

## Theoretical Modelling of Molecular Mechanisms in Stimuli-Responsive Polymers

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**Abstract :** Context: Thermo-responsive polymers are materials that undergo significant changes in their physical properties in response to temperature changes. These polymers have gained significant attention in research due to their potential applications in various industries and medicine. However, the molecular mechanisms underlying their behavior are not well understood, particularly in relation to cosolvency, which is crucial for practical applications. Research Aim: This study aimed to theoretically investigate the phenomenon of cosolvency in long-chain polymers using the Flory-Huggins statistical-mechanical framework. The main objective was to understand the interactions between the polymer, solvent, and cosolvent under different conditions. Methodology: The research employed a combination of Monte Carlo computer simulations and advanced machine-learning methods. The Flory-Huggins mean field theory was used as the basis for the simulations. Spinodal graphs and ternary plots were utilized to develop an initial computer model for predicting polymer behavior. Molecular dynamic simulations were conducted to mimic real-life polymer systems. Machine learning techniques were incorporated to enhance the accuracy and reliability of the simulations. Findings: The simulations revealed that the addition of very low or very high volumes of cosolvent molecules resulted in smaller radii of gyration for the polymer, indicating poor miscibility. However, intermediate volume fractions of cosolvent led to higher radii of gyration, suggesting improved miscibility. These findings provide a possible microscopic explanation for the cosolvency phenomenon in polymer systems. Theoretical Importance: This research contributes to a better understanding of the behavior of thermo-responsive polymers and the role of cosolvency. The findings provide insights into the molecular mechanisms underlying cosolvency and offer specific predictions for future experimental investigations. The study also presents a more rigorous analysis of the Flory-Huggins free energy theory in the context of polymer systems. Data Collection and Analysis Procedures: The data for this study was collected through Monte Carlo computer simulations and molecular dynamic simulations. The interactions between the polymer, solvent, and cosolvent were analyzed using the Flory-Huggins mean field theory. Machine learning techniques were employed to enhance the accuracy of the simulations. The collected data was then analyzed to determine the impact of cosolvent volume fractions on the radii of gyration of the polymer. Question Addressed: The research addressed the question of how cosolvency affects the behavior of long-chain polymers. Specifically, the study aimed to investigate the interactions between the polymer, solvent, and cosolvent under different volume fractions and understand the resulting changes in the radii of gyration. Conclusion: In conclusion, this study utilized theoretical modeling and computer simulations to investigate the phenomenon of cosolvency in long-chain polymers. The findings suggest that moderate cosolvent volume fractions can lead to improved miscibility, as indicated by higher radii of gyration. These insights contribute to a better understanding of the molecular mechanisms underlying cosolvency in polymer systems and provide predictions for future experimental studies. The research also enhances the theoretical analysis of the Flory-Huggins free energy theory.

**Keywords :** molecular modelling, flory-huggins, cosolvency, stimuli-responsive polymers

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