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Determination of the Diffusion Coefficient of Butylparaben and Bisphenol-A via UV-Vis Spectrometry †

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Abstract

Bisphenol-A (BPA) and butylparaben (BP) are recognized as emerging contaminants due to their extensive use in plastics and personal care products, posing significant risks to ecosystems and human health. Understanding their transport behavior is vital for predicting environmental fate and designing mitigation measures. This study quantifies the diffusion coefficients of BPA and BP under infinite dilution conditions to simulate realistic environmental scenarios. Laboratory experiments employed a UV-Visible spectrophotometer to monitor concentration changes over time at four initial BP concentrations (0.0005–0.0025 M) and at temperatures between 294.85 K and 304.15 K. Experimental data show that BP concentrations at lower initial values (0.0005 M and 0.00075 M) remained constant, indicating minimal diffusion. Theoretical estimations using the Stokes–Einstein equation yielded diffusion coefficients at 299.38 K of 1.51×10^{-13} m^2/s for BP and 8.47×10^{-14} m^2/s for BPA. The Wilke–Chang equation estimated higher values: 1.21×10^{-10} m^2/s for BP and 1.18×10^{-10} m^2/s for BPA at the same temperature. Results confirm that temperature increases enhance diffusion, while molecular size differences cause BP to diffuse faster than BPA. The robust experimental dataset produced here supports the refinement of predictive models for contaminant mobility. These insights are critical for risk assessment and for developing targeted strategies to minimize the persistence and spread of endocrine-disrupting chemicals in aquatic and terrestrial systems.

Keywords: diffusion coefficient; bisphenol-A; butylparaben; UV-Vis spectrophotometry; emerging contaminants

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1. Introduction

Cosmetics have become integral to daily life, often incorporating antimicrobial agents like butylparaben to enhance product safety and shelf life [1]. Butylparaben, a paraben commonly used as a food additive, is widely used in cosmetics as a preservative due to its antimicrobial properties. While the FDA regulates cosmetic safety generally, the increasing use of antimicrobials contributes to the growing problem of antimicrobial resistance (AMR), a critical global health challenge linked to millions of deaths annually. The overuse of such compounds necessitates a deeper understanding of their behavior in various applications.

Another prevalent chemical, bisphenol-A (BPA), is a diphenylmethane derivative used extensively in manufacturing various products, including food packaging [2]. BPA is crucial in the plastics industry, particularly in producing polycarbonates and synthetic polymers, finding its way into numerous consumer products like pipes, toothpaste, food packaging, and personal care items. However, the widespread use of BPA-containing plastics contributes to environmental pollution, especially in aquatic ecosystems where plastic debris can leach BPA and other toxic substances, posing risks to both the environment and human health [3]. Furthermore, conventional water treatment plants often struggle to fully remove BPA, leading to increasing concentrations in water sources [4].

BPA and parabens are classified as endocrine-disrupting chemicals capable of mimicking estrogenic activity, potentially affecting reproductive, developmental, and metabolic processes in humans and aquatic organisms. Environmental monitoring studies report their frequent detection in wastewater, rivers, sediments, and even drinking water due to incomplete removal during treatment processes. Continuous low-level exposure increases ecological risk and human health concerns, emphasizing the importance of understanding their physicochemical transport behavior, including molecular diffusion in liquid systems.

Understanding the diffusion of these compounds, butylparaben, and bisphenol-A, is crucial for assessing their potential impact. Diffusion, the movement of molecules from high to low concentration, plays a key role in many biological and chemical processes. Accurate determination of diffusion coefficients is essential for evaluating dermal absorption of butylparaben in cosmetics and understanding BPA's behavior in polycarbonate plastics, allowing for better assessment of safety and efficacy. Fick's First Law provides a foundation for calculating diffusion coefficients by relating diffusion flux to concentration gradients, a principle used in environmental science to study pollutant dispersal (e.g., butylparaben in ecosystems and BPA's effects on the human body). This research aims to experimentally determine the diffusion coefficients of butylparaben and BPA at varying concentrations and temperatures.

2. Methodology

2.1. Preparation of Solution and Samples

Analytical-grade butylparaben and bisphenol-A were used as model pharmaceutical-related compounds in this study. Individual concentrated stock solutions of each analyte were prepared by accurately weighing the required amount of compound and dissolving it in absolute ethanol (99.9% purity), selected based on its high solvation capacity and compatibility with both analytes. The stock solution concentrations were defined according to the solubility limits of each compound to ensure complete dissolution and chemical stability. Working standard solutions were prepared by serial dilution of the stock solutions with ethanol to achieve the desired concentrations for diffusion experiments. All solutions were freshly prepared prior to analysis and stored in amber containers to minimize photodegradation.

2.2. Calibration of Instrument

The cuvette was thoroughly washed with deionized water and dried completely before each trial to minimize errors and ensure the accuracy of the experiment. Additionally, an absorbance reading of a cuvette containing deionized water was performed to confirm the removal of impurities. The analytical wavelengths of 256 nm for butylparaben and 214 nm for bisphenol-A were selected based on their maximum absorption wavelengths (λ_{max}) determined from preliminary spectral scanning (200–400 nm), ensuring maximum sensitivity and minimal spectral interference.

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2.3. Diffusion Coefficient Measurement

The diffusion coefficient of butylparaben and bisphenol-A was determined using a diffusion cell experiment. A known concentration of the compound was introduced into one side of the diffusion cell, while the other side was filled with pure ethyl alcohol. The diffusion of the compound across the cell was monitored over time by measuring the absorbance of the solution in the receiving compartment at the appropriate wavelength. The results are compared to the theoretical concepts using the Stoke–Einstein Equation,

$$D = \frac{k_B T}{6\pi\eta r} \tag{1}$$

where D is the diffusion coefficient, k_B is the Boltzmann constant, T is the temperature in Kelvin, η is the fluid's viscosity, and r is the particle radius. Also, Wilke–Change Equation,

$$D = \frac{7.4 \times 10^{-8}\sqrt{M_b T}}{\eta v_A^{0.6}} \tag{2}$$

where D is the diffusion coefficient, M_b is the molecular weight of the solvent, T is the temperature in Kelvin, η is the fluid's viscosity, and v_A is the molar volume of the solute at its boiling point.

2.4. Experimental Set-Up

The experiment involved preparing donor solutions of butylparaben and bisphenol-A at five different concentrations (0.0005 M, 0.00075 M, 0.001 M, 0.0025 M, and 0.005 M). Pure ethanol was placed in five separate beakers to serve as receptor compartments. Semi-permeable membrane diffusion cells were used to contain the donor solutions.

Each diffusion cell was filled with one of the prepared donor solutions at a specific concentration. These cells were then submerged in the corresponding beakers of pure ethanol, initiating the diffusion process of the analytes from the donor compartment, across the membrane, and into the ethanol. All diffusion experiments were conducted under controlled temperature conditions using a thermostatically regulated water bath (±0.5 K accuracy). The diffusion cells were immersed in the bath throughout the experiment to maintain constant temperature and minimize viscosity-related variations in diffusion behavior.

The concentration of the analytes in the receptor compartment was monitored every 5 min. At each interval, a small sample was extracted from the ethanol in the beaker, placed in a cuvette, and analyzed using a UV-Visible spectrophotometer, as presented in Figure 1. This process was repeated over a set period to gather kinetic data on the diffusion.

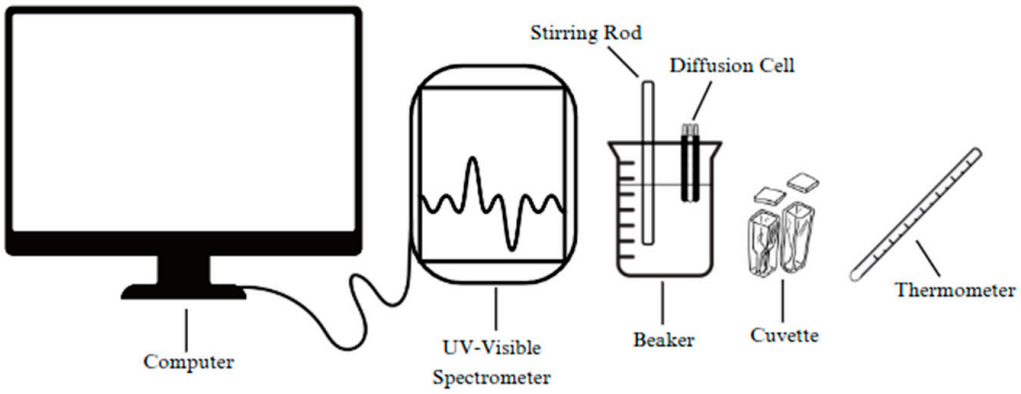


Figure 1. Experimental Set-up for UV Vis Analysis.

2.5. Statistical Analysis

A time-course analysis, conducted in triplicate, examined the relationship between concentration and the diffusion coefficient, with mean and standard deviation used for data presentation. A two-way ANOVA was employed to investigate the effects of time interval and molarity on solution concentration throughout the experiment. The significance of these effects was determined by comparing the calculated F-value to the critical F-value, with $F > F_{crit}$ indicating a statistically significant effect. Similarly, a *p*-value of less than 0.05 was considered statistically significant.

3. Results and Discussion

3.1. Absorbance of Butylparaben and Bisphenol-A at Varying Concentrations

Both butylparaben and bisphenol-A demonstrate a concentration-dependent increase in absorbance at 256 nm and 214 nm, consistent with Beer-Lambert's Law presented in Figure 2. While butylparaben solutions show stable absorbance over time, bisphenol-A exhibits greater variability, indicating possible photochemical degradation, adsorption onto the membrane surface, or solvent-mediated transformation processes occurring during the experiment. The presence of negative absorbance values in bisphenol-A data is anomalous and may be attributed to baseline correction issues, calibration errors, or data processing artifacts. These values require careful investigation and may need to be excluded from further analysis.

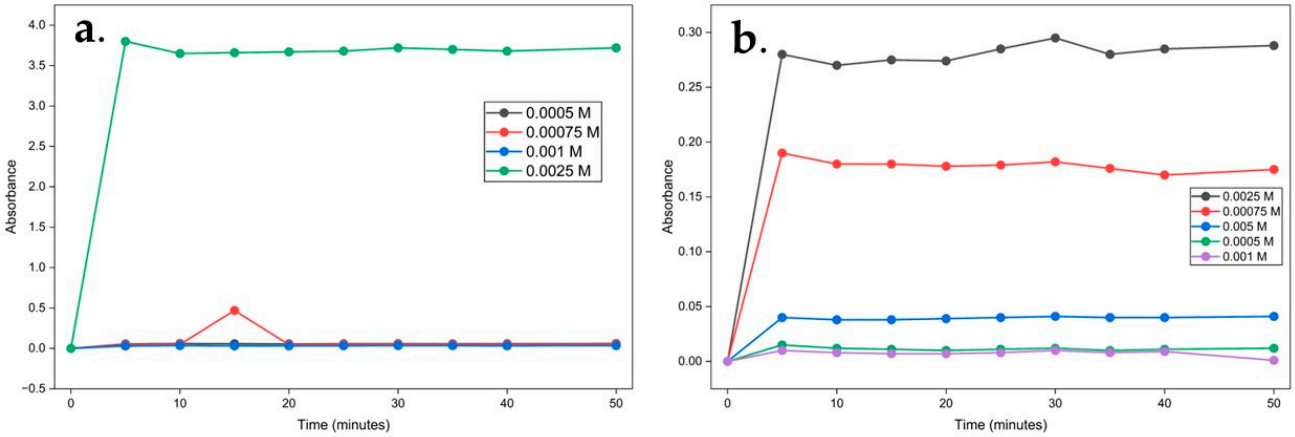


Figure 2. Time-Course Absorbance of (**a**) butylparaben, and (**b**) bisphenol-A.

Across a 50 min experiment, the absorbance of butylparaben solutions at 0.005 M and 0.00075 M remained consistently low (around 0.064), with overall absorbance remaining relatively stable, suggesting minimal chemical change. This stability aligns with previous research indicating butylparaben's general stability under appropriate conditions, though other studies highlight potential influences from factors like additional ingredients or UV exposure [5].

The gradual decrease in absorbance observed for bisphenol-A across all concentrations indicates a progressive reduction in dissolved BPA concentration, which may result from photodegradation, adsorption onto the membrane surface, or chemical transformation in the ethanol medium. This decrease was concentration-dependent, with higher initial concentrations showing a more steady degradation rate [6]. This pattern is consistent with bisphenol-A photodegradation, as supported by existing literature, which also notes degradation through chemical reactions and microbial activity [7].

The reduction in BPA absorbance may be attributed to photochemical oxidation processes initiated by UV exposure, generating phenoxy radicals that subsequently undergo

hydroxylation or cleavage reactions. These transformation pathways reduce the concentration of the parent BPA molecule, thereby lowering the measured absorbance over time [7].

3.2. Concentration Changes over Time Using Initial Molarity

The absorbance-derived concentration profiles indicate that butylparaben remained stable across all initial concentrations (0.0005–0.005 M) over the 50 min experimental period presented in Figure 3. At lower concentrations (0.0005 M and 0.00075 M), the concentration remained constant at approximately 4.27×10^{-5} M, while intermediate concentrations (0.001 M and 0.0025 M) exhibited minimal temporal variation, indicating that any diffusion-driven transport was below the detection limit of the UV–Vis method. Minor fluctuations observed at 0.0025 M are attributed to experimental variability rather than changes in diffusion behavior. A gradual decrease followed by stabilization at 0.00075 M suggests the attainment of diffusion equilibrium, where net mass transfer becomes negligible as concentration gradients diminish. The highest concentration tested (0.005 M) remained stable throughout the experiment, indicating that increasing the initial concentration did not significantly enhance measurable transport. Overall, the weak dependence of concentration on time suggests slow, equilibrium-controlled diffusion of butylparaben in ethanol under the studied conditions [8].

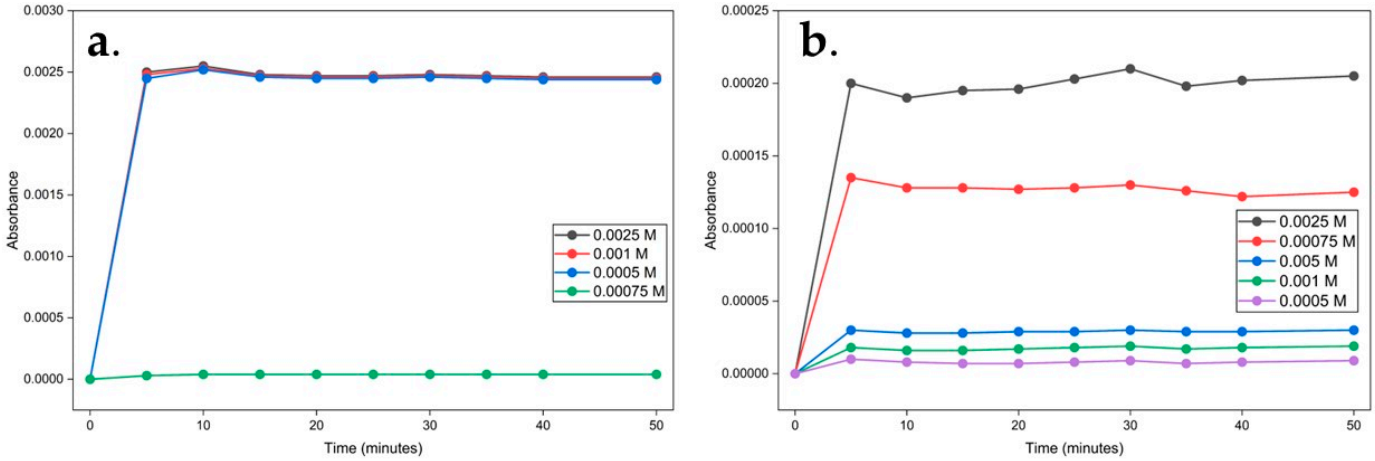


Figure 3. Computed Concentration using Absorbance value of (**a**) butylparaben, and (**b**) bisphenol-A.

3.3. Calculated Diffusion Coefficients

3.3.1. Stokes-Einstein Equation

Diffusion coefficients estimated using the Stokes–Einstein equation increased with temperature over the range 294.85–304.15 K, consistent with the theoretical dependence of molecular diffusion on thermal energy and solvent viscosity. As temperature increases, the reduction in solvent viscosity and the enhancement of molecular Brownian motion collectively promote higher diffusivity. At 299.38 K, butylparaben exhibited a higher diffusion coefficient (1.51×10^{-13} m^2/s) than bisphenol-A (8.47×10^{-14} m^2/s), indicating faster molecular mobility in ethanol, as presented in Table 1.

Table 1. Diffusion Coefficients via Stokes-Einstein.

Contaminant	Temperature (K)	Stokes-Einstein (m^2/s)
butylparaben	299.38	1.5110×10^{-13}
Bisphenol-A	299.38	8.4701×10^{-14}

The higher diffusivity of butylparaben can be attributed to its smaller effective hydrodynamic radius compared with bisphenol-A. The Stokes–Einstein model treats diffusing

species as spherical particles and assumes continuum hydrodynamics; thus, molecules with smaller hydrodynamic dimensions experience reduced frictional resistance and diffuse more rapidly [9]. However, it should be noted that the absolute diffusion coefficients predicted by this model are relatively low, reflecting the limitations of applying Stokes–Einstein to non-spherical, molecular-scale solutes in low-viscosity organic solvents [9]. Consequently, these values should be interpreted as qualitative indicators of relative diffusivity rather than exact experimental measurements.

3.3.2. Wilke-Change Equation

Diffusion coefficients estimated using the Wilke–Chang equation were approximately three orders of magnitude higher than those predicted by the Stokes–Einstein equation, with values of 1.21×10^{-10} m^2/s for butylparaben and 1.18×10^{-10} m^2/s for bisphenol-A at 299.38 K. This difference arises from the Wilke–Chang model explicitly accounting for solvent properties and solute molar volume, making it more suitable for predicting molecular diffusion in liquid systems [10]. Consistent with theoretical expectations, butylparaben exhibited slightly higher diffusivity than bisphenol-A, which can be attributed to its smaller molar volume (151.74 cm^3/mol versus 190.24 cm^3/mol) is presented in Table 2. Smaller solute molecules generally experience lower hydrodynamic drag within the solvent matrix, resulting in enhanced mobility.

Table 2. Diffusion Coefficients via the Wilke–Chang Equation.

Contaminant	Temperature (K)	Wilke-Chang (m^2/s)
Butylparaben	299.38	1.2100×10^{-10}
Bisphenol-A	299.38	1.1800×10^{-10}

The relatively small difference between the diffusion coefficients of the two compounds suggests that, while molecular size influences diffusivity, both solutes experience comparable solvent–solute interactions in ethanol [11]. Overall, the Wilke–Chang predictions fall within the typical range reported for small organic molecules diffusing in liquid solvents (10^{-10}–10^{-9} m^2/s), whereas the Stokes–Einstein estimates are substantially lower. This discrepancy highlights the importance of model selection when estimating diffusion coefficients and reinforces that the values reported here should be considered theoretical estimates [12]. The consistent trend observed across both models, the higher diffusivity of butylparaben relative to bisphenol-A supports the conclusion that molecular size and hydrodynamic resistance are key factors governing diffusion behavior in ethanol.

The diffusion coefficients predicted using the Wilke–Chang model ($\approx 10^{-10}$ m^2 s^{-1}) fall within the range commonly reported for small organic molecules in liquid solvents (10^{-10}–10^{-9} m^2 s^{-1}), consistent with previously published diffusion measurements for phenolic compounds in alcohol media [10–12].

Previously reported diffusion coefficients of phenolic organic compounds in ethanol typically range from 0.8×10^{-10} to 2.5×10^{-10} m^2 s^{-1}, indicating that the Wilke–Chang estimates obtained in this study fall within experimentally observed ranges, whereas the Stokes–Einstein predictions significantly underestimate molecular diffusivity due to continuum-assumption limitations.

3.4. Statistical Analysis of Absorbance by Concentration and Time

The two-way analysis of variance (ANOVA) conducted for butylparaben absorbance (Table 3) revealed that time did not exert a statistically significant effect within the 5 min sampling intervals ($F = 2.34$, $p = 0.054$). Although the p-value approaches the conventional significance threshold, the result indicates that short-term temporal variations did not

produce systematic changes in absorbance over the 50 min experimental duration. This finding suggests that butylparaben remained chemically stable in ethanol and that any diffusion-driven concentration changes in the receptor phase were too small to be detected by the UV–Vis method within the studied timeframe [8].

Table 3. ANOVA Analysis of Butylparaben.

Source of Variation	SS	df	MS	F	*p*-Value	F-Crit
Time	0.0016	8	0.00012	2.3356	0.0542	2.3551
Concentration	120.5762	3	40.1921	815,965.1	2.0×10^{-54}	3.0088
Error	0.0019	24	8.0913×10^{-5}			
Total	120.5798	35				

In contrast, concentration had an overwhelmingly significant effect on absorbance ($F = 8.16 \times 10^5$, $p \approx 0$), demonstrating a strong linear dependence between absorbance and concentration. This result provides robust statistical confirmation of the Beer–Lambert law and validates the reliability of the UV–Vis calibration used in this study. The very large F-value indicates that variability in absorbance is dominated by differences in concentration rather than by experimental noise or time-dependent effects. The relatively small error term further supports the precision and reproducibility of the absorbance measurements for butylparaben.

Similarly, the two-way ANOVA results for bisphenol-A (Table 4) showed that time had no statistically significant influence on absorbance ($F = 2.52$, $p = 0.288$), indicating that absorbance variations over time were not systematic. This suggests that, within the experimental resolution, temporal effects such as diffusion, degradation, or instrumental drift did not produce statistically detectable changes. However, as with butylparaben, concentration exerted a highly significant effect on absorbance ($F = 1.09 \times 10^4$, $p \approx 0$), confirming that concentration remains the primary determinant of UV–Vis response for bisphenol-A.

Table 4. ANOVA Analysis of Bisphenol-A.

Source of Variation	SS	df	MS	F	*p*-Value	F-Crit
Time	0.0006	9	7.0074×10^{-5}	2.5175	0.2879	2.1526
Concentration	1.1103	4	0.2776	10,858.9119	7.0562×10^{-1}	2.6335
Error	0.0010	36	2.6464×10^{-5}			
Total	1.1119	49				

The lower F-value for concentration in the bisphenol-A system compared with butylparaben may reflect greater data variability, potentially arising from baseline correction issues or the presence of negative absorbance values observed in some measurements. Nonetheless, the strong statistical significance confirms that the Beer–Lambert relationship remains valid for bisphenol-A under the experimental conditions. Importantly, the statistical insignificance of time for both compounds should not be interpreted as evidence of the absence of diffusion; rather, it indicates that diffusion-related concentration changes were small relative to the sensitivity of the analytical method and the experimental timescale.

4. Conclusions and Recommendations

This study evaluated the diffusion behavior of butylparaben and bisphenol-A in ethanol using UV–Vis spectroscopy. Both compounds followed Beer–Lambert's law, confirming reliable concentration measurements. Butylparaben remained stable over time, while bisphenol-A showed decreasing absorbance, suggesting possible degradation or transformation. Diffusion coefficients increased with temperature, and butylparaben diffused faster than bisphenol-A due to its smaller molecular size. Overall, the results show

that molecular size, temperature, and chemical stability strongly influence contaminant transport in liquid systems. Further studies using direct diffusion methods and broader environmental conditions are recommended.

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