THEORETICAL FOUNDATION FOR PREDICTING DISPERSION EFFECTIVENESS DUE TO WAVES

Michel C. Boufadel(*)
and Erik Wickley-Olsen
Dept. of Civil and Environmental Engineering, Temple University,
Ph: (215) 204-7871; Fax: (215) 204-4696, boufadel@temple.edu; http://www.temple.edu/environment.

Tom King, Zhengkai Li, Ken Lee
Center for Offshore Oil and Gas Environmental Research, Bedford Institute of Oceanography, Fisheries and Oceans Canada, Dartmouth, NS, Canada, , and

Albert D. Venosa
National Risk Management Research Laboratory, US EPA, Cincinnati, Ohio.

ABSTRACT
The studies of dispersion of oil in wave tanks have reached their maturity in terms of analytical techniques for measuring and quantifying dispersion. However, there does not seem to be a theoretical framework for predicting or even interpreting the results based on the physics of the problem. One of the reasons is that the oil breakup studies were based on chemical reactors where the energy input is constant with time whereas the energy input to droplets varies with time under waves. For this reason, we present a holistic approach that accounts for the duration over which the oil is subjected to various intensities along with a droplet kinetics model that uses a variable energy dissipation rate function. A salient advantage of the droplet model is that it accounts for the effects of scale of problem, because it has been observed that large systems produce smaller droplets than smaller systems with the same average kinetic energy dissipation rate. We illustrate the usage of the model using simulated wave data.

INTRODUCTION
A wave tank facility at the Bedford Institute of Oceanography (BIO) was designed and built collaboratively by the U.S. Environmental Protection Agency (EPA) and Fisheries and Oceans Canada (DFO) to specifically address these factors in controlled oil dispersion studies over a range of sea states (i.e., energy dissipation rates) obtained by causing waves to break in the tank. The basic method is to generate a train of small period waves (1.18 s herein) and follow it by a train of long period waves (2.0 s). The second train catches up to the first one injecting momentum into it, causing the waves to break. The theory is that long period waves propagate faster than small period waves. Further details about the approach could be found in Wickley-Olsen et al. (2007). Our work herein relies on the new results presented in Wickley-Olsen et al.(2008), where a plunging breaker resulted.

It is reasonable to assume that the dispersion of oil due to waves occurs primarily near the water surface, where water velocity is usually highest for any type of waves, and especially breaking waves as can be noted from the results of Rapp and Melville (1990) and our own results (Wickley-Olsen et al., 2007). Thus, one may neglect additional dispersion from deep zones in the wave tank. Our assumption is similar to that commonly adopted in mixing in reactor studies, where the dispersion near the blade of the impeller (the impeller zone) is considered the major (even the sole) source of oil dispersion (Tsouris and Tavlarides, 1994; Baldyga and Podgorska, 1998).

As the oil moves at sea or in a wave tank near the water surface, it gets subjected to various mixing intensities for different durations. Thus, dispersion has to account not only for the intensity of mixing but also to the duration at which the oil was subjected to such a mixing. Thus, it is conceivable that a moderate mixing energy for a long duration would engender the same (or even more) dispersion as a high mixing energy for short duration. This is a problem not encountered in reactor studies where the large-scale hydraulics is assumed at steady-state. Therefore, for one to quantify the dispersion, one needs to account for the residence time of the oil plume in various zones of the tank (near the free surface), the mixing energy at those zones, and a model for the evolution of the droplet size distribution with time.

The layout of this paper is as follows: First we explain how we used velocity measurements along with simulations using the Computational Fluid Dynamics (CFD) program FLUENT (www.fluent.com) to estimate both the transport properties of the plume and the mixing energy at various locations near the water-air interface. The mixing energy is quantified by the dissipation rate of kinetic energy per unit water mass, which was estimated following the approach of Wickley-Olsen et al. (2007) for a smaller tank with different wave conditions. For more discussion on , the reader is urged to consult the works of (Kaku et al., 2002; Kaku et al., 2006a; Kaku et al., 2006b). Second we present a model for the dispersion rate of oil droplets. The model is a state of the science from a theoretical point of view, because it is based on the multifractal representation of turbulent velocity fluctuations, which is the most rigorous approach. Multifractals is a new mathematics introduced in the mid-eighties (Frisch and Parisi, 1985) specifically to model and turbulent velocity. The model poses some challenges from a practical point of view, and these are elucidated in the manuscript.
TRANSPORT OF OIL IN THE TANK

We used the model FLUENT to simulate the superposition and breaking of waves. The model is computationally demanding; for the simulation of a 20 seconds of waves accurately, one needs a grid containing 800,000 nodes. The simulation time was around a week on 16 processors running in parallel. The model provides the net water velocity and the energy dissipation rate throughout the tank for 20 s, which could be used directly to evaluate the breakup of droplets. Figures 1 and 2 report results immediately prior to the breaker and 0.5 s later. The value of the dissipation rate of kinetic energy per unit water mass, ε, ranged from 0.1 to 0.0001 watt/kg near the surface. Observations of the oil slick placed in the breaking zone revealed that the oil moves downstream at the approximate velocity of 0.030 m/s. We assumed this to the velocity of the centroid of the oil plume, and we used FLUENT results to obtain the values of ε that the centroid is subjected to as it travels downstream horizontally in the tank (we neglected downward motion). The results are reported in Figure 3, where one notes that ε decreases by two orders of magnitude within 2 seconds (approximately 2 waves periods of the short waves). A model to predict dispersion based on each value of ε is presented next.

OIL DISPERSION MODEL

The model that we are proposing for droplet formation (i.e., dispersion) does not account for coalescence of droplets. This is not a problem when dealing with dispersion of oil at sea or in large tanks (the added oil was 300 ml in a 27 m³ of water). In such situations, there is very little interaction (and coalescence) between droplets. Much of the model theory was developed by Baldyga and Podgorska (1998). Our contribution in this part is to better explain the evasive multifractal approach based on our application of multifractal for analyzing geophysical data (Boufadel et al., 2000; Tennekoon et al., 2003) and to adapt their approach to droplet dispersion due to waves. In the process, we also highlight some inconsistencies in Baldyga and Podgorska (1998) that greatly hindered us early on.

The evolution of the number of droplets is governed by:

\[ \frac{\partial n(\delta,t)}{\partial t} = -D(\delta,t) + B(\delta,t) \]  

where \( n(\delta,t) \) is the number density of (spherical) droplet of diameter \( \delta \) at time \( t \) in the control volume of interest; \( D(\delta,t) \) and \( B(\delta,t) \) represent the death rate and birth rate of the number concentration of droplets of size \( \delta \), respectively. The death rate is commonly represented as proportional to the number concentration:

\[ D(\delta,t) = g(\delta)n(\delta,t) \]  

where \( g(\delta) \) is the breakup frequency of drops of diameter \( \delta \) (discussed below).

If one considers that birth is only due to breakup of droplets of larger size (i.e., no coalescence), then one may write:

\[ B(\delta,t) = \int_{\delta'}^{\infty} \beta(\delta',\delta)m(\delta')D(\delta',t)d\delta' \]  

Where \( D(\delta',t) \) represents the death rate of the number concentration of drops of diameter \( \delta' > \delta \); \( m(\delta') \) is the number of droplets formed from the breakup of a drop of volume \( \delta' \); and \( \beta(\delta,\delta') \) is the probability density of forming drops of diameter \( \delta' \) from drops of diameter \( \delta \). Equation 3 can be read as \( B(\delta,t) \) is the sum of the outcome of breaking of all droplets of diameters \( \delta' \) larger than \( \delta \).

The upper limit of infinity should imply the largest size diameter in the system. Considering that there is no coalescence, the largest diameter would be encountered at the initial time (i.e., prior to mixing).

Following Baldyga and Podgorska (1998), we adopt for \( \beta(\delta,\delta') \) the U-shaped probability density function of Tsouris and Tavlarides (1994). It is given as follows:

\[ \beta(\delta,\delta') = \frac{\epsilon_{\text{min}} + (\epsilon_{\text{max}} - \epsilon)}{\sum_{i>1} \epsilon_{\text{min}} + (\epsilon_{\text{max}} - \epsilon)} \]  

where \( \beta(\delta,\delta') \) is the probability density to produce droplets of diameter \( \delta = \delta + \Delta \delta \) from breakup of a droplets of diameter \( \delta' = \delta + \Delta \delta \). \( \Delta \delta \) and "e" represents the formation energy of a droplet. Recalling that the droplets are treated as spherical:

\[ \epsilon_{\text{min}} = \pi(\delta')^2 \]  

\[ \epsilon_{\text{max}} = \pi(\delta^2 - \delta')^2 \]  

where \( \sigma \) is the surface tension between oil and water, assumed constant for all droplets. Note that the value of the surface tension does not affect the value of \( \beta(\delta,\delta') \). However, its presence in Eqs. 4 and 5 is convenient from a physical point of view. An illustration of the shape \( \beta(\delta,\delta') \) is given in Figure 4. This probability density function is appropriate, because more energy is required to form two equal-sized drops than to form drops of different sizes. Hence, the probability of equal-sized drops is minimal when approaching half the size of the largest drop. In Figure 1, the minimum value is not at half the maximum size (i.e., not 10 micron) because the lowest diameter is not zero.

In the multifractal framework, the characteristic velocity of an eddy of size \( \delta \) is:

\[ u(\delta,\alpha) = \left[ \langle \epsilon \delta \rangle \right]^{\frac{1}{\alpha-1}} \]  

Where \( L \) is the largest scale of the system; \( \langle \epsilon \rangle \) is the average kinetic energy dissipation rate per unit mass, and \( \alpha \) is a positive parameter, whose value determines the value of the velocity at scale \( \delta \). The values of \( \alpha \) range from a minimum, \( \alpha_{\text{min}} \), to a maximum value of approximately 1.7. The minimum value was estimated by She and Leveque (1994) to be 0.33, though it was estimated by Meneveau and Sreenivasan (1987) to be \( \alpha_{\text{min}} = 0.12 \), a more common value, and is thus adopted herein. Note that a decrease in \( \alpha \) below 1.0 corresponds to an increase in the velocity, because \( \gamma^2 \) is less than 1.0. This means that the maximum velocity in the system corresponds to \( \alpha_{\text{min}} \). In the traditional framework, \( \alpha = 1.0 \), and all eddies of a given size have the same velocity. The frequency (inverse of turnover time) of eddies of diameter \( \delta \) is given by:

\[ g(\delta,\alpha) = \frac{u(\delta,\alpha)}{\delta} \]

The probability density function for eddies of size \( \delta \) is given by (Baldyga and Podgorska, 1998):

\[ P(\delta,\alpha) = C_\alpha \left[ \frac{\delta}{L} \right]^{\alpha} \left[ \frac{\delta}{L} \right]^{-\gamma^{2}(\alpha)} \]  

Where \( C_\alpha \) is a constant. The quantity \( f(\alpha) \) is known as the “multifractal spectrum” (it has nothing to do with the Fourier spectrum), and is commonly estimated based on turbulent velocity data. An empirical expression for \( f(\alpha) \) was given by Baldyga and Podgorska (1998):
Podgorska (1998) based on the data provided by Meneveau and Sreenivasan (1987):

\[ f(\alpha) = a + b \alpha + c \alpha^2 + d \alpha^3 + e \alpha^4 + f \alpha^5 + g \alpha^6 + h \alpha^7 + i \alpha^8 \]  

(9)

Where \( a = -3.510, b = 18.721, c = -55.918, d = 120.900, e = -162.540, f = 131.510, g = -62.572, h = 16.100, \) and \( i = -1.7264. \)

Summing up the collision frequency from all eddies of size \( \delta, \) one obtains (Baldyga and Podgorska, 1998):

\[ g(\delta) = \int_{-\infty}^{\infty} g(\delta, \alpha) P(\delta, \alpha) d\alpha \]  

(10)

The upper limit, \( \delta_{\text{L}} \), results from the fact that eddies of scale \( \delta \) who have small turbulence velocity (i.e., large \( \alpha \)) do not contribute to the breakup of droplets. The evaluation of \( \delta_{\text{L}} \) is provided later in the manuscript.

In reactors’ studies, where an impeller is stirring the water, there are terms introduced to account for the inhomogeneity of mixing between the high intensity zone near to the blade and the relatively low intensity zone in the bulk of the reactor. Such terms are not directly applicable for mixing at sea, and we thus lump them along with the constant \( C_0 \) above in a constant \( C_1. \) The breakup frequency becomes:

\[ g(\delta) = C_1 \left[ \ln \left( \frac{L}{\delta} \right) \right]^{0.8} \delta^{2 + \gamma} \int \frac{d\alpha}{\alpha} \]  

(11)

The multifractal representation appears through the terms \( \alpha \) and \( f(\alpha). \) The presence of \( \ln \) in the integral indicates that mixing is scale-dependent. Hence, conserving the average value of \( \varepsilon \) (i.e., \( \langle \varepsilon \rangle \)) is not sufficient, and one needs to correct by accounting for the scale.

The term \( \left[ \ln \left( \frac{L}{\delta} \right) \right]^{0.8} \) does not indicate strong scale-dependence, because the logarithm “compresses” all numbers to a narrow range (the square root play a similar, though weaker role).

For example, for \( \delta \) equal to 100 and 10,000, the term above takes the values 2.14 and 3.03, respectively.

**EVALUATION OF \( \alpha_x \)**

The equilibrium of forces on a droplet states that the destructive forces are equal to the stabilizing forces:

\[ F_P = B + T \]  

(12)

Where \( F_P \) is the force due to the dynamic pressure (destructive); \( B \) is the resistant force due to the stress tensor in the droplet (due the viscosity within the droplet); and \( T \) is the resistant force due to surface tension between the droplet and the surrounding liquid. If one assumes that the stress in the elongation direction of the droplet is the dominant term, and if one reports the equilibrium per unit area of the droplet, then one obtains:

\[ p(\delta) = \mu_s \frac{\partial \delta}{\partial x} + C_s \frac{\sigma}{\delta} \]  

(13)

Where \( p(\delta) \) is the dynamic pressure on the droplet of diameter \( \delta, \mu_s \) is the dynamic viscosity of the dispersed phase (i.e., within the droplet), and \( T \) is the velocity along the major axis of the droplet, \( \mu_s \alpha \) is the surface tension between the dispersed phase and the continuous phase, and \( C_s \) is an empirical coefficient discussed later.

Assuming that the rate of elongation is constant, one obtains:

\[ p(\delta) = \mu_s \frac{1}{x} \frac{\delta}{\delta t} + C_s \frac{\sigma}{\delta} \]  

(14)

With \( x(t=0) = \delta. \) Integrating the equation and rearranging results in:

\[ \ln \left( \frac{\delta}{\delta_0} \right) = \frac{1}{\mu_s} \left[ p(\delta) - C_s \frac{\sigma}{\delta} \right] t \]  

(15)

where \( \left( \frac{\delta}{\delta_0} \right) \) is the value at breaking. Because \( p(\delta) \) is a dynamic pressure, it can be represented as the product of density and the square of the velocity of eddies at scale \( \delta. \) This gives:

\[ p(\delta) = C_P \rho u(\delta)^2 \]  

(16)

Where \( \rho \) is a dimensionless constant that varies between 0.5 and 0.7 according to Hinze (1959, p242). Baldyga and Bourne (1995) and Baldyga and Podgorska (1998) report a range from 0.7 to 2.0, which is more common. \( C_P \)

Using the expression of velocity from Eq. 6, the pressure is:

\[ p(\delta, \alpha) = C_P \rho \left[ (\varepsilon)^\frac{2}{3} \right] \left( \delta \right)^\frac{2}{3} \frac{\delta}{L} \]  

(17)

The drop will break when the elongation time “t” is equal to or larger than the Lagrangian time, \( T_L, \) over which the dynamic pressure is applied. The value of \( T_L \) could be approximated based on the Eulerian turnover time by:

\[ T_L = \beta \tau_c = \beta \frac{\delta}{u(\delta, \alpha)} \]  

(18)

The constant \( \beta \) is equal to 1/3 (Tennekes and Lumley, 1972, p278) and is usually less than 1.0 at high Reynolds number (Hinze, 1975, p424). Baldyga and Podgorska (1998) reported it erroneously equal to 3.0 on page 466 of their article.

In the framework of multifractals, one has the velocity from Eq. 6, which results in:

\[ T_L = \beta \tau_c = \beta \frac{\delta^{2/3} \langle \varepsilon \rangle^{1/3} \delta \left( \frac{L}{\delta} \right)^{1/3}}{u(\delta, \alpha)} \]  

(19)

By setting “t” equal to the maximum time of elongation of the droplet, \( T_L, \) and by using the expression for pressure (Eq. 17), one can compute the value of \( \alpha \) below which all droplets would break. That value labeled \( \alpha_x \) is given by:

\[ \alpha_x = 3 - 3 \ln \left( \frac{L}{\delta} \right) \left( \frac{2}{\beta \rho C_s^{5/3} \mu_s} \right)^{1/3} \left( \frac{\beta C_s^{5/3} \nu_s}{\rho \langle \varepsilon \rangle^{13/3} L^{11/3} \delta} \right)^{1/3} \]  

(20)

Where: \( \left[ \frac{x}{\delta} \right] \) is the elongation of the droplet immediately prior to breaking. A parameter of great significance emerges:

\[ C_s = (C_0/C_P) 0.6 \]  

(21)

With \( C_s = 0.725 \) based on the theory of Hinze (1955, p295). Baldyga and Podgorska (1998) report \( C_s = 0.23, \) which appears to be an error. Based on an average value of 1.4, one obtains \( C_0/C_P = 0.82. \) Also:

\[ \beta \tau_c = \frac{\ln(x/\delta)}{\beta C_s^{5/3} C_P} = \frac{\ln(x/\delta)}{\beta C_s^{5/3} C_P} \]  

(22)

It is worth noting that some of the constants used herein were developed to provide an order of magnitude information about the physics. For example, the value of \( \beta \) is not necessarily equal to 1/3, and it could be for example 0.15 or 0.6. Thus, it is important
to estimate these values from experiments. In addition, a weakness of the above model is that values of $\alpha$ greater than $\alpha_c$ do not contribute at all to breakup, which is not physical. For example if $\alpha_c$ gave a value of $u(\alpha, \alpha_c)$ of 0.40 m/s that induces breaking, the model predicts that a velocity value of 0.39 m/s which results from a slightly larger value of $\alpha$ does not contribute to the breakup of a droplet. This is too restrictive a cutoff considering the uncertainty in the constants' values. The exponentially decaying breakup frequency of Tsouris and Tavlarides (1994) is advantageous from that point of view, and we will be explored it in future works.

A FORTRAN code was written to solve Equation 1. It is based on forward Euler in time. Integration was done using the trapezoid method. The values of parameters used for the simulation are:

$\mu=0.01 \text{ kg/(m.s)}, \sigma=0.07 \text{ N/m}, C_v=0.725, C_p=2.0, \left[\alpha\right]=2.0, L=1.0$

$m$ representing the half length of wave. Figure 5 presents droplet size results for selected sizes (for brevity). The figure clearly shows the sudden change in the number concentration as the energy dissipation rate (Figure 3) is changed.

**CONCLUSIONS**

This paper presented a holistic approach for estimating the dispersion of oil at sea and/or in wave tanks. Our approach required that we developed a droplet kinetics model that is capable of accounting for the variation of the energy dissipation rate with time (due to the fact that waves are transient). The model accounts for the effect of scale because it relies on the multifractal representation of turbulence. We illustrated our approach using wave tank data of velocity and energy dissipation rate.

**FIGURE 1:** VELOCITY VECTORS AND CONTOURS OF TURBULENT ENERGY DISSIPATION RATE PRE-BREAKER (T=0).

**FIGURE 2:** VELOCITY VECTORS AND CONTOURS OF TURBULENT ENERGY DISSIPATION RATE AT TIME = 0.5 SEC.

**FIGURE 3:** VALUES OF THE ENERGY DISSIPATION RATE THAT THE CENTROID OF THE OIL PLUME is subjected to as it travels downstream in the tank. The breaker occurred around $t=3$ s (zero second in Figures 1 and 2).

**FIGURE 4:** THE PROBABILITY DENSITY FUNCTION $\beta(\delta, \delta')$ OF BREAKAGE OF A DROP OF DIAMETER 20 MICRON INTO SMALLER DROPLETS (DIAMETERS SHOWN). NOTICE THE U-SHAPE.

**FIGURE 5:** VARIATION WITH TIME OF THE NUMBER OF SELECT OIL DROPLETS. THE SYSTEM HAD INITIALLY 1000 OIL DROPLET OF DIAMETER 500 MICRONS. NOTE THE SUDDEN CHANGE IN THE NUMBER CONCENTRATION AS THE ENERGY DISSIPATION RATE CHANGES (FIGURE 3). THE NUMBER CONCENTRATION SEEMS TO BE INVERSELY PROPORTIONAL TO THE DROPLET SIZE.
REFERENCES


