droplets adhered and hydrocarbons adsorbed to suspended particulate matter in the water; hydrocarbons on and in the sediments; dissolved MAHs and PAHs in the sediment pore water; and hydrocarbons on and in the shoreline sediments and surfaces.

1.3 Oil Fates Algorithms

1.3.1 Transport

Lagrangian particles (spillets) are moved in three dimensions over time. For each model time step, the new vector position of the spillet centre is calculated from the old plus the vector sum of east-west, north-south, and vertical components of advective and diffusive velocities:

$$X_t = X_{t-1} + \Delta t \, (U_t + D_t + R_t + W_t)$$

where X_t is the vector position at time t, X_{t-1} is the vector position the previous time step, Δt is the time step, U_t is the sum of all the advective (current) velocity components in three dimensions at time t, D_t is the sum of the randomized diffusive velocities in three dimensions at time t, R_t is the rise or sinking velocity of whole oil droplets in the water column, and W_t is the surface wind transport ("wind drift"). The magnitudes of the components of D_t are scaled by horizontal and vertical diffusion coefficients (Okubo and Ozmidov, 1970; Okubo, 1971). The vertical diffusion coefficient is computed as a function of wind speed in the surface wave-mixed layer (which ranges from centimetre scales in rivers and near lee shorelines to potentially metres in large water bodies away from shore when wind speeds are high), based on Thorpe (1984). R_t is computed by Stokes law, where velocity is related to the difference in density between the particle and the water, and to the particle diameter. The algorithm developed by Youssef and Spaulding (1993) is used for wind transport in the surface wave-mixed layer (W_t, described below).

1.3.2 Shoreline Stranding

The fate of spilled oil that reaches the shoreline depends on characteristics of the oil, the type of shoreline, and the energy environment. The stranding algorithm is based on work by CSE/ASA/BAT (1986), Gundlach (1987), and Reed and Gundlach (1989) in developing the COZOIL model for the U.S. Minerals Management Service. In SIMAP, deposition occurs when an oil spillet intersects shore surface. Deposition ceases when the volume holding capacity for the shore surface is reached. Subsequent oil coming ashore is not allowed to remain on the shore surface. It is refloated by rising water, and carried away by currents and wind drift. The remaining shoreline oil is then removed exponentially with time. Data for holding capacity and removal rate are taken from CSE/ABA/BAT (1986) and Gundlach (1987), and are a function of oil viscosity and shore type. The algorithm and data are in French et al. (1996a).

1.3.3 Spreading

Spreading determines the areal extent of the surface oil, which in turn influences its rates of evaporation, dissolution, dispersion (entrainment) and photo-oxidation, all of which are functions of surface area. Spreading results from the balance among the forces of gravity, inertia, viscosity, and surface tension (which increases the diameter of each spillet); turbulent diffusion (which spreads the spillets apart); and entrainment followed by resurfacing, which can spatially separate the leading edge of the oil from resurfaced oil transported in a different direction by subsurface currents.

For many years Fay's (1971) three-regime spreading theory was widely used in oil spill models (ASCE, 1996). Mackay et al. (1980; 1982) modified Fay's approach and described the oil as thin and thick slicks. Their approach used an empirical formulation based on Fay's (1971) terminal spreading behaviour. They assumed the thick slick feeds the thin slick and that 80-90% of the total slick area is represented by the thin slick. In SIMAP, oil spillets on the water surface increase in diameter according to the spreading algorithm empirically-derived by Mackay et al. (1980; 1982). Sensitivity analyses of this algorithm led to the discovery that the solution was affected by the number of spillets used. Thus, a formulation was derived to normalize the solution under differing numbers of surface spillets (Kolluru et al., 1994). Spreading is stopped when an oil-specific terminal thickness is reached.

1.3.4 Evaporation

The rate of evaporation depends on surface area, thickness, vapour pressure and mass transport coefficient, which in turn are functions of the composition of the oil, wind speed and temperature (Fingas, 1996; 1997; 1998; 1999; Jones, 1997). As oil evaporates its composition changes, affecting its density and viscosity as well as subsequent evaporation. The most volatile hydrocarbons evaporate most rapidly, typically in less than a day and sometimes in under an hour (McAuliffe, 1989). As the oil continues to weather, and particularly if it forms a water-in-oil emulsion, evaporation will be significantly decreased.

The evaporation algorithm in SIMAP is based on accepted evaporation theory, which follows Raoult's Law that each component will evaporate with a rate proportional to the saturation vapour pressure and mole fraction present for that component. The pseudo-component approach (Payne et al., 1984; French et al., 1996a; Jones, 1997; Lehr et al., 2000) is used, such that each component evaporates according to its mean vapour pressure, solubility, and molecular weight (Table 2-3). The mass transfer coefficient is calculated using the methodology of Mackay and Matsugu (1973), as described in French et al. (1996a).

1.3.5 Entrainment

As oil on the water surface is exposed to wind and waves, or if oil moves into a turbulent area of a stream or river, it is entrained (or dispersed) into the water column. Entrainment is a physical process where globules of oil are transported from the water surface into the water column due to breaking waves or other turbulence. It has been observed that entrained oil is broken into droplets of varying sizes. Smaller droplets spread and diffuse in the water column, while larger ones rise back to the surface.

Entrainment by Breaking Surface Wave Action

In open waters, breaking waves created by the action of wind and waves on the water surface are the primary sources of energy for entrainment. Entrainment is strongly dependant on turbulence and is greater in areas of high wave energy (Delvigne and Sweeney, 1988).

Delvigne and Sweeney (1988), using laboratory and flume experimental observations, developed a relationship for entrainment rate and oil droplet size distribution as a function of turbulent energy level and oil viscosity. Entrained droplets in the water column rise according to Stokes law, where velocity is related to the difference in density between the particle and the water, and to the particle diameter. The data and relationships in Delvigne and Sweeney (1988) are used in SIMAP to calculate mass and particle size distribution of droplets entrained. Particle size decreases with higher turbulent energy level and lower oil viscosity. The natural dispersion particle sizes observed by Delvigne and Sweeney (1988) are confirmed by field observations by Lunel (1993a,b).

Use of chemical dispersants (not modelled in the scenarios examined here) decrease the median particle size, increasing the number of droplets in the <70 μm range (Daling et al., 1990; Lunel, 1993a,b). Particle size distributions for dispersed oil are available for several oils from these studies. When dispersant is applied, the model entrains surface oil, creating subsurface droplets in the appropriate size distribution for dispersant use. The median particle size for permanently dispersed droplets is set at 20 microns, the median size observed by Lunel (1993a,b). The fraction of oil permanently dispersed is set by the assumed dispersant efficiency. The IKU/SINTEF studies provide data on the viscosity range where oils may be dispersed chemically. Typically, dispersants are effective up to about 10,000 cp (Aamo et al., 1993; Daling and Brandvik, 1988; 1991; Daling et al., 1997). In the model, oil is dispersed up to 10,000 cp.

Entrained oil is well mixed in (i.e., mixed uniformly throughout) the wave-mixed zone. Vertical mixing is simulated by random placement of particles within the wave-mixed layer each time step. Settling of particles does not occur in water depths where waves reach the bottom (taken as 1.5 times wave height). Wave height is calculated from wind speed, duration and fetch (distance upwind to land), using the algorithms in CERC (1984). Wave height is on the scale of centimetres in small rivers and streams, and near lee shorelines; whereas it may increase to metres in open waters under windy conditions.

1.3.6 Emulsification (Mousse Formation)

The formation of water-in-oil emulsions, or mousse, depends on oil composition and turbulence level. Emulsified oil can contain as much as 80% water in the form of micrometre-sized droplets dispersed within a continuous phase of oil (Daling and Brandvik, 1988; Fingas et al., 1997). Viscosities are typically much higher than that of the parent oil. The incorporation of water also dramatically increases the oil/water mixture volume.

The Mackay and Zagorski (1982) emulsification scheme is implemented in SIMAP for floating oil. Water content increases exponentially, with the rate related to the square of wind speed and previous water incorporation. Viscosity is a function of water content. The change in viscosity feeds back in the model to the entrainment rate.

1.3.7 Dissolution

Dissolution is the process by which soluble hydrocarbons enter the water from a surface slick or from entrained oil droplets. The lower molecular weight hydrocarbons tend to be both more volatile and more soluble than those of higher molecular weight. For surface slicks, since the partial pressures tend to exceed the solubilities of these lower molecular weight compounds, evaporation accounts for a larger portion of the mass than dissolution (McAuliffe, 1989), except perhaps under ice. Dissolution and evaporation are competitive processes. The dissolved component concentration of hydrocarbons in water under a surface slick shows an initial increase followed by a rapid decrease after some hours due to the evaporative loss of components. Most soluble components are also volatile and direct evaporation (volatilization) from the water column depletes their concentrations in the water. Dissolution is particularly important where evaporation is low (dispersed oil droplets and ice-covered surfaces). Dissolution can be significant from entrained droplets because of the lack of atmospheric exposure and because of the higher surface area per unit of volume.

The model developed by Mackay and Leinonen (1977) is used in SIMAP for dissolution from a surface slick. The slick (spillet) is treated as a flat plate, with a mass flux (Hines and Maddox, 1985) related to solubility and temperature. It assumes a well-mixed layer with most of the resistance to mass transfer lying in a hypothetical stagnant region close to the oil. For subsurface oil, dissolution is treated as a mass flux across the surface area of a droplet (treated as a sphere) in a calculation analogous to the Mackay and Leinonen (1977) algorithm. The dissolution algorithm was developed in French et al. (1996a).

1.3.8 Volatilization from the Water column

The procedure outlined by Lyman et al. (1982), based on Henry's Law and mass flux (Hines and Maddox, 1985), is followed in the SIMAP fates model. The volatilization depth for dissolved substances is limited to the maximum of one half the wave height. Wave height is computed from the wind speed and fetch (CERC, 1984). The volatilization algorithm was developed in French et al. (1996a).

1.3.9 Adsorption and Sedimentation

Aromatics dissolved in the water column are carried to the sediments primarily by adsorption to suspended particulates, and subsequent settling. The ratio of adsorbed (C_a) to dissolved (C_{dis}) concentrations is computed from standard equilibrium partitioning theory as

$$C_a / C_{dis} = K_{oc} C_{ss}$$

K_{oc} is a dimensionless partition coefficient and C_{ss} is the concentration of suspended particulate matter (SPM) in the water column expressed as mass of particulate per volume of water. As a default, the model uses a mean value of total suspended solids of 10 mg/l (Kullenberg, 1982); alternatively suspended sediment concentration is specified as model input.

Sedimentation of oil droplets occurs when the specific gravity of oil increases over that of the surrounding water. Several processes may act on entrained oil and surface slicks to increase density: weathering (evaporation, dissolution and emulsification), adhesion or sorption onto suspended particles or detrital material, and incorporation of sediment into oil during interaction with suspended particulates, bottom sediments, and shorelines. Rates of sedimentation depend on the concentration of suspended particulates and the rates of particulate flux into and out of an area. In areas with high suspended particulate concentrations, rapid dispersal and removal of oil is found due to sorption and adhesion (Payne and McNabb, 1984).

Kirstein et al. (1987) and Payne et al. (1987) used a reaction term to characterize the water column interactions of oil and suspended particulates. The reaction term represents the collision of oil droplets and suspended matter, and both oiled and unoiled particulates are accounted for. The model formulation developed by Kirstein et al. (1987) is used to calculate the volume of oil adhered to particles. In the case where the oil mass is larger than the adhered sediment (i.e., the sediment has been incorporated into the oil) the buoyancy of the oil droplet will control its settling or rise rate. The Stoke's law formulation is used to adjust vertical position of these particles. If the mass of adhered droplets is small relative to the mass of the sediment it has adhered to, the sediment settling velocity will control the fate of the combined particulate.

1.3.10 Degradation

Degradation may occur as the result of photolysis, which is a chemical process energized by ultraviolet light from the sun, and by biological (bacterial) breakdown, termed biodegradation. In the model, degradation occurs on the surface slick, deposited oil on the shore, the entrained oil and aromatics in the water column, and oil in the sediments. A first order decay algorithm is used, with a specified (total) degradation rate for each of surface oil, water column oil and sedimented oil (French et al., 1999).

1.4 Habitat Type

Ecological habitat types (Table 2) are broadly categorized into two zones within SIMAP: shoreline and submerged (or intertidal versus subtidal in estuarine and marine areas, where intertidal habitats are those above spring low water tide level, with subtidal being all water areas below that level). In modelled scenarios, the shoreline habitats may become oiled as surface oil makes contact with these cells. Submerged or subtidal cells are always underwater. Intertidal/shoreline areas may be extensive, such that they are wide enough to be represented by an entire grid cell at the resolution of the grid. These are typically either mud flats or wetlands, and are coded 20 (seaward mudflat), 21 (seaward wetland), 50 (landward mudflat), or 51 (landward wetland). All other intertidal/shoreline habitats are typically much narrower than the size of a grid cell. Thus, these fringing intertidal/shore types (indicated by F in Table 2) have typical (for the region, e.g., French et al., 1996a for estuarine and marine areas) widths associated with them in the model. Boundaries between land and water are fringing habitat types. On the waterside of fringing grid cells, there may be extensive intertidal/shoreline grid cells if the wetlands or mudflats are extensive. Otherwise, subtidal/submerged habitats border the fringing cells.

Table 2. Classification of habitats. seaward (Sw) and landward (Lw) system codes are listed. (fringing types indicated by (F) are only as wide as the intertidal zone or shoreline width where oiling might occur. Others (W = water) are a full grid cell wide and have a fringing type on the land side.)

Habitat Code (Sw,Lw)	Ecological Habitat	F or W
	Intertidal / Shore	
1,31	Rocky Shore	F
2,32	Gravel Shore	F
3,33	Sand Beach or Shore	F
4,34	Fringing Mud Flat	F
5,35	Fringing Wetland (Emergent or Forested)	F
6,36	Macroalgal Bed	F

Habitat Code (Sw,Lw)	Ecological Habitat	F or W
7,37	Mollusk Reef	F
8,38	Coral Reef (marine only)	F
	Subtidal / Submerged	
9,39	Rock Bottom	W
10,40	Gravel Bottom	W
11,41	Sand Bottom	W
12,42	Silt-mud Bottom	W
13,43	Wetland (submerged areas)	W
14,44	Macroalgal Bed	W
15,45	Mollusk Reef	W
16,46	Coral Reef (marine only)	W
17,47	Submerged Aquatic Vegetation Bed	W
	Intertidal / Shore	
18,48	Man-made, Artificial	F
19,49	Ice Edge	F
20,50	Extensive Mud Flat	W
21,51	Extensive Wetland (Emergent or Forested)	W

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1.6 References – SIMAP Example Applications and Validations

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2 OILMAP Deep Model Description

OILMAP Deep was used to characterize the near field blowout conditions for use in the SIMAP model, which characterized the far field effects. OILMAP Deep contains two sub-models, a plume model and a droplet size model. The plume model predicts the evolution of plume position, geometry, centerline velocity, and oil and gas concentrations until the plume either surfaces or reaches a terminal height at which point the plume is trapped. The droplet model predicts the size and volume (mass) distribution of the oil droplets. Provided below is an overview of blowout theory and modeling implementation.

2.1 Blowout Model Theory

RPS ASA's oil blowout model is based on the work of McDougall (gas plume model, 1978), Fanneløp and Sjøen (1980a, plume/free surface interaction), Spaulding (1982, oil concentration model), Kolluru, (1993, World Oil Spill Model implementation), Spaulding et.al. (2000, hydrate formation) and Zheng et.al. (2002, 2003, gas dissolution). A simplified integral jet theory is employed for the vertical as well as for the horizontal motions of the gas-oil plume. The necessary model parameters defining the rates of entrainment and spreading of the jet are obtained from laboratory studies (Fanneløp and Sjøen 1980a). The gas plume analysis is described in McDougall (1978), Spaulding (1982), and Fanneløp and Sjøen (1980a). The hydrate formation and dissociation is formulated based on a unique equilibrium kinetics model developed by R. Bishnoi and colleagues at the University of Calgary. A brief description of the governing equations used in RPS ASA's blowout model and the solution methodology are described in Spaulding et al., 2000. The core components of this model are conservation of water mass, conservation of oil mass, conservation of momentum, and conservation of buoyancy.

Oil droplet size distribution calculations are based on the methodology presented by Yapa and Zheng (2001a&b) and Chen and Yapa (2007), which uses a maximum diameter calculation and the associated volumetric droplet size distribution. The maximum diameter can is determined using Hinze (1955) and coefficients consistent with Chen and Yapa (2007). The droplet size distribution is defined using a Rosin-Rammler (1933) function.

2.2 Blowout Model Implementation

The results of the near-field blowout model provide information to the far field fates model about the plume (the three dimensional extent of the mixture of gas/oil/water) and a characterization of the initial dispersion / mixing of the oil discharged during the blowout. Key factors in this analysis are the volume flux of oil and gas, gas to oil ratio (GOR), depth, exit flow velocity and environmental water column conditions (the profile of water temperature and density), which affect both the trap height and the potential for hydrate formation. Other factors such as duration of the blowout and ambient currents are also included but are less important.

The OILMAP Deep blowout model implementation is done in two parts; the first is the plume model described in the previous section, based on the McDougall bubble plume model; the second is the oil droplet size distribution and volume fraction calculation. While they are based on the same scenario blowout specifications (e.g. oil type and flow rate, gas oil ratio and depth), the model predictions are treated separately and do not interact. The two parts of the model predictions only come together at the collapse of the near field plume, at the trap height, where the depth and droplet distribution predictions are used for initialization of the far field particle model simulation.

The blowout plume model solves equations for conservation of water mass, momentum, buoyancy, and gas mass as described in Section 2.1 of the OILMAP Deep Technical Documentation, using integral plume theory. An additional equation for the conservation of oil at the plume centerline is also solved.

The plume model prediction is defined externally by a small set of parameters including:

- Blowout release depth
- Oil discharge rate
- Oil density
- Gas : oil ratio (GOR) at the surface
- Atmospheric pressure
- Ambient seawater density profile
- Plume spreading coefficient (□)
- Entrainment parameter (α)
- Slip velocity of gas bubbles in the oil plume
- Ambient current velocity
- Water column profile of temperature and density

The blowout plume models the evolution of the plume within the water column, solving for the position, radius, velocity and oil and gas concentrations along the centerline. The blowout droplet model solves for the distribution of mass within droplet sizes associated with the turbulence of the release. Typically, the near-field model is on the timescale of seconds and length scale of hundreds of metres, where the far-field model is on the scales of hours/days and kilometres. The details of the near field modelling that are passed along to the far field model include the distribution of the release mass in different droplet sizes at the appropriate initial position in the water column.

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