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Comparison of Mathematical Models for the Diffusivity of Crude Oil in Water: Implications for Oil Spills and Global Warming

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Abstract - Understanding the influence of temperature on the diffusion coefficient of crude oil in water is crucial for assessing environmental impact of oil spills, particularly under conditions of climate change. Oil spills can have catastrophic consequences on ecosystems, harming or killing fish, dolphins, whales and other marine animals, as well as damaging delicate habitats such as coral reefs and mangroves. This study compares the predictions of an empirical model with those of the fundamental Stokes-Einstein equation for the temperature dependence of crude oil diffusion. The diffusion coefficient was calculated using both an empirical model and the Stokes-Einstein model for temperatures ranging from 1°C to 100°C using both models. Results indicate that the Stokes-Einstein equation predicts higher diffusivity at lower temperatures, whereas the empirical model predicts significantly greater diffusivity at higher temperatures. At elevated temperatures, the empirical model estimates diffusion rates nearly twice as high as those predicted by the Stokes-Einstein model. These results are critical for predicting the rapidity of spread of oil spills with global warming. Specifically, during non-steady state diffusion, the time required for oil to travel a specific distance is inversely related to the diffusion coefficient. This means that as temperature increases and diffusivity rises, oil spreads more rapidly and in turn reduces the time to contaminate swaths of ocean, a problem worsened by warming ocean temperatures. Given the limitations of current models and the fact that the empirical model was developed using distilled water, future research will require more experimental data at higher temperatures under conditions that mimic actual seawater. This can enable the development of more accurate diffusion models and improve predictive tools for managing the impact of oil spills.

Keywords**:** Climate Change, Diffusivity, Global Warming, Oil Spills, Stokes-Einstein Model

1. Introduction

Understanding the influence of temperature on the diffusion coefficient of crude oil in water is critical for predicting the environmental impact of oil spills, particularly in the context of rising global temperatures due to climate change. The Deepwater Horizon spill, for example, resulted in the deaths of 4,900–7,600 large juvenile and adult sea turtles and caused a 50% decline in some marine mammal populations due to oil exposure and habitat destruction in the proximity [1]. Further, long-term environmental monitoring revealed that over 770 square miles of the Gulf seafloor remain contaminated with oil residues, which have a detrimental impact on deep sea ecosystems and decrease biodiversity [2].

Diffusion is the movement of particles in a fluid due to random motion. The diffusion coefficient, also known as the diffusivity, is a parameter that quantifies the rate at which a substance spreads or moves from an area of higher concentration to an area of lower concentration within another medium. In the context of oil spills, the diffusion coefficient describes how quickly crude oil molecules disperse within water. A higher diffusion coefficient indicates faster spreading, while a lower value suggests slower dispersion. This property can be modeled as the partial differential equation

$$\frac{\delta C(x,t)}{\delta t} = D\frac{\delta^2 C(x,t)}{\delta x^2}$$

where C represents concentration, t represents time, and x represents the location where diffusion is occurring with respect to the starting point. Assuming that diffusion occurs in the downward direction toward a boundary at x=L, the boundary conditions for this differential equation are

$$C = 0 \text{ at } x = 0$$
$$\frac{\delta C}{\delta t} = 0 \text{ at } x = L.$$

The solution to this partial differential equation is

$$C = C_0\left(1 - \frac{4}{\pi} sin\left(\frac{\pi x}{2L}\right) \cdot e^{-\left(\frac{\pi}{2L}\right)^2 Dt}\right)$$

for large values of t. Using this model, Hamam [3] estimated the diffusion coefficient D of crude oil in distilled water, by measuring the concentration C versus time t at three different temperatures: 25°C, 35°C, and 45°C. Hamam found that the diffusion coefficient D varied with temperature T (measured in °C) to the 1.53 power

$$D = 4.13 \cdot 10^{-3}\ T^{1.53}\ \frac{cm^2}{hr}.$$

This finding differs from the predictions of the Stokes-Einstein equation, which is based on fundamental principles and states that

$$D = \frac{k_b T}{6\pi\mu R_0}$$

where k_b is the Boltzmann constant, T is absolute temperature (measured in °K), μ is viscosity of the solvent in which particles are diffusing, and R_o is the solute radius of the diffusing particles. It follows from the Stokes-Einstein equation that the diffusion coefficient will vary with temperature according to

$$\frac{D_{T_1}}{D_{T_2}} = \frac{T_1}{T_2} \cdot \frac{\mu_{T_2}}{\mu_{T_1}}$$

where T_1 is the initial temperature and T_2 is the final temperature. This equation is typically used to model the dependence of diffusion coefficient on temperature and assumes that the diffusion coefficient is linearly related to absolute temperature and inversely related to viscosity. The objective of this research is to compare the predictions of the empirical Hamam model to those of the fundamental Stokes-Einstein model for the temperature dependence of the diffusion coefficient of crude oil in water.

2. Methods

The predicted diffusion coefficient D for crude oil in seawater was calculated to three significant figures for temperatures ranging from 1°C to 100°C (274°K to 373°K) using the Hamam model and the Stokes-Einstein equation. For the Stokes-Einstein model, the viscosity of water at temperatures ranging from 1°C to 100°C was obtained from the International Association for the Properties of Water and Steam [4]. For both models, the diffusivity D of crude oil in water at 25°C (298°K) was assumed to be 0.604 cm²/hr, as measured experimentally by Hamam [3]. According to the IAPWS, the dynamic viscosity of water is 0.000891 Pa · s at 25°C.

For the Hamam Model, the diffusion coefficients at different temperatures were determined by the equation

$$D = 4.13 \cdot 10^{-3}\ T^{1.53}\ \frac{cm^2}{hr}.$$

The diffusion coefficients for the Stokes Einstein model were determined by the equation

$$D = 0.604 \cdot \frac{T}{298} \cdot \frac{8.91 \cdot 10^{-4}}{\mu_T},$$

which follows from the Stokes-Einstein equation.

3. Results

The Hamam empirical model and the Stokes-Einstein fundamental model predict distinct trends at low and high temperatures for the diffusivity of crude oil in water (Figure 1). It is evident that at lower temperatures (below 25°C), the Stokes-Einstein equation predicts a higher diffusion coefficient of crude oil in water compared to the Hamam model. In contrast, the Hamam model predicts a lower diffusion coefficient than does the Stokes-Einstein model at lower temperatures, but the Hamam model also predicts greater growth in the diffusion coefficient with increases in temperature than does the Stokes-Einstein model.

However, at higher temperatures (above 45°C), the Hamam model predicts a significantly larger diffusion coefficient than the Stokes-Einstein equation. For example, at 80°C, the Hamam model predicts a diffusivity of 3.370 cm²/hr, which is almost twice the Stokes-Einstein model prediction of 1.695 cm²/hr (Table 1). This discrepancy can be attributed to the nonlinear factors influencing diffusion at higher temperatures, which could be related to crude oil's chemical structure and interactions in water.

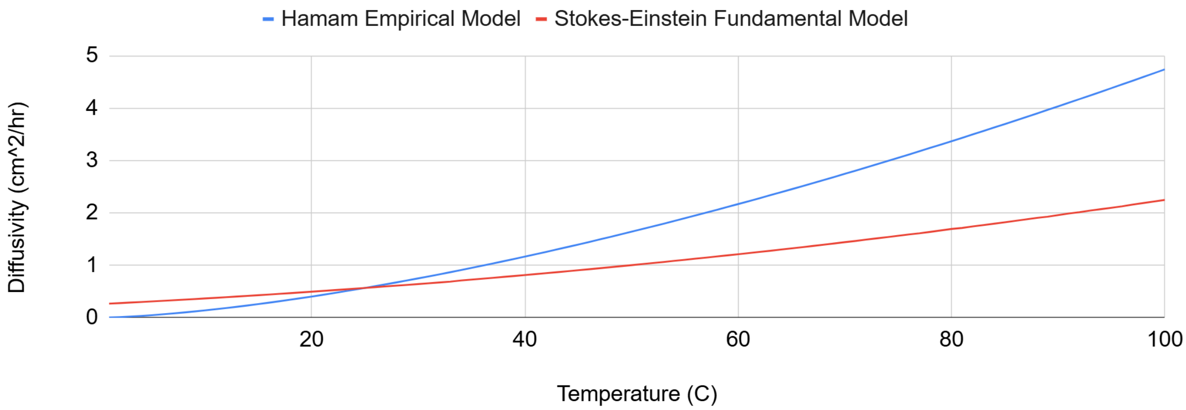

Fig. 1: Diffusivity versus temperature for crude oil in water according to two different models.

Table 1: Calculated diffusivity values for crude oil in water.

Temperature (°C)	Diffusivity from Hamam Model (cm^2/hr)	Diffusivity from Stokes-Einstein Model (cm^2/hr)
10	0.1399	0.3678
20	0.4041	0.4966
30	0.7515	0.6431
40	1.167	0.8149
50	1.642	1.004
60	2.17	1.212
70	2.748	1.443
80	3.37	1.695
90	4.036	1.959
100	4.742	2.248

4. Discussion

A limitation of this study is that Hamam's empirical model is based on diffusion measurements from distilled water and not seawater. Because seawater contains salts and organic matter (Table 2) that can alter viscosity and diffusion behavior [5,6], these results may be inconsistent with real-life oil spills. Additionally, Hamam's experimental data only covers the range from 25°C to 45°C while the Stokes-Einstein equation can extrapolate a broader temperature range, which means there may be a need for more extensive experimental data.

The time required for crude oil to travel a certain distance is inversely related to diffusivity. During non-steady state diffusion, the time t required for oil to spread over a distance d is estimated by the equation

$$t = \frac{d^2}{D}.$$

This means that a doubling of the diffusion coefficient will halve the time required for oil to spread over the same distance. As shown in Figure 1, the Hamam model predicts a significantly higher diffusivity at elevated temperatures, which means that oil spills in warmer conditions could spread much faster than estimated by the Stokes-Einstein equation. This has important implications for environmental response efforts, as faster spreading creates a shorter time frame to address spills before they invariably affect marine ecosystems.

Table 2: Comparison of thermophysical properties of water and seawater

Property	Pure Water	Seawater	Relevance to Diffusion
Density	Lower	Higher	Higher density can create resistance mixing
Dynamic Viscosity	Lower	Higher	Higher viscosity → lower diffusion coefficient (Stokes-Einstein equation)
Diffusion Coefficient	Higher	Lower	Diffusion is slower in seawater due to higher viscosity and ionic interactions
Specific Heat Capacity	Higher	Lower	Lower heat capacity → heats faster → acceleration of diffusion

5. Conclusion

Because oil spills disrupt ecosystems and regularly reach sediments [7], it is critical to understand the rapidity of spread of crude oil in water. This research evaluated the predictions of an empirical model and a fundamental Stokes-Einstein model for the diffusivity of crude oil in water, and found that the empirical predicts a significantly higher diffusivity at higher temperatures than does the fundamental model. These results are important since they show that a purely fundamental approach may underestimate the rate of spread of oil in water at higher temperatures. Specifically, at 80^oC, the diffusivity of crude oil as predicted by the Hamam model is almost twice as high as that predicted by the Stokes-Einstein model; this emphasizes the limitation of the theoretical approach. While the Stokes-Einstein model is based on fundamental principles, it may not fully capture the complexities of oil motion, especially in seawater. This difference could potentially be exacerbated by the lack of experimental data, including that of the Hamam model, that accounts for the salinity of seawater and its effect on diffusivity. Overall, these combined findings demonstrate that further experimentation will be necessary to refine predictions and ensure oil spill mitigation efforts are effective enough to address the problem. It is essential to be prepared for a worst-case scenario that accounts for discrepancies with fundamental physics, particularly in the context of climate change.

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