INDIAN INSTITUTE OF TECHNOLOGY GUWAHATI
SHORT ABSTRACT OF THESIS

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Thesis Title: **Atomistic Insights Into the Transport of Solvents and Salt Ions in Polymer-based Membranes Constructed via an Interfacial Polymerization**

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Thesis Submitted to the Department/ Center	:	**Chemical Engineering**
Date of completion of Thesis Viva-Voce Exam	:	**24/06/2025**
Key words for description of Thesis Work	:	Membrane Technologies, Molecular Dynamics

SHORT ABSTRACT

Membrane technology is vital for desalination and wastewater treatment, yet further performance enhancements are essential. This thesis presents a comprehensive computational study of polymer-based membranes—including polyamide, semi-aromatic, polyester, and polyimine—using equilibrium and non-equilibrium molecular dynamics simulations under various conditions. We evaluate their behavior in forward osmosis (FO) and nanofiltration (NF) processes to gain atomistic insights into solvent and solute transport. A semi-aromatic polyamide (SAPA) membrane was investigated in the FO process using Na_2SO_4 as the draw solute and pure water as the feed. The SAPA membrane showed excellent water permeability with no reverse solute flux. Additional equilibrium simulations with NaCl and Na_2SO_4 revealed selective ion transport mechanisms, offering insights for textile wastewater treatment. Cyclodextrin (CD)-based membranes were studied for water and hexane permeation. Contrary to expectations, both solvents bypassed the CD cavity, instead diffusing through polar ester-linked aggregate pores, with water showing significantly higher flux. This suggests the need to reassess the role of the CD cavity in transporting polar and non-polar solvents. For dye-contaminated wastewater, a polyimine membrane model was constructed and tested in NF simulations. It demonstrated high water flux, strong dye rejection, and good NaCl permeability, highlighting its potential for textile industry applications. Finally, solvent transport in polyamide nanofilm membranes was examined, focusing on solvent activation. DMF treatment enhanced methanol permeance by 300% via structural changes, which reversed upon drying. These findings elucidate solvent-membrane interactions and structural dynamics, offering pathways to energy-efficient separations.