![KBC - A Yokogawa Company logo]

Petro-SIM Polymers Powered by PREDICI

Petro-SIM® Polymer Modeling, powered by Predici polymer kinetic software, offers a comprehensive solution to address the complexities of polymerization reactions and polymer properties.

Seamlessly integrated with KBC Process Twin and Yokogawa's advanced process control technologies, this solution enables clients to analyze and monitor KPIs, both manually and with automated Petro-SIM digital twin, calibrate models, and optimize plant performance across the petrochemical-polymer supply chain, including polymer recycling for the circular economy. It also provides tools to track carbon intensity and decarbonize the supply chain from end-to-end.

Bringing **DECARBONIZATION** *to Life* ™

To remain competitive and meet required product specifications, polymer companies must address several key challenges in polymer production, including:

- **Understanding Polymer Chemistry** and polymerization reaction networks.
- **Analyzing Reaction Kinetics** and operating conditions on polymer properties.
- **Overcoming Lab-Scale and Scale-Up Issues** for developing new polymer grades and innovative technologies.
- **Monitoring Key Performance Indicators** and polymer grade changes, in both steady-state and dynamic modes.

Petro-SIM Polymers Modeling

Petro-SIM polymers, powered by Predici, offer the premier simulation package for modeling both steady-state and dynamic polymer processes, including depolymerization. Predici provides kinetic polymerization software. Additionally, it excels in modeling depolymerization and polymer degradation kinetics from radical copolymerization to living polymerizations in emulsion, suspension polymerizations, Ziegler-Natta catalyzed systems, and other polymerization kinetics. The unique Galerkin h-p-method enables the rigorous computation of complete molecular weight distributions of any form and up to any degree of polymerization with many additional properties.

Petro-SIM software allows you to control system challenges and manage the production and scheduling of desired polymer grades. By simulating the entire petrochemical-polymer supply chain in both steady-state and dynamic modes, you can optimize polymer grade transitions and operating conditions while enhancing profit margins.
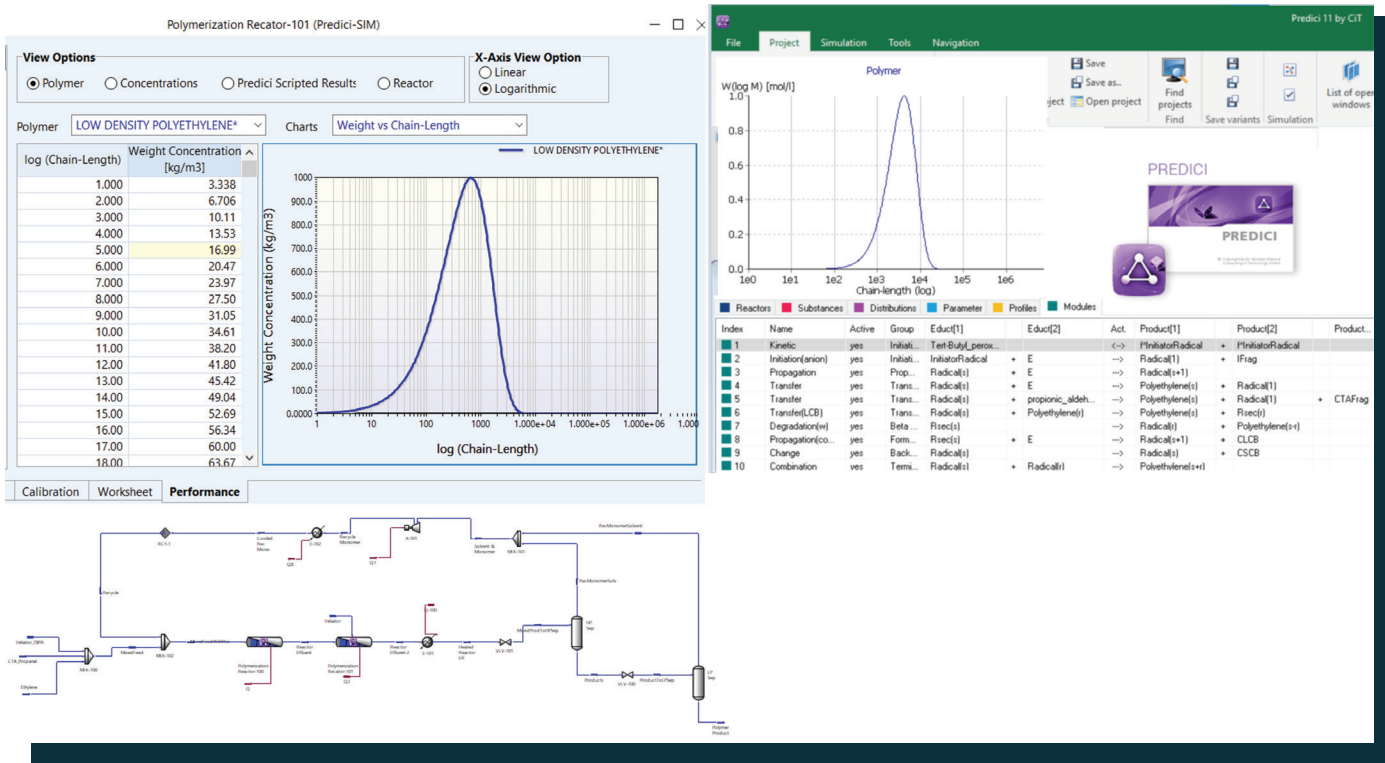
Key Features

Polymerization Reaction
Comprehensive kinetic packages with open mathematical structure for various reaction steps, propagation, termination, transfer (monomer, agent, polymer), depolymerization and polymer degradation, description of oligomers, chain-length dependent reactions, and many more.

Versatile Reactor Options
Support for different reactor types, multiple injection points for monomers, initiators, and solvents as well as multiple coolant streams.

Molecular Weight Distribution Analysis
Rigorous treatment of complete molecular weight distribution for all kinetic systems.

Kinetic Calibration & Parameter Estimation
Manipulate kinetic rate coefficients through parameter estimation and Petro-SIM software calibration, manually or automatically, with an automated Petro-SIM digital twin.

Polymerization Reactor Outputs
Presents polymerization reactor outputs including monomer conversion, polymer molecular properties (e.g. number, weight, polydispersity) and Melt Flow Index (MFI), polymer weight versus chain length, and temporal change of component concentration.

Advanced Thermodynamic Modeling
Integrates KBC Multiflash® Thermodynamic PC-SAFT EOS model in Petro-SIM process simulation for accurate predictions.

Polymer Components Databases and Polymer Stream Type
Integrates KBC Multiflash polymer database with Petro-SIM and defines Petro-SIM polymer stream type to present polymerstream properties such as weight average molecular weight (WAMW), Melt Flow Index (MFI), and particle size distribution (PSD).

Key Benefits

Gain Insights

Easily Analyze Polymer Production
Predict the impact of changing feeds (monomer, initiators, catalysts) and reactor operating conditions on yields, polymer specifications, and downstream facilities.

Confidently Accelerate Learning and Decision-Making
Evaluate cause-and-effect results through immersive simulation runs in both steady and dynamic modes.
Leverages a customizable Excel workbook to drive calibration, prediction, and optimize case runs.
Automatically generated and customizable Excel facilitates data analysis.

Monitor & Optimize Performance

Simplify Complex Processes
First principle modeling within plant-wide simulation containing polymerization, depolymerization reactor, heat exchanger, recycles, steam cracker furnace and column allows you to track mass and heat balances across your entire petrochemical-polymer plant. Petro-SIM digital twin can monitor and predict key process indicators to improve polymerization reactor performance and optimize feed, catalyst consumptions, and operating conditions.

Increase Efficiency and Profitability While Improving Polymer Product Specification
Perform real-time optimization by integrating Petro-SIM digital twin and RTO withAPC. This integration minimizes grade change time and downgraded products while maximizing production rates and product quality control (e.g., MFI).

Improve Yield, Reduce Energy Consumption, and Reduce Emissions
A high-fidelity Petro-SIM digital twin with real-time plant historian data enables plant-wide optimization and energy integration across your entire petrochemical-polymer-plastic recycling plant on a single platform. Applying Petro-SIM tools such as Meter, Historian, and Explorer for visualization and monitoring provides process insights that lead to effective, efficient decision-making. The digital twin can monitor and predict key process indicators to improve polymerization reactor performance and optimize processes and explore strategies to maximize profitability.

Research & Development

Accelerate New Technology Development
Virtually prototype and produce new product grades to develop new products.

Reduce Scale-Up Risks and Experiment Time for Plastic Circularity
Enhance efficiency in research and development for polymer and depolymerization processes.

A Unique Focus
Design. Operate. Improve. Sustain.

Design
Process Engineering
Engineering Design
CapEx Study
Feasibility Studies

Design With auto-configuration options, setting up the simulation environment is easy. Configure your component lists and choose the most relevant property package. Purpose-built with industry relevant technology, Petro-SIM software adapts to unit operations, utility options, and default stream property lists to suit your process simulation needs.

Improve
Debottlenecking
Process Engineering
Troubleshooting
Improvement Projects
Process Optimization

Improve At its core, Petro-SIM software's delivers reliable results to propel excellence. Its open platform architecture fosters seamless integration and collaboration, enabling your entire company to enhance efficiencies in process modelling workflows.

Operate
Process Engineering
Target Setting
Operating Standards
Environment & Safety

Operate Petro-SIM technology streamlines your process to provide access to relevant features, saving you valuable time and effort during model configuration. Petro-SIM simplifies complexity, giving you more time for analyzing results.

Sustain
Process Engineering
Performance Monitoring
Fouling Monitoring
Staff Training

Sustain Backed by industry-leading consulting expertise, we deliver tailored solutions to a wide range of clients. Additionally, our commitment to technical support via maintenance agreements ensures you're never alone to navigate challenges.

Fit-For-Purpose Process Simulation

Petro-SIM digital twin is a strategic tool designed to maximize your assets' value. Empowering you with the confidence to make informed decisions to improve your facility's performance, drive organizational excellence and bring decarbonization to life. Partner with us to reach the full potential of your assets and move your business toward success in the dynamic petrochemical-polymer industry.