# *Comparison of the Effect of Poly (N-vinyl Caprolactam) and Poly (N-isopropyl Acrylamide) trimers on the Stability of Hydrated Na-montmorillonite: A Molecular Dynamics Study*

**Moussa Camara[1], Hualin Liao[1], Jiafang Xu[*1], Jun Zhang[2*]**

1. *Shandong Provincial Key Laboratory of Oilfield Chemistry, Key Laboratory of Unconventional Oil & Gas Development, School of Petroleum Engineering, China University of Petroleum, Qingdao, China*
2. *School of Material Science & Engineering*

** Corresponding authors. Email: xjiafang@upc.edu.cn, dynamic_zh@163.com*

## *Abstract*

In the present study, we performed a molecular dynamics (MD) simulation of the intercalation of poly (N-isopropyl acrylamide) $(NIPAM)_3$ and poly (N-vinyl caprolactam) $(NVCL)_3$ trimers into Na-montmorillonite (Na-Mt) to evaluate their effect on the interlayer structure and the stability of hydrated Na-Mt. The impact of both trimers on the interlayer species and their dynamics properties at different temperature in a canonical ensemble (NVT) were investigated. The results showed that the electrostatic forces exerted by Na cations on $H_2O$ molecules and the interlayer $H_2O$ molecules arrangement are not affected by the rise in temperature after adding both trimers. Trimers addition reinforced the structure of interlayer $H_2O$ molecules so that the effect of temperature increase on them became negligible. The structural dynamics evolution of the radius of gyration of both trimers showed the existence of conformation changes when temperature increased. These conformational changes are more complex in the case of $(NVCL)_3$ than $(NIPAM)_3$ due to its large monomers. Both trimers reduced the mobility of interlayer particles with a better inhibition effect obtained for $(NVCL)_3$ compared to $(NIPAM)_3$. The concentration profile of interlayer's species showed the affinity of Na cations for clay mineral surfaces while $H_2O$ molecules moved away. Compared these two trimers, the most stable state of Na-Mt is achieved with $(NVCL)_3$. These results could help highlight the inhibition properties of $(NIPAM)_3$ and $(NVCL)_3$ on hydrated Na-Mt and to predict its stability against environmental condition changes.

***Key words:*** Na-Mt, Trimer, Thermosensitive polymers, Molecular dynamics, Radial distribution function, Self-diffusion coefficient, Radius of gyration, Concentration profile.