

EPSRC Centre for Doctoral Training in Industrially Focused Mathematical Modelling

Modelling the Breakup of Droplets in a Turbulent Jet

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Figure 1 – **The Deepwater Horizon oil spill in 2010 released 800 million litres of oil and formed an oil slick which covered an area of up to 175,000** km² **.**

Figure 2 – **Turbulent oil jet in a deep-sea oil spill.**

1 Introduction

Background information

Deep-sea oil spills can pose a significant threat to the environment (see Figure [1\)](#page-2-4). Therefore, it is important to understand what happens in an oil spill and how best to clean them up.

In a deep-sea oil spill, a pipe transporting oil ruptures hundreds of metres below the sea surface and a highly turbulent oil jet is released into the sea (see Figure [2\)](#page-2-5). The jet's turbulent mixing breaks the oil up into smaller droplets, which are then eaten by microbes. It is highly desirable to produce small oil droplets (with a diameter less than 50- 70 microns). These small droplets provide a greater surface area for microbial degradation and rise less rapidly so they lead to a thinner oil slick forming. To facilitate the breakup of oil drops, chemicals called dispersants are injected into the jet to reduce the oil-water surface tension. Injecting dispersants directly into the rising jet (rather than the more traditional approach of spraying them at the sea surface) makes use of the jet's highly turbulent motion to break up droplets more effectively.

Our aim is to understand the breakup of droplets in a turbulent jet. Once this is understood, we investigate the effect of adding of surfactants. The two main questions of interest are how much surfactant should be added and where.

Approach

Our modelling framework is illustrated in Figure [3.](#page-2-6) We initially consider what happens when no dispersant is added. We examine models for the large-scale turbulent jet and the small-scale droplet breakup. These are combined to produce drop size distributions at different locations in the jet. We then explore droplet-dispersant interactions and their effect on the drop size distribution.

Figure 3 – **Modelling framework.**

Drops are broken up because of the vigorous mixing in the turbulent jet. The energy dissipation is a measure of the intensity of the turbulent mixing and so, is often used as a measure of the energy controlling droplet breakup.

2 Turbulent Jets

We first examine a turbulent oil jet. There are a number of simplifying assumptions made:

- We consider a momentum driven jet and neglect buoyancy. This is a good assumption for approximately the first 50 nozzle diameters from the release point of the oil spill.
- We consider a turbulent water jet with a low oil fraction.

The evolution of the jet, namely its velocity and energy dissipation, are modelled. The energy dissipation is an important element in our models. It dictates the turbulent energy of the eddies in the jet which deform and break up the droplets. Therefore, it is a measure of the energy controlling drop breakup.

CFD

We perform CFD (computational fluid dynamics) numerical simulations of the turbulent jet. They capture the entirety of the jet's motion and provide detailed insights into its behaviour. We see in Figure [4\(](#page-3-2)a) that the jet's velocity decreases with height and width. The arrows in Figure [4\(](#page-3-2)a) show water being entrained into the jet, diluting the oil. The energy dissipation in Figure [4\(](#page-3-2)b) very rapidly decreases away from the source. However, these are complicated simulations. Computations take up to 30 minutes and simulations must be recomputed for different nozzle diameters, flow rates, oil properties etc.

Figure 4 – **Motion and energy in jet from CFD. (a) Velocity magnitude with direction shown by arrows. (b) Energy dissipation, with a log scale.**

Self-similar models

How can we simplify and unify these turbulent jet models? We use the fact that the fully developed flow of a jet has self similar or scale-invariant behaviour. This means that if we rescale properties of the flow, for example its velocity, the variation of velocity with rescaled width will look the same at different heights. A similarity solution refers to the rescaled solution which is the same for all heights.

Figure 5 – **Similarity solutions. At different height, we plot the rescaled velocity and energy dissipation from the CFD results. These are shown in blue. Because of self-similarity, these rescaled quantities lie on the same line at different heights. This line is approximated in red.**

We plot the similarity solution for the velocity and turbulent energy dissipation in the fully developed jet flow in Figures [5\(](#page-3-3)a) and [5\(](#page-3-3)b) respectively. For instance in Figure [5\(](#page-3-3)a) we take the jet's vertical velocity from CFD simulations at different fixed heights and rescale. The rescaled velocity versus rescaled width lie on the same line. This line can be very simply calculated using self similar models and accurately describes the full CFD results.

A turbulent jet's vertical velocity decreases like 1/z with height z. The energy dissipation decreases more rapidly, like $1/z⁴$.

Droplet breakup is a function of:

- Drop size.
- Energy dissipation.
- Surface tension.

Total oil fraction decreases like $1/z$ with height z due to dilution with water.

Drops break up and drop size decreases with increasing height and width in the jet.

A self-similar approach give a universal description of the macroscopic jet properties, which is independent of particular values of the nozzle diameter, flow rate etc. For example, the self-similar model shows that the jet's vertical velocity decreases like $1/z$ with height z, and the energy dissipation decreases more rapidly, like $1/z⁴$. These models, however, cannot fully canture the region at the hase of the jet however, cannot fully capture the region at the base of the jet.

We use the self-similar jet models in two-dimensions and also average them across jet width to obtain simpler one-dimensional models which only vary along the jet's height.

3 Droplet breakup

We now turn our attention from the macroscopic scale to the microscopic droplet scale. We assume the breakup rate of a droplet depends on (i) its size, (ii) the energy dissipation in the surrounding turbulent flow, and (iii) the oil-water surface tension. The energy of the jet's turbulent flow causes the drops to deform and break up whilst surface stresses make droplet breakup more difficult. We use scaling laws to determine an appropriate form for the breakup rate. This must satisfy the following physical laws:

- The rate of droplet breakup increases with increased energy dissipation and decreased surface tension.
- Resistive surface stresses make it difficult for smaller droplets to break up. Surface tension forces increase with decreased drop size.
- Some small droplets cannot break up. The energy dissipation required to break up these droplets is not sufficient to overcome the resistive surface stresses.

4 Combining jet and drop models

We combine our large-scale jet and small-scale droplet models to examine the drop size distribution at different locations in the jet. We make the simplifying assumption that the coupling of macroscopic and microscopic scales is one way. Whilst the droplets move with the jet flow and break up due to the energy in the jet, we assume the motion and breakup of droplets has a negligible influence on the macroscopic flow.

Total oil fraction

We begin by modelling the total volume fraction of oil in the jet. We find that it is proportional to the jet's vertical velocity so the oil is advected and diffused in the same way as the jet flow. This was illustrated in Figure [5\(](#page-3-3)a). We can see that as we move away from the source, the oil is diluted by water and its volume fraction decreases significantly.

Full numerical solutions of drop size distribution

Full numerical simulations are used to examine how the size of the oil droplets varies with height and width in the jet. Figure [6\(](#page-5-3)a) shows the variation of drop size distribution with height, at a fixed width in the jet. We see that the droplets break up and decrease in size with increasing height. At lower heights, the distribution is bimodal; this means that there is one peak corresponding to the smaller droplets produced by breakup and another peak corresponding to the largest drops which still remain. With increasing height, we observe that the mode drop size increases. This phenomenon may seem counter-intuitive. It arises because, higher up in the jet, only larger drops can break up. With increasing height the energy in the jet decreases, and it is not sufficient to overcome the large surface stresses of smaller drops. (Lower down the jet, these smaller droplets would have been able to break up.) Therefore the size of drops which break up increases and they produce large drops upon breakup. Similar behaviour is seen in the evolution of the drop size distribution with increasing width (see Figure [6\(](#page-5-3)b)).

At large heights, the energy dissipation is too low for droplet breakup to occur and the drop size distribution stops evolving; it reaches a fully developed state. After this point, the drop size distribution does not vary with either height or width. This fully-developed distribution is very important for oil production companies. We can investigate how it varies with different parameters and for different surfactant applications to gain useful insights.

Figure 6 – **The volume fraction of oil drops of different sizes versus drop diameter, . We have divided by the total oil to eliminate the effect of dilution. Drop size distribution (a) for varying heights at fixed** $r = 0.1$; (b) for varying widths at fixed $z = 10$;

Simplified width-averaged models

To simplify the problem, we can average our two-dimensional models over the width of the jet to produce simpler models which only vary along the jet's height. Our widthaveraged models agree fairly well with the two-dimensional models discussed in the previous section. In particular, the fully developed distribution agrees relatively well with results from the full two-dimensional models. However, we cannot, capture the variation of droplet size distribution with jet width.

Analytical results

We predominantly use numerical simulations to determine the drop size distributions. However, under certain assumptions, it is possible to also find analytical solutions, which enable us to write down the exact form of the drop size distribution. These arise due to the self-similarity of the turbulent jet. Under certain conditions, they provide accurate solutions for the full two-dimensional problem with very little computational effort.

5 Effect of dispersant

We now consider the effect of adding dispersants to the system. Currently, other models do not exist for the evolution of drop size distribution with varying surface tension.

The active ingredient in dispersants are chemicals called surfactants. When they are added to the system, they exist as either single monomers (illustrated in the second panel in Figure [7\)](#page-5-4) or aggreggates of these monomers, called micelles (illustrated in the first panel in Figure [7\)](#page-5-4). The micelles can disassociate into monomers and the monomers can aggregate into micelles. Only free monomers can adsorb or stick onto the surface of an oil droplet (see the third panel in Figure [7\)](#page-5-4). These adsorbed monomers can also disassociate from the droplet surface into the bulk, becoming free monomers. By adsorbing onto the surface of droplets, the surfactant monomers reduce the oil-water surface tension.

Figure 7 – **Schematic of interactions between surfactant micelles and monomers (grey), and oil drops (orange).**

By reducing the surface tension, the surfactant promotes droplet breakup and the drop size distribution shifts towards smaller droplets. In turn, since smaller droplets are produced, the droplet surface area increases. There is more droplet surface that the surfactant must be spread over and, as a result, the effect of surfactant eventually wanes. We model these droplet-surfactant interactions and combine them with our width-averaged jet models. We observe, in Figure [8\(](#page-6-2)a), the shift towards smaller drop sizes with the addition of

When dispersants are added, surfactant monomers stick to oil droplets, reducing the oil-water surface tension. This makes it easier for them to break up.

 10 1 8 0.8 $d^2\phi/\Phi$ 6 $6.0.6$ 4 0.4 \circ $\begin{matrix} 0 \\ 10 \end{matrix}$ 0.2 10^{-3} 10^{-2} 10^{-1} 10^{0} 0 5 10 15 20

surfactant. This is caused by the decrease in surface tension seen in Figure [8\(](#page-6-2)b). At later heights, surface tension increases mainly due to dilution of the surfactant with water.

(a) Drop size distribution

Figure 8 – **(a) Drop size distribution without dispersant (blue) and with dispersant (red), and (b) the evolution of surface tension with jet height due to the addition of dispersant.**

(b) Surface tension

Comparisons to experiments

Figure 9 – **Comparisons to experiments by SINTEF with different dispersant to oil ratios (DOR).**

We fit our jet-drop-surfactant model to small-scale experiments by SINTEF [\[1\]](#page-8-1). There are three fitting parameters. One refers to the rate of droplet breakup. Another measures the strength of resistive surface stresses compared to the energy dissipation which causes droplets breakup. The third relates to the rate at which the surfactant sticks or adsorbs onto the drops. The model is fitted to two experiments, one without dispersant and the other with dispersant to oil ratio 1:50. As seen in Figure [9,](#page-6-3) the fitted cases and cases with other dispersant concentrations agree well with the model.

How much surfactant should be injected?

Now that we have constructed accurate models of drop-surfactant interactions in a turbulent jet, we seek to answer two key questions of interest to BP: how much surfactant should be added and where? We find that increasing the surfactant concentration, C_0 , allows greater droplet breakup. However, increasing the surfactant monomer However, increasing the surfactant monomer concentration beyond a certain concentration (beyond around $C_0 = 1$) has diminishing returns. This can be seen in Figure [10\(](#page-7-2)b), where the fraction of small droplets produced starts to stagnate at larger dispersant concentrations.

The reason for this phenomenon is that, beyond surfactant concentrations of around $C_0 = 1$, the additional surfactant aggregates with itself, forming micelles. Higher up the jet, these disassociate into monomers which can adsorb onto the droplet surface and reduce the surface tension. However, by this height, the energy dissipation is much smaller

The droplet-surfactant dynamics occurs over three distinct regions, seen in Figure [8\(](#page-6-2)b). At small heights, surface tension rapidly decreases. It then stays roughly constant at its minimum value. Higher up the jet the surface tension increases due to dilution.

and the surface tension is increasing. As a result, the opportunity for significant droplet breakup has been missed. This can be seen in Figure [10\(](#page-7-2)a), comparing the cases with C_0 = 0.75 and C_0 = 1.5. For $z < 5$, where the energy controlling droplet breakup is large, the surface tension is the same for $C_0 = 1.5$ and $C_0 = 0.75$. Only at later heights, for $z > 10$ is the surface tension considerably smaller for $C_0 = 1.5$, but here the energy available for droplet breakup is small so it does not lead to a great deal of additional droplet breakup.

Figure 10 – **Effect of adding different concentrations of surfactant.**

Where should the surfactant be injected?

We now investigate the effect of injecting surfactant at different heights in the jet. We find that it is best to inject the dispersant as close to the jet source as possible. This is because the evolution of surface tension is essentially independent of the height at which the dispersant is injected, as seen in Figure [11\(](#page-7-3)a). Additionally, the energy controlling droplet breakup decreases rapidly with height. At low heights the fraction of small drops produced decreases relatively slowly with height, as seen in Figure [11\(](#page-7-3)b). However, beyond a small height in the jet, droplet breakup efficiency decreases exponentially with height. Eventually, injecting the dispersant high up the jet has little advantage over injecting no dispersant at all. In this example it takes around 13 jet diameters.

Figure 11 – **Effect of injecting dispersant at different heights in the jet.**

6 Discussion, conclusions and recommendations

We have modelled a turbulent jet of oil escaping into water, along with the consequent break-up of the oil into droplets, assisted by the injection of dispersant. Our models produce drop size distributions at different locations in the jet, which agree well with small-scale experiments.

We find that increasing the concentration of dispersant we add increases the efficiency of droplet breakup and allows more small droplets to be produced. However, there are diminishing returns after a certain amount, namely after the critical micelle concentration.

We also find that it is best to inject the dispersant as low down the jet as possible. Beyond a short height above the release point, the fraction of small droplets produced decreases exponentially with height. This suggests that it may be more important to focus on injecting the dispersant low down the jet than adding vast amounts of dispersant. Our model can be used to discuss and investigate different oil spill situations and how best to apply dispersant in these cases.

The model could be extended to provide more accurate predictions in a wider range of circumstances. A number of modelling assumptions have been used to make progress. The effect of gas has not been included. Furthermore, the oil is assumed to not be very viscous. These assumptions could be relaxed in further work. In addition, only relatively small-scale lab-based experiments were used to develop the model. Results from any future subsea incidents or larger scale experiments could be incorporated to improve accuracy.

7 Potential impact

The application of sub-sea dispersant is a key spill response tool for the oil and gas industry. Dispersant is usually applied at a fixed dispersant to oil ratio. There is no known technique for optimising dispersant dose when applied subsea, to conserve dispersant stocks. There are also no models which predict the variation in the efficiency of the dispersant when it is injected at different heights. Understanding the effect of different dispersant application methods is important not only in guiding oil spill responders but also in obtaining regulatory approval to use the dispersant.

Dan Touzel, Environmental Specialist at BP said: "*The Droplet Breakup in a Turbulent Jet, PhD undertaken by Rachel Philip as part of BP's Modelling the use of Dispersants on Oil Spills project under Oxford's Industrially FocusedMathematicalModelling (Centre for Doctoral Training) delivered a model which successfully resolved the complex physical processes of a subsea oil plume, including the effect of dispersant injection. The use of simple reduced models and demonstration of their potential for assessing key parameters was considered a key success. This outcome generated the opportunity for development of an operational tool that could be used by oil spill responders and crisis management professionals to assess and optimise subsea dispersant injection. Such a tool would be widely applicable to industry oil spill planning and response. The PhD is considered to have realised the potential, and provided a proof of concept, for development of a Sub Sea Injection Dispersant tool.*"

References

[1] P. J. Brandvik, Ø. Johansen, U. Farooq, G. Angell, and F. Leirvik. *Sub-Surface Oil Releases - Experimental Study of Droplet Distributions and Different Dispersant Injection Techniques - Version 2. A Scaled Experimental Approach Using the SINTEF Tower Basin.* SINTEF report no: A26122. Trondheim Norway, 2014.