

## **Appendix A: SIMAP Model Description**

This appendix provides a discussion of the SIMAP model and its important oil fates model algorithms. It is intended to supplement information provided in the spill modeling technical report and help the reader understand the application of the model to the spill simulations performed. It includes an extensive reference list for oil spill modeling in general and a supplementary list of model application and validation study references.

SIMAP includes (1) an oil physical fates model, (2) interfacing to a hydrodynamics model for simulation of currents, (3) a biological effects model, (4) an oil physical, chemical and toxicological database, (5) environmental databases (winds, currents, salinity, temperature), (6) geographical data (in a GIS), (7) a biological database, (8) a response module to analyze effects of response activities, (9) graphical visualization tools for outputs, and (10) exporting tools to produce text format output.

SIMAP originated from the oil fates and biological effects sub-models in the Natural Resource Damage Assessment Model for Coastal and Marine Environments (NRDAM/CME), which ASA developed in the early 1990s for the US Department of the Interior for use in Natural Resource Damage Assessment (NRDA) regulations under the Comprehensive Environmental Response, Compensation and Liability Act of 1980 (CERCLA). 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. (1996a,b,c). This technical development involved several in-depth peer reviews, as described in the Final Rule.

While the NRDAM/CME was 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. SIMAP may be run in stochastic mode to evaluate a distribution of spill results, rather than just a single result for a specific hind-cast. 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 modeling, and facilitate analysis of results. The consideration of the impacts of subsurface oil is important, particularly in the evaluation of impacts on aquatic organisms. Surface floating oil primarily impacts wildlife and intertidal biota, and not aquatic biota in subtidal habitats. At higher wind speeds than about 12 knots (or at lower wind speeds if dispersant is applied), oil will entrain into the water column, unless it has become too viscous to do so after weathering and the formation of mousse. Once oil is entrained in the water in the form of small droplets, monoaromatics (MAHs) and polynuclear aromatic hydrocarbons (PAHs) dissolve into the water column. The dissolved MAHs and PAHs are the most bioavailable and toxic portion of the oil. The dissolution rate is very sensitive to the droplet size (because it involves mass transfer across the surface area of the droplet), and the amount of hydrocarbon mass dissolved is a function of the mass entrained and droplet size distribution. These are in turn a function of soluble hydrocarbon content of the oil, the amount of evaporation of these components before

entrainment, oil viscosity (which increases as the oil weathers and emulsifies), oil surface tension (which may be reduced by surfactant dispersants), and the energy in the system (the higher the energy the smaller the droplets). Large droplets (greater than a few hundred microns in diameter) resurface rapidly, and so dissolution from those is also inconsequential. Dispersant application facilitates the entrainment of oil into the water in a smaller size distribution than would occur naturally, with the median droplet size about 20  $\mu\text{m}$  (Lunel, 1993a,b).

Thus, the fate of MAHs and PAHs in surface oil is primarily volatilization to the atmosphere, rather than to the water. If wind speeds exceed 12 knots, entrainment of the surface oil into the water becomes significant. Dispersant application can also facilitate entrainment into the water column. If oil is entrained before it has weathered and lost the lower molecular weight aromatics to the atmosphere, dissolved MAHs and PAHs in the water can reach concentrations where they can affect water column organisms or bottom communities (French McCay and Payne, 2001).

Below is a brief description of the physical fates model implemented in SIMAP. Detailed descriptions of the algorithms and assumptions in the model are in published papers (French McCay 2002, 2003, 2004). The model has been validated with more than 20 case histories, including the Exxon Valdez and other large spills (French and Rines, 1997; French McCay, 2003, 2004; French McCay and Rowe, 2004) as well as test spills designed to verify the model (French et al., 1997).

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 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 semi-soluble aromatics to suspended sediments, sedimentation, and degradation.

Oil is a mixture of hydrocarbons of varying physical, chemical, and toxicological characteristics. Thus, oil hydrocarbons have varying fates and impacts on organisms. In the model, oil is represented by component categories, and the fate of each 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.

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 eight components (defined in Table A-1). Six of the components (all but the two non-volatile residual components) 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, with the MAHs the most soluble, the 2-ring PAHs semi-soluble, and the 3-ring PAHs slightly soluble Mackay et al. (1992a,b,c,d). 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 A-1. DEFINITION OF FOUR DISTILLATION CUTS AND THE EIGHT PSEUDO-COMPONENTS IN THE MODEL (MONOAROMATIC HYDROCARBONS, MAHs; BENZENE + TOLUENE + ETHYBENZENE + XYLENE, BTEX; POLYNUCLEAR AROMATIC HYDROCARBONS, PAHs).**

Characteristic	Volatile and Highly Soluble	Semi-volatile and Soluble	Low Volatility and Slightly Soluble	Residual (non-volatile and insoluble)
Distillation cut	1	2	3	4
Boiling Point (°C)	< 180	180 - 265	265 - 380	>380
Molecular Weight	50 - 125	125 - 168	152 - 215	> 215
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 $\log(K_{ow}) > 5.6$ (insoluble)

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 impact analyses because the impacts to water column organisms are caused by MAHs and PAHs, which have specific properties that differ from the other volatile and soluble compounds. Use of more pseudo components does not improve accuracy, as the major constituents of concern are well characterized (sufficiently similar in properties within the pseudo-component group of chemicals) by the modeled component properties used in SIMAP. 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 on 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.

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 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. The physical fates model creates output files recording the distribution of a spilled substance in three dimensional space and time. The quantities recorded are:

- area covered by oil and thickness on the water surface ("swept area");
- volumes in the water column at various concentrations of dissolved aromatics;
- volumes in the water column at various concentrations of total hydrocarbons in suspended droplets;
- total hydrocarbon concentrations and dissolved aromatic concentrations in surface sediment;
- lengths and locations of shoreline impacted and volume of oil ashore in each segment.

### **Important Oil Fates Processes**

The following section describes the details of the important processes simulated in the SIMAP model.

#### Wind Drift

If the wind drift of the surface wave-mixed layer is not included in three-dimensional and time varying current data supplied to the fates model, wind drift is added to the advective particle velocity within the oil fates model. Wind drift for surface slicks may be added as a user-specified, constant percentage of wind speed, with the option of including a drift angle clockwise of the down wind direction. Alternatively, wind drift is calculated in the SIMAP fates model.

The wind drift rate is the ratio of oil drift speed relative to the wind speed. Drift velocities due to a wind,  $u_{wc}$  and  $v_{wc}$  (m/sec), toward the east and north, respectively, are

$$u_{wc} = C_w u_w$$

$$v_{wc} = C_w v_w$$

where

- $u_w$  - east component of wind speed (m/sec)
- $v_w$  - north component of wind speed (m/sec)
- $C_w$  - drift factor (fraction)

The drift factor,  $C_w$ , may be set by the user as a constant (Lange and Hufnerfuss, 1978; Wu, 1980; Samuels et al., 1982), where  $C_w$  varies between 2.5 and 4.5%. These are values based on observations. The default value in the model is 3.5%, which may be reset by the user.

The wind drift angle is the angle the oil drifts clockwise (to the right in the northern hemisphere, use negative values for southern hemisphere) of the wind direction. The drift angle may be entered by the user as a constant angle in degrees. The default value is zero. For open waters a small positive value may be appropriate. A mean of 20° has been observed in several spills in mid-latitudes. The angle increases with latitude.

### Oil Degradation

Degradation may occur as the result of photolysis, which is a chemical process energized by ultraviolet light from the sun, and by biological breakdown, termed biodegradation.

Most studies of microbe-hydrocarbon interactions have been carried out under controlled laboratory conditions and results are not always applicable to the marine environment. Several parameters can limit biodegradation including the microbial population, temperature, oil composition, toxicity and state of weathering; and availability of nutrients and dissolved oxygen.

In the SIMAP model, degradation occurs on the surface slick, oil on the shore and the entrained oil and aromatics in the water column. A first order decay algorithm is used.

The degradation rate,  $\overset{\circ}{M}_b$  (g/sec), can be defined as:

$$\overset{\circ}{M}_b = \frac{dM_{b,i}}{dt} = -K_i M_i$$

$i$	environmental compartment (water or shoreline surface, water column, and sediments)
$M_{b,i}$	mass of oil lost by degradation from $i$ (g)
$M_i$	mass of oil subjected to degradation from $i$ (g)
$K_i$	degradation constant for compartment $i$ (1/day)

Many types of marine organisms ingest, metabolize and utilize oil as a carbon source, producing carbon dioxide and water as by-products. The biodegradable fraction of various

crude oils ranges from 11 to 90% (NRC, 1985, 1989). A typical degradation rate results in the loss of 1% of the available oil mass per day.

### Shoreline Interactions

The fate of spilled oil that reaches the shoreline depends on characteristics of the oil, the type of shoreline, and the energy environment (Reed et al., 1986, 1988, 1989; Gundlach, 1987; Reed and Gundlach, 1989; Harper and Harvey-Kelly, 1994; Humphrey, 1994). Even when beached, oil will continue to weather. However, several additional processes become important: refloating, penetration into the substrate, and retention/transport in the beach-groundwater system. Erosion of oiled substrate from the beach to offshore sediments may also occur. Considerable study of shoreline oiling, fates and removal processes was performed as part of the development of the COZOIL model for the U.S. Minerals Management Service (Reed et al., 1986, 1988, 1989; Gundlach, 1987; Reed and Gundlach, 1989). The shoreline interaction algorithms in SIMAP are based on this model.

The maximum oil holding thickness is a function of oil viscosity and shore type (CSE/ASA/BAT, 1986; Gundlach, 1987). Oil removal from the shoreline is by water penetration and flushing, and by wave erosion. Thus, removal is faster on exposed coasts than sheltered shorelines. Each shoreline cell in the SIMAP model grid has an oil holding capacity based on oil type, shore type, beach slope, beach width (Table A2) and shoreline grid length.

Oil deposition occurs when oil intersects the shore surface. Deposition ceases when the holding capacity for the shore surface is reached. Subsequent oil deposited is not allowed to remain on the shore surface, and is refloated as slicks that continue to move along shore. After stranding permanently, the shoreline oil is removed exponentially with time. The removed oil is returned to the water column on a rising tide (sufficiently high to wet the oiled surface) and offshore winds.

**TABLE A2: TYPICAL BEACH WIDTHS BY SHORE TYPE (CERC, 1984; FRENCH ET AL, 1996).**

Shore Type	Mean Beach Width (m)				
	East Coast <sup>2</sup>	Gulf of Mexico <sup>3</sup>	California <sup>4</sup>	Pacific NW <sup>5</sup>	Gulf of Alaska <sup>6</sup>
1. Exposed rocky	2	1	2	3	3
2. Wave cut platform	2	1	2	3	3
3. Fine sand	10	5-15	10	15	20
4. Coarse sand	10	5	10	15	20
5. Mixed sand/gravel	5	5	5	7	10
6. Gravel	3	2	3	4	6
7. Exposed tidal flats	10	10	10	15	20
8. Sheltered rocky	2	1	2	3	3
9. Sheltered tidal flats	140	20	120	210	300
10. Sheltered marsh	140	50	120	210	300
11. Glacier edge	-	-	-	-	3
12. Artificial <sup>1</sup>	0.1	0.1	0.1	0.1	0.1

<sup>1</sup> Assumed value for vertical bulkhead

<sup>2</sup> These shore widths, as well as the data in Tables 3-4 and 3-5, are included in the default data file "CME-East\_Coast.SHR" supplied with the model.

<sup>3</sup> These shore widths, as well as the data in Tables 3-4 and 3-5, are included in the default data file "CME-Gulf\_of\_Mexico.SHR" supplied with the model.

<sup>4</sup> These shore widths, as well as the data in Tables 3-4 and 3-5, are included in the default data file "CME-California.SHR" supplied with the model.

<sup>5</sup> These shore widths, as well as the data in Tables 3-4 and 3-5, are included in the default data file "CME-Pacific\_NW.SHR" supplied with the model.

<sup>6</sup> These shore widths, as well as the data in Tables 3-4 and 3-5, are included in the default data file "CME-Gulf\_of\_Alaska.SHR" supplied with the model.

### Oil Entrainment

As oil on the sea surface is exposed to wind and waves, it is entrained (and dispersed) into the water column. Entrainment is a physical process where globules of oil are transported from the sea surface into the water column by breaking waves. 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 rapidly back to the surface (Delvigne and Sweeney, 1988; Delvigne, 1991). Breaking waves created by the action of wind and waves on the ocean surface are the primary sources of energy for entrainment, although other sources of turbulence can entrain oil (Delvigne et al., 1994). Entrainment is strongly dependent on turbulence and is greater in areas of high wave energy.

It has been observed that entrained oil is subjected to enhanced dissolution and biodegradation processes. The increased surface area represented by these droplets increases the rates of dissolution and photo-oxidation.

Delvigne and Sweeney (1988), using laboratory and flume experimental observations, developed relationships for oil entrainment rate and resulting suspended oil droplet size distribution as functions of turbulent energy level and oil viscosity. Droplet sizes decrease and entrainment rate increases with increasing turbulence. The higher the oil viscosity, the larger is the maximum droplet size and the lower the entrainment rate. Oil viscosity is increased by emulsification, which slows entrainment rate (Spaulding et al., 1992; French et al., 1996; Dahling et al., 1997). The data and relationships in Delvigne and Sweeney (1988) are used to calculate mass and particle size distribution of droplets entrained in SIMAP (as it is in the NRDAM/CME, French et al., 1996). Particle size decreases with higher turbulent energy level and lower oil viscosity, from a low-turbulence and high-viscosity condition where droplet sizes range up to a maximum of 5 mm, to a high-turbulence and low-viscosity condition where droplet sizes range up to a maximum of 0.2 mm (200  $\mu$ m). The natural dispersion particle sizes observed by Delvigne and Sweeney (1988) are confirmed by field observations by Lunel (1993a,b).

Entrained droplets in the water column rise according to Stokes Law, where velocity is related to the difference in density between the particle (droplet) and the water, and to the particle diameter. In addition to rising according to Stoke's Law, entrained droplets are transported by currents and mixed vertically by randomized turbulent diffusion. When droplets intersect the water surface, if their buoyancy can overcome vertical mixing they surface and form sheens and tar balls (modeled as surface spilletts of <0.1mm average thickness).

### Oil Evaporation

Evaporation can result in the transfer of 20-40% of spilled oil from the sea surface to the atmosphere, depending on the type of oil (Gundlach and Boehm, 1981). The rate of evaporation depends on surface area, thickness, vapor pressure and mass transport coefficient, which in turn are functions of the composition of the oil, wind speed and temperature. As oil evaporates its composition changes, affecting its density and viscosity as well as subsequent evaporation. The most volatile hydrocarbons (low carbon number) 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.

Evaporation models assume the oil to be well-mixed within the slick. For thick, viscous slicks, the well-mixed assumption is not valid, and virtually fresh oil may remain for several days or even weeks, trapped within viscous oil-water emulsions. A diagram of the evaporative process is in Figure A1.

The Mackay evaporative exposure algorithm (Stiver and Mackay, 1984) is used in many oil spill models such as the Mackay et al. models (Mackay and Leinonen 1977; Mackay et al. 1980a,b, 1982), ADIOS (Lehr et al. 1992), OILMAP (Spaulding et al. 1992), and earlier versions of SIMAP (French et al. 1999). The algorithm is based on accepted evaporation theory, which follows Raoult's Law that each component will evaporate with a rate proportional to the saturation vapor pressure and mole fraction present for that component. For the evaporative exposure model the assumption is that the oil mixture behaves as a single component. It uses an analytical approach to predict the volume fraction evaporated, using distillation data to estimate parameters needed for the analytic equation.



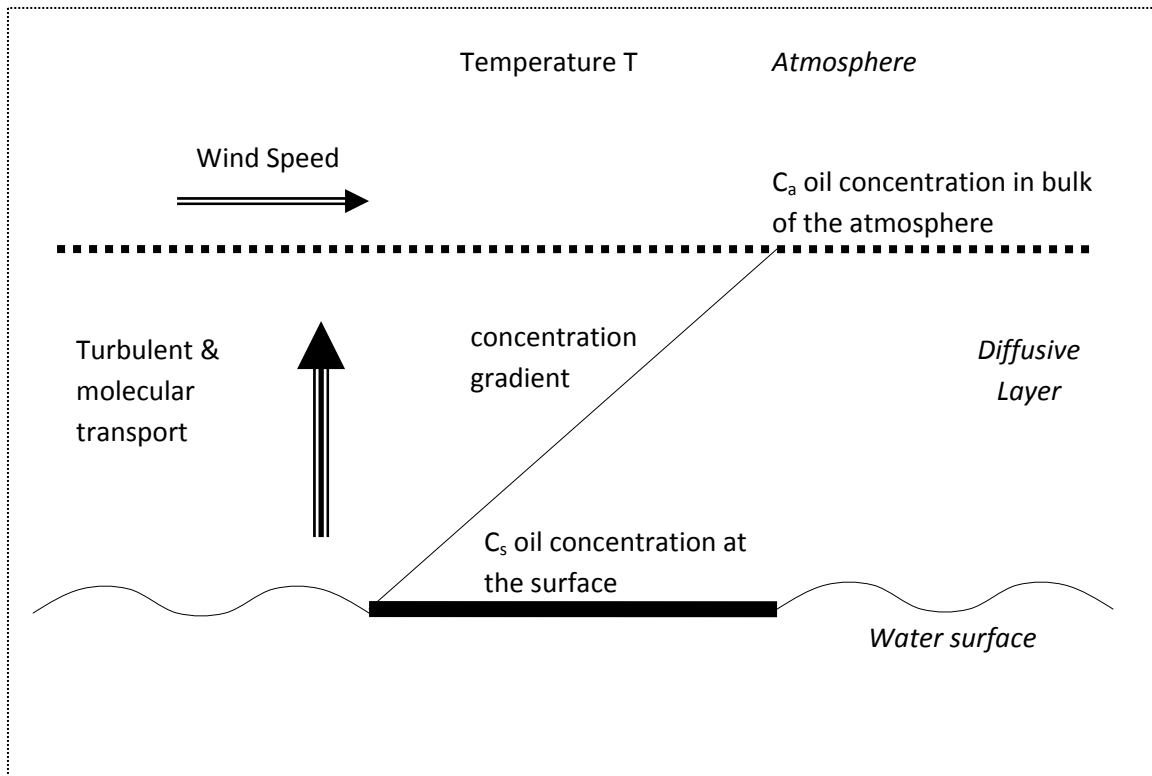


FIGURE A1. SCHEMATIC DIAGRAM OF EVAPORATION PROCESS.

In other models (Payne et al. 1984, 1987; Kirstein et al. 1985; French et al. 1996; Jones 1997; Lehr et al. 2000; Reed et al. 2000) and in SIMAP, so-called pseudo-components (chemical component classes) are evaporated according to an analogous evaporative exposure algorithm, where the flux to the atmosphere is specific to the component's molar volume, vapor pressure, and molecular weight. Jones (1997) simplified this approach into a simplified pseudo-component (SPC) model, relating molar volume, vapor pressure, and molecular weight to the boiling point of the component. Thus, only the boiling points and initial volume fractions of the components need to be specified to implement the model.

#### Oil/Ice Interactions

The SIMAP model accounts for the presence of ice when calculating surface oil advection, evaporation, entrainment into the water column and surface oil spreading. Table A3 briefly summarizes how the model deals with oil advection and weathering in the presence of different ice concentrations.

**TABLE A3: SUMMARY OF OIL-IN-ICE ADVECTION AND WEATHERING EFFECTS ACCOUNTED FOR IN THE SIMAP MODEL.**

<b>Ice Cover (Percent)</b>	<b>Advection</b>	<b>Evaporation</b>	<b>Entrainment</b>	<b>Spreading</b>
0 – 30	No change	No change	No change	No change
30 – 80	15° to right	Linear reduction with ice cover	Linear reduction with ice cover	Terminal thickness increased in proportion to ice coverage
80 - 100	Oil moves with pack ice	No weathering	No weathering	Oil thickness computed as a function of ice thickness

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