DHI Oil Spill Model

Oil Spill Template

Scientific Description

DHI headquarters
Agern Allé 5
DK-2970 Hørsholm
Denmark

+45 4516 9200 Telephone
mike@dhigroup.com
www.mikepoweredbydhi.com

Company Registration No.: DK36466871

CONTENTS

DHI Oil Spill Model
Oil Spill Template
Scientific Description

1 Introduction 1

2 What is Oil? 3
2.1 Introduction 3
2.2 Weathering Processes 3
2.3 Oil Components 5

3 Weathering Processes in the DHI Oil Spill Model 7
3.1 State Variables 7
3.1.1 Volatile oil mass 7
3.1.2 Heavy oil mass 8
3.1.3 Amount of asphaltenes 8
3.1.4 Water fraction of oil 8
3.1.5 Droplet diameter 9
3.1.6 Area of oil 9
3.1.7 Immersed state 10
3.2 Evaporation 10
3.2.1 Description of the detailed evaporation process 10
3.2.2 Simple time-dependent expression of the evaporation process 11
3.3 Dissolution 12
3.4 Emulsification 13
3.5 Sedimentation 14
3.6 Biodegradation 15
3.7 Photooxidation 15
3.8 Vertical Dispersion 16
3.9 Physical Properties of Oil 17
3.9.1 Dynamics of viscosity 18
3.9.2 Dynamics of density 18

4 Oil Booms, Movement Block 20

5 Beaching, Shore Lock-Reflection Conditions 22

6 Detergents 24

7 Drift 26
7.1 Bed Shear Profile (Logarithmic Profile) 26
7.2 Wind Induced Profile 27
7.3 Wind Acceleration of Surface Particles 28
7.3.1 Wind drift angle 29

8 Parameterisation of an Oil Type 30
8.1 Evaporation 30
8.2 Distribution into Different Model Components 31
8.3 Dynamic Viscosity 33
8.4 Specific Density, Volumetric Expansion Coefficient 34
8.5 Final Parameterisation for STATFJORD 35

9 References 38

APPENDICES

APPENDIX A
Evaporation Parameters for Different Oils

APPENDIX B
Parameterisation Values for Different Oils

1 Introduction

An oil spill is the release of a liquid petroleum hydrocarbon into the environment due to human activity, and is a form of pollution. The term often refers to marine oil spills, where oil is released into the ocean or coastal waters. The oil may be a variety of materials, including crude oil, refined petroleum products (such as gasoline or diesel fuel) or by-products, ships' bunkers, oily refuse.

DHI's Oil Spill Model is a tool for predicting fate of marine oil spills, covering both the transport and the changes in chemical composition. The model is a Lagrangian model that runs decoupled from hydrodynamics. The prerun hydrodynamic results from the hydrodynamic model that can be applied in the model are contained in 2D or 3D result files.

The changes in chemical composition of oil residues over time is a result of physical and biological processes and is often referred to as 'weathering' of the oil. The more closely the chemical composition of a residue resembles that of the unspilled oil, the 'fresher' it is.

The weathering processes included in the model depends on the user's choice. Most simulated weathering process can be separately enabled or disabled.

In the model; the oil is divided into two oil fractions; a light volatile fraction and a heavier fraction.

2 What is Oil?

2.1 Introduction

Crude oil is a complex mixture of many chemical components. The relative compositions vary, resulting in many crude oil types with different chemical and physical properties.

The refinery distillation processes at an oil refinery converts the crude oil into a number of refined products, as shown in Figure 2.1 below.

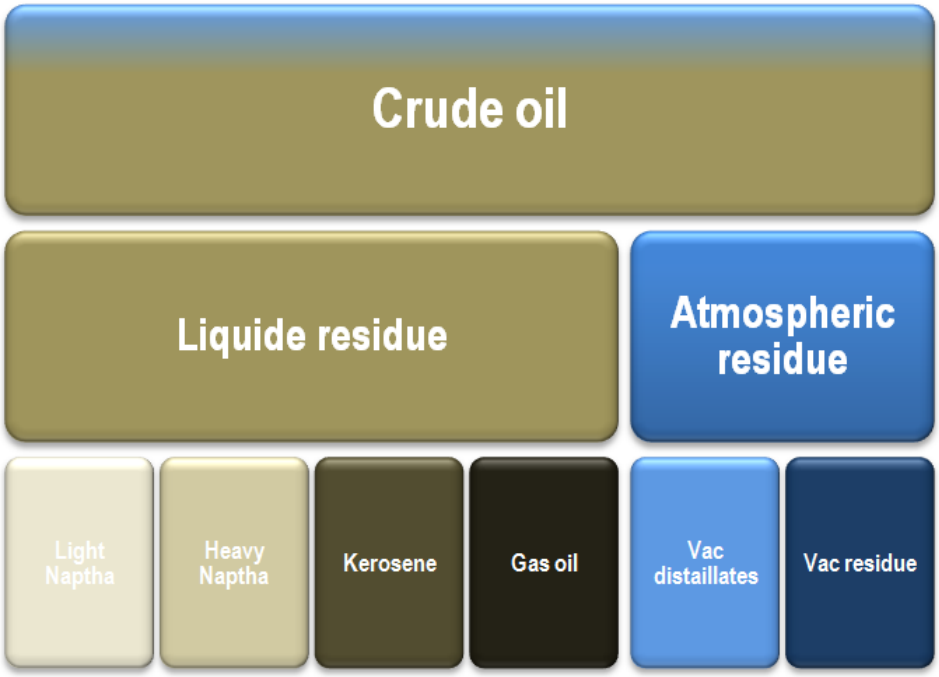

Figure 2.1 Conversion of crude oils into refined oil products by distillation

2.2 Weathering Processes

Oil spilled in the water surface immediately spreads over a slick of few millimetres. The spreading is especially promoted by gravity and surface tension, however many spills of varying size quickly reach a similar average thickness of about 0.1 mm. Advection of currents and wind affects both surface oil and droplets dispersed in the water body.

Due to evaporation, emulsification, dispersion, dissolution, photooxidation, sedimentation and biodegradation the oil changes its physical and chemical properties and may disappear from the sea surface. All mentioned processes are dependent on each other and are referred to as oil weathering.

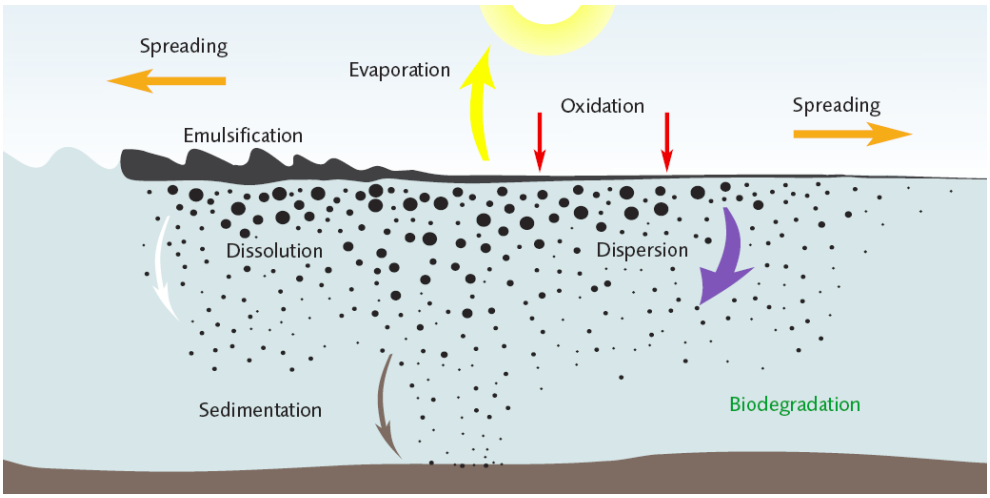

Figure 2.2 Processes acting on spilled oil (from Fate of Marine Oil Spills (2002))

Spreading, evaporation, dispersion and dissolution can be defined as short-term weathering processes, whereas emulsification, biodegradation and photochemical oxidation are recognised as long-term weathering processes.

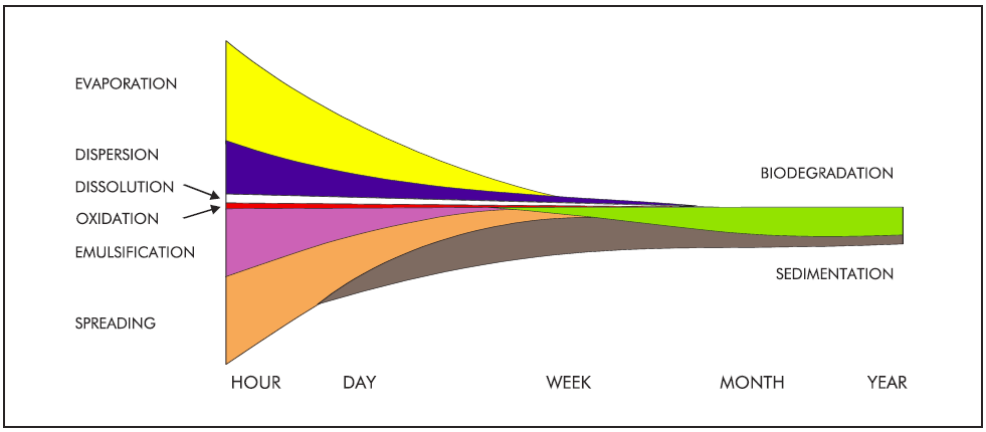

Figure 2.3 A schematic representation of the fate of a crude oil spill showing changes in the relative importance of weathering processes with time - the width of each band indicates the importance of the process (from Fate of Marine Oil Spills (2002))

The different chemical components in the oil are described by, among other things, the molecular weight which is an indication of how volatile the component is and how it is affected by the weathering process. A schematic presentation of how these processes are dependent on each other and the oil components is given in Figure 2.4.

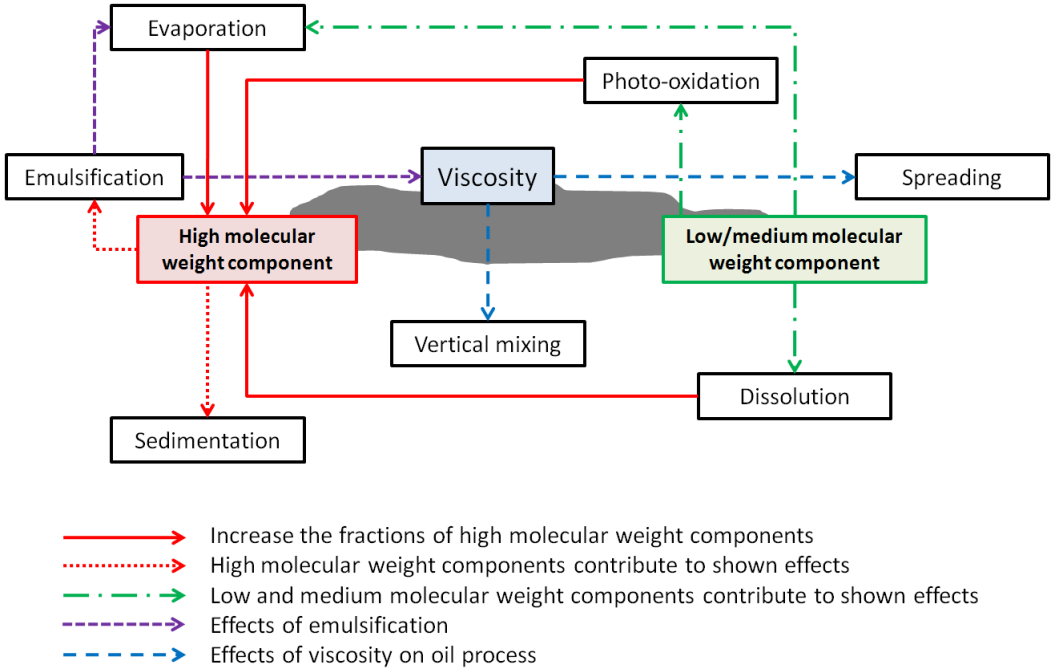

Figure 2.4 Effect of oil components and property on oil processes (from Xie et. al (2007))

2.3 Oil Components

For better prediction of the weathering processes the oil is often split up into fractions of certain properties (so-called pseudo-components). This usually requires detailed knowledge about the oil properties such as content of each pseudo-component and its properties. Therefore, for modelling purposes it is required to find specific oil characteristics, either from a database or by performing additional calculations.

An example of such a division of bulk liquid into pseudo-components of certain properties is shown in Chapter 8.

The oil spill templates used in DHI Oil weathering model describes the oil by two fractions only: a light volatile fraction and a heavier fraction. The light volatile fraction is defined as the mass of hydrocarbons with molecular weight below 160 g/mol and an boiling point well below 300°C. The heavy fraction is defined as hydrocarbons of molecular masses above 160 g/mol and boiling points from 250°C - 300°C and upwards, including wax and asphaltene components.

Each crude oil type has a different composition of the various components and it may be difficult to obtain the characteristics for the composition used in the DHI oil weathering model. If available the distillation data will provide valuable information.

Table 2.1 contains an estimated composition for the four groups of the ITOPF classification, see Fate of Marine Oil Spills (2002). The ITOPF classification is defined by the density of the oil. At the end of the table estimates for the relative distribution into the two oil fraction types used in the DHI Oil Spill model are given.

Table 2.1 Estimated composition of 4 generic oil groups

	ITPOF Group	I	II	III	IV
	Density (g/cm^3)	**< 0.8**	**0.8 – 0.85**	**0.85 – 0.95**	**> 0.95**
	°API	**> 45**	**35 - 45**	**17.5 – 35**	**< 17.5**
8	**Examples**	Gasoline, Kerosene	Gas oil, Brent Blend, Ekofisk	Crude oil, Arabian Heavy	Heavy fuel
	DHI oil fractions				
1	Light volatile	100	70	55	35
1	Heavy	0	30	45	65

3 Weathering Processes in the DHI Oil Spill Model

The oil is divided into two main fractions; a light volatile fraction of aromatics and other oil components with molecular weight less than approximately 160 g/mol and a boiling point well below 300°C, and a more heavy fraction (> 160 g/mol) with a boiling point above 250°C-300°C, covering the residuals. Wax and asphaltenes components are considered as special fractions of the oil, and they are assumed not to degrade, evaporate neither dissolve in the water.

In general the model describes the total amount of spilled oil as an assemblage of smaller oil amounts represented by individual oil track particles. These oil track particles are subject to weathering and drift process, working solely on the represented oil.

3.1 State Variables

There are 8 internal state variables for each oil track particle. The first five describe the oil loading, whereas the last three represent physical properties:

- Volatile oil mass [kg]
- Heavy oil mass [kg]
- Amount of asphaltenes [kg]
- Amount of wax [kg]
- Water fraction of oil [kg/kg]
- Droplet diameter [m]
- Area of oil [m^2]
- Immersed state [logical (0/1)]

Each state variable has an ordinary differential equation describing its rate of change.

3.1.1 Volatile oil mass

This state variable is defined as the mass of aromatics with molecular weight below 160 g/mol and a boiling point well below 300°C, e.g. the light and volatile fraction of the oil. This component is subject to evaporation, dissolution, biodegradation and photooxidation.

The rate of change is given as:

$$\frac{dVolatile_Oilmass}{dt} = -EVAP - DISSOL_volatile - BIOD_volatile - PHOT_volatile \quad (3.1)$$

Where:

EVAP	Evaporation, see Section 3.2
DISSOL_volatile	Dissolution, see Section 3.3
BIOD_volatile	Biodegradation of volatile fraction of oil, see Section 3.6
PHOT_volatile	Photooxidation of volatile fraction of oil, see Section 3.7

3.1.2 Heavy oil mass

This state variable is defined as the mass of the oil components with a molecular weight above 160 g/mol and a boiling point above 300°C. This component is subject to dissolution, biodegradation and photooxidation. Note that there is no evaporation in this component.

The rate of change expression is given as:

$$\frac{dHEAVY_oilmass}{dt} = \begin{aligned} &-DISSOL_heavy \\ &-BIOD_heavy \\ &-PHOT_heavy \end{aligned} \tag{3.2}$$

Where:

DISSOL_heavy	Dissolution of heavy fraction of oil, see Section 3.3
BIOD_heavy	Biodegradation of heavy fraction of oil, see Section 3.6
PHOT_heavy	Photooxidation of heavy fraction of oil, see Section 3.7

3.1.3 Amount of asphaltenes

This state variable is defined as the amount of asphaltenes in the oil. Asphaltenes are considered to be conservative, i.e. the component does neither degrade, evaporate nor dissolve.

$$\frac{dAsphaltenes}{dt} = 0 \tag{3.3}$$

Amount of wax
This state variable is defined as the amount of wax in the oil. Wax components are also considered to be conservative, i.e. the component does neither degrade, evaporate nor dissolve.

$$\frac{dWax}{dt} = 0 \tag{3.4}$$

3.1.4 Water fraction of oil

This state variable is defined as the water content in the oil particle.

The rate of change expression is given as:

$$\frac{dY_W}{dt} = \begin{aligned} &+wateruptake \\ &-waterrelease \end{aligned} \tag{3.5}$$

Where:

wateruptake	Uptake of water in oil (emulsification), see Section 3.4
waterrelease	Release of water from oil, see Section 3.4

3.1.5 Droplet diameter

The droplet diameter can be significantly altered by wave action.
The change is described as:

$$\frac{dDropletDiameter}{dt} = DiameterChange \tag{3.6}$$

The diameter change is only computed when wave dissipation is enabled. See Section 3.9 for details.

The change rate is set to match the mean droplet diameter *d* as calculated according to French-McCay (2004):

$$d = 1.818\,E^{-0.5}\;N^{0.34} \tag{3.7}$$

Where:

E	Energy dissipation rate for breaking wave ($J/m^3/s$) set equal to $10e^3$
N	kinematic viscosity (10^{-6} centistokes)

3.1.6 Area of oil

This state variable is defined as the area of contact with the sea surface. It represents the equivalent area of a circular slick for the oil loading of an individual oil track particle. Please note that this area does not describe the total, by all particles covered area. Also this total covered area is not equivalent to the sum of all particle track areas as single particle track areas can overlap. However, the sum of all particle track areas gives an upper bound for the total covered area.

The change in this area with time is expressed by Mackay et al. (1980):

$$\frac{dA}{dt} = K_{Spread} \cdot A^{\frac{1}{3}} \cdot \left[\frac{V}{A}\right]^{\frac{4}{3}} \tag{3.8}$$

Where:

K_{spread}	is a rate constant [s^{-1}]
V	volume of oil [m^3]
A	area of the oil particle [m^2]

3.1.7 Immersed state

The immersed state is used to separate oil particles that are in the water phase or stranded on the shore line. It will be '1' for a particle in the water phase and '0' for a particle not in the water phase.

If a track particle is thrown on land it may be absorbed (the position will be locked and no further movement is allowed) or reflected into the sea again. The probability of getting absorbed can be a single, global value or be specified as 2D map. Certain process will be only active if a track particle is immersed and not beached (i.e. area and water content change, dissolution and dispersion processes).

3.2 Evaporation

In the first hours and days of the spill, evaporation at the surface of the slick is the dominant weathering process. If the spill consists of a lightweight, highly refined product like gasoline, evaporation can very effectively remove nearly all of the spill contamination in as little as 24 hours. For spills of most medium-weight crudes the removal is less complete but substantial nevertheless. Typically, 10-30% of the material from these spills can be removed through evaporation in the first 24 hours.

Other factors effecting the evaporation of a spill include the amount of the spill exposed at the surface of the slick, wind and sea surface conditions.

Two options for the modelling of the evaporation are included:
1. Detailed boundary regulated evaporation
2. Simple time-dependent expression

3.2.1 Description of the detailed evaporation process

In the detailed description of the evaporation, the evaporation process for one particle that is in contact with the water surface (within 5 cm from surface) is calculated according to the 'Model of Reed', see Betancourt et al. (2005) and Reed (1989):

$$EVAP = \frac{K_2 \cdot P_{vp} \cdot A}{R \cdot T} \cdot f \cdot MW \tag{3.9}$$

Where:

K_2	Mass transfer coefficient is defined as [m/h]
P_{VP}	Vapor pressure [atm.]
A	Slick area of each particle in contact with water surface [m^2]
R	Gas constant $8.206 \cdot 10^{-5}$ atm m^3/ mol K
T	Temperature [K]
f	fraction of the evopartive oil component
MW	Molecular weight [g/mol]

The mass transfer coefficient is calculated according to Mackay et al. (1980) as:

$$K_2 = 0.0292 \cdot wspd^{0.78} \cdot D^{-0.11} \cdot Sc^{-0.67} \cdot \sqrt{\frac{MW + 29}{MW}} \quad (3.10)$$

Where:

wspd	Wind speed [m/h]
MW	Average molecular weight of fraction [g/mol]
Sc	Schmidt number (dim.less)
D	Diameter of each particles area in contact with water surface [m]

The assumed diameter has a lower limit of 0.5 m and the minimum applied wind speed is 1m/h.

The Schmidt number *Sc* characterises the relative proportions of momentum and mass diffusion convection process. It can be interpreted as surface roughness information. Traditionally the Schmidt number *Sc*=2.7 for cumene evaporation is used in oil spill modelling, Mackay et al. (1980).

3.2.2 Simple time-dependent expression of the evaporation process

The time-dependent correlations for evaporation loss as suggested by Fingas (1996) and (1997) are also included in the DHI oil spill model. Based on empirical studies on the evaporation of oil and petroleum products, Fingas determined best-fit equations for both the percentage loss by time and absolute weight loss for various oil types. Most oils were found to follow logarithmic loss curves, but a smaller amount fitted square root loss curves with time for periods up to about 5 days. The derived relationships are of the general structure:

Evaporation curve type: logarithmic form

$$loss(\%weight) = (A + B * T) * \ln(t) \quad (3.11)$$

Evaporation curve type: square root form

$$loss(\%weight) = (A + B * T) * \sqrt{t} \quad (3.12)$$

Where:

A	Oil specific constant (called *evapA* in the DHI model)
B	Oil specific constant for temperature dependency (called *evapB* in the DHI model)
T	Oil temperature [°C]
t	Age of the oil [minutes]

The oil specific constants **A** and **B** as well as the type of the evaporation curve are often available for specific oils and can be found in literature. A list for common oils can be found in APPENDIX A.

The oil temperature is assumed to be equal to the ambient water temperature.

Generic evaporation formulas

The loss equation constants were found to correlate fine with the percentage distilled at 180°C (r2 between 0.74 and 0.98, Fingas (1996). If the specific values for A and B are not known, the distillation loss at 180°C can be used instead. The model allows specifying this distillation loss at 180°C directly. In this case some generic forms for the evaporation loss equations are used:

Evaporation curve type: logarithmic, generic form

$$loss(\%weight) = (0.165 * D + 0.045 * (T - 15)) * \ln(t) \quad (3.13)$$

Evaporation curve type: square root, generic form

$$loss(\%weight) = (0.0254 * D + 0.01 * (T - 15)) * \sqrt{t} \quad (3.14)$$

Where:

D	distillation loss (weight %) at 180°C (called *evap180* in the DHI model)
T	Oil temperature [°C]
t	Age of the oil spill [minutes]

Please note that a value (> 0%) for the constant ***D*** (distillation loss at 180°C) in the model parameterisation will override any specific values ***A*** and ***B***. There are possible temperature constrains when applying the simplified evaporation scheme; the generic forms should not be used below a temperature of 15°C.

3.3 Dissolution

Some part of the oil slick is removed as the water-soluble portion of the petroleum hydrocarbons are dissolved into the surrounding seawater. Although this reduces the size of the slick it presents an environmental problem since the water-soluble spill components and breakdown products are those that are most toxic to marine life. Small aromatic hydrocarbons like benzene and toluene, and somewhat larger polycyclic aromatic hydrocarbons (PAHs) like naphthalene, are among the water-soluble petroleum components known to have toxic effects.

Other factors affecting the dissolution of a spill include the amount of the spill exposed at the surface of the slick, wind and sea surface conditions, air temperature, and insolation intensity. Another factor is emulsification of the slick, which significantly retards the rate of evaporation.

The dissolution processes for the volatile and heavy oil fractions are calculated as:

$$DISS_volatile = k_{disl} \cdot A \cdot M_{volatile} / M_{total} \cdot \rho_{volatile} \cdot f_{Disp} \cdot C^{sat}_{volatile} \quad (3.15)$$

$$DISS_heavy = k_{dish} \cdot A \cdot M_{heavy} / M_{total} \cdot \rho_{heavy} \cdot f_{Disp} \cdot C^{sat}_{heavy} \quad (3.16)$$

Where:

k_{disl}	Dissolution rate for light, volatile fraction [m/s]
k_{dish}	Dissolution rate for heavy fraction [m/s]
$M_{volatile}$	Volatile mass of oil particle [kg]
M_{heavy}	Heavy mass of oil particle [kg]

M_{total}	Total mass of oil particle [kg]
$\rho_{volatile}$	density of volatile fraction [kg/m^3]
ρ_{heavy}	density of heavy fraction [kg/m^3]
A	Slick area of each particle in contact with water surface [m^2]
f_{DISP}	Effect of chemical dispersant, enhancing the solubility
$C^{sat}_{volatile}$	Water solubility of volatile fraction [kg/kg]
C^{sat}_{heavy}	Water solubility of heavy fraction [kg/kg]

3.4 Emulsification

Emulsification is the formation of a mixture of two distinct liquids, seawater and oil in the case of a marine spill. Fine oil droplets are suspended within (but not dissolved into) the water and the emulsification formed occupies a volume that can be up to four times that of the oil it formed from. Moreover, the viscous emulsion is considerably more long-lived within the environment than the source oil, and its formation slows subsequent weathering processes.

Emulsification tends to occur under conditions of strong winds and/or waves and generally not until an oil spill has persisted on the water for at least several hours. A persistent, partially emulsified mixture of water in oil is sometimes referred to as a 'mousse.' Mousse is resistant to biodegradation, the important final weathering stage, and in shallow marsh environments it can persist within sediments for years to decades.

The present model describes the emulsification as an equilibrium process between the two stages oil + water and water in oil. Stability of emulsions is an important factor determining ability of emulsions to demulsify, as unstable and mesostable emulsions will release water. A first order water release formula is used to describe the process, Xie et al. (2007):

$$wateruptake = K_{em} * (U+1)^2 * \frac{(Y_{\max} - Y_w)\cdot}{Y_{\max}} \tag{3.17}$$

$$waterrelease = -\alpha \cdot Y_w \tag{3.18}$$

Where:

Y_w	water fraction [kg/kg]
Y_{max}	maximum water fraction [kg/kg]
U	wind speed [m/s]
K_{em}	emulsification rate constant. A typically of 2×10^{-6} s/m^2 is given in Sebastião & Soares (1995).
α	water release rate, α=0 for stable emulsions; α>0 for mesostable emulsions [s^{-1}]

The water release rate α is related to the parameter for emulsion stability S.

$$\alpha = \begin{cases} \alpha_0 - (\alpha_0 - \alpha_{0.67})S/0.67 & for \quad S < 0.67 \\ \alpha_{0.67}\left[(1.22 - S)/(1.22 - 0.67)\right] & for \quad 0.67 \le S < 1.22 \\ 0 & for \quad S \ge 1.22 \end{cases} \tag{3.19}$$

Where:

α_0	water release rate for unstable emulsion with S=0. It is set equal to $\ln(Y_{max}/0.1)/3600$ s^{-1} corresponding to that the emulsion breaks down within a few hours at very low wind speeds
$\alpha_{0.67}$	water release rate for the mesostable emulsion with S=0.67. It is set equal to: $\ln(Y_{max}/0.1)/(24 \cdot 3600)$ s^{-1} corresponding to that the a mesostable emulsion breaks down within a few days at very low wind speeds

In the oil spill model, the stability index formulated by Mackay and Zagorski (1982) is used:

$$S = X_a \cdot \exp\left[K_{ao} \cdot (1 - X_a - X_w)^2 + K_{aw} \cdot X_w^2\right] \cdot \exp\left[-0.04 \cdot (T - 293)\right] \quad (3.20)$$

Where:

a	subscript represents asphaltenes
w	subscript represents wax
o	subscript represents other chemical components
K_{ao}	3.3 at 293 K
K_{aw}	200 at 293 K
X_a	fraction of asphaltenes
X_w	fraction of wax
T	temperature, K

Emulsions with S>1.22 are considered stable, whereas oils with a S value between 0.67 – 1.22 are considered to form mesostable emulsions and oils with a S below 0.67 form unstable emulsion, Xie et al. (2007).

3.5 Sedimentation

Very few crudes are dense enough to sink on their own in seawater, and few of them weather fully enough to yield a residue dense enough to do so either (unless the oil is ignited, in which case sufficiently dense residues may be formed). The model can however handle the oils vertical movement driven by buoyancy forces from differences in oil density and water density in both upward and downward direction. The implementation is based on Stokes Law:

$$setv = \frac{(\rho_{oil} - \rho_{water}) \cdot d^2 \cdot g}{18 \cdot \eta_{water}} \quad (3.21)$$

Where:

Setv	is the sedimentation rate [m/s]
ρ_{water}	Density of water [kg/m^3]
ρoil	Density of oil [kg/m^3]
d	Average grain diameter of oil droplets [m]
g	Gravitational acceleration [9.81 m/s^2]
η water	Viscosity of water [kg/m/s]

3.6 Biodegradation

Microbial oil degradation is a critical late-stage step in the natural weathering of petroleum spills, as it is the stage that gradually removes the last of the petroleum pollutants from the marine environment.

Microbial degradation of petroleum compounds occurs most rapidly via the oxidative metabolic pathways of the degrading organisms. As such, biodegradation is predicted to occur fastest in environments with ample oxygen as well as a diverse and healthy oil-degrading flora. Conversely, oxygen-depleted marine sediments that are often sites of petroleum contamination are among the habitats where aerobic metabolism is severely limited and microbial oil breakdown must therefore proceed via slower anaerobic pathways. Even though degradation within these sites is slow, it may still have a substantial cumulative impact over time.

The biodegradation process is calculated as a simple 1st order process:

$$BIOD_volatile = k_{bio,volatile} \cdot M_{volatile} \tag{3.22}$$

$$BIOD_heavy = k_{bio,heavy} \cdot M_{heavy} \tag{3.23}$$

Where:

$k_{bio,volatile}$	Biodegradation rate for the volatile fraction[1/s]
$k_{bio,heavy}$	Biodegradation rate for the heavy fraction[1/s]
$M_{volatile}$	Volatile mass of oil particle [kg]
M_{heavy}	Heavy mass of oil particle [kg]

3.7 Photooxidation

Chemical oxidation of the spilled oil also occurs, and this process is facilitated by exposure of the oil to sunlight. Oxidation contributes to the total water-soluble fraction of oil components. Less complete oxidation also contributes to the formation of persistent petroleum compounds called tars. The overall contribution of photooxidation to oil spill removal is small. Even exposed to strong sunlight (approximately 700 W/m^2 in Europe), photooxidation only breaks down about a tenth of a percent (0.1%) of an exposed slick in a day.

The photooxidation process is calculated as a simple 1st order process:

$$PHOT_volatile = i \cdot k_{photo,volatile} \cdot M_{volatile} \tag{3.24}$$

$$PHOT_heavy = i \cdot k_{photo,heavy} \cdot M_{heavy} \tag{3.25}$$

Where:

$k_{photo,volatile}$	Photooxidation rate for the volatile fraction at sea surface[1/d] at a light intensity of 100 W/m²
$k_{photo,heavy}$	Photooxidation rate for the heavy fraction at sea surface [1/d] at a light intensity of 100 W/m²
$M_{volatile}$	Volatile mass of oil particle [kg]
M_{heavy}	Heavy mass of oil particle [kg]
I	Solar radiation at given distance from surface [normalised to 100 W/m^2], calculated with Lambert Beer expression:

$$i = \frac{i_0}{100} \cdot e^{-\beta \cdot dsurf} \quad (3.26)$$

Where:

i_0	Solar radiation at surface [W/m^2]
100	*normalisation constant to 100 W/m²*
β	Light extinction coefficient [1/m]
dsurf	Distance from particle to water surface [m]

3.8 Vertical Dispersion

An important factor moving the oil into the water column is vertical dispersion. Strong winds, currents, and turbulent seas facilitate the process of dispersion.

Breaking waves cause the oil droplets to be moved far into the water column. This is by far the most important dispersion mechanism. The entrainment of oil from the sea surface into the water column is based on, Delvigne and Sweeney (1988):

$$Q_d = CD^{0.57} SFd^{0.7} \Delta d \quad (3.27)$$

Where:

C	entrainment coefficient
D	dissipation wave energy [J/m^2)]
S	fraction of sea surface covered by oil (assumed to be 1 around each particle)
F	fraction of sea surface covered by breaking waves per unit time [s^{-1})]
d	mean diameter of droplet size
Δd	droplet size interval

The entrainment coefficient ***C*** is calculated as:

$$C = 4450N^{-0.4} \quad (3.28)$$

Where:

N	kinematic viscosity (10^{-6} centistokes)

The dissipation energy ***D*** [*μm*] is calculated as:

$$D = 0.0034\rho_w g H_{rms}^{\ 2} \quad (3.29)$$

Where:

ρ_w	density of sea water [kg/m^3]
g	acceleration due to gravity [m^2/s]
H_{rms}	r.m.s. value of the wave height

The fraction ***F*** of sea surface covered by breaking waves is calculated as:

$$F = 0.032 \frac{(U_w - U_{th})}{T_w} \quad (3.30)$$

Where:

U_w	wind speed [m/s]
U_{th}	threshold wind speed for onset of breaking waves [m/s]
F	zero for $U_w < U_{th}$.

The mean droplet diameter d is calculated according to French-McCay (2004) as:

$$d = 1818\, E^{-0.5}\, N^{0.34} \tag{3.31}$$

Where:

E	Energy dissipation rate for breaking wave [$J/m^3/s$] set equal to $10e^3$

The entrainment depth is approximated according to Delvigne and Sweeney (1988) as:

$$z = (1.5 \pm 0.35) H_b \tag{3.32}$$

Where:

H_b	breaking wave height ≈1.67*H_s

The probability of individual particles to disperse vertically due to wave breaking is determined as:

$$p_{wbreak} = MIN\left(1, \frac{Q_d}{M_{Total}}\right) \tag{3.33}$$

Where:

M_{Total}	Total oil mass of the particle.

If a particle becomes dispersed the distance that the oil droplets are dispersed into the water column $disp_{wbreak}$ is determined by a standard normal distribution N (μ, σ^2)

$$disp_{wbreak} = N(\mu, \sigma^2) \tag{3.34}$$

Where:

μ	average depth ≈ 1.5 * Hb
σ^2	standard deviation ≈ 0.35 * Hb

Redispersion of oil

Usually the oil density is smaller than the water density. The dispersed oil droplets therefore tend to resurface. However, they can remain dispersed for a long time, due to water turbulence.

3.9 Physical Properties of Oil

The term oil describes a broad range of hydrocarbon-based substances. Hydrocarbons are chemical compounds composed of the elements hydrogen and carbon. This includes substances that are commonly thought of as oils, such as crude oil and refined petroleum products, but it also includes animal fats, vegetable oils, and other non-petroleum oils.

Each type of oil has distinct physical and chemical properties. These properties affect the way oil will spread and break down, the hazard it may pose to aquatic and human life, and the likelihood that it will pose a threat to natural and man-made resources.

3.9.1 Dynamics of viscosity

Change in viscosity as a result of emulsification can be calculated using Mooney equation, Sebastião and Guedes Soares (1995):

$$\mu = \mu_0 \cdot \exp\left[\left(\frac{2.5 \cdot Y_w}{1 - C \cdot Y_w}\right)\right] \tag{3.35}$$

Where:

μ_0	parent oil viscosity [cP].
C	viscosity constant ('*Mooney constant*'), final fraction of water content, 0.7 for crude oil and heavy fuel oil, 0.25 for home heating oil
Y_w	water fraction [kg/kg]

The **parent viscosity *μ0*** is calculated as temperature corrected viscosity of the fresh spilled oil. In the model a simple exponential temperature dependency is assumed:

$$\mu_0 = \frac{\mu_{ref}}{\exp(b * T_{ref})} * \exp(b * T) \tag{3.36}$$

Where:

B	coefficient for temperature dependency [1/°C]
T	Temperature [°C]
μ_{ref}	oil viscosity [cP] at given reference temperature.
T_{ref}	reference temperature [°C]

3.9.2 Dynamics of density

The oil physico-chemical properties also vary with the temperature, and the fluid dynamics are therefore strongly temperature dependent. As the temperature of the spilled oil has temperature above the pour point immediately after the spill, the density is rather low, making the oil buoyant and therefore the oil slick is forced towards the water surface in the beginning. However as the oil slick cools down, the density increases and minimises the density difference to the enclosing water, and therefore the slick can react to turbulent waters by dispersing under the surface.

The temperature dependency of the fluid density is based on the volumetric thermal expansion of a fluid:

$$\rho_T = \frac{\rho_0}{1 + \beta(T - T_0)} \tag{3.37}$$

Where:

ρ_T	final density [kg/m^3]
T	temperature [°C]

ρ_0 reference density [kg/m^3]
T_0 reference temperature [°C]
β volumetric temperature expansion coefficient [1/°C]

It is assumed that the density of sea water is correctly given in the model inputs; no temperature correction is applied to this value. The initial density for the light and heavy oil fraction has to be given at 20°C and is corrected to the ambient temperature using the above formula. The expansion coefficients for the fractions can be parameterised independently. Table 3.1 lists some generic values for common fluids.

Table 3.1 Example of volumetric temperature expansion coefficients for various liquids

Liquid	Volumetric temperature expansion coefficient [1/°C]
Water	0.00018
Petroleum	0.001
Oil	0.0007
Kerosene, Gasoline	0.001

As a result of emulsification and temperature the density of oil slick changes. The general density of the emulsion is calculated as:

$$\rho_e = Y_w \rho_w + (1 - Y_w)\rho_c \tag{3.38}$$

Where:
ρ_e emulsion density [kg/m^3]
ρ_w seawater density [kg/m^3]
ρ_c oil density [kg/m^3]
Y_w water content

The oil density is calculated as

$$\rho_c = \frac{M_{volatile}\rho_{volatile} + (M_{heavy} + M_{Asph} + M_{Wax})\rho_{heavy}}{M_{total}} \tag{3.39}$$

Where:
ρ_c oil density [kg/m^3]
$\rho_{volatile}$ temperature corrected volatile fraction density [kg/m^3]
ρ_{heavy} temperature corrected heavy fraction density [kg/m^3]
$M_{volatile}$ Mass volatile fraction [kg]
M_{heavy} Mass heavy fraction [kg]
M_{Asph} Mass asphaltene fraction [kg]
M_{Wax} Mass wax fraction [kg]
M_{total} total oil mass [kg]

4 Oil Booms, Movement Block

The DHI oil weathering model includes a simple oil barrier model.
The user can supply a spatial 2D map for the probability to block the movement of an oil particle for each time step.

Internally for each time step a random number [0..1] is drawn and compared with the given block probability for the current grid element. If the random number is smaller than the block probability the movement vectors for the particle are cleared and the particle does not perform any movement in this step.

Please note that the probabilities work on a per time step base.

5 Beaching, Shore Lock-Reflection Conditions

The DHI oil weathering model includes a simple beaching model.
The user can supply a spatial 2D map for the probability to lock an oil particle when it is washed on land. Once a particle gets locked on shore no further movement is allowed an only the following weathering process are applied:

Weathering processes for beached particles
- Biodegradation
- Photo-Oxidation
- Evaporation

By providing different values for the probability to get locked on shore it is possible to represent the different shore properties. A hard bottom shore or a harbour with sheet pilings will not absorb much oil, thus the locking probability is low whereas wetlands will entrain most of the oil (thus have a high probability). The principal mechanism works the same way as described for the movement block (Section 4).

Please note that the beaching lock works on a per beaching event base, and is thus also dependent on the time step.

6 Detergents

The DHI oil weathering model includes a simple mechanism for oil detergents. The user can supply a spatial 2D map for local enhancements of the oil break down when using detergents. See Section 3.3 (Dissolution) for details.

7 Drift

The combined effects of current, wind drag and bed drag cause the drift of the oil particles.

The drift vector is normally varying in space. It represents the combined effects of current and wind drag that cause the advection of the particles.

$$\vec{a}(x,y,z,t) = f\left(current, wind\ drag, bed\ drag\right) \tag{7.1}$$

The drift profile is a description of the vertical variation of the drift regime that influences the particles. It will normally be the currents and the wind that governs the shape of the drift profile. Currents and wind are already calculated in the hydrodynamic setup, but for 2D hydrodynamics it is the depth average values that are the output of the hydrodynamic setup. By assuming some shapes of the vertical drift profile it is possible to get a more realistic current profile than just a depth integrated value, and therefore a more realistic drift of particles.

7.1 Bed Shear Profile (Logarithmic Profile)

The shape of the velocity profile within a turbulent boundary layer is well established by both theory and experiment. The profile has specific characteristics very close to the bed where viscosity controls the vertical transport of momentum, and different characteristics farther from the bed where turbulence controls the vertical transport of momentum.

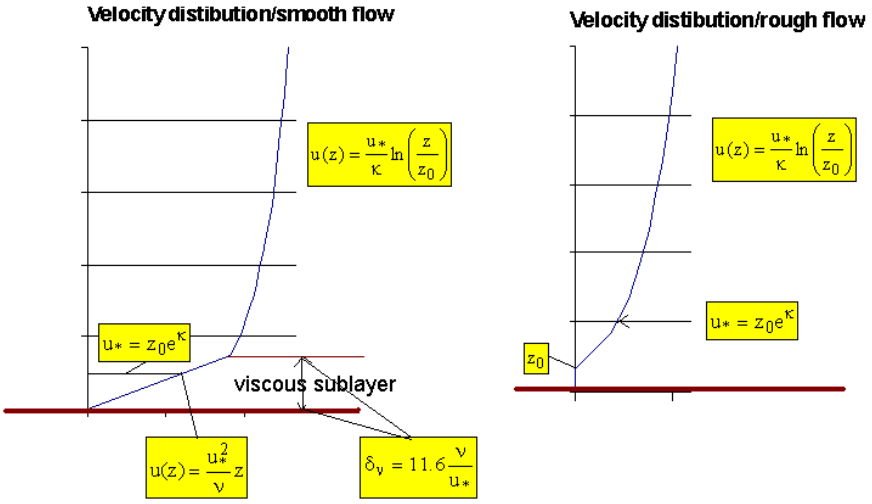

Figure 7.1 Example of bed shear profile applied from 2D flow fields

The region closest to the bed boundary is called the laminar sub-layer or viscous sub-layer, because within the region turbulence is suppressed by viscosity. The viscous, laminar sub-layer only plays a significant role for smooth flows, where a typical thickness of the viscous layer is about 2 cm, whereas for rough flows the viscous sub layer is typically less than 1 mm, and instead the flow is set to zero for z smaller than z0.

Logarithmic layer (z >= δ_v smooth flow**) (z >=** z0 rough flow**)**

$$u = \frac{2.3}{k} \cdot u^* \cdot \log_{10} \frac{z}{z_0} \tag{7.2}$$

Smooth flow: Laminar bed shear layer (**z <** δ_s)

$$u = \left(u^*\right)^2 \cdot \frac{z}{\nu} \tag{7.3}$$

Where:

κ	Von Karman empirical constant 0.4
z_0	Characteristic roughness
z	Coordinate from bed towards water surface [m]
u^*	Friction velocity
δ_v	Thickness of viscous bed shear layer
ν	Kinematic viscosity of water

7.2 Wind Induced Profile

The wind drag can also cause increased flow velocities in the upper part of the water column, and corresponding velocities in the opposite direction in the lower part. In 3D hydrodynamics this effect is included in the hydrodynamic output, but that is not the case with the depth averaged 2D hydrodynamics. So if this flow regime should be described with 2D hydrodynamics, a wind induced profile must be applied, which will distribute the depth averaged flow in the water column.

This has been done by calculating a wind drift vector that is multiplied with the current velocity vector.

The magnitude of the surface wind drift vector c_w^* is commonly assumed to be proportional to the magnitude of the wind speed 10 m above the sea surface. This factor c_w^* has a common value that varies from 3 to 4 per cent of the wind speed 10 m above the sea surface (from Al-Rabeh (1994)).

The vertical distribution of the wind drift vector consists of an offshore part and an onshore part. The onshore distribution is based on a parabolic vertical profile and is able to produce backflow at depths, where the offshore logarithmic profile does not.

The parabolic profile acts in shallow waters with a water depth less than a specified water depth, h_{sep}, which is a positive value (in metres) and measured from the free water surface.

The vertical distribution of the parabolic onshore profile is given by:

$$c_w(z) = c_w^* \left(1 - 3\frac{z}{h}\right)\left(1 - \frac{z}{h}\right) \tag{7.4}$$

Where:

h	Local water depth in meter
z	Vertical particle co-ordinate, measured from sea surface
c_w^*	Wind drift factor (input)

The parabolic profile causes the wind-generated flow in the upper third of the water column to be in the same direction as the current and the flow in the lower part to be in the opposite direction of the wind. There is no net depth averaged mass transport due to the wind.

The vertical distribution of the offshore wind drift vector is given by:

$$c_w(z) = c_w^* \exp\left(-k_0\, z\right) \tag{7.5}$$

Where:

k_0	3/hw [m-1]
h_w	Depth of wind influence [m]
z	Vertical co-ordinate measured from sea surface
c_w^*	Wind drift factor [-]

7.3 Wind Acceleration of Surface Particles

Particles that are exposed to wind in the water surface are affected according to the wind regime in 2 ways: indirectly via the currents that include the wind, but also directly as an extra force directly on the particle. How much of the wind speed that is transferred to the particle speed depends on the nature of the particle: how much is the particle exposed, etc. Therefore, it is a calibration factor that expresses how much of the wind speed that is added to the particle speed.

In the Particle Tracking Module the wind acceleration of surface particles affect the drift with the following modification:

When the particle is in the top 5 cm of water column:

$$U_{particle} = U_{current} + windweigth \cdot W \cdot \sin\left(Winddirection - \pi + \theta_w\right) \tag{7.6}$$

$$V_{particle} = V_{current} + windweigth \cdot W \cdot \cos\left(Winddirection - \pi + \theta_w\right) \tag{7.7}$$

Where:

θ_w	Wind drift angle
windweight	Calibration factor for wind drag on particle

7.3.1 Wind drift angle

The Coriolis force is normally included in the hydrodynamic currents, but also for the wind acceleration of surface particles the Coriolis force must be considered.

Due to the influence from the Coriolis force, the direction of the wind drift vector is turned relatively to the wind direction. The angle θw of deviation is termed with the wind drift angle. It turns to the right on the Northern Hemisphere and to the left on the Southern Hemisphere. From Al-Rabeh (1994), it is assumed that

$$\theta_w = \beta \exp\left(\frac{\alpha |U_w|^3}{g\gamma_w}\right) \tag{7.8}$$

Where:

α	$-0.3 \cdot 10^{-8}$
β	$28^o\ 38'$
γ_w	Kinematic viscosity [kg/(ms)]
g	Acceleration due to gravity [m/s^2]

The magnitude of the wind drift angle varies with the geographical location and wind speed and it is often estimated at 12-15 degrees in the North Sea.

8 Parameterisation of an Oil Type

It is always difficult to find a proper parameterisation for an oil type.
The DHI Oil weathering model describes the oil by two fractions only: a light volatile fraction and a heavy, non-volatile fraction. The light fraction is defined as the mass of hydrocarbons with molecular weight below 160 g/mol and a boiling point (well) below 300°C. The heavy fraction is defined as hydrocarbons of molecular masses above 160 g/mol and boiling points from 300°C and upwards, including wax and asphaltene components.

Each crude oil type has a different composition of the various components and it may be difficult to obtain the characteristics for the composition used in the DHI oil weathering model. If available the distillation data will provide valuable information.

As an example on how to derive input parameters for an oil spill model, the oil type 'STATFJORD' from the Norwegian North Sea is used. You can find a data sheet on this oil type at the 'Oil Properties Database' of the Environmental Technology Center Canada[1] . The information from this data sheet is exemplarily used to find a parameterisation for the DHI oil weathering model. Similar information may be obtained for other oils from different sources, see APPENDIX B.

8.1 Evaporation

The data sheet lists the following equation for predicting the evaporation:

$$\%Ev = (2.67 + 0.060 * T) * \ln(t) \qquad (8.1)$$

Where:

%Ev	the weight percent evaporated
T	the surface temperature
t	the time in minutes

These data can be directly used for the model constant when using a simple evaporation formulation. Obviously this is a logarithmic evaporation type, thus the constant 'Simple Evaporation, select logarithmic or quadratic type' has to be set to '0' and the constants 'Simple Evaporation: 1st oil specific constant'=2.67 and 'Simple Evaporation: 2nd oil specific constant for temperature dependency'=0.06. In APPENDIX A you can find a list of further common oil types and values for the simple evaporation parameterisation.

Table 8.1 Input Lagrange constants for evaporation in oil spill model setup

Description	Value
Simple Evaporation: 1st oil specific constant	2.67
Simple Evaporation: 2nd oil specific constant for temperature dependency	0.06.
Simple Evaporation, select logarithmic or quadratic type	0

[1] Environmental Technology Center Canada, http://www.etc-cte.ec.gc.ca/databases/spills_e.html

8.2 Distribution into Different Model Components

It is often difficult to find good estimates how the oil can be represented by the oil fractions defined in the weathering model. The distillation data can provide good information for this task. The different oil fractions of the template are defined by the molecular mass and boiling points. Note that due to the chemical structures of hydrocarbons these properties are well correlated.

The data sheet contains the following distillation information for the fresh oil:

Table 8.2 'STATFJORD' boiling point distribution and distillation yields.
Values in italic are considered as 'light' and values in bold as the 'heavy' fraction (values in normal are ambivalent and may belong to both fractions)

Boiling point ºC	Weight %
40	*2*
60	*3*
80	*3*
100	*5*
120	*17*
140	*20*
160	*23*
180	*26*
200	*30*
250	*39*
300	**49**
350	**59**
400	**68**
450	**77**
500	**84**
550	**89**
600	**94**
650	**97**
700	**99**

Fraction	Temperature [ºC]	Yields weight %
Light ends	-	*4*
Gasoline	5-65	*3*
Light naphtha	65-90	*4*
Naphtha	90-150	*12*
Heavy naphtha	150-180	*6*
Light gas oil	180-240	*10*
Gas oil	240-320	16
Gas oil	320-375	**10**
Heavy gas oil	375-420	**6**
Heavy gas oil	420-525	**17**
Heavy gas oil	525-565	**4**
Residue	>565	**10**

This data could be used to parameterise the general for of simple evaporation equation (taking the percent loss at 180°C, in this case 26% as shown in Figure 8.1). However, luckily the specific constants are given explicitly in the data sheet and can be entered directly into the model, see Table 8.3.

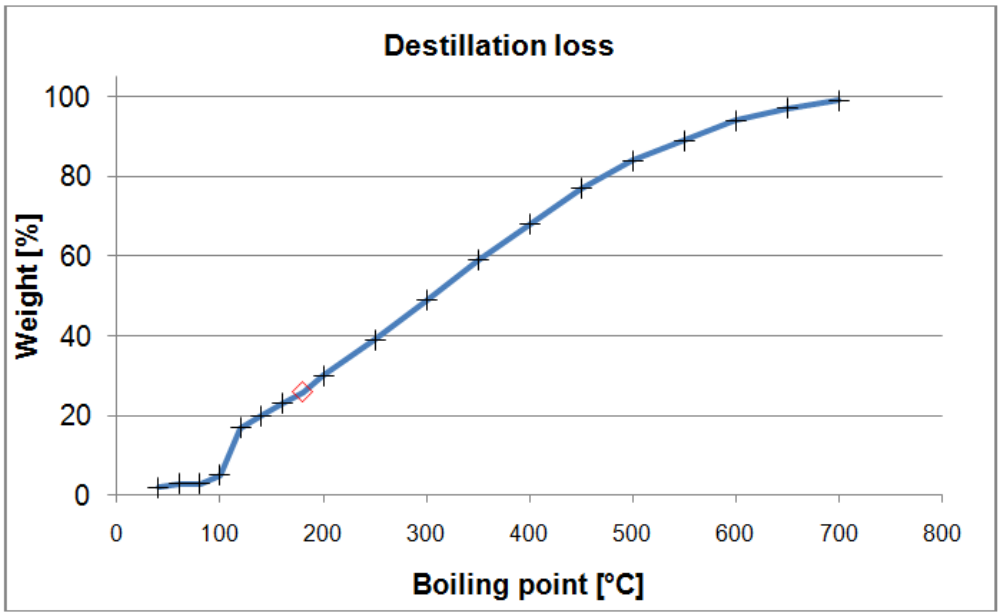

Figure 8.1 Distillation loss for oil type 'STATFJORD', marked point evaporation loss at 180°C

Table 8.3 Input Lagrange constant for evaporation

Description	Value
Simple evaporation, distillation percentage at 180ºC	26%

From the data it can be derived that roughly 40%-50% of the oil has a boiling point below or well below 300°C. This will be used as 'light' fraction in the weathering model. The remaining mass has to be split up between the 'heavy' and the conservative wax and asphaltene fractions. For the later the data sheet lists contents of 8% for wax and 2% for asphaltene in the fresh oil. The data sheet does contain information on the water content as being '< 0.05% volume', thus we assume a negligible water amount in the fresh oil. From the yield table for the crude oil similar information can be derived. Here the 'light' fraction will sum up to about 55%. Thus the volatile fraction is assumed to represent 50% of the total oil mass.

The information will lead to the mass distribution for the fresh oil as shown in Table 8.4.

Table 8.4 Input state variables for oil

Model component	Fraction	Per 1000 kg
Volatile fractions	50 %	500 kg
Heavy fractions	40 %	400 kg
Wax mass	8 %	80 kg
Asphaltene mass	2 %	20 kg
Water fraction	0 %	0.0 kg

8.3 Dynamic Viscosity

The data sheet lists the following information for the dynamic viscosity at different temperatures:

Table 8.5 Dynamic viscosity 'STATFJORD'

Temperature [ºC]	Dynamic viscosity [cP]
0	31
13	7
15	6

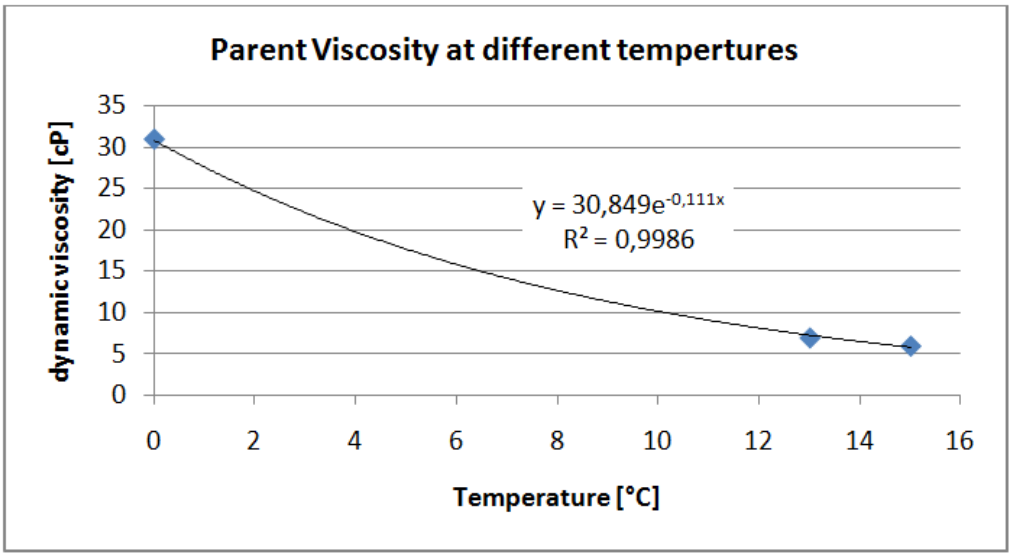

Figure 8.2 Dynamic viscosity at different temperatures

This leads to an input for the reference viscosity and temperature:

- Dynamic viscosity at reference temperature: 6 cP
- Reference temperature for dynamic viscosity: 15°C

From the exponential fit the exponent for the exponential temperature dependency of the viscosity can be read as: -0.111. thus the input parameters for viscosity are defined as in Table 8.6.

Table 8.6 Input Lagrange constant for viscosity

Description	Value
Dynamic viscosity at reference temperature	6 cP
Reference temperature for dynamic viscosity	15ºC
Coefficient for exponential temperature dependency	-0.111

8.4 Specific Density, Volumetric Expansion Coefficient

The data sheet lists the specific density of the oil for two different temperatures:

0°C 0.8478 g/cm³ ≈ 848 kg/m³
15°C 0.8354 g/cm³ ≈ 835 kg/m³

However, this is for the fresh oil and the model need information on the density at 20°C for both the 'light' and the 'heavy' components. The data sheet information can be used to compute these values. First the volumetric expansion coefficient can be determined:

$$\begin{aligned}\beta &= \left(\frac{\rho_{T0}}{\rho_{T1}} - 1\right) / \left(T_1 - T_0\right) \\ &= \left(\frac{848}{835} - 1\right) / \left(15 - 0\right) \\ &\approx 0.001\end{aligned} \tag{8.2}$$

For simplicity reason it is assumed that volatile and heavy components have the same expansion coefficient. This leads to a total density of:

$$\begin{aligned}\rho(total)_{20°C} &= \left(\frac{\rho_T}{1 + \beta\left(20°C - T\right)}\right) \\ &= \left(\frac{835}{1 + 0.001 * \left(20°C - 15°C\right)}\right) \\ &\approx 831\end{aligned} \tag{8.3}$$

Assuming a density for the light fraction of 755 kg/m³ and a mass fraction of 50% the remaining heavy fraction must have a density of 907 kg/m³:

$$\rho_{heavy} = \frac{\rho_{total} - f * \rho_{light}}{(1-f)} = \frac{831 - 0.5 * 755}{(1-0.5)} = 907 \quad (8.4)$$

This leads to the input parameters given in Table 8.7

Table 8.7 Input Lagrange constant for density and volumetric expansion coefficients

Description	Value
Buoyancy: Density of original oil at 20°C, volatile fraction	755 kg/m³
Buoyancy: Density of original oil at 20°C, heavy fraction	907 kg/m³
Volumetric temperature expansion coefficient volatile fraction	0.001
Volumetric temperature expansion coefficient heavy fraction	0.001

8.5 Final Parameterisation for STATFJORD

Table 8.8 Composition of the different fractions

Model component	Fraction	Per 1000 kg
Volatile fractions	50 %	500 kg
Heavy fractions	40 %	400 kg
Wax mass	8 %	80 kg
Asphaltene mass	2 %	20 kg
Water fraction	0 %	0.0 kg

Table 8.9 Model constants

Description	Value
Simple evaporation, distillation percentage at 180ºC	26%
Simple Evaporation: 1st oil specific constant	2.67
Simple Evaporation: 2nd oil specific constant for temperature dependency	0.06.
Buoyancy: Density of original oil at 20°C, volatile fraction	755 kg/m³
Buoyancy: Density of original oil at 20°C, heavy fraction	907 kg/m³
Volumetric temperature expansion coefficient volatile fraction	0.001
Volumetric temperature expansion coefficient heavy fraction	0.001
Dynamic viscosity at reference temperature	6 cP
Reference temperature for dynamic viscosity	15ºC
Coefficient for exponential temperature dependency	-0.111
Simple Evaporation, select logarithmic or quadratic type	0

9 References

/1/ Al-Rabeh, A., 1994. Estimating surface oil spill transport due to wind in the Arabian Gulf. Ocean Engineering 21:461-465. doi: 10.1016/0029-8018(94)90019-1.

/2/ Betancourt F., A. Palacio, and A. Rodriguez, 2005. Effects of the Mass Transfer Process in Oil Spill. American Journal of Applied Science 2:939-946.

/3/ Delvigne, G., and C. Sweeney, 1988. Natural dispersion of oil. Oil and Chemical Pollution 4:281-310. doi: 10.1016/S0269-8579(88)80003-0.

/4/ Fate of Marine Oil Spills, 2002. Page 8. Technical Reports, The International Tanker Owners Pollution Federation Limited (ITOPF), London.

/5/ Fingas, M. F., 1996. The evaporation of oil spills: Prediction of equations using distillation data. Spill Science & Technology Bulletin 3:191-192. doi: 10.1016/S1353-2561(97)00009-1.

/6/ Fingas, M. F., 1997. Studies on the evaporation of crude oil and petroleum products: I. the relationship between evaporation rate and time. Journal of Hazardous Materials 56:227-236. doi: 10.1016/S0304-3894(97)00050-2.

/7/ Fingas, M.F., 2004. Modeling evaporation using models that are not boundary-layer regulated. Journal of Hazardous Materials, Volume 107, 2004, pp. 27-36.

/8/ French-McCay, D. P.,2004. Oil spill impact modeling: Development and validation. Environmental Toxicology and Chemistry 23:2441-2456. doi: 10.1897/03-382.

/9/ Mackay, D., I. Buist, R. Mascarenhas, and S. Paterson, 1980. Oil spill processes and models. Environmental Emergency Branch, Department of Fisheries and Environment, Environment Canada, Ottawa, ON.

/10/ Mackay, D., and W. Zagorski, 1982. Water-in-oil emulsions: a stability hypothesis. Proceedings of the Fifth Annual Arctic Marine Oilspill Program Technical Seminar:61-74.

/11/ Reed, M., 1989. The physical fates component of the natural resource damage assessment model system. Oil and Chemical Pollution 5:99-123. doi: 10.1016/S0269-8579(89)80009-7.

/12/ Sebastião, P., and C. Guedes Soares, 1995. Modeling the fate of oil spills at sea. Spill Science & Technology Bulletin 2:121-131. doi: 10.1016/S1353-2561(96)00009-6.

/13/ Xie, H., P. D. Yapa, and K. Nakata, 2007. Modeling emulsification after an oil spill in the sea. Journal of Marine Systems 68:489-506. doi: 10.1016/j.jmarsys.2007.02.016.

APPENDICES

APPENDIX A

Evaporation Parameters for Different Oils

Oil-type	Curve type	A	B	T [°C] >
Adgo	1	0.11	0.013	---
Adgo-long term	0	0.68	0.045	---
Alberta Sweet Mixed Blend	0	3.24	0.054	---
Amauligak	0	1.63	0.045	---
Amauligak-f24	0	1.91	0.045	---
Arabian Heavy	0	1.31	0.045	---
Arabian Heavy	0	2.71	0.045	---
Arabian Light	0	2.52	0.037	---
Arabian Light	0	3.41	0.045	---
Arabian Light (2001)	0	2.4	0.045	---
Arabian Medium	0	1.89	0.045	---
ASMB - Standard #5	0	3.35	0.045	---
ASMB (offshore)	0	2.2	0.045	---
Av Gas 80	0	15.4	0.045	---
Avalon	0	1.41	0.045	---
Avalon J-34	0	1.58	0.045	---
Barrow Island	0	4.67	0.045	---
BCF-24	0	1.08	0.045	---
Belridge Cruide	1	0.03	0.013	---
Bent Horn A-02	0	3.19	0.045	---
Beta	1	-0.08	0.013	6
Beta - long term	0	0.29	0.045	---
Boscan	1	-0.15	0.013	12
Brent	0	3.39	0.048	---
Bunker C Anchorage	1	-0.13	0.013	10
Bunker C Anchorage - long term	0	0.31	0.045	---
Bunker C -long term	0	-0.21	0.045	5
Bunker C -short term	1	0.35	0.013	---
Bunker C-Light (IFO-250)	1	0.0035	0.0026	---
California API 11	1	-0.13	0.013	10
California API 15	1	-0.14	0.013	11
Cano Limon	0	1.71	0.045	---
Carpenteria	0	1.68	0.045	---
Cat cracking feed	1	-0.18	0.013	14
Chavyo	0	3.52	0.045	---
Combined Oil/gas	1	-0.08	0.013	6
Compressor Lube Oil (new)	0	-0.68	0.045	15
Cook Inlet - Swanson River	0	3.58	0.045	---
Cook Inlet - Granite Point	0	4.54	0.045	---
Cook Inlet Trading Bay	0	3.15	0.045	---
Corrosion Inhibitor Solvent	1	-0.02	0.013	2
Cusiana	0	3.39	0.045	---
Delta West Block 97	0	6.57	0.045	---
Diesel - long term	0	5.8	0.045	---
Diesel Anchorage - Long	0	4.54	0.045	---
Diesel Anchorage - Short	1	0.51	0.013	---
Diesel Fuel - southern - long term	0	2.18	0.045	---
Diesel Fuel - southern - short term	1	-0.02	0.013	2
Diesel Mobil 1997	1	0.03	0.013	---
Diesel Mobil 1997 - long term	1	-0.02	0.013	2
Diesel Regular stock	1	0.31	0.018	---
Dos Cuadros	0	1.88	0.045	---
Edicott	0	0.9	0.045	---
Ekofisk	0	4.92	0.045	---
Empire Crude	0	2.21	0.045	---
Esso Spartan EP-680 Industrial Oil	0	-0.66	0.045	15
Eugene Island 224 - condensate	0	9.53	0.045	---
Eugene Island Block 32	0	0.77	0.045	---
Eugene Island Block 43	0	1.57	0.045	---
Evendell	0	3.38	0.045	---
FCC Heavy Cycle	1	0.17	0.013	---
FCC Light	1	-0.17	0.013	13
FCC Medium Cycle	1	-0.16	0.013	12
FCC-VGO	1	2.5	0.013	---
Federated	0	3.47	0.045	---
Federated (new- 1999)	0	3.45	0.045	---
Garden Banks 387	0	1.84	0.045	---
Garden Banks 426	0	3.44	0.045	---
Gasoline	0	13.2	0.21	---
Genesis	0	2.12	0.045	---
Green Canyon Block 109	0	1.58	0.045	---
Green Canyon Block 184	0	3.55	0.045	---
Green Canyon Block 65	0	1.56	0.045	---
Greenplus Hydraulic Oil	0	-0.68	0.045	15
Gullfaks	0	2.29	0.034	---
Heavy Reformate	1	-0.17	0.013	13
Hebron MD-4	0	1.01	0.045	---
Heidrun	0	1.95	0.045	---
Hibernia	0	2.18	0.045	---
High Viscosity Fuel Oil	1	-0.12	0.013	9
Hondo	0	1.49	0.045	---
Hout	0	2.29	0.045	---
IFO-180	1	-0.12	0.013	9
IFO-30 (Svalbard)	0	-0.04	0.045	1
IFO-300 (old Bunker C)	1	-0.15	0.013	12
Iranian Heavy	0	2.27	0.045	---
Issungnak	0	1.56	0.045	---
Isthmus	0	2.48	0.045	---
Jet 40 Fuel	0	8.96	0.045	---
Jet A1	1	0.59	0.013	---
Jet Fuel (Anch)	0	7.19	0.045	---
Jet Fuel (Anch) short term	1	1.06	0.013	---
Komineft	0	2.73	0.045	---

Oil-type	Curve type	A	B	T [°C] >
Lago	0	1.13	0.045	---
Lago Tecco	0	1.12	0.045	---
Lucula	0	2.17	0.045	---
Main Pass Block 306	0	2.28	0.045	---
Main Pass Block 37	0	3.04	0.045	---
Malongo	0	1.67	0.045	---
Marinus Turbine Oil	0	-0.68	0.045	15
Marinus Value Oil	0	-0.68	0.045	15
Mars TLP	0	2.28	0.045	---
Maui	1	-0.14	0.013	11
Maya	0	1.38	0.045	---
Maya crude	0	1.45	0.045	---
Mississippi Canyon Block 194	0	2.62	0.045	---
Mississippi Canyon Block 72	0	2.15	0.045	---
Mississippi Canyon Block 807	0	2.05	0.045	---
Nektroalik	0	0.62	0.045	---
Neptune Spar (Viosca Knoll 826)	0	3.75	0.045	---
Nerlerk	0	2.01	0.045	---
Ninian	0	2.65	0.045	---
Norman Wells	0	3.11	0.045	---
North Slope - Middle Pipeline	0	2.64	0.045	---
North Slope - Northern Pipeline	0	2.64	0.045	---
North Slope - Southern Pipeline	0	2.47	0.045	---
Nugini	0	1.64	0.045	---
Odoptu	0	4.27	0.045	---
Oriente	0	1.32	0.045	---
Oriente	0	1.57	0.045	---
Orimulsion plus water	0	3	0.045	---
Oseberg	0	2.68	0.045	---
Panuke	0	7.12	0.045	---
Pitas Point	0	7.04	0.045	---
Platform Gail (Sockeye)	0	1.68	0.045	---
Platform Holly	0	1.09	0.045	---
Platform Irene - long term	0	0.74	0.045	---
Platform Irene - short term	1	-0.05	0.013	4
Point Arguello - co-mingled	0	1.43	0.045	---
Point Arguello Heavy	0	0.94	0.045	---
Point Arguello Light	0	2.44	0.045	---
Point Arguello Light -b	0	2.3	0.045	---
Port Hueneme	0	0.3	0.045	---
Prudhoe Bay (new stock)	0	2.37	0.045	---
Prudhoe Bay (old stock)	0	1.69	0.045	---
Prudhoe stock b	0	1.4	0.045	---

Oil-type	Curve type	A	B	T [°C] >
Rangely	0	1.89	0.045	---
Sahara Blend	1	0.001	0.013	---
Sahara Blend - long term	0	1.09	0.045	---
Sakalin	0	4.16	0.045	---
Santa Clara	0	1.63	0.045	---
Scotia Light	0	6.87	0.045	---
Scotia Light	0	6.92	0.045	---
Ship Shoal Block 239	0	2.71	0.045	---
Ship Shoal Block 269	0	3.37	0.045	---
Sockeye	0	2.14	0.045	---
Sockeye co-mingled	0	1.38	0.045	---
Sockeye Sour	0	1.32	0.045	---
Sockeye Sweet	0	2.39	0.045	---
South Louisiana	0	2.39	0.045	---
South Pass Block 60	0	2.91	0.045	---
South Pass Block 67	0	2.17	0.045	---
South Pass Block 93	0	1.5	0.045	---
South Timbalier Block 130	0	2.77	0.045	---
Statfjord	0	2.67	0.06	---
Sumatra Heavy	1	-0.11	0.013	8
Sumatra Light	0	0.96	0.045	---
Taching	1	-0.11	0.013	8
Takula	0	1.95	0.045	---
Tapis	0	3.04	0.045	---
Tchatamba Crude	0	3.8	0.045	---
Terra Nova	0	1.36	0.045	---
Terresso 150	0	-0.68	0.045	15
Terresso 220	0	-0.66	0.045	15
Terresso 46 Industrial oil	0	-0.67	0.045	15
Thevenard Island	0	5.74	0.045	---
Turbine Oil STO 120	0	-0.68	0.045	15
Turbine Oil STO 90	0	-0.68	0.045	15
Udang	1	-0.14	0.013	11
Udang - long term	0	0.06	0.045	---
Vasconia	0	0.84	0.045	---
Viosca Knoll Block 826	0	2.04	0.045	---
Viosca Knoll Block 990	0	3.16	0.045	---
Voltesso 35	1	-0.18	0.013	14
Waxy Light and Heavy	0	1.52	0.045	---
West Delta Block 30 w/water	1	-0.04	0.013	3
West Texas Intermediate	0	2.77	0.045	---
West Texas Intermediate	0	3.08	0.045	---
West Texas Sour	0	2.57	0.045	---
White Rose	0	1.44	0.045	---
Zaire	0	1.36	0.045	---

Oil-type: Common oil name (brand)
Curve type: logarithmic (0)
square root (1)
A, B: Oil specific evaporation parameters

Please note:
These tables are based on the information provided by Fingas (2004). The parameter 'Curve type' corresponds to model parameter 'evap_type', the specific constants A and B to the model parameters '**evapA**' and '**evapB**'. Some evaporation equations will not work for ambient water temperatures below the given minimum temperature in °C. Sometimes you find multiple entries for the same oil type. In this case usually a long- and a short-term behaviour are described or the data is based on different sources.

If no oil specific constants are available alternatively the percent evaporated at 180 °C can be used (model parameter '**evap180**'). Then a generic evaporation scheme is used. In this case the ambient temperature should not be below 15°C.

APPENDIX B

Parameterisation Values for Different Oils

Please note:
The values in the table below are based on the information provided in the DHI Spill Analysis Data Sheets (cf. DHI_SpillAnalysisDataSheets.pdf).

Representative oil type			Light oil	Middle oil, Low aromatics	Middle oil, High aromatics	Medium crude oil	Heavy fuel oil
Source magnitude	**State variables**	**unit**					
Weight	Volatile oil fractions	wt%	72.9	30	30	8	7.5
	Heavy oil fractions	wt%	26.09	68.99	68.99	78.3	77.5
	Asphaltene	wt%	0.01	0.01	0.01	11.5	8
	Wax	wt%	1	1	1	2.2	7
Processes	**Class constants**						
	Schmidt number		2.7	2.7	2.7	2.7	2.7
	Average molecular weight of volatile fraction	g/mol	123	123	116	121	123
	Vapore pressure of volatile fraction (atm)	atm	0.005	0.005	0.006	0.005	0.005
Simple evaporation	Distillation percentage at 180oC	%	22.5	10	10	5	5
Spreading	terminal thickness	m	0.0001	0.0001	0.0001	0.0001	0.0001
Biodegradation	Decay rate, volatile fraction	per day	0.005	0.005	0.005	0.005	0.005
	Decay rate, in-volatile fraction	per day	0	0	0	0	0
Emulsification	Maxiumum water fraction	m^3/m^3	0.5	0.5	0.5	0.85	0.85
	Kao constant		3.3	3.3	3.3	3.3	3.3
	Kaw constant		200	200	200	200	200
	Emulsion rate	s/m^2	2.00E-06	2.00E-06	2.00E-06	2.00E-06	2.00E-06
Buoyancy	Density of oil at 20oC, volatile fraction	kg/m^3	789	796	796	813	787
	Density of oil at 20oC, heavy fraction	kg/m^3	878	886	886	997	1011
Water solubility	Water solubility, volatile fraction	kg/kg	2.00E-05	2.00E-05	2.00E-05	2.00E-05	2.00E-05
	Water solubility, heavy fraction	kg/kg	2.00E-07	2.00E-07	2.00E-07	2.00E-07	2.00E-07
Volumentric temperature	Volatile oil fraction	$1/^oC$	0.0007	0.0007	0.0007	0.0007	0.0007
expansion coefficient	In-volatile oil fraction	$1/^oC$	0.0007	0.0007	0.0007	0.0007	0.0007
Photooxidation	Decay rate, volatile fraction	per day	0	0	0	0	0
	Decay rate, heavy fraction	per day	0	0	0	0	0
	Light extinction coefficient	1/m	1	1	1	1	1
Dissolution	Dissolution rate, Light fraction	per day	0.4	0.4	0.4	0.4	0.4
	Dissolution rate, heavy fraction	per day	0.4	0.4	0.4	0.4	0.4
Vertical dispersion	Wind speed for wave breaking	m/s	5	5	5	5	5
	Wave energy dissipation rate	$J/m^3/s$	1000	1000	1000	1000	1000
Vertical limits	Max distance below surface for surface amount	m	0.05	0.05	0.05	0.05	0.05
	Max distance above bed for bottom amount	m	0.05	0.05	0.05	0.05	0.05
Viscosity	Mooney constant		0.25	0.25	0.25	0.7	0.7
	Dynamic oil viscosity at reference temperature	cP	1.62	1.68	1.68	1283	209
	Reference temperature for dynamic oil viscosity	^oC	40	40	40	40	50
	Coeff. exponential temperature dependency		-0.136	-0.136	-0.136	-0.136	-0.136
Oil_area	Oil_area growth rate constant	per sec	150	150	150	150	150