Advancing fossil-free polymers through AI-powered polymer development

Society urgently requires polymers that are both safe and sustainable, yet current portfolios are dominated by fossil-based materials with environmental or toxicological concerns. Polymer Informatics (PI) – the fusion of polymer science with AI and machine learning – offers a promising route to accelerate the discovery of fossil-free, CO_2- and biobased polymers, reducing development cycles from years to months. Building on TNO's earlier work on data pipelines, AI models, and BigSMILES-based polymer fingerprinting, this presentation highlights how AI can now begin to handle the true complexity of real-world polymers, moving beyond homopolymers toward copolymers.

The presentation will outline remaining scientific and practical challenges, including data scarcity, polymer topology representation, formulation & processing, biodegradability prediction, and safety & sustainability. With respect to sustainability, predictability of Life Cycle Assessments is of particular interest, in order to align with policy-metrics. This makes renewable-carbon compliance a design variable rather than a reporting exercise. Finally, this presentation will demonstrate an end-to-end AI-guided design loop, specifically for polyesters, targeting textile applications.