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Polimer Çözeltilerinde Statik Işık Saçılmasının Simülasyon Temelli Bir İncelemesi: Rayleigh, Mie, Debye ve Guinier Modellerinin Araştırılması

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Öz

Bu çalışmada, bir polimer çözeltisindeki polimer parçacıklarının saçılma davranışı simülasyon temelli bir yaklaşımla incelenmiştir. 635 nm dalga boyuna sahip bir lazer kaynağı kullanılmış ve saçılma, açıları 0° ile 175° aralığında hesaplanmıştır. Çözücü ve polimer parçacıklarının kırılma indisleri sırasıyla 1.33 (su için tipik) ve 1.59 (polimerler için yaygın) olarak ayarlanmıştır. Hidrodinamik çaptan tahmin edilen jirasyon yarıçapı 58.5 nm olarak alınmıştır. Saçılma davranışını analiz etmek için dört model—Rayleigh, Mie, Debye ve Guinier uygulanmıştır. Küçük parçacıklar için geçerli olan Rayleigh saçılması, 0°'de düşük bir yoğunlukla başlamış ve 100°'ye kadar artan açıyla azalmış, ardından daha yüksek açılarda simetrik olarak artmıştır. Daha büyük parçacıklar için uygun olan Mie saçılması, 0°'de en yüksek yoğunluğu göstermiş ve açı arttıkça keskin bir şekilde azalmıştır. Debye saçılması, normalleştirilmiş 1.0 yoğunluğuyla başlamış ve açıyla birlikte düzgün bir şekilde azalarak polimer zincirlerinin rastgele sarmal yapısını analiz etmedeki etkinliğini göstermiştir. Öte yandan, Guinier yaklaşımı düşük açılarda etkili olmuş ve yoğunluk açı arttıkça üstel olarak azalmıştır, bu da onu parçacık boyutunu belirlemede kullanışlı bir yöntem haline getirmiştir. Bu karşılaştırma, her bir modelin açısal bağımlılıklarını ve uygulama alanlarını vurgulamıştır. Mie saçılması büyük parçacıklar için, Debye saçılması polimer zincirleri için, Rayleigh saçılması küçük parçacıklar için ve Guinier yaklaşımı düşük açılarda parçacık boyutunu ve jirasyon yarıçapını belirlemek için en uygun bulunmuştur. Bu çalışma, polimer çözeltilerinin saçılma davranışını anlamada bu modellerin güçlü ve zayıf yönlerini ortaya koymaktadır.

Anahtar Kelimeler
Debye modeli; Guinier modeli, Mie modeli; Polymer çözeltileri; Rayleigh modeli; Statik ışık saçılması.

A Simulation-Based Study of Static Light Scattering in Polymer Solutions: Exploring Rayleigh, Mie, Debye, and Guinier Models

Abstract

This study investigated the scattering behavior of polymer particles in a solvent using a simulation-based approach. A laser source with a wavelength of 635 nm was employed, and scattering angles were calculated within the range of 0° to 175°. The refractive indices of the solvent and polymer particles were set to 1.33 (typical for water) and 1.59 (commonly observed for polymers), respectively. The radius of gyration, estimated from the hydrodynamic diameter, was taken as 58.5 nm. Four models—Rayleigh, Mie, Debye, and Guinier—were applied to analyze the scattering behavior. Rayleigh scattering, valid for small particles, started with a lower intensity at 0° and decreased with increasing angle up to 100°, after which it symmetrically increased at higher angles. Mie scattering, suitable for larger particles, exhibited the highest intensity at 0° and sharply decreased as the angle increased. Debye scattering began with a normalized intensity of 1.0 and decreased smoothly with angle, demonstrating its effectiveness in analyzing the random coil structure of polymer chains. On the other hand, the Guinier approximation was most effective at low angles, where the intensity decreased exponentially with increasing angle, making it a useful method for determining particle size. This comparison highlighted the angular dependencies and application areas of each model. Mie scattering was found to be most appropriate for large particles, Debye scattering for polymer chains, Rayleigh scattering for small particles, and the Guinier approximation for determining particle size and radius of gyration at low angles. This study underscores the strengths and limitations of these models in understanding the scattering behavior of polymer solutions.

Keywords
Debye model; Guinier model; Mie model; Polymer solutions; Rayleigh model; Static light scattering.

1. Introduction

Polymers are long-chain molecules widely found in natural and synthetic environments. They play critical roles in nearly every aspect of life and technology, ranging from biological macromolecules like DNA and proteins to industrial materials such as plastics, rubbers, fibers, and resins. The extensive range of applications for polymers stems from their unique physical and chemical properties, which arise from the repetitive bonding of small structural units called monomers into long chains. These properties are determined by various microscopic parameters, including molecular weight, molecular weight distribution, chain architecture (linear, branched, cyclic, star-shaped, comb-like, etc.), chain flexibility (or rigidity), chemical composition, and interactions between polymer chains (Findik, 2025)

Polymer solutions, formed when polymers dissolve in a solvent, are important in fundamental scientific research and industrial applications. These systems are widely used in drug delivery systems (controlled release and targeted delivery of drugs), biomedical applications (tissue engineering, implants, biosensors), coating and paint technologies (surface protection, adhesion, rheological control), the food industry (thickeners, emulsifiers, gelling agents), cosmetic products (shampoos, creams, lotions), and the petroleum industry (drilling fluids, viscosity modifiers), among many others. In each of these applications, the macroscopic properties of the polymer solution (e.g., viscosity, elasticity, surface tension, phase behavior, film-forming ability) are closely linked to the microscopic structure and dynamics of the polymer chains (Mansuri et al., 2025).

For instance, in a drug delivery system, the molecular weight and solubility of the polymer chains directly influence the drug release rate and bioavailability. In a coating formulation, the molecular weight distribution and chain architecture of the polymer determine the mechanical strength, adhesion properties, and drying behavior of the coating. In a food product, the concentration and flexibility of the polymer chains affect the product's texture, mouthfeel, and shelf life. These examples highlight the critical importance of accurately characterizing the structural and thermodynamic properties of polymer chains at the microscopic level to control and optimize the macroscopic properties of polymer solutions (Thakkar and Bhattacharya, 2025; Hsissou, 2021; Zhang et al., 2020).

Among the experimental techniques used to study the structural and thermodynamic properties of polymer solutions, static light scattering (SLS) stands out due to its unique advantages. SLS is a non-invasive technique, meaning that the structure or properties of the polymer solution remain unchanged during the measurement. It is a relatively fast method, with typical measurements completed within minutes. SLS provides information over a wide size range (from a few nanometers to micrometers), enabling the characterization of individual polymer chains and larger aggregates. It can be applied to dilute and concentrated solutions, allowing the study of systems ranging from those where polymer chains interact minimally to those where chains are densely entangled and exhibit complex interactions. Furthermore, SLS is an absolute method, meaning structural parameters such as molecular weight can be determined directly without calibration or reference standards (Schärtl,2007; Minton, 2016; Takahashi, 2020).

The fundamental principle of SLS involves scattering monochromatic (single-wavelength) light from a laser source as it passes through a polymer solution. This scattering occurs due to fluctuations in density (or refractive index) within the solution, which arises from the thermal motion of polymer chains (Brownian motion), concentration differences in dilute solutions, or interactions between polymer chains and solvent molecules in concentrated solutions (Fischer and Abetz,2018).

The intensity of the scattered light, denoted as I(θ), is measured depending on the scattering angle θ. This intensity can also be expressed in terms of the magnitude of the scattering vector q, which is related to the scattering angle, the refractive index of the solvent (n_{ref}), and the wavelength of the light (λ) in a vacuum. By mathematically analyzing I(q), researchers can extract valuable information about the structural and thermodynamic properties of the polymer solution. This includes details about the particles or molecules' size, shape, and interactions within the solution (Schärtl,2007; Wyatt,1993).

To accurately interpret SLS data and extract meaningful results, it is essential to use appropriate theoretical models that physically and mathematically describe the scattering process. These models relate the scattering structures' size, shape, and concentration (e.g., individual polymer chains, chain coils, spherical aggregates, rod-like structures) to the angular dependence of the scattering intensity. However, due to the structural complexity of polymer solutions and the coexistence of structures of different scales, it is clear that no single "universal" SLS model can account for all scenarios. As a result, other theoretical approaches have been developed for various size regimes, polymer architectures, and solvent conditions.

The primary objective of this study is to provide a comprehensive and comparative analysis of the theoretical models commonly used in the literature to interpret static light scattering data from polymer solutions. This analysis examines the applicability, fundamental assumptions, strengths, and limitations of these models, their relationships, and their ability to fit experimental data. This work focuses on four fundamental theoretical approaches:

- **Rayleigh Scattering**: This is the simplest model, applicable when the size of the scattering structures is much smaller than the wavelength of light (Miles et al., 2001).
- **Mie Scattering**: A more complex theory that describes the scattering from spherical particles based on the exact solution of Maxwell's equations (Cheong and Woon, 2011).
- **Debye Scattering**: A specialized approach for modeling the scattering from ideal, randomly coiled polymer chains (Scardi et al, 2016).
- **Guinier-Porod Model**: This is a more general and flexible approach capable of modeling data at low and high scattering angles (Hammouda, 2010).

Each model is better suited to specific polymer solutions and size regimes. In some cases, a combination of multiple models or more advanced approaches (e.g., the Zimm model, Random Phase Approximation (RPA) theory, or blob models) may be required.

Static light scattering has emerged as a critical analytical technique for characterizing the molar mass, size, topology, and optical properties of particles in fields ranging from materials science to atmospheric studies. In recent years, efforts to improve the accuracy and applicability of this method have elucidated scattering dynamics in systems ranging from polymeric structures to colloidal systems and even complex atmospheric particles. The computational modeling revolution that began in the 2000s transformed the capacity of static light scattering to generate reliable data even in highly polydispersive systems and complex environments, and the advances of this period have laid the foundation for today's industrial and scientific applications. Below is a chronological overview of some of the work carried out in this context.

Schure and Palkar investigated the combination of static light scattering-based multi-angle measurements and field-flow fractionation to provide accurate characterization of narrowly dispersed particle systems and showed that Mie theory gives more accurate results for large particles than the Rayleigh-Gans-Debye approach (Schure and Palkar, 2002).

Svaneborg and Pedersen developed parameterized scattering functions using Monte Carlo simulations for static light scattering data analysis in complex liquids and applied this method to semi-flexible polymers and worm-like micelle systems with/without electrostatic interaction (Svaneborg and Pedersen, 2004).

Wolf and Voshchinnikov developed an extensible computer program for Mie scattering simulations of spherical particles with arbitrarily large size parameters based on static light scattering. By calculating scattering matrix elements, efficiency factors, cross sections, and asymmetry parameters, the study enables the analysis of single particles as well as ensembles with multiple components and large-size distributions, highlighting its applicability in areas such as cosmic dust, atmospheric optics, and industrial particle characterization (Wolf and Voshchinnikov, 2004).

Bunge et al. analyzed the static light scattering properties of polymer optical fibers using side illumination and horizontal and angular scanning methods. The study revealed that about 95% of the standard scattering is due to Rayleigh scattering in the core, while in high temperature fibers, 40% was due to Mie scattering at the core-cladding interface (Bunge et al.,2006).

Tang et al. developed a mathematical model for static light scattering analysis in polymers based on Mie scattering theory and integrated with Monte Carlo method. By simulating the scattering processes of individual photons, this model aims to statistically predict the light distribution inside the polymer from light sources such as laser or CCFL (Ma et al., 2007).

Tacx and Iedama investigated the use of the 3D cross-correlation technique to reduce errors caused by multiple scattering effects in static light scattering measurements. The study verified through Monte Carlo simulations that this method can directly quantify the angular dependence of the individual scattered light intensity even in turbid environments and is consistent against optical path length variations. The results prove that, unlike conventional methods, multiple scattering distortions can be neutralized, and measurement accuracy can be improved without the need for detailed experimental parameter information (Tacx and Iedema, 2017).

Molnar et al. have developed a new model for static light scattering analysis in semi-crystalline polymers using the full Mie scattering theory of radially anisotropic spheres. By modeling the optical behavior of polycrystalline systems in isotactic polypropylene films over different sample thicknesses and crystal structures, this study successfully predicted the turbidity values of multiple light interactions at scattering centers (Molnár et al., 2020).

Balderas-Cabrera and Castillo modeled the optical behavior of large and inhomogeneous particles using Mie scattering theory in the static light scattering analysis of colloidal particles with core-shell structure. The study successfully predicted the scattering intensity of structures containing a core with a constant refractive index and a shell with a solvent-compatible graded decreasing refractive index profile by numerically approximating the Gaussian refractive index profile with multilayer spherical models. The developed open-source software produced results in agreement with experimental form factor functions and proved the wide applicability of this method for understanding photonic properties or characterizing similar symmetric particles such as superabsorbing agents (Balderas-Cabrera and Castillo,2024).

Matson et al. detailed the basic principles and SEC-MALS applications of the static light scattering technique for standard-free absolute molar mass, size and topology analysis of polymers. In particular, the study emphasized how the accuracy of experimental parameters such as refractive index variation affects the results, the role of chromatographic separation quality on the numerical molar mass, and the effect of contaminants/aggregates in the sample on the scattering data (Matson et al., 2024).

Su et al. presented a scattering model developed with the Monte Carlo method to improve the accuracy of static light scattering-based analysis in highly concentrated mixed particle systems. The model significantly reduced the measurement errors compared to conventional methods by considering the multiple scattering and absorption effects of non-aligned laser beams and demonstrated that the particle size distribution can be precisely determined from spectral data with the differential evolution algorithm (Su et al., 2025).

This study was intended to contribute to the field by providing a practical methodology for analyzing the scattering behavior of polymer solutions. The main novel contributions can be summarized as follows: Comparison of Rayleigh, Mie, Debye, and Guinier models under a single framework, clarifying the limits of their validity in polymer systems and providing a simple guide for model selection. The analyses, supported by controlled simulations, increased model reliability by visualizing the behavior of the theoretical assumptions.

2. Materials and Method

This study conducted four simulations to examine the light-scattering behavior of polymer particles in solution. A laser with a wavelength of 635 nm, which falls within the visible spectrum and is commonly used in light scattering studies, was employed as the light source. Scattering intensities were calculated at specific angles—0°, 25°, 50°, 75°, 100°, 125°, 150°, and 175°—and these angles were converted into radians for computational accuracy. The refractive index of the solvent (n_s), representing water, was set to 1.33. In contrast, the refractive index of the polymer particles (n_p), typical for many polymeric materials, was assigned a value of 1.59. The radius of gyration (R_g), which characterizes the spatial size distribution of the polymer particles, was derived from the hydrodynamic diameter and determined to be 58.5 nm (calculated as Rg = 117 nm / 2). For simplicity, the intensity of the incident light (I_0) was normalized to 1 at 0°.

Four different theoretical approaches were applied to model the scattering behavior. Rayleigh scattering was used to describe the behavior of small particles relative to the wavelength of light. In contrast, Mie scattering was applied to particles whose sizes are comparable to or larger than the wavelength. Debye scattering was utilized to account for the internal structure and interactions of polymer chains, and the Guinier approximation was used to analyze the low-angle scattering region, providing insights into the radius of gyration and the overall size of the polymer particles. By employing these models and the defined parameters, the simulations enabled a detailed analysis of the scattering patterns and a comparative evaluation of the different theoretical frameworks. This approach facilitated extracting structural information about the polymer particles in solution, offering a comprehensive understanding of their scattering behavior (Cheong and Woon,2011; Hammouda, 2010; Miles et al., 2001; Xu,2001).

Rayleigh scattering refers to the scattering of light by particles significantly smaller than the wavelength of the incident light, such as molecules or tiny particles. This phenomenon is closely associated with natural events, such as the scattering of sunlight by atmospheric gas molecules, which gives the sky its blue color. Rayleigh scattering is applicable when the particle diameter (d) is much smaller than the wavelength of light ($d \ll \lambda$), making it a fundamental example of the interaction between electromagnetic waves and small particles. One of the key characteristics of Rayleigh scattering is its strong wavelength dependence, as the intensity of scattered light is inversely proportional to the fourth power of the wavelength (λ^{-4}). This explains why shorter wavelengths, such as blue and violet light, are scattered much more than longer wavelengths, like red and yellow light. During the day, sunlight passing through the atmosphere scatters blue light more effectively, resulting in the blue appearance of the sky. At sunset, however, sunlight travels a longer path through the atmosphere, causing most of the blue light to scatter out of view, leaving behind the red and orange hues. Another important feature of Rayleigh scattering is its relationship to particle size. It is valid when the particle size is much smaller than the wavelength of light, typically d<λ/10, making it particularly suitable for modeling molecular-level scattering. More complex models, such as Mie scattering, are required for larger particles. Rayleigh scattering generally exhibits an isotropic profile, meaning the light is scattered equally in all directions. However, polarization effects can also occur depending on the scattering angle, with light scattered at a 90° angle being completely polarized. This polarization effect is significant in studying atmospheric scattering phenomena and has important applications in optical technologies. Rayleigh scattering is widely used to explain various natural and scientific phenomena. For instance, atmospheric science accounts for the blue color of the sky and the reddish hues of sunsets. Additionally, it is a valuable tool in fields such as optics, laser technology, biophysics, and astronomy. Understanding Rayleigh scattering has contributed to significant advancements in fundamental and applied sciences. The expressions for Rayleigh scattering are given below, where σ is the Rayleigh scattering cross-section, m is the relative refractive index of the particle, I_0 is the intensity of the incident light, and r is the distance between the observer and the particle (Miles et al.,2001; Xu, 2001; He et al., 2009; Jonasz and Fournier, 2011).

$$\sigma = \left[\frac{2\pi^5 d^6}{3\lambda^4}\right]\left(\frac{m^2-1}{m^2+1}\right)^2 \qquad (1)$$

$$I(\theta)=I_0\,\frac{[1+\cos^2(\theta)]\sigma}{2r^2} \qquad (2)$$

In the Rayleigh scattering code developed for this study, a function was defined to calculate the scattering intensity for small particles. This function expresses the angular dependence of the scattering intensity using the formula $I(\theta)\propto(1+\cos^2(\theta)$. This formula reflects the symmetric angular dependence of Rayleigh scattering and the low scattering intensity characteristic of small particles. Another important factor affecting the scattering intensity is the contrast between the refractive indices of the particle and the solvent. This contrast is calculated using the formula $((n_p^2-n_s^2)/(n_p^2+2n_s^2))^2$, where n_p represents the refractive index of the particle, and n_s represents the refractive index of the solvent. This calculation was performed to accurately model the effect of the optical difference between the particle and the solvent on the scattering intensity. The code provided the scattering angle in degrees and converted it to radians for calculations. This conversion was performed using the np.radians() function from the NumPy library. Subsequently, the defined Rayleigh scattering function was called to calculate the scattering intensity for each scattering angle. These intensities exhibit angular dependence consistent with the theoretical expectations of Rayleigh scattering, particularly when the particle size is much smaller than the wavelength of light. The calculated scattering intensities were normalized to make them comparable with other scattering models. The normalization process was performed by dividing the scattering intensity at each angle by the intensity at 0°, as described by the formula $I_{normalized}(\theta)=I(\theta)/I(0)$. This process ensured that all models could be evaluated on the same scale, allowing for a clearer comparison of angular dependencies.

Mie scattering refers to the phenomenon of light scattering by spherical particles whose sizes are comparable to or larger than the wavelength of the incident light. This process has significant applications in various fields, including atmospheric optics, colloid chemistry, biomedical imaging, and materials science. The theory developed by Gustav Mie in 1908 is based on solving Maxwell's equations in spherical coordinates. Mie theory enables the calculation of the intensity, polarization, and angular distribution of scattered light as functions of parameters such as particle size, refractive index, and the wavelength of the incident light. The foundation of Mie's theory involves several key steps. First, the Helmholtz equation, which describes the propagation of electromagnetic waves, is solved in spherical coordinates. The incident and scattered electromagnetic fields are then expanded into partial waves using spherical harmonics. Boundary conditions, which require the continuity of the electric and magnetic fields at the particle's surface, are applied to derive equations for the amplitudes of the partial waves. Mie coefficients (a and b) amplitudes are calculated from the boundary conditions. The scattering amplitudes ($S_1(\theta)$ and $S_2(\theta)$), representing the two orthogonal components of the scattered electric field, are determined using the Mie coefficients and angular functions. Finally, the scattering intensity, proportional to the sum of the squares of the scattering amplitudes, is computed. The mathematical expressions for Mie scattering are given as follows. In these expressions, the scattering cross-section is denoted by σ, m is the particle's refractive index, x is the size parameter of the particle, ξ' and their derivatives are the Riccati-Bessel functions, and γ, τ are the Legendre polynomials(Jonasz and Fournier, 2011; Cheong and Woon, 2011; Horvath, 2009; He et al., 2009).

$$\sigma = \frac{\lambda^2}{2\pi}\sum_{n=1}^{\infty}(2n+1)(\left|a_n\right|^2+\left|b_n\right|^2) \tag{3}$$

$$a_n = \frac{m\psi_n(mx)\psi'_n(x) - \psi_n(x)\psi'_n(mx)}{m\psi_n(mx)\xi'_n(x) - \xi_n(x)\psi'_n(mx)} \tag{4}$$

$$b_n = \frac{\psi_n(mx)\psi'_n(x) - m\psi_n(x)\psi'_n(mx)}{\psi_n(mx)\xi'_n(x) - m\xi_n(x)\psi'_n(mx)} \tag{5}$$

$$S_1(\theta)=\sum_{n=1}^{\infty}\frac{2n+1}{n(n+1)}(a_n\gamma_n(\cos\theta)+b_n\tau_n(\cos\theta)) \tag{6}$$

$$S_2(\theta)=\sum_{n=1}^{\infty}\frac{2n+1}{n(n+1)}(a_n\tau_n(\cos\theta)+b_n\gamma_n(\cos\theta)) \tag{7}$$

$$I(\theta) = \frac{1}{2}(\left|S_1(\theta)\right|^2+\left|S_2(\theta)\right|^2) \tag{8}$$

In this study, the Mie scattering code implements a detailed mathematical model to calculate the scattering intensity for spherical particles whose size is comparable to or larger than the wavelength of light. At its core, the code uses Mie theory, which describes the interaction of electromagnetic waves with spherical particles. The function mie_scattering_intensity takes three main parameters: the complex refractive index, the size parameter, and the scattering angle. The size parameter is calculated using the formula x=2πr/λ. This parameter is critical in determining the scattering behavior and has been accurately implemented in the code. The Mie coefficients (an and bn) are calculated using Riccati-Bessel functions, which are essential for determining the amplitude of the scattered electromagnetic field. Additionally, angular functions are computed for each scattering angle to determine the angular distribution of the scattered light. The series summation is terminated using the Wiscombe criterion, max ≈ x+4x1/3+2, ensuring convergence and computational efficiency. As a result, the Mie scattering model successfully captures the characteristic features of large particles, such as strong forward scattering, sharp angular dependencies, and interference patterns. The code normalizes the results to the intensity at 0° to enable comparison with other scattering models.

Debye scattering is a phenomenon that arises from the interaction of light with small particles, such as polymer molecules, colloidal particles, or macromolecules. It is particularly applicable when the size of the particles is much smaller than the wavelength of the incident light (d≪λ) and is often considered a generalization of Rayleigh scattering. This type of scattering is widely used to study key physicochemical parameters in polymer solutions, including molecular weight, structural properties, particle size distribution, and interparticle interactions. One of the defining characteristics of Debye scattering is its applicability to small particles, making it especially relevant for systems such as polymer chains, colloidal particles, and nanostructures. It provides valuable insights into structural features such as particle size, shape, radius of gyration (Rg), and molecular weight (Mw). It can also reveal information about chain flexibility and branching for polymer chains. In dilute solutions, where interparticle interactions are negligible, the scattering intensity is directly related to the form factor (P(q)), allowing for particle structure and dynamics analysis. Beyond polymers, Debye scattering is extensively applied in colloidal systems to determine particle size, shape, and interactions and assess stability and aggregation behavior. Biophysics and biochemistry investigate the structural properties of proteins, DNA, and other biomolecules and the behavior of macromolecular complexes in solutions. In materials science, Debye scattering is crucial in characterizing nanomaterials and composites, providing insights into particle size distribution and surface properties. With its broad range of applications, Debye scattering is an indispensable tool in fundamental research and industrial applications. It is particularly valuable in fields such as polymer science, colloidal systems, biophysics, and materials science, where understanding and controlling the structural properties of particles is essential. The formulas for Debye scattering are given below, where q is the scattering vector, n is the refractive index of the medium, P(q) is the form factor dependent on interparticle interactions, S(q) is the structure factor dependent on particle shape (equal to 1 in dilute solutions), R is the particle radius, and Rg is the radius of gyration for polymers (Shen and Wang,2010; Jones,1999;Wieder and Fuess,1997;Wyatt, 1993).

$$q = \frac{4\pi n}{\lambda}\sin(\theta/2) \qquad (9)$$

$$I(q) = I_0 P(q) S(q) \qquad (10)$$

$$P(q) = \left[\frac{3(\sin(qR) - qR\cos(qR)}{(qR)^3}\right]^2 \qquad (11)$$

$$P(q) = \left[\frac{2(e^{-(qR_g)^2} + (qR_g)^2 - 1}{(qR_g)^4}\right] \qquad (12)$$

$$S(q) = \frac{1}{1 + \beta(q)\Phi} \qquad (13)$$

$$I(q) = I_0\left[\frac{2(e^{-(qR_g)^2} + (qR_g)^2 - 1}{(qR_g)^4}\right] \qquad (14)$$

In this study, the Debye scattering code is based on the assumption that polymer chains consist of randomly oriented segments, and it calculates the scattering intensity using the Debye form factor. The function debye scattering takes the scattering vector's magnitude and the gyration's radius as input parameters. The scattering form factor is computed; for very small (qRg)2 values, a Taylor series expansion is applied to improve accuracy. This ensures precise calculations for small q values correspond to low scattering angles.

The Debye scattering model successfully represents the random coil structure of polymer chains and their internal interactions. After calculating the scattering intensity, the results are normalized to the intensity at 0° to allow for direct comparison with other models. This normalization ensures that the angular dependence of Debye scattering can be effectively visualized and analyzed. Overall, the Debye scattering model provides a robust framework for understanding polymer chains' internal structure and behavior in solutions.

The Guinier-Porod model is a widely used framework for interpreting the scattering behavior of polymers and similar soft materials in experiments such as small-angle X-ray scattering (SAXS) or small-angle neutron scattering (SANS). It describes how the intensity of scattered radiation or light changes as a function of the scattering vector, denoted as q. This model effectively combines two distinct scattering regimes: observed at low q values (small angles) and high q values (large angles). In laser light scattering, Guinier analysis can be applied to study the size and structural properties of polymers or particles, particularly at small angles and in dilute solutions. However, the range of the scattering vector q and the measurement conditions in this technique determine the limitations of the analysis. In the low q regime, the scattering intensity provides information about the overall size and shape of the polymer. This is called the Guinier regime, where the intensity decreases exponentially with increasing q. The rate of this exponential decay is related to the polymer's radius of gyration, which quantifies the spatial distribution of the polymer chain. At high q values, the scattering intensity follows a power-law decay known as the Porod regime. In this region, the intensity decreases as a power of q, and the exponent of this decay reveals details about the polymer's surface structure or fractal properties. For instance, a smooth surface typically corresponds to a specific exponent, while a rough or fractal surface results in a different value. The Guinier-Porod model seamlessly bridges these two regimes, enabling researchers to analyze scattering data across the entire range of q. By fitting experimental data into this model, key structural parameters of the polymer, such as its size, shape, and surface characteristics, can be extracted. This makes the model an essential tool for studying the structural properties of polymers and other complex materials. The mathematical expression for the Guinier approximation is provided in equation (15) (Marangoni and Pensini,2025; Wei and Hore, 2021; Zheng and Best, 2018; Hammouda, 2010).

$$I(q) = I(0).e^{\left(\frac{-q^2 R_g^{\,2}}{3}\right)},\ q \ll 1/R_g \qquad (15)$$

The Guinier scattering code applies a simplified approach to determine particle size at low scattering angles. The function guinier_scattering calculates the scattering intensity using the scattering vector, the radius of gyration, and the intensity at zero angles. Guinier approximation is based on the equation (15). he code implements this formula to model the scattering behavior at low angles with high precision. The Guinier scattering model is particularly effective for determining particle size in the low-angle regime. The calculated intensities are normalized to the value at 0° to facilitate comparison with other scattering models. This normalization ensures that the characteristic features of Guinier scattering can be visualized and analyzed. As a result, the Guinier approximation provides a reliable and efficient method for estimating particle size in polymer solutions.

3. Results and Discussion

Rayleigh scattering (Figure 1) exhibits a distinct angular dependence and behavior, particularly for small particles relative to the wavelength of light. At 0°, the scattering intensity starts at 0.031329, which is relatively low compared to other scattering models. This indicates that Rayleigh scattering primarily applies to small particles, which scatter light less effectively. As the angle increases, the intensity decreases, reaching values such as 0.028532 at 25°, 0.022137 at 50°, and 0.016714 at 75°. However, at higher angles, such as 150° and 175°, the intensity begins to rise again, increasing from 0.027413 at 150° to 0.031210 at 175°. This behavior reflects the symmetric nature of Rayleigh scattering, which follows the angular dependence described by the formula $1+\cos^2(\theta)$. As a result, the intensity decreases with increasing angles but shows a characteristic rise at larger angles due to the symmetry of the scattering pattern. Physically, Rayleigh scattering is most relevant for small particles, where the particle size is much smaller than the wavelength of light. This makes it suitable for modeling the scattering behavior of small polymer aggregates or individual molecules. The low intensity and symmetric angular dependence observed in Rayleigh scattering highlight that small particles scatter light less efficiently, and the scattering pattern is primarily determined by the angular dependence rather than the particle size. This symmetry and low scattering efficiency are key characteristics of Rayleigh scattering, making it distinct from other scattering models.

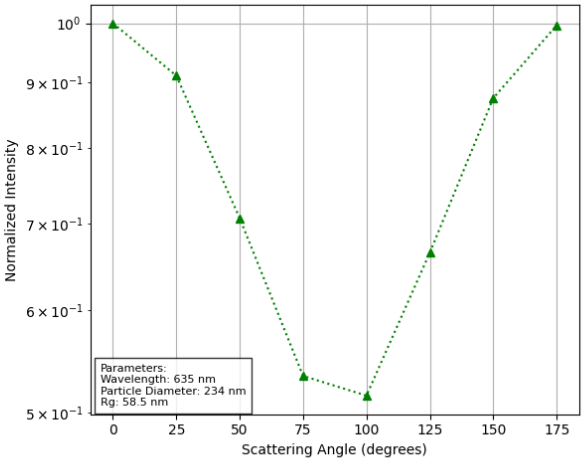

Figure 1. Rayleigh scattering intensity as a function of angle.

Mie scattering (Figure 2) demonstrates a distinct angular dependence and behavior, particularly for larger particles where the particle size is comparable to or greater than the wavelength of light. At 0°, the scattering intensity is 1.204984, the highest initial intensity compared to other scattering models. This indicates that Mie scattering is highly effective for large particles as they scatter light more strongly. As the angle increases, the intensity decreases, reaching values such as 1.065229 at 25°, 0.757242 at 50°, and 0.490584 at 75°. However, at certain angles, such as 125° and 150°, the intensity shows an increase, rising from 0.412427 at 125° to 0.496620 at 150°. These fluctuations in intensity are characteristic of Mie scattering and arise due to interference effects caused by the interaction of light waves scattered from different parts of the particle. This makes the angular dependence of Mie scattering more complex compared to other models. Physically, Mie scattering is most relevant for large particles, where the particle size is comparable to or larger than the wavelength of light. This makes it suitable for modeling the scattering behavior of large polymer aggregates or colloidal particles. The observed fluctuations in intensity result from interference effects, where light waves reflected from the particle's surface interact constructively or destructively. These interference patterns provide valuable insights into how the size and shape of particles influence the scattering intensity, making Mie scattering a powerful tool for studying larger particles.

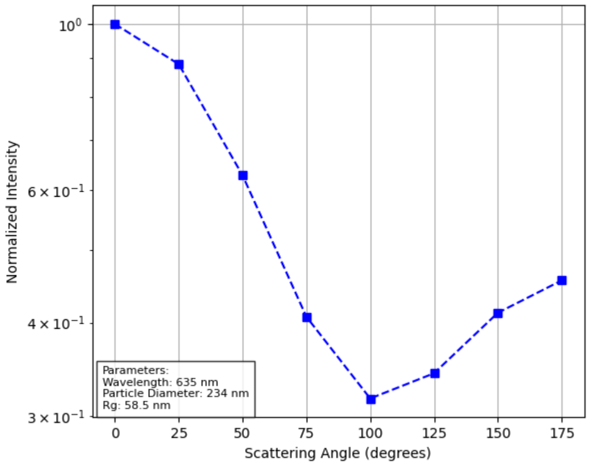

Figure 2. Mie scattering intensity as a function of angle.

Debye scattering (Figure 3) exhibits a smooth and predictable angular dependence, reflecting polymer chains' random structure and segmental correlations. At 0°, the scattering intensity starts at 1.000000, which, although not normalized, is lower than other scattering models' initial intensities. As the angle increases, the intensity decreases steadily, with values such as 0.963985 at 25°, 0.872616 at 50°, 0.761630 at 75°, and 0.661322 at 100°. This consistent decline in intensity is characteristic of Debye scattering and highlights the random coil structure of polymer chains and the correlations between their segments. Unlike other models, Debye scattering does not exhibit fluctuations in intensity, indicating that interference effects are negligible and that the polymer chains are uniformly distributed. Physically, Debye scattering is particularly suited for analyzing the molecular size and shape of polymer chains in solution. It accounts for the random arrangement of polymer segments and their correlations, making it an effective model for studying polymer solutions. The smooth decrease in intensity with increasing angle reflects the homogeneous distribution of polymer chains and the influence of segmental correlations on the scattering behavior. This regularity and lack of interference effects distinguish Debye scattering from other models, providing valuable insights into the structural properties of polymers in solution.

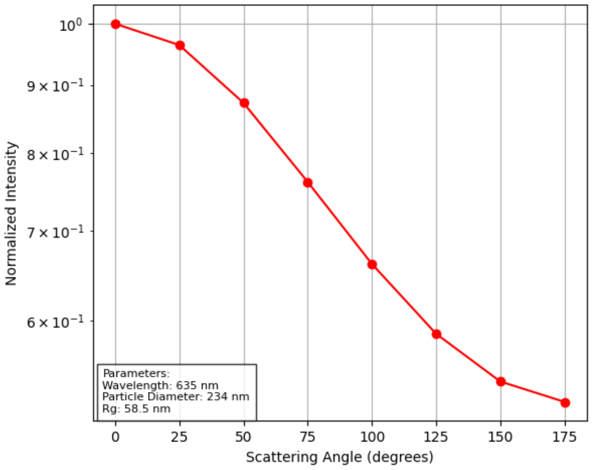

Figure 3. Debye scattering intensity as a function of angle.

The Guinier approximation demonstrates a smooth and exponential angular dependence, which is particularly effective at low angles for understanding particle size. At 0°, the scattering intensity starts at 1.000000, indicating a relatively high initial intensity compared to other models. As the angle increases, the intensity decreases steadily, with values such as 0.963657 at 25°, 0.868364 at 50°, 0.746127 at 75°, and 0.628927 at 100°. This consistent decline reflects the exponential nature of the Guinier approximation, which is most accurate at low angles. The regular decrease in intensity highlights the model's suitability for analyzing particle size and its limitations at higher angles, where the approximation becomes less reliable. Physically, the Guinier approximation is particularly useful for determining particle size in the low-angle scattering regime. The exponential decrease in intensity with increasing angle provides insights into the overall size and distribution of particles. The model's accuracy at low angles makes it a valuable tool for studying the structural properties of particles. In contrast, its limitations at higher angles emphasize the need for complementary models to describe scattering behavior fully. The smooth and predictable nature of the Guinier approximation underscores its effectiveness in analyzing particle size in systems where low-angle scattering dominates.

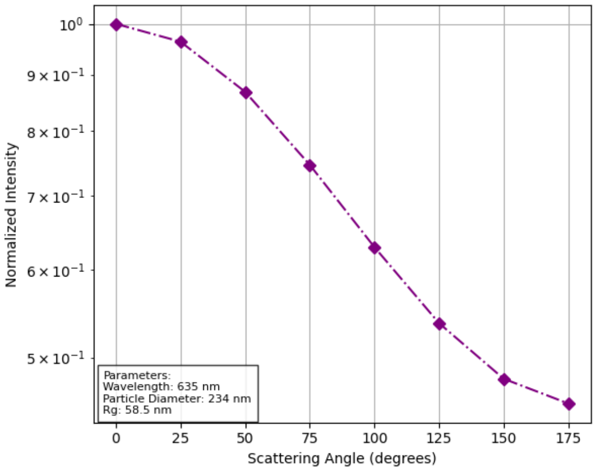

Figure 4. Guinier scattering intensity as a function of angle.

Figure 5 compares four scattering models—Mie scattering, Debye scattering, Rayleigh scattering, and the Guinier approximation—applied to polymer solutions. The graph shows the normalized scattering intensity as a function of the scattering angle, ranging from 0° to 175°. The parameters used in the simulation include a wavelength of 635 nm, a particle diameter of 234 nm, and a radius of gyration (Rg) of 58.5 nm. Rayleigh scattering, which is relevant for small particles, begins with a lower intensity at 0° and decreases with angle until around 100°, after which it increases symmetrically at higher angles, following the $1+\cos^2(\theta)$ angular dependence. Mie scattering exhibits the highest initial intensity at 0°, reflecting its applicability to large particles. The intensity decreases sharply with increasing angle, showing characteristic fluctuations at higher angles due to interference effects caused by the particle size being comparable to the wavelength of light. In contrast, Debye scattering starts at a normalized intensity of 1.0. It decreases smoothly and consistently with the angle, highlighting its suitability for analyzing the random coil structure and segmental correlations of polymer chains. Finally, the Guinier approximation also starts at a normalized intensity of 1.0. It exhibits an exponential decrease in intensity with increasing angle, demonstrating its effectiveness for low-angle scattering analysis and particle size determination. This comparison highlights the distinct angular dependencies and applications of each model. Mie scattering is ideal for large particles, Debye scattering is suited for polymer chains, Rayleigh scattering is effective for small particles, and the Guinier approximation is most accurate at low angles for determining particle size and radius of gyration.

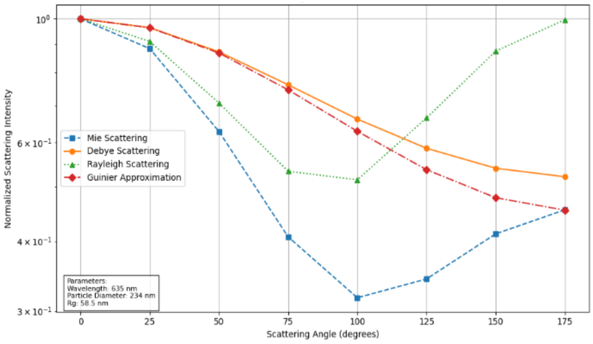

Figure 5. Comparison of different scattering models for polymer solutions.

Considering the references given in the introduction, this study, supported by controlled simulations, has increased model reliability by visualizing the behavior of theoretical assumptions in experimental scenarios. In particular, investigations over an angular range of 0°-175° revealed dynamics such as symmetric density variations at high angles. Moreover, the relationship established between hydrodynamic diameter and gyration radius provides a methodological contribution that strengthens the theoretical bridge in particle size determination, while the validation of the Debye model for random sequestered structures highlights its effectiveness in polymer characterization. The proposed multiscale analysis approach with Guinier-Mie integration at low angles and observations on the angular dependence of the models are considered important in the study.

4. Conclusion

The results of this study provide a comprehensive comparison of the angular dependencies of different scattering models—Rayleigh, Mie, Debye, and the Guinier approximation—applied to polymer solutions. Each model represents distinct physical conditions and particle characteristics, offering valuable insights into the scattering behavior of particles under various scenarios. Rayleigh scattering is most applicable to small particles, where the particle size is significantly smaller than the wavelength of light. The angular dependence is symmetric, with scattering intensity starting low at 0°, decreasing to 100°, and then increasing symmetrically at higher angles. This behavior highlights the limited scattering efficiency of small particles and the symmetric nature of their interaction with light. Mie scattering is particularly suitable for large particles, exhibiting a complex angular dependence with noticeable fluctuations. These fluctuations arise from interference effects, which cause alternating increases and decreases in scattering intensity at higher angles. This makes Mie scattering an effective model for analyzing the optical properties of large particles or aggregates. Conversely, Debye scattering reflects the random coil structure of polymer chains. Its angular dependence is smooth and regular, with scattering intensity decreasing steadily as the angle increases. This model is well-suited for studying the molecular size, shape, and interactions of polymer chains in solution, making it a reliable tool for analyzing polymer solutions. The Guinier approximation is particularly effective at low angles, providing accurate insights into particle size and the radius of gyration. The angular dependence is characterized by an exponential decrease in intensity as the angle increases. However, the model's reliability diminishes at higher angles, making it most suitable for low-angle scattering analysis.

In conclusion, this comparison underscores the importance of selecting the appropriate scattering model based on the particle size, structure, and experimental conditions. Rayleigh scattering is effective for small particles, Mie scattering is ideal for large particles, Debye scattering is best for polymer chains, and the Guinier approximation excels at low-angle particle size analysis. These models collectively serve as powerful tools for interpreting experimental data and understanding the scattering behavior of polymer solutions.

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