

## Appendix A: SIMAP Model Description

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.

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 A2 briefly summarizes how the model deals with oil advection and weathering in the presence of different ice concentrations.

**TABLE A2: 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

## References

- French, D., M. Reed, K. Jayko, S. Feng, H. Rines, S. Pavignano, T. Isaji, S. Puckett, A. Keller, F. W. French III, D. Gifford, J. McCue, G. Brown, E. MacDonald, J. Quirk, S. Natzke, R. Bishop, M. Welsh, M. Phillips and B.S. Ingram, 1996a. The CERCLA type A natural resource damage assessment model for coastal and marine environments (NRDAM/CME), Technical Documentation, Vol. I - Model Description. Final Report, submitted to the Office of Environmental Policy and Compliance, U.S. Dept. of the Interior, Washington, DC, April, 1996, Contract No. 14-0001-91-C-11.
- French, D., M. Reed, S. Feng and S. Pavignano, 1996b. The CERCLA type A natural resource damage assessment model for coastal and marine environments (NRDAM/CME), Technical Documentation, Vol. III - Chemical and Environmental Databases. Final Report, Submitted to the Office of Environmental Policy and Compliance, U.S. Dept. of the Interior, Washington, DC, April, 1996, Contract No. 14-01-0001-91-C-11.
- French, D., S. Pavignano, H. Rines, A. Keller, F.W. French III and D. Gifford, 1996c. The CERCLA type A natural resource damage assessment model for coastal and marine environments (NRDAM/CME), Technical Documentation, Vol.IV - Biological Databases. Final Report, Submitted to the Office of Environmental Policy and Compliance, U.S. Dept. of the Interior, Washington, DC, April, 1996, Contract No. 14-01-0001-91-C-11.
- French, D.P., and H. Rines, 1997. Validation and use of spill impact modeling for impact assessment. Proceedings, 1997 International Oil Spill Conference, Fort Lauderdale, Florida, American Petroleum Institute Publication No. 4651, Washington, DC, pp-829-834.
- French, D.P., H. Rines and P. Masciangioli, 1997. Validation of an Orimulsion spill fates model using observations from field test spills. In: Proceedings of the Twentieth Arctic and Marine Oilspill Program (AMOP) Technical Seminar, Vancouver, Canada, June 10-13, 1997, Emergencies Science Division, Environment Canada, Ottawa, Ontario, Canada, pp.933-961.
- French McCay, D.P., 2002. Development and Application of an Oil Toxicity and Exposure Model, OilToxEx. *Environmental Toxicology and Chemistry* 21(10): 2080-2094.
- French McCay, D.P., 2003. Development and Application of Damage Assessment Modeling: Example Assessment for the North Cape Oil Spill. *Marine Pollution Bulletin*, Volume 47, Issues 9-12, September-December 2003, pp. 341-359.
- French McCay, D.P., 2004. Oil spill impact modeling: Development and validation. *Environmental Toxicology and Chemistry* 23(10): in press.
- French McCay, D. and James R. Payne, 2001. Model of oil fate and water concentrations with and without application of dispersants. In: Proceedings of the Twenty-fourth Arctic and Marine Oil spill Program (AMOP) Technical Seminar, Emergencies Science Division, Environment Canada, Ottawa, Ontario, Canada, pp.611-645.

- French McCay, D.P., and J.J. Rowe, 2004. Evaluation of Bird Impacts in Historical Oil Spill Cases Using the SIMAP Oil Spill Model. In Proceedings of the 27th Arctic and Marine Oil Spill Program (AMOP) Technical Seminar, Emergencies Science Division, Environment Canada, Ottawa, ON, Canada, pp. 421-452.
- Jones, R.K., 1997. A Simplified Pseudo-Component of Oil Evaporation Model, in Proceedings of the 20<sup>th</sup> Arctic and Marine Oil Spill Program (AMOP) Technical Seminar, Environment Canada, pp. 43-61.
- Lehr, W.J., D. Wesley, D. Simecek-Beatty, R. Jones, G. Kachook and J. Lankford, 2000. Algorithm and interface modifications of the NOAA oil spill behavior model. Proceedings of the 23rd Arctic and Marine Oil Spill Program (AMOP) Technical Seminar, Vancouver, BC, Environmental Protection Service, Environment Canada, pp. 525-539.
- Lunel, T. 1993a. Dispersion: Oil droplet size measurements at sea. in Proceedings of the 16<sup>th</sup> Arctic Marine Oilspill Program (AMOP) Technical Seminar, Environment Canada, Calgary, Alberta, June 7-9, 1993, pp. 1023-1056.
- Lunel, T. 1993b. Dispersion: Oil droplet size measurements at sea. in Proceedings of the 1993 Oil Spill Conference, pp. 794-795.
- Mackay, D., S. Paterson and K. Trudel, 1980. A mathematical model of oil spill behavior, Department of Chemical and Applied Chemistry, University of Toronto, Canada, 39p.
- Mackay, D., W.Y. Shiu, and K.C. Ma, 1992a. Illustrated Handbook of Physical-Chemical Properties and Environmental Fate for Organic Chemicals, Vol. I, Monoaromatic Hydrocarbons, Chlorobenzenes, and PCBs. Lewis Publ., Chelsea, Michigan, 668p.
- Mackay, D., W.Y. Shiu, and K.C. Ma, 1992b. Illustrated Handbook of Physical-Chemical Properties and Environmental Fate for Organic Chemicals, Vol. II, Polynuclear Aromatic Hydrocarbons, Polychlorinated Dioxins, and Dibenzofurans. Lewis Publ., Chelsea, Michigan, 566p.
- Mackay, D., W.Y. Shiu, and K.C. Ma, 1992c. Illustrated Handbook of Physical-Chemical Properties and Environmental Fate for Organic Chemicals, Vol. III, Volatile Organic Chemicals. Lewis Publ., Chelsea, Michigan, 885p.
- Mackay, D., W.Y. Shiu and D.C. Ma, 1992d. Illustrated Handbook of Physical-Chemical Properties and Environmental Fate for Organic Chemicals. Volume IV Oxygen, Nitrogen, and Sulfur containing compounds. Lewis Publishers, Inc. Chelsea, Michigan, 930p.
- Payne, J.R., B.E. Kirstein, G.D. McNabb, Jr., J.L. Lambach, R. Redding R.E. Jordan, W. Hom, C. deOliveria, G.S. Smith, D.M. Baxter, and R. Gaegel, 1984. Multivariate analysis of petroleum weathering in the marine environment – sub Arctic, Environmental Assessment of the Alaskan Continental Shelf, OCEAP, Final Report of Principal Investigators, Vol. 21 and 22, Feb. 1984, 690p.

Payne, J.R., B.E. Kirstein, J.R. Clayton, Jr., C. Clary, R. Redding, G.D. McNabb, Jr., and G. Farmer, 1987. Integration of suspended particulate matter and oil transportation study. Final Report. Minerals Management Service, Environmental Studies Branch, Anchorage, AK. Contract No. 14-12-0001-30146, 216 p.

Stiver, W. and D. Mackay, 1984. Evaporation rate of oil spills of hydrocarbons and petroleum mixtures. *Environmental Science and Technology* 18: 834-840.