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**For a Safe Diamide Extraction Process, Elucidated by Atomistic Simulations** BAOFU QIAO, Department of Materials Science and Engineering, Northwestern University, ROSS J. ELLIS, Chemical Sciences and Engineering Division , Argonne National Libboratory, MONICA OLVERA DE LA CRUZ[1], Department of Materials Science and Engineering, Northwestern University — The diamide extraction process has been successfully employed in separating trivalent actinides from used nuclear fuels. The extractant, which is an amphiphilic molecule with a metal-binding polar headgroup and hydrophobic tail, binds the actinides, thus extracting them from the aqueous phase into the oil phase. However, the oil phase will split into two phases, once a critical concentration of actinide is reached. This phase splitting is suspected to have caused the Red Oil events, which can decompose explosively. Therefore, it is extremely important for an extractant to have a high extraction efficiency, on one hand, and resist phase splitting, on the other. In comparison with DMDBTDMA, DMDOHEMA has both higher extraction efficiency and phase stability, which we suspect stem from the supramolecular aggregated structures influenced by the different extractant tails. To test our hypothesis, atomistic molecular dynamics simulations were performed on DMDBTDMA in bulk oil system and DMDOHEMA in bulk oil system. Our preliminary results indicate that DMBTDMA is more disposed toward formation of chain-like aggregates, especially at lower water concentration, in comparison with the branched structures observed in DMDOHEMA.

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