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Adjusting the Quantity of Surfactants in Decontamination Solutions

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***Abstract*— A comparative analysis of non-ionic, anionic, and cationic surfactants was conducted to evaluate their potential use in the decontamination of radioactive contamination. The study produced both graphical and analytical representations of the relationship between surfactant concentration and surface tension. These findings enable precise control over the selection and concentration of surfactants in decontamination solutions, optimizing their effectiveness for specific application.**

***Keywords*— CBRN decontamination, surface tension, surfactant, effectiveness, Wolfram Mathematica, radioactive contamination.**

I. Introduction

The limited capabilities for providing adequate and timely protection to the population and infrastructure necessitate improving the effectiveness of mitigating the consequences of chemical, radiological, and biological events. [1]-[10] The relevance of this report arises from the increased requirements for the characteristics of solutions used in specialized decontamination processes, emphasizing both the thoroughness of the decontamination and environmental protection. Surfactants are a critical component of decontamination solutions for radiological, chemical, and biological agents, enhancing their wetting properties. It is therefore advisable to explore alternatives to the currently used compositions that contain surfactants. Studies on the surface tension of special treatment solutions are particularly relevant, as surface tension directly affects their performance characteristics [11, 12].

The lack of qualitative and quantitative characterization of the performance properties of surfactants and detergents in decontamination formulations, which could potentially replace synthetic base products, represents a significant scientific challenge addressed in this report.

The report presents studies on the surface tension of various formulations containing surfactants, aiming to achieve optimal wetting properties in decontamination solutions. Selecting the appropriate surfactant requires consideration of various factors. From the studies conducted, it can be concluded that surfactants must be carefully chosen for each specific application. To streamline the selection process, surfactants can be compared to identify a few that are more effective than others. Typically, surfactants are used in combination with other surfactants and decontaminating agents. These combinations aid in removing a wide range of radiological, chemical, and biological contaminants.

Surfactants are a vital component of decontamination solutions as they enhance wetting properties. One of the primary requirements for decontamination solutions is the effective removal of pollutants from contaminated surfaces. Adding a surfactant to water decreases the surface tension of the solution and improves its wetting ability. [13]

Aqueous surfactant solutions are used to decontaminate radioactive contamination. In the Bulgarian Army, the decontamination composition DV-2 is in use, which contains alkylphenol polyglycol ethers, sodium tripolyphosphate, and sodium sulphate. This study aimed to conduct a comparative analysis of the wetting capabilities of water solutions containing DV-2 and alternative surfactant-based solutions under varying temperature and concentration conditions.

The purpose of this report is to develop a methodology for qualitative and quantitative assessment on the wetting action of solutions to eliminate radiological, chemical and biological agents.

Objects of the research are water solutions DV-2 (Alkylphenolpolyglycol Ethers, Sodium three Polyphosphate and Sodium Sulphate), water solutions on Diethanolamide of Coconut Oil Acids ($C_{(7+n)}H_{(15+2n)}NO_3$, n

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= 5, 7, 9, 11, 13, 15), n-Alkyl Dimethyl Benzyl Ammonium Chloride ($C_9H_{13}NClR$, where R = $C_{12}H_{25}$, $C_{14}H_{29}$ or $C_{16}H_{33}$), Sodium Lauryl ether Sulphate ($C_{12}H_{25}O.(C_2H_4O)2.SO_3.Na$).

II. Materials and Methods

The report describes an experimental setup using the "Maximum Pressure When Blowing a Bubble from the Capillary" method, which is widely applied in practice. This method has been modified by incorporating a tempering coil to regulate the solution's temperature. A schematic representation of the setup is shown in Fig. 1.

The essence of the method lies in determining the maximum pressure (p_max) required to blow a bubble from the end of the capillary. A schematic diagram of the apparatus used for measuring surface tension is presented in Fig. 1. The dimensions of Rebinder's vessel are as follows: height – 10 cm, diameter – 12 cm.

The key component of Rebinder's vessel is the capillary (4)—a pipette graduated from 0.1 cm³, with an inner radius of 0.00043 m. The capillary is positioned inside the vessel (1) so that its end is immersed 5 mm into the liquid being tested. When a vacuum is created in the system, an air bubble will emerge from the capillary once the external pressure becomes sufficient to overcome the surface tension of the liquid. [14, 15]

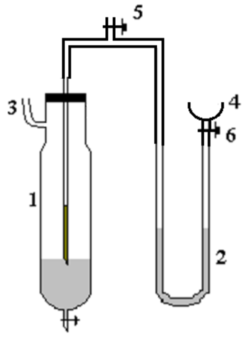

Fig. 1. Schematic of an experimental set-up for determining the surface tension by the "Maximum pressure when blowing a bubble from the capillary" method.

1) Rebinder's vessel, 2) water pressure gauge 3) hole for charging the system with the solution under study; 4) pressure vessel; 5) and 6) taps.

Before starting the measurements, the tightness of the vessel is checked. To do this, tap (7) is closed, and tap (5) is opened.

The capillary constant is determined as follows: Vessel (1) is washed several times and then filled up to the mark. Tap (5) is opened, allowing water to be drawn through tube (3) from the side hole, after which the tube is sealed with a plug. Then, tap (6) is opened, and by removing the pressure vessel (4), the water level in both legs of the manometer is adjusted to zero on the scale. After closing tap (6), the manometer tube is raised again until the water level aligns with the uppermost divisions on the manometer scale. At this point, tap (5) is closed.

By slowly and carefully opening tap (6), the water in the pressure vessel flows into the pressure gauge, creating a difference in liquid levels between the two legs of the manometer. As a result, the liquid in the manometer shifts to the left leg. Now when an air bubble separates from the capillary, the difference in liquid levels between the two legs of the manometer is recorded as h_0.

The surface tension of water (σ_0) at the corresponding temperature is taken from a reference book. After determining the capillary constant, the differences in liquid levels between the two legs of the manometer for the tested liquids (h) are measured. When the maximum difference in levels is reached, a bubble is blown, causing the difference to decrease. However, for calculations, the maximum difference is required, not the difference after the bubble is blown.

For the purposes of the dissertation experiment, the working temperatures of the solutions were controlled by cooling to 10°C and heating with a heater, with the liquid passing through a tempering tube in vessel (1). [15]

When blowing a bubble from the capillary, the surface tension (σ) and maximum pressure (P_{max}) required to detach the bubble from the capillary are related by the following equation:

$$\sigma = \frac{r}{2}(p_{max} - hpg) \quad (1)$$

where:

- r – radius of the capillary (m)
- h – depth of capillary immersion (m)
- g – gravitational acceleration (9.80665 m/s² at sea level)
- ρ – liquid density (kg/m³)
- σ – surface tension (N/m)

Equation (1) is expressed in terms of quantities that can be directly measured. The maximum pressure (P_{max}) is determined using a water manometer. Since accurately measuring the capillary radius (r) can be challenging, this measurement can be bypassed if the experiment is conducted with a liquid of known surface tension (e.g., distilled water):

$$\sigma_0 = \frac{r_0}{2}(P_{0max} - h\rho_0 g) \quad (2)$$

where the index "0" indicates the values that apply to water. By eliminating r_0 from (1.) and (2.), the dependence is obtained:

$$\sigma = \sigma_0 \frac{P_{max} - h\rho g}{P_{0max} - h\rho_0 g} \quad (3)$$

To calculate the maximum pressure required to blow a bubble out of the capillary (3) one can write:

$$\sigma = \sigma_0 \frac{H - h}{H_0 - h} \quad (4)$$

Where:

- H – difference in water manometer levels for the investigated solution (m)
- H_0 – difference in water manometer levels for distilled water (dH_2O) (m)
- h – capillary immersion depth (m)
- σ – surface tension (N/m)

One advantage of this method is that surface tension is determined at a moment when the contact angle is zero. This eliminates the need to account for the θ-parameter, whose determination is often associated with significant error.

The method is dynamic and should be conducted as slowly as possible to ensure an accurate determination of P_{max}. To minimize errors, it is recommended to perform the experiment at least five times. If variations occur in the measurements, the reported differences should be averaged to improve reliability. We used Wolfram Mathematica to create the mathematical models. Wolfram Mathematica is a powerful computational software system used across various fields such as mathematics, science, engineering, and data analysis. It combines symbolic and numerical computation, data visualization, and the creation of interactive interfaces all in one platform.

The software allows for algebraic manipulations like simplifying expressions, differentiation, and solving equations symbolically. It also supports numerical computations with high precision, optimization, and numerical integration. Mathematica offers strong data analysis capabilities, including statistics and machine learning. For visualization, it can generate both 2D and 3D graphics of high quality.

Wolfram Language is the programming language of Mathematica, enabling the development of functions, scripts, and interactive applications. This makes it extremely useful in academia, research, and various industrial sectors. [16]-[18]

III. RESULT AND DISCUSSION

The research was conducted over a concentration range using three types of surfactants, each in different concentration intervals due to their varying rates of surface tension reduction.

Figures 2, 3, and 4 present charts illustrating the correlation between surface tension (σ) and concentration (c) as σ = f(c). Figure 5 shows a chart of DV-2.

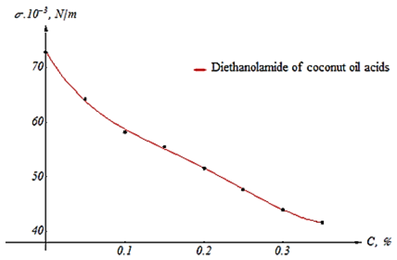

Fig. 2. Surface Tension versus Concentration of Diethanolamide of Coconut Oil Acids.

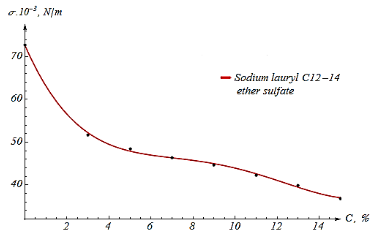

Fig. 3. Surface Tension versus Concentration of Sodium Lauryl Ether Sulphate.

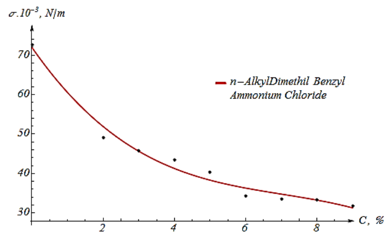

Fig. 4. Surface Tension versus Concentration of n-Alkyl Dimethyl Benzyl Ammonium Chloride.

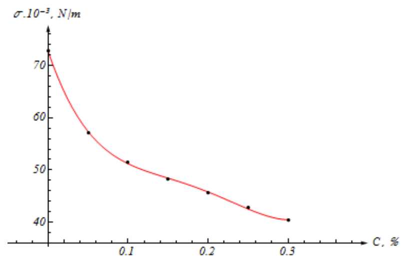

Fig. 5. Surface Tension versus Concentration of DV-2.

If DV-2 is used within a concentration range of 0.1% to 0.2%, it may be replaced with Diethanolamide of Coconut Oil Acids at a concentration of no less than 0.28%.

The other surfactants shown in Figures 2 and 4 exhibit a decrease in surface tension over higher concentration intervals. Therefore, if Sodium Lauryl Ether Sulfate or n-Alkyl Dimethyl Benzyl Ammonium Chloride is used, a larger amount must be added to the decontamination solution.

Analytically, the interdependence between surface tension and concentration can be described using regression equations, formulated with the Wolfram Mathematica software [11, 12, 13]. Statistically processed correlation data for DV-2 and Diethanolamide of Coconut Oil Acids, along with their regression equations at 20°C, are presented in equation (5).

$$\sigma = a[0] + a[1].C + a[2].C^2 + a[3].C^3 + a[4].C^4 \quad (5)$$

where:

σ - surface tension [N/m],

C- concentration [%],

a – coefficients.

TABLE 1. STATISTICAL EVALUATION OF EXPERIMENTAL DATA ON DV-2.

	Estimate	Standard Error	t-Statistic	P-Value
a[0]	72.6875	0.385222	188.69	0.0000280856
a[1]	−449.783	21.8892	−20.5482	0.00236001
a[2]	3457.58	337.974	10.2303	0.00942006
a[3]	−12775.8	1762.44	−7.24891	0.0185041
a[4]	16848.5	2916.26	5.77744	0.0286767

TABLE 2. STATISTICAL EVALUATION OF EXPERIMENTAL DATA FOR DIETHANOLAMIDE DERIVED FROM COCONUT OIL FATTY ACIDS.

	Estimate	Standard Error	t-Statistic	P-Value
a[0]	72.8218	0.407361	178.765	3.85991×10^{-7}
a[1]	−238.533	19.0153	−12.5442	0.00109218
a[2]	1402.4	246.499	5.68926	0.0107645
a[3]	−4933.11	1095.24	−4.50413	0.02044
a[4]	6129.09	1552.61	3.94761	0.0289901

Diethanolamide of Coconut Oil Acids offers numerous benefits, making it a preferred choice for radioactive decontamination solutions. It belongs to the group of non-ionic surfactants, which play a crucial role in surface tension reduction and improving wetting properties.

One of the key characteristics of non-ionic surfactants is their ability to adsorb onto a negatively charged water/air interface, effectively reducing the surface load and film thickness. This process creates conditions for electrostatic destabilization, which can enhance contaminant removal. However, due to this property, non-ionic surfactants often require combination with ionic surfactants to achieve better control over surface charge and film stability. This synergy between non-ionic and ionic surfactants ensures optimal detergency and wetting efficiency in decontamination solutions.

IV. CONCLUSIONS

Various substances and formulations can be used in radioactive decontamination solutions to lower surface tension, provided they undergo a preliminary quantitative and qualitative assessment of their wetting ability. The empirical correlations established between surface tension and concentration can be effectively applied after statistical processing of experimental data. These correlations are crucial for optimizing the efficacy and performance of decontamination solutions.

It is recommended to use aqueous solutions of Diethanolamide of Coconut Oil Acids in the concentration range of 0.2% to 0.3%, as they exhibit wetting properties like DV-2 at a concentration of 0.1% to 0.2%.

Additionally, the Wolfram software can be utilized to generate graphical and analytical dependencies for various surfactants, allowing for a more precise evaluation of their surface tension behaviour and effectiveness in decontamination applications.

V. ACKNOWLEDGEMENTS

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VI. DISCLOSURE OF INTERESTS

The author has no competing interests.

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