



The oil spill model OILTRANS and its application to the Celtic Sea

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ABSTRACT

This paper describes details of an oil spill model, OILTRANS, developed by the authors. The model is an off-line particle-transport model coupled to the most up to date operational met-ocean model forecasts. Formulations for the dominant oil fate processes of spreading, advection, diffusion, evaporation, emulsification and dispersion have been encoded, providing the model with the ability to accurately predict the horizontal movement of surface oil slick, the vertical entrainment of oil into the water column and the mass balance of spilled oil. The application of the OILTRANS model to an accidental release during a ship-to-ship fuel transfer in the Celtic Sea in February 2009 is presented to validate the system. Comparisons with aerial observations of the oil slick at the time of the incident, and subsequent model simulations, indicate that the OILTRANS model is capable of accurately predicting the transport and fate of the oil slick.

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1. Introduction

Oil spills are an inevitable and undesirable consequence of producing and transporting petroleum and associated refined products. More than two thirds of all large (>700 ton) oil spills in the past forty years have occurred whilst vessels have been underway in open or inland waters and although the incidence of large and medium (7–700 ton) oil spills from vessels has significantly reduced in the past forty years, the trade in seaborne oil transportation has increased steadily since the mid 1980s (ITOPF, 2011). Whilst there has only been a limited number of oil spills around the Irish coast in the past forty years, recent data showing 12–13 million tonnes of oil and petroleum products transiting through Irish ports per annum (IMDO, 2010, 2011) indicates that the risk persists of a large oil spill incident occurring.

The three questions of most importance at the time of any oil spill incident are; where will it go, when will it get there, and what will it be like when it arrives? The first two questions are critical in relation to the response operations for combating the spill and the answers to those questions rely on having accurate models for the hydrodynamics and wind fields for the relevant water body (Al Rabeah et al., 2000). The third question, the weathered state of the oil, is important for potential removal operations and depends on using reliable oil fate and weathering algorithms. The processes through which oil weathers often occur simultaneously with each other, and the rate and significance of the weathering processes on the ultimate fate of the oil are dependent on the type of oil spilled, the spill location and the weather conditions at the time of the spill

(API, 1999). Mackay and McAuliffe (1988) postulated that if oil is well characterised and the environmental conditions of wind speed and direction, sea state, currents, salinity and temperature are known, it should be possible to calculate the rates of many of the dominant oil weathering processes and thus establish how oil changes with time. Unfortunately, the rates of the oil spill processes are understood with different levels of confidence, and can be described by mathematical models that are partially based and calibrated on empirical results from laboratory or small scale field tests (Sebastiao and Guedes Soares, 1995).

In spite of these limitations, a large number of oil spill models have been developed over the past forty years (Aamo et al., 1995; Al Rabeah et al., 1995, 2000; Ambjorn, 2007; Carracedo et al., 2006; Chao et al., 2003; CONCAWE, 1983; Daling et al., 1997; French-McKay, 2004; Guo and Wang, 2009; Howlett, 1998; Inan and Balas, 2010; Lehr et al., 2002; Mackay et al., 1980a; Pollani et al., 2001; Reed, 1989; Reed et al., 1995; Spaulding et al., 1992; Tkalic and Xiaobo, 2001; Wang and Shen, 2010) and the state of the art in oil spill modeling has been reviewed by various authors (ASCE, 1996; Reed et al., 1999; Spaulding, 1988).

Oil spill models can be classified with respect to their stages of evolution as: first, second and third generation models (Cekirge et al., 1995). First generation models are transport models with limited fate algorithms. Second generation models consist of limited two-dimensional hydrodynamics and fate algorithms. The third generation model or the comprehensive oil spill model consists of a set of algorithms to simulate the fate and transport of oil in three dimensions, including the processes of advection, diffusion, surface spreading, vertical mechanical dispersion, evaporation, emulsification and stranding (Cekirge et al., 1995).

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the type of oil, the volume of oil spilled and the weather conditions during a spill event. After Fingas (2011), the order of importance of the weathering processes encoded in the model are: evaporation, emulsification and natural dispersion. Implementation of the weathering process algorithms chosen for the OILTRANS model are detailed in subsequent sections.

2.2. OILTRANS oil fate governing equations

The processes encoded in OILTRANS to describe the physical and chemical weathering processes of spilled oil include: advection of the slick due to currents and wind drift, diffusion of the oil particles due to random motions, the mechanical spreading of the slick under gravity and viscous forces, the evaporation from the slick of the lighter components of the spilled oil, the entrainment of water into the oil slick forming emulsions, and the dispersion of the smaller droplets of oil into the water column through the action of breaking waves. These processes are considered by the authors to be the dominant mechanisms through which oil is removed from the marine environment. The processes of dissolution, biodegradation, sedimentation and photo-oxidation have not been encoded in the current version of OILTRANS as it is considered that they represent the removal of only a very small fraction of spilled oil during the first 3 days of a spill, the period of the operational oil spill forecast system. In a novel departure from other oil spill modelling systems, OILTRANS allows for user to select a number of different algorithms for the processes of mechanical spreading, evaporation and emulsification. Details of the algorithms for the current implementation of OILTRANS are presented below, with the alternate encoded formulations referenced briefly.

2.2.1. Mechanical spreading

Oil will spread on the surface of a water body even without external forces such as tidal currents or wind stresses. The spreading of the oil on calm waters is due to the force of gravity and the interfacial tension between oil and water, with the oil viscosity and inertia retarding the spreading forces (Fay, 1969). The most widely used formulations for determining the rate of spread of oil on the water's surface are the equations proposed by Fay (1971), or versions thereof. Fay divided spreading into three phases. The first phase known as the gravity-inertial phase generally lasts for less than an hour, except for the largest of spills and is not modelled by OILTRANS. As the time for the first gravity-inertial phase is so short, OILTRANS begins the oil weathering processes once the end time, t_o , of this first phase has been reached, which was determined by Fay (1971) to be:

$$t_o = \left(\frac{k_2}{k_1} \right)^4 \left(\frac{V_o}{v_w g \Delta \rho} \right)^{1/3} \quad (1)$$

where k_1 and k_2 are empirical coefficients (1.14 and 1.45, respectively, after Fay (1971)), V_o is the original volume of spilled oil (m^3), v_w is the kinematic viscosity of water (m^2/s), g is gravitational acceleration (m/s^2), and $\Delta \rho$ is the relative density difference between water and oil given by:

$$\Delta \rho = \frac{\rho_w - \rho_{oil}}{\rho_w} \quad (2)$$

where ρ_w is the density of water (g/cm^3) and ρ_{oil} is the density of oil (g/cm^3). The area (m^2) over which the oil slick has spread at the end of this first spreading phase was determined by Fay (1971) to be:

$$A_o = \pi \frac{k_2^4}{k_1^2} \left(\frac{V_o^5 g \Delta \rho}{v_w^2} \right) \quad (3)$$

The second stage of slick spreading known as the gravity-viscous phase is governed by the balance between the viscosity of the oil and the oil–water interfacial tension. The viscous spreading

phase continues to such a time that the slick gets so thin that surface tension forces alone play a role in spreading the slick, leading to the third, surface-tension, phase. This third phase is not modelled in OILTRANS as it occurs at much later stages in slick spreading, rather a terminal oil film thickness is defined in OILTRANS to denote the end of the gravity viscous phase after which no further mechanical spreading occurs. Generally, by this time significant weathering will have occurred and the slick is allowed to disperse horizontally or break into smaller slicks due to surface current shears.

The general spreading formulae proposed by Fay (1971) only deal with an idealized spreading of a slick in a radial manner on calm seas. They take no account of wind conditions, which play an important role in determining the shape and area of actual spills. Results of field experiments on the spreading of oil slicks have been reported by Elliott et al. (1986), Jeffrey (1973) and Lehr et al. (1984), all of which found that slicks developed elongated shapes, with the major axis orientated in the direction of the wind. Lehr et al. (1984) devised a Fay-type formula to account for the elongation of the oil slick in the direction of the wind.

Using the assumptions adopted by previous researchers (Al Rabeh et al., 2000; Chao et al., 2003; Gou and Wang, 2009; Inan and Balas, 2010; Nagheeb and Kolahdoozan, 2008), that the slick is elliptical in shape with the major axis orientated in the direction of the wind, the area, A ($\times 10^3 m^2$), of the oil slick once the gravity-viscous spreading phase has commenced, can be represented as:

$$A = 1/4\pi QR \quad (4)$$

where Q and R are the lengths of the minor and major ellipse axis respectively, given by:

$$Q = 1.7(\Delta \rho V_o)^{1/3} t^{1/4} \quad (5)$$

$$R = Q + 0.03 U_{wind}^{4/3} t^{3/4} \quad (6)$$

where in this case, V_o is the volume of the spill (bbl), t is the time after the oil slick commences spreading (min) and U_{wind} is the wind speed (kts). Following the method adopted by Al Rabeh et al. (1989, 1995, 2000), the slick can be conceptualised as a series of concentric ellipses in a local Cartesian reference frame X^*Y^* with the centre of mass of the slick located at the local coordinates of $(x^*, y^*) = (0,0)$, see Fig. 2. The local X^* axis of the slick is orientated in the direction of the wind. The elliptical spreading of the slick over time is assumed to be uniform, in that;

$$\frac{r}{R} = \frac{r + \Delta r}{R + \Delta R} \quad (7)$$

$$\frac{q}{Q} = \frac{q + \Delta q}{Q + \Delta Q} \quad (8)$$

$$\frac{q}{Q} = \frac{r}{R} \quad (9)$$

where r and q are the lengths of the major and minor axis of an interior ellipse, Δr and Δq are the increases in length of the major and minor axis of an interior ellipse in time-step Δt (min), and ΔR and ΔQ are the increases in length of the major axis and minor axes of the outer ellipse in time-step t (min).

Any oil particle constituting the slick will therefore be subjected to a displacement proportional to the increase in the length of the respective axes with time. Given the location of a particle on an interior ellipse at coordinates, x_t^*, y_t^* which can be rewritten as $x_t^* = r \cos \theta$ and $y_t^* = q \sin \theta$, the displacement of the particle outwards by Δx^* and Δy^* by spreading has been calculated by Al Rabeh et al. (2000) to be:

$$\Delta x^* = \Delta r \cos \theta = \Delta r (x_t^*/r) = x_t^* (\Delta R/R) \quad (10)$$

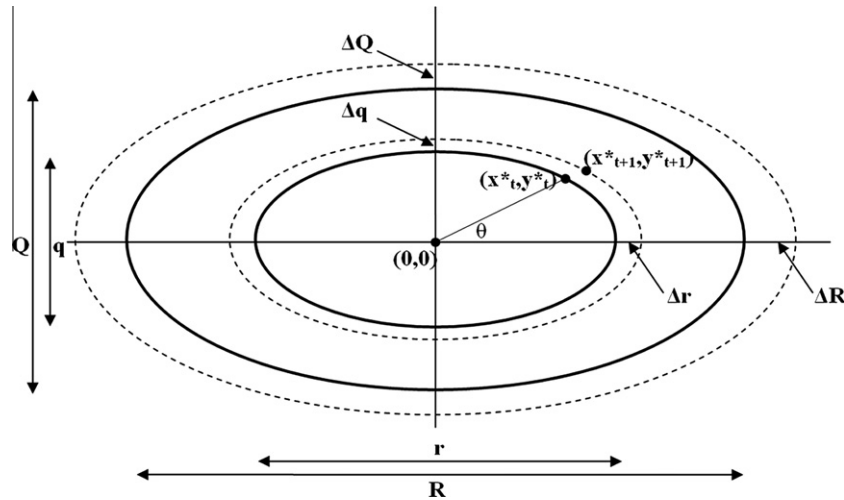


Fig. 2. Elliptical spreading of a surface slick.

$$\Delta y^* = \Delta r \sin \theta = \Delta r (y_t^*/q) = y_t^* (\Delta Q/Q) \quad (11)$$

where the values of ΔQ and ΔR are given by the formulae;

$$\Delta Q = 1.7(\Delta \rho V_0)^{1/3} 1/4t^{-3/4} \cdot \Delta t \quad (12)$$

$$\Delta R = \Delta Q + 0.03U_{wind}^{4/3} 3/4t^{-1/4} \cdot \Delta t \quad (13)$$

with units as those in Eqs. (5), (6). As the local Cartesian reference frame for the slick is orientated in the direction of the wind, the coordinates must be converted to the global Cartesian coordinate system used by the OILTRANS model by means of the following transformations;

$$X = (\cos \varphi)x^* + (\sin \varphi)y^* \quad (14)$$

$$Y = (-\sin \varphi)x^* + (\cos \varphi)y^*$$

where φ is the angle between the wind direction and the positive x-axis of the OILTRANS model domain. After each time-step in the OILTRANS model, the centre of mass of the oil slick is re-calculated and becomes the origin of a new local coordinate system for a new set of concentric ellipses, the extent of which is calculated from Eqs. (5), (6).

The classical Fay (1971) formulation for mechanical spreading, in the absence of wind effects, is also encoded in the OILTRANS system for sensitivity analyses and to give end users the options to choose an alternative algorithm for local implementations. The calculation of the elliptical spreading of the oil slick is undertaken during the gravity-viscous phase of the spreading of the oil slick and only until the terminal oil slick thickness is reached. Once the terminal oil slick thickness is reached the spreading assumption is removed and the slick is allowed to spread under the influence of horizontal diffusion, surface winds and water current shears, as detailed below, to represent complex, realistic surface slicks.

2.2.2. Advection and diffusion

The movement of an oil slick at the water surface can be considered as being composed of the advection of the oil slick by both surface currents ($U_{current}$), wind effects (U_{wind}), and the diffusion of oil particles as a result of random processes (ASCE, 1996; Ambjorn, 2007; Guo and Wang, 2009; Carracedo et al., 2006; Cheng et al., 2011; Jordi et al., 2006). The advection of the oil slick due to surface currents is taken to be the current velocity as predicted

in the surface layer of the water column by the authors' oceanographic model, $U_{current}$.

There are a number of processes that are associated with wind effects and most oil spill models represent them with a simple wind drift factor (Guo and Wang, 2009; French-McKay, 2004; Nagheeb and Kolahdoozan, 2008; Perianez and Caravaca, 2010). Most oceanographic models do not adequately resolve the uppermost centimeter of the water column at the air–water interface and thus tend to underpredict the actual wind induced surface current. Allowance is made for this through incorporation into the wind drift factor, as in Ambjorn (2007). Based on sensitivity testing the cumulative wind drift factor was set at 3.5% of the wind speed, which is in keeping with values found in published literature (Carracedo et al., 2006; Guo and Wang, 2009; French-McKay, 2004; Perianez and Caravaca, 2010). In addition to the advective wind drift factor, a Coriolis force correction is also introduced, whereby the surface slick is deflected to the right by a drift angle, which is set to 5°.

It follows therefore that the centre of mass of the oil slick is advected by surface currents and wind effects according to:

$$U_a = U_{current} + 0.035U_{wind} \quad (15)$$

where U_a is the advective velocity of the oil slick (m/s). By modelling the oil spill as a large number of discrete lagrangian particles in an XY planar reference frame at the water surface such that (x_t, y_t) represents the location of a particle at time-step t , the location of that particle at time-step $t+1$ due to advective and diffusive transport processes will be (x_{t+1}, y_{t+1}) where:

$$X_{t+1} = x_t + u_a(x_t, y_t)\Delta t + \Delta x_{diff} \quad (16)$$

$$Y_{t+1} = y_t + v_a(x_t, y_t)\Delta t + \Delta y_{diff}$$

where $u_a(x_t, y_t)$ and $v_a(x_t, y_t)$ are the u and v components of the interpolated advective velocity U_a at location x, y in the X and Y directions respectively (m/s), Δt is the time-step interval (s), Δx_{diff} and Δy_{diff} are the diffusive displacements of the particle in the X and Y directions respectively due to random process. Based on the work by Al Rabeh et al. (1989) the values of Δx_{diff} and Δy_{diff} can be calculated as:

$$\Delta x_{diff} = [R]_0^1 \sqrt{12D_h \Delta t} \cos \theta \quad (17)$$

$$\Delta y_{diff} = [R]_0^1 \sqrt{12D_h \Delta t} \sin \theta$$

where $[R]_0^1$ is a random number uniformly distributed between 0 and 1, D_h is the horizontal diffusion coefficient (m^2/s) and is user-definable, and θ is the directional angle assumed to be uniformly distributed between 0 and 2π (i.e. $\theta = 2\pi[R]_0^1$).

2.2.3. Evaporation

Evaporation is the primary weathering process involved in the natural removal of oil from the sea surface, with the rate of evaporation being determined by the oil properties and increasing due to the spreading of the oil, seawater temperature and wind speed (CONCAWE, 1983). The evaporation process in OILTRANS is modelled using the pseudo-component approach adopted by Jones (1997) where the oil is approximated as an ideal mixture of a small number of components. Each component is characterised by a mole fraction and vapour pressure. The total evaporation rate for the oil is the sum of the evaporation rates of each component, i , which is expressed as:

$$\frac{dV_i}{dt} = \frac{K_i A(t) P_i \bar{V}_i \chi(t)_i}{RT} \quad (18)$$

Where A is the area of the oil slick (m^2), at time t , R is the gas constant, T is the oil temperature, assumed equal to the water temperature ($^\circ\text{K}$), K_i is the mass transfer coefficient, expressed after Mackay and Matsugu (1973) as:

$$K_i = 0.0048 U_{\text{wind}}^{7/9} X^{-1/9} Sc^{-2/3} \quad (19)$$

Where X is the downwind length of the oil slick axis (m), Sc is the Schmidt number based on the mole weighted average of the oil (MW_{avg}), and calculated after Lehr et al. (2002) to be:

$$Sc = 1.3676 \left(\frac{0.018}{MW_{\text{avg}}} \right)^{-1/2} \quad (20)$$

\bar{V}_i

is the molar volume of each component i , correlated by Jones (1997) to boiling point data to give:

$$\bar{V}_i = 7.0 \times 10^{-5} - (2.102 \times 10^{-7} BP_i) + (1.0 \times 10^{-9} BP_i^2) \quad (21)$$

where BP_i is the boiling point cut for each component, i , P_i , the vapour pressure of component i , is given by Antoine's equation as:

$$\ln \frac{P_i}{P_a} = \frac{\Delta S_i (BP_i - C_2)^2}{R BP_i} \left[\frac{1}{BP_i - C_2} - \frac{1}{T - C_2} \right] \quad (22)$$

where P_a is atmospheric pressure (Pa), C_2 is a coefficient = $0.19(BP_i - 18.0)$, ΔS_i is a coefficient = $8.75 + 1.987 \log(BP_i)$, $\chi(t)_i$ is the mole fraction of component, i , at time, t , which can be expressed in terms of volumes and molar volumes as:

$$\chi(t)_i = \frac{V_i / \bar{V}_i}{\sum_{j=1}^{i_{\text{max}}} V_j / \bar{V}_j} \quad (23)$$

Substituting Eqs. (19)–(21) into Eq. (18) gives:

$$\frac{dV_i}{dt} = \frac{0.0656 U_{\text{wind}}^{7/9} (0.018 / MW_{\text{avg}})^{1/3}}{X^{1/9}} \cdot \frac{A(t) P_i}{RT} \cdot \frac{V_i}{\sum_{j=1}^{i_{\text{max}}} V_j / \bar{V}_j} \quad (24)$$

This equation is solved in each time step to determine $\frac{dV_i}{dt}$. The final term in Eq. (24), the volumetric mole fraction term, is recalculated at the end of each time-step to account for the losses from each component, i , in that time-step. The total fraction of oil evaporated, F_{evap} , is then the sum of the volumes of the components evaporated divided by the initial volume of the oil.

The evaporation algorithms of both Stiver and Mackay (1984) and Fingas (1999) are also encoded in the OILTRANS system for use in sensitivity analyses and to give end users the options to

choose an alternative algorithm for local implementations. Emulsification will affect the evaporation rate; therefore a factor of $(1-Y)$ is applied to account for the fraction of oil that is in emulsion, where Y is the water content of the emulsified oil, (see Section 2.2.4)

2.2.4. Emulsification

Emulsification is the second most important weathering process after evaporation (Fingas and Fieldhouse, 2001). Emulsification is the process by which water droplets are incorporated into an oil slick. The most important characteristic of a water-in-oil emulsion is its stability (Fingas et al., 1999). The classification of stability is important before one can identify the properties of the emulsion, as they change significantly for each type of emulsion (Fingas and Fieldhouse, 2001). Extensive studies on over four hundred oil types have classified water-in-oil emulsions into four stability types; stable, mesostable, entrained and unstable. Emulsion formation in the OILTRANS model is modelled using the approach of Fingas and Fieldhouse (2004), subsequently improved by Fingas (2011) where the stability class is directly predicted from empirical data, and herein referred to as the Fingas method. To the best of the author's knowledge, this is the first implementation of the Fingas method in an operational oil spill modelling system.

The first step in this method is to calculate the oil properties at the weathering condition of concern, which is accomplished internally in the OILTRANS model's evaporation, density, viscosity and dispersion subroutines. A review of knowledge on water in oil emulsions (Fingas and Fieldhouse, 2006) found that the asphaltene and resin content are primarily responsible for stability whilst a previous study (Fingas and Fieldhouse, 2003) determined that while the wax content showed some correlation to viscosity, it was not associated with the formation of any state of emulsion. The oil properties required for the Fingas method are thus the density, viscosity, and saturate, resin and asphaltene contents of the weathered oil. These values are then transformed in the manner of Fingas (2011) and substituted into the following equation to determine the stability class:

$$\begin{aligned} \text{Stability}C = & 12.3 + 0.259St - 1.601Rt - 17.2(A/Rt) \\ & - 0.50Vt^3 + 0.002Rt^3 + 0.001At^3 + 8.51(A/Rt)^3 \\ & - 1.12\log(Vt) + 0.7\log(Rt) + 2.97\log(A/Rt) \\ & + 6.0 \times 10^{-8} (\exp(Vt))^2 - 1.96(\exp(A/Rt))^2 \\ & - 4.0 \times 10^{-6} \log(Dt)/(Dt)^2 \\ & - 1.5 \times 10^{-4} \log_{10}(A/Rt)/(A/Rt)^2 \end{aligned} \quad (25)$$

where: *Stability C* is the stability classification, *St* is the transformed saturate content (%), *Rt* is the transformed resin content (%), *A/Rt* is the transformed asphaltene/resin ratio, *Vt* is the transformed natural logarithm of viscosity (mPas), *At* is the transformed asphaltene content (%), and *Dt* is the transformed exponential of the oil density (g/cm^3). The calculated values of *Stability C* are then related to the emulsion state, with associated conditions where applicable, according to (Fingas, 2011). In addition, the viscosity of the resulting emulsion has been determined as a multiplicative factor on the starting oil viscosity and can be taken as the average value for the emulsions types at a given time, following the values provided by Fingas (2011). The water content of the resulting emulsion type at given times has also been determined by Fingas (2011) and is included in the OILTRANS formulations. The time to formation of the emulsions has previously been studied by Fingas and Fieldhouse (2004), who related the time to formation of each emulsion type to the energy required for formation (expressed as equivalent wave height) and expressed as:

$$y = a + (b/x^{1.5}) \quad (26)$$

where y is the time to formation (min), a and b are coefficients depending on emulsion type after [Fingas \(2011\)](#), and x is the wave height (cm). The emulsification algorithms of [Mackay et al. \(1980a,b\)](#) are also encoded in the OILTRANS system for use in sensitivity analyses and to give end users the options to choose an alternative algorithm for local implementations.

2.2.5. Dispersion

Natural dispersion, or entrainment, of oil slicks at sea occurs when droplets of oil are mixed into the water column by breaking waves. If the droplets are small enough natural turbulence in the water will prevent the oil from resurfacing whilst larger droplets tend to rise and will not stay in the water column for more than a few minutes. The droplets that stay in the water column are considered to be permanently dispersed. The natural dispersion process within the OILTRANS model is based on the classic method of [Delvigne and Sweeney \(1988\)](#) who developed a relationship for entrainment rate, Q_d , as a function of droplet size and oil viscosity, as:

$$Q_d = C^* D_d^{0.57} S F d^{0.7} \Delta d \quad (27)$$

where: Q_d is the entrainment rate, (kg/m²s), for droplet diameter d , (m), C^* is an empirical entrainment constant which depends on oil type and weathering state. Using a series of experimental data by [Delvigne and Hulsen \(1994\)](#), the entrainment constant, C^* , was fit to the following equations by [French-McCay \(2004\)](#):

$$\begin{aligned} C^* &= \exp(-0.1023 \ln(\nu_{oil}) + 7.575) & \text{for } \nu_{oil} < 132(\text{cSt}) \\ C^* &= \exp(-1.8927 \ln(\nu_{oil}) + 16.313) & \text{for } \nu_{oil} > 132(\text{cSt}) \end{aligned} \quad (28)$$

where: ν_{oil} is the viscosity of the oil, (cSt). D_d is the dissipated breaking wave energy per unit surface area, (J/m²), and is given by:

$$D_d = 0.0034 \rho_w g H_b^2 \quad (29)$$

where H_b is the breaking wave height, assumed to be equal to $1.5H_{sig}$ using the simple estimate of [Liungman and Mattsson \(2011\)](#) where H_{sig} is the significant wave height (m), and assuming a fully developed sea-state, can be calculated according to [CERC \(1984\)](#) as:

$$H_{sig} = \left(\frac{0.243 U_*^2}{g} \right) \quad (30)$$

Where $U_*^2 = 0.71 U_{wind}^{1.23}$, is the wind stress factor associated with the 10 m wind speed U_{wind} (m/s). S is the fraction of sea surface covered by oil (assumed as 0.75). F is the fraction of sea surface hit by breaking waves and is parameterised as:

$$\begin{aligned} F &= 3.0 \times 10^{-6} (U_{wind}^{3.5} / T_w) & \text{for } U_{wind} < U_{th} \\ F &= 3.0 \times 10^{-2} [(U_{wind} - U_{th}) / T_w] & \text{for } U_{wind} > U_{th} \end{aligned} \quad (31)$$

where U_{th} is the threshold 10 m wind speed for onset of breaking waves assumed as 5 m/s, T_w is the significant wave period and assuming a fully developed sea-state can be calculated according to [CERC \(1984\)](#) as:

$$T_w = 8.13 \left(\frac{U_{wind}}{g} \right) \quad (32)$$

Δd is the oil droplet interval diameter, (m), equally spaced between d_{max} and d_{min} . After [Reed et al. \(1995\)](#) the maximum and minimum droplet size diameters are calculated as:

$$\begin{aligned} d_{max} &= 3400 E^{-0.4} (\nu_0)^{0.34} \\ d_{min} &= 500 E^{-0.4} (\nu_0)^{0.34} \end{aligned} \quad (33)$$

where E is the wave energy dissipation rate per unit volume, (J/m³s) set as 5.0×10^3 after [Delvigne and Sweeney \(1988\)](#) as an intermediate value for breaking waves. The oil particle interval

diameter was then constructed by adopting ten size classes between d_{min} and d_{max} , equally spaced on diameter, as:

$$\Delta d = (d_{max} - d_{min}) / 10.0 \quad (34)$$

The OILTRANS model randomly assigns a droplet diameter to each of the lagrangian particles based on the droplet distribution profile calculated from Eqs. (33), (34). The depth, to which the dispersed oil droplets mix, Z_{mix} , is expressed as:

$$Z_{mix} = \max(D_v / w_d, Z_i) \quad (35)$$

where D_v is the vertical diffusion coefficient (m²/s), equal to $0.0015 U_{wind}$ after [Thorpe \(1984\)](#), w_d is the rise velocity (m/s) for droplet diameter d , and Z_i is the intrusion depth (m) of the breaking wave equal to $1.5H_b$ after [Delvigne and Sweeney \(1988\)](#). The rise velocity, w_d , of the droplets is calculated based on the droplet Reynolds number with Stokes Law applied for small droplets and Reynolds Law applied for larger droplets, after [Tkachik and Chan \(2002\)](#). The total entrainment rate of oil into the water column, Q_{total} (kg/m²s), for all droplet size classes is:

$$Q_{total} = \sum_{d=1}^{10} Q_d \quad (36)$$

and the total mass entrained, M_{ent} (kg), per time step is equal to:

$$M_{ent} = Q_{total} A_t \Delta t \quad (37)$$

The droplet sizes determine whether dispersed oil will re-surface and at what rate. Large droplet sizes will resurface faster than small droplets, which may remain permanently dispersed in the water column. Droplets which do not re-surface within the model time-step are assumed to be permanently dispersed within the water column. The current version of OILTRANS does not model the subsurface transport of dispersed oil droplets.

2.2.6. Density

The initial oil density is obtained from either the API gravity of the oil, or the density value and reference temperature, both contained within an oil database. Only oils with densities lower than water are modelled, as more dense oils will sink. The change in oil density over time is related to three different processes; changing water temperature, evaporation, and emulsification. The change in density due to changing temperature can be expressed as:

$$\rho_{oil} = \rho_{ref} (1.0 - C_{DensT} (T - T_{ref})) \quad (38)$$

where ρ_{oil} is density of oil (g/cm³), at temperature T (°K) (assumed equal to the water temperature), ρ_{ref} is the reference density of oil (g/cm³), at reference temperature T_{ref} (°K), C_{DensT} is an empirical constant equal to 8.0×10^{-4} after [Lehr et al. \(2002\)](#). The change in density due to evaporation can be expressed as:

$$\rho_{oil} = \rho_{ref} (1.0 + C_{Dense} F_{Evap}) \quad (39)$$

where C_{Dense} is an empirical constant equal to 1.8×10^{-2} after [Lehr et al. \(2002\)](#), F_{Evap} is the fraction of oil evaporated from the slick. The change in density due to emulsification can be expressed as:

$$\rho_{oil} = (Y \rho_w) + \rho_{ref} (1.0 - Y) \quad (40)$$

Where Y is the water content of the emulsion. Eqs. (38)–(40) can be combined into one single equation to give the total change in density of the oil as ([Buchanan and Hurford, 1988](#)):

$$\rho_{oil} = (Y \rho_w) + \rho_{ref} (1.0 - Y) (1.0 + C_{Dense} F_{Evap}) (1.0 - C_{DensT} (T - T_{ref})) \quad (41)$$

2.2.7. Viscosity

The change in oil viscosity over time is related to three different processes; changing water temperature, evaporation,

and emulsification. The change in density due to changing temperature can be expressed using Andrade's correlation as:

$$\nu_{oil} = \nu_{ref} \exp \left(C_{Temp} \left(\frac{1}{T} - \frac{1}{T_{ref}} \right) \right) \quad (42)$$

Where ν_{oil} is viscosity of oil (cSt) for given water temperature, T (°K) (assumed equal to the water temperature), ν_{ref} is the reference viscosity of oil at reference temperature T_{ref} (°K), C_{Temp} is an empirical constant equal to 5.0×10^3 after Lehr et al. (2002). The change in viscosity due to evaporation can be expressed as (Mackay et al., 1980a,b):

$$\nu_{oil} = \nu_{ref} \exp(C_{Evap} \cdot F_{Evap}) \quad (43)$$

where F_{Evap} is the fraction of oil evaporated from the slick, C_{Evap} is an empirical constant equal to 10.0 after Reed (1989). The change in viscosity due to emulsification can be determined with reference to Table 2, above, after Fingas (2011) where:

$$\nu_{oil} = \nu_{ref} \text{Visc}_{Emul} \quad (44)$$

Where ν_{ref} is the oil viscosity at the onset of emulsification and is calculated from Eqs. (42), (43), Visc_{Emul} is the interpolated viscosity multiplier from Table 2.

3. Application to a spill incident in the Celtic Sea

The previous sections were focussed on the components of the OILTRANS modelling system and the general model formulations for oil transport and fate processes. In this section, the capability of the OILTRANS model is demonstrated through its application to an actual oil spill incident which occurred in the Celtic Sea on 14th February 2009.

3.1. Background

The spill incident in the Celtic Sea involved the accidental release of oil during a ship-ship fuel transfer to the Russian naval vessel Admiral Kuznetsov. At the time of the incident it was estimated that 400–500 tonnes of a light crude oil was discharged (EMSA, 2010). The quantity of the spill was later revised down to 300 tonnes with the type of oil confirmed to be Mazut, which is a heavy, low quality crude oil (Irish Coastguard, *pers. comm.*). This incident represented the largest accidental spill in European waters in 2009 and the largest spill in waters around the British Isles since the Sea Empress ran aground off Milford Haven, Wales in 1996 (EMSA, 2010).

On Saturday the 14th February 2009 at 10:54 am, the European Maritime Safety Agency (EMSA) satellite surveillance programme CleanSeaNet detected an oil slick 100 km southeast of Ireland's most southerly point, Mizen Hd., Co. Cork and notified the Irish and UK Coastguard agencies. Upon notification of the event, both the Irish and UK coastguard agencies tracked the evolution of the slick on an almost daily basis by aerial reconnaissance until 2nd March by which time the surface slick was no longer visible.

The OILTRANS model was employed to simulate the transport and fate of the spilled oil for a 10 day period from the 14th to 23rd February. The area of interest for this case study, within the authors' larger Northeast Atlantic operational model domain, is presented in Fig. 3, and highlights the location of the Kuznetsov incident and the M3 databuoy which recorded wind speeds, directions and wave heights throughout the course of the incident.

3.2. Environmental conditions

Accurate environment information is essential for the reliable prediction of the transport and fate of oil pollution. The three most

important sets of environmental information required are the spatially and temporally varying fields of wind, water current and waves. Accurate definition of these dynamic forcing conditions is fundamental to producing an accurate oil spill trajectory model.

The wind fields defined to the OILTRANS model were obtained from the GFS re-analysis model predictions for the period in question. The winds at the location of the incident over the period were interpolated from the 0.5° GFS model predictions to the incident location and are shown in Fig. 4(a). The wind blew predominantly in a north–northeasterly direction, though the wind rotated through all points of the compass throughout the 10 day time period with wind speeds of 5.5 m/s–8.8 m/s experienced for greater than 50% of the time.

The dynamic wave fields were defined to the OILTRANS model using the CERC (1984) deepwater wave formulations based on wind speeds predicted by the GFS re-analysis model for the period in question. The calculated significant wave heights at the incident location are presented in Fig. 4(b). The surface currents at the incident location over the 10 day period are shown in Fig. 4(c), with surface current direction shown in Fig. 4(d).

The surface current speeds defined to the OILTRANS model were obtained from the authors' operational Northeast Atlantic oceanographic model at hourly intervals. Maximum surface current speeds at the incident location were approximately 0.5 m/s on the spring tide of the 14th February, with highest neap tide surface currents approximately 0.15 m/s occurring on the 19th February.

3.3. Model simulation

The OILTRANS model was used to simulate the trajectory and fate of the spilled oil over a 10 day period, from the 14th to 23rd February 2009. The model was initialised at 00:00 h on 14th February with the hydrodynamic fields from the authors Northeast Atlantic oceanographic model, wind fields from the pre-interpolated GFS re-analysis model and wave fields based on the CERC (1984) formulations. Thereafter, the above spatially and temporally varying met-ocean forcing fields were updated within the OILTRANS model at hourly intervals. It was assumed that the oil spill incident occurred instantaneously at 00:00 h on 14th February with a discharge of 300 tonnes of Mazut crude oil. The exact time and duration of the spill incident was never established (Irish Coastguard, *pers. comm.*). The Mazut crude oil properties defined to the model are presented in Table 1. The trajectory of the oil spill particles were calculated at 5 min intervals and the evolution of the oil weathering process were calculated at hourly intervals. The OILTRANS model simulation was executed until 00:00 h on 24th February.

4. Results and discussion

As is often the case in validating oil spill models, a lack of sufficient field data at the time of an oil spill event hampers the efforts to accurately calibrate model predictions. In the case of the incident in the Celtic Sea, daily reconnaissance over-flights of the oil slick were conducted thereby allowing the predicted oil slick trajectories from the OILTRANS model simulation be compared against the actual observations of the oil slick positions. Unfortunately, limited sampling of the actual spilled oil for analysis was undertaken. Only one sample from the 21st February was available for comparison against OILTRANS model predictions. Therefore, for validation of the oil fates component of OILTRANS for the incident in question, recourse was made to comparing the predictions from the OILTRANS model against predictions from the publicly available ADIOS v2.0.1 oil weathering model (NOAA, 2012).

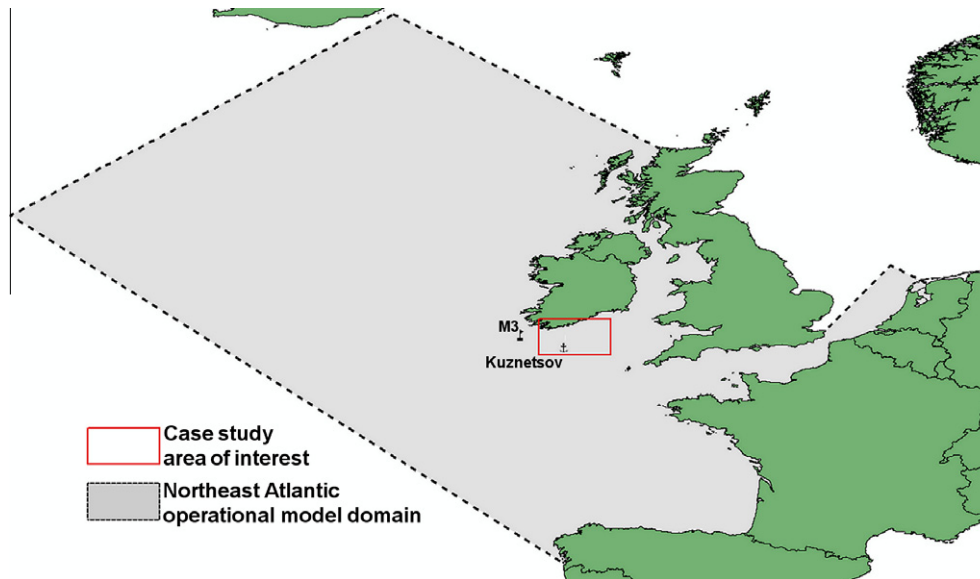


Fig. 3. Operational Northeast Atlantic model domain showing the case study area of interest.

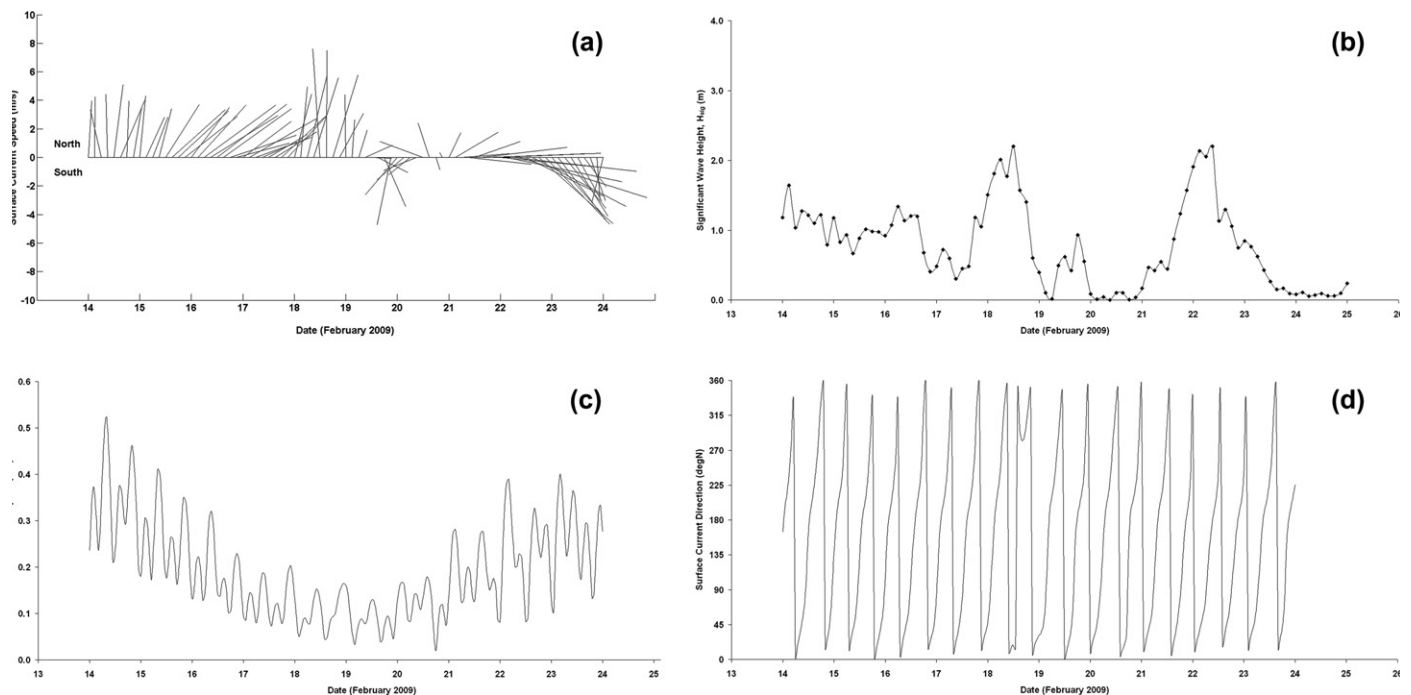


Fig. 4. Time history of (a) wind speed, (b) wave height, (c) current speed and (d) current direction at incident location.

4.1. Oil slick trajectory

The OILTRANS oil slick trajectory predictions were compared against available aerial reconnaissance observations of the slick location for the period from the 14th to 23rd February 2009 and are presented in Fig. 5. In general, the predictions from the OILTRANS model showed close agreement with both the observed slick locations and the overall trajectory of the oil slick throughout the 10 days of model simulation.

From the beginning of the oil spill incident both the observed slick and the predicted slick travelled in a northeasterly direction until the 15th February. The trajectory of the predicted slick was offset parallel to the observed slick by approximately 5 km during

this time. From the 15th to 18th February the observed slick travelled in an east-northeasterly direction, with the predicted slick travelling in an easterly direction. The trajectory of the predicted slick intersected that of the observed slick on the 17th February. During this period from 15th to 18th February the average difference between the observed slick and the predicted slick locations was approximately 4.5 km. From the 18th to 19th February, both the observed and predicted slicks travelled in a northeasterly direction. During the period from the 19th to 21st February both slicks circulated in a clockwise manner with very close agreement between the positions of the observed and predicted slick locations. From the 21st to 23rd February, when the OILTRANS model simulation ended, both slicks travelled in an east-southeasterly

Table 1
Mazut oil properties.

Parameter	Value	Units
Density at 15 °C	0.89	g/ml
Kinematic viscosity at 80 °C	118	cSt
Asphaltenes	3.6	%
<i>Distillation</i>		
5% recovered	259	°C
10% recovered	310	°C
20% recovered	358	°C
30% recovered	445	°C
40% recovered	502	°C
50% recovered	534	°C
60% recovered	538	°C
75% recovered	545	°C
78% recovered	550	°C

direction. The difference between the location of the observed slick and predicted slick on the 22nd February varied from 2.5 to 5.5 km, whilst on the 23rd February the difference between the locations of the observed slick and predicted slick varied from 4.5 to 11 km due to the 'comet' nature of the predicted slick shape.

4.2. Oil slick weathering

The predictions from the OILTRANS oil weathering modules were compared against predictions from the publicly available ADIOS v2.0.1 oil weathering model. The ADIOS model was executed with time varying wind fields from Fig. 4(a) and time varying wave heights from Fig. 4(b). The Mazut oil was defined as custom oil to ADIOS using the specifications from Table 1. The maximum simulation time possible for the ADIOS model is 5 days. Comparison between the OILTRANS oil weathering module and the ADIOS oil model are presented in Fig. 6 for a 5 day period.

Both the OILTRANS and ADIOS models predict that dispersion due to wave action is the primary mechanism through which the oil was removed from the water surface. OILTRANS predicted that 238 m³ (70.64%) of the oil was removed by natural dispersion, whilst the ADIOS model predicted that 223 m³ (66.17%) was

removed by dispersion. The model predictions are broadly in keeping with reports from on-scene observers on the 21st February who stated “the slick is now quite dispersed and only a light sheen appears to remain at this time” (Irish Coastguard, pers. comm.) The volume of oil predicted to have evaporated from the oil slick by the OILTRANS model was 34 m³ (10.18%) whilst the ADIOS model predicted 13 m³ (3.86%) to have evaporated. The differences between the OILTRANS and ADIOS model predictions for volumes of oil evaporated and dispersed from the slick were seen in the volumes of oil remaining on the sea surface at the end of the model simulations as predicted by both models. The OILTRANS model predicted 64 m³ (19.18%) of oil remained on the water surface, whilst ADIOS predicted that 101 m³ (29.97%) remained.

In addition to volumes of oil evaporated, dispersed and remaining on the water surface, OILTRANS also predicted the slick thickness, viscosity, density and water content throughout the course of the 10 day simulation from 14th to 23rd February as presented in Fig. 7. The OILTRANS model predicted the oil slick viscosity to increase gradually over the first 24 h from the starting oil viscosity of 118cSt to 190cSt. After the first 24 h, during which evaporation of the lighter components of the oil had occurred, the viscosity of the oil increased significantly from 190cSt to 72,000cSt signifying the emulsification of the oil due to the incorporation of water droplets. With the onset of emulsification, the OILTRANS model predicted a large increase in the water content of the oil, from a starting value of 0.06 to an emulsified value of 0.8, signifying that the oil had formed a stable emulsion. Thereafter, the water content of the oil decreased slightly to a long term value of 0.77. OILTRANS also predicted an increase in density of the oil over the same time frame, from a starting value of 0.890 g/cm³ to an eventual value of 1.001 g/cm³. The OILTRANS model predicted the thickness of the initial oil slick to be approximately 1 cm, with the slick thickness reducing over time to a final value of 0.132 mm (132 µm).

4.3. Model limitations and further development

Accurate environment information is essential for the reliable prediction of the transport and fate of oil pollution. The three most important sets of environmental information required are the

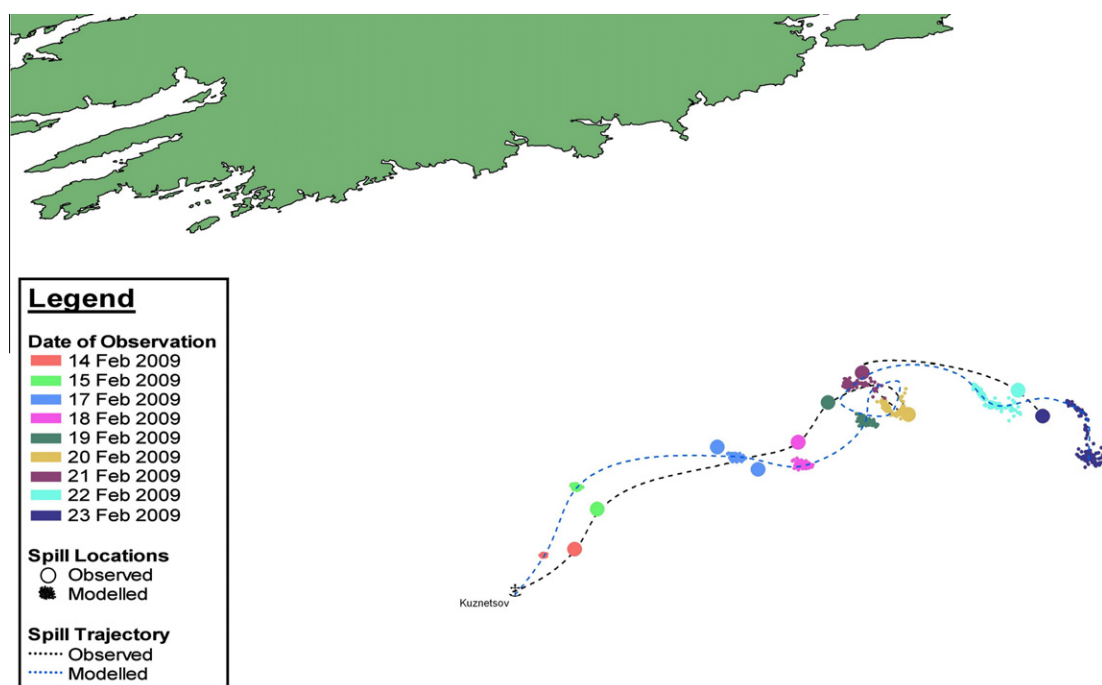


Fig. 5. Comparison of OILTRANS model against observed slick positions from 14th – 23rd February 2009.

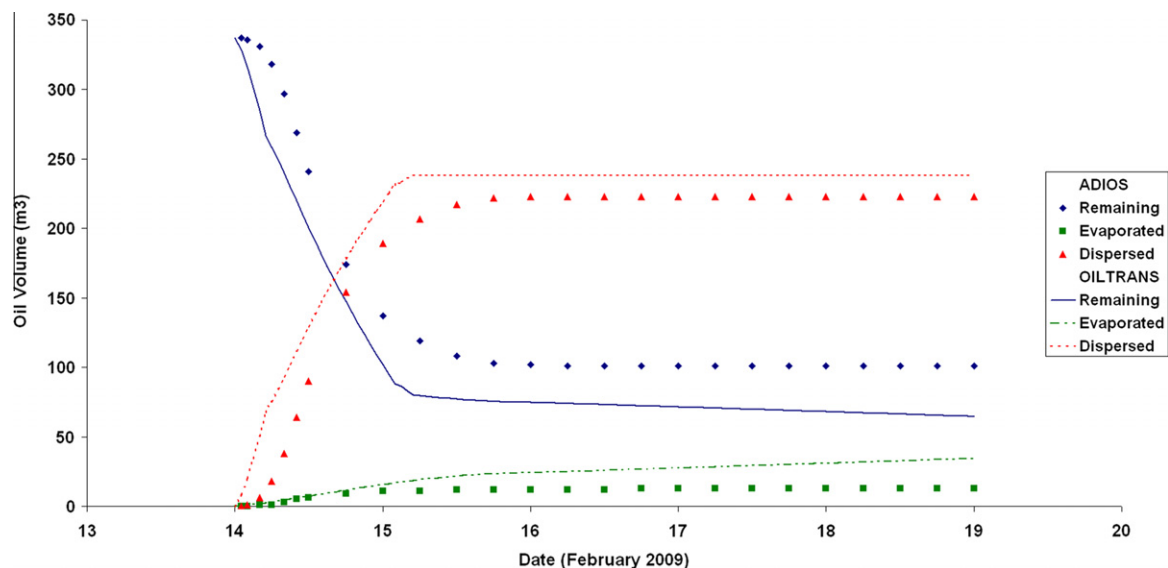


Fig. 6. Comparison of OILTRANS predictions against ADIOS v2.0.1 predictions.

spatially and temporally varying fields of wind, water current and waves. OILTRANS can seamlessly incorporate operational model predictions for both wind fields (GFS) and water currents (ROMS) but currently has only limited capability to incorporate operational predictions of wave fields (SWAN). The limited capability relates to those instances of wave models which have a computational grid in common with the oceanographic ROMS model. Some effort is required to implement generic algorithms to interpolate native SWAN grids to the OILTRANS grid to overcome this limitation.

The ability of an oil spill model to accurately account for wave processes which disperse oil vertically into the water column during wave breaking is very important. In the application of the OILTRANS model to the oil spill incident in the Celtic Sea, the wave fields were calculated internally using the CERC (1984) deepwater wave equations for fully developed sea-states, Eq. (30) and Eq. (32). It was found that these equations under-predicted the significant wave height and significant wave period respectively when compared with actual field observations from the M3 databuoy. The

M3 databuoy located just outside the case study area of interest, see Fig. 3, recorded wind speeds, significant wave heights and periods on an hourly basis during the time of the Celtic Sea incident. Eq. (30) was used to calculate significant wave heights at the M3 databuoy location using the M3 buoy recorded wind speeds. The superposition of the Eq. (30) computed significant wave heights with the M3 databuoy observed significant wave heights in Fig. 8 shows a consistent under-prediction by Eq. (30) in almost all instances. Increased accuracy can be expected in the OILTRANS model's dispersion algorithms by incorporating operational wave model predictions into OILTRANS in place of the CERC (1984) formulations. This is highlighted in Fig. 9 which presents the comparison of significant wave heights as predicted by the authors' recent SWAN model with the M3 databuoy observations of significant wave heights for a 30 day period in November 2011.

Another limitation of the OILTRANS modelling system which is linked to the vertical dispersion of oil droplets due to wave action is the inability of the model to simulate the subsurface transport of

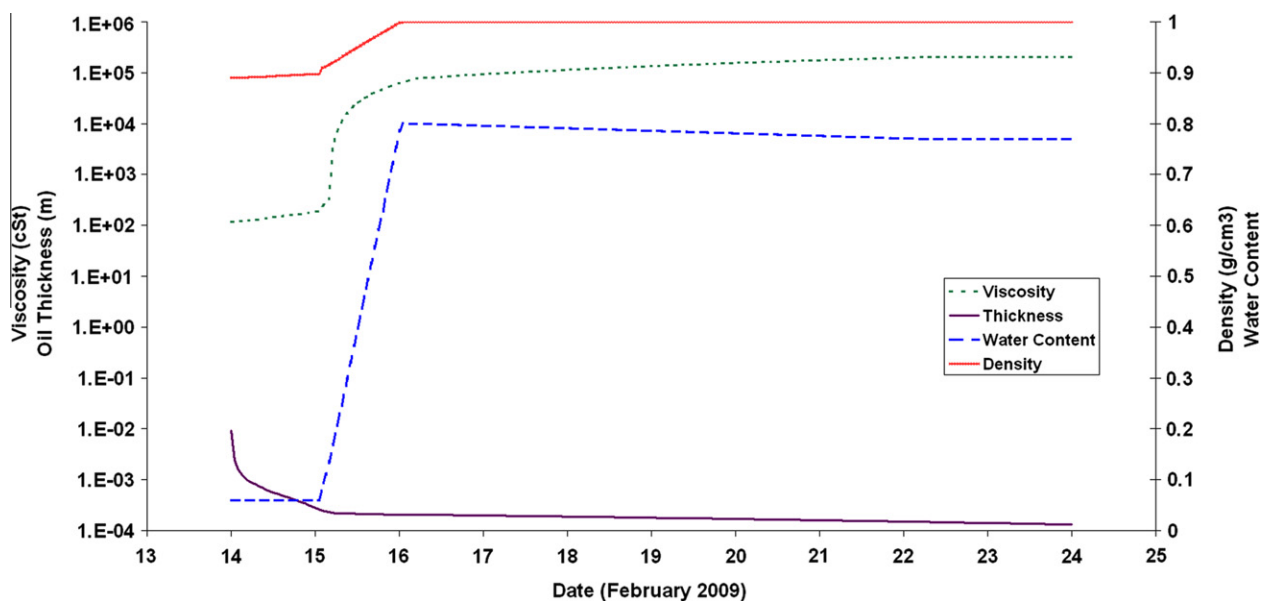


Fig. 7. OILTRANS model prediction of oil slick viscosity, thickness, water content and density.

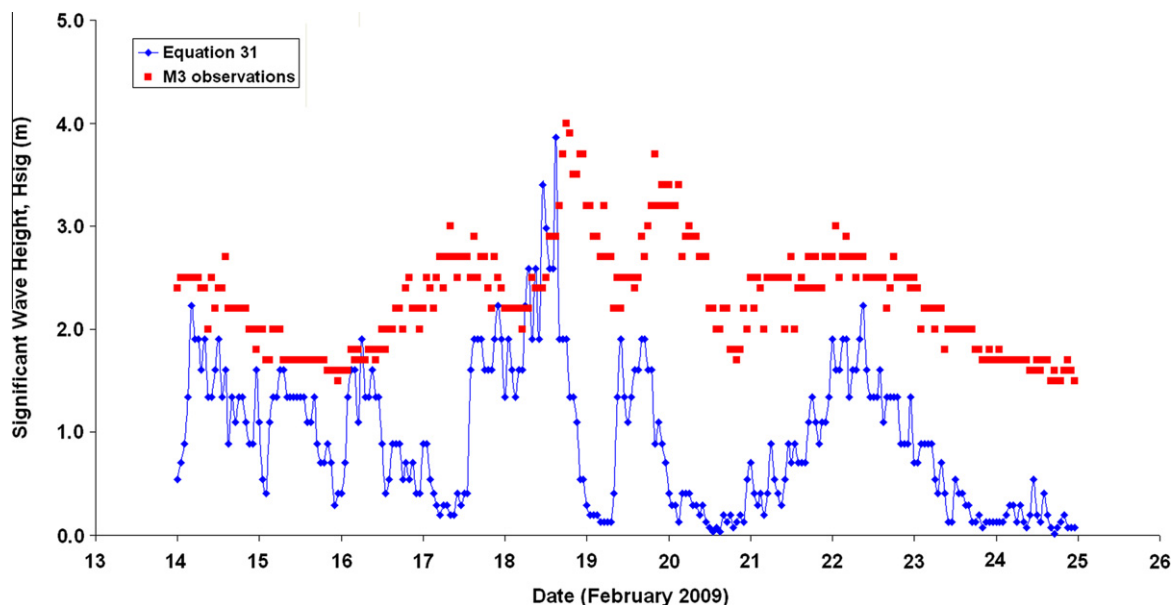


Fig. 8. Comparison of Eq. (30) against M3 buoy recorded significant wave height, H_{sig} .

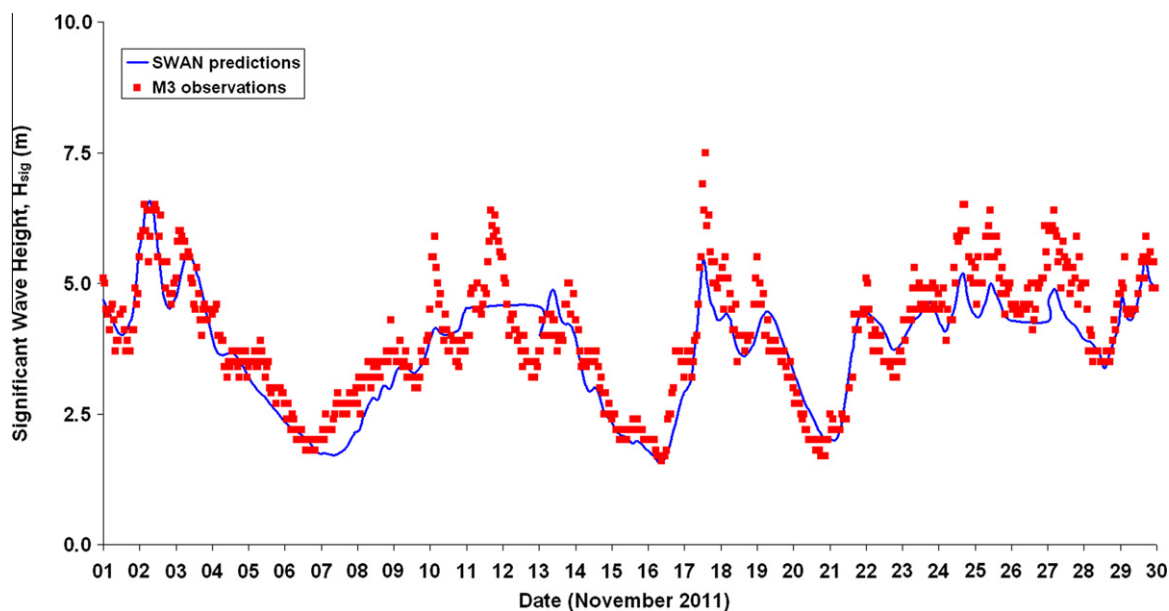


Fig. 9. Comparison of SWAN predictions against M3 buoy recorded significant wave height, H_{sig} .

dispersed oil droplets. Future development of the modelling system will see the incorporation of subsurface oil transport functionality.

Although the OILTRANS model's predictions for the various fate process of evaporation, emulsification and dispersion could not be compared against observations from the actual oil spill event due to insufficient data availability, the model's predictions were compared against one of the standard oil fate modelling applications, ADIOS. The OILTRANS model predicted volumes of oil evaporated, dispersed and remaining on the water which were close to those predicted by the ADIOS model, though differences were evident. The differences in model predictions were due to the adoption of different formulations for the process of emulsification and different parameterisation of formulae for natural dispersion. Reed et al. (1999) stated that two models purporting to contain the same

algorithms may give quite different results from the same input data, and that the performance of one algorithm will be affected by performance of other algorithms in the model. Therefore, it was to be expected that the OILTRANS model would give different results to the ADIOS model owing to the adoption of different formulations and implementations. However, the broad similarity in results between the OILTRANS and ADIOS models provided confidence that the OILTRANS modelling system has accurately accounted for the dominant oil weathering processes.

5. Conclusions

A new oil spill transport and fate model, OILTRANS, which forms the basis of a newly developed operational oil spill forecasting

system for Irish waters, has been developed. The OILTRANS model consists of a set of algorithms based on the most widely used equations and empirical datasets to quantify the processes of advection, diffusion, mechanical spreading, evaporation, dispersion and emulsification. The model facilitates the implementation of differing algorithms for the processes of evaporation, emulsification and mechanical spreading of the oil slick. The model incorporates surface currents from an operational ROMS oceanographic model and wind fields from the operational GFS meteorological model. The OILTRANS model was applied to simulate the case of the accidental release of approximately 300 tonnes of Mazut heavy crude oil in the Celtic Sea on 14th February 2009. The aerial reconnaissance data acquired at the time of the oil spill incident was used to perform a validation test of the OILTRANS transport model. The trajectory and timing of the simulated oil slick's movement compared very well with the reconnaissance data. The main obstacle in presenting validation of the OILTRANS fate model algorithms was the difficulty in obtaining field data for the physical properties of the spilled oil during the course of the incident. Validation of the oil fates component of OILTRANS was made against the ADIOS oil model. The validation exercise verified that the model algorithms provided an encouraging level of accuracy when compared against results from the ADIOS oil model application. Further developments have been identified to improve the accuracy and functionality of the OILTRANS system.

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