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# Advanced simulation of polyolefin production

## Minimise grade transition times and reduce off-grade products using polymer modelling, process digital twins, and sensitivity analysis

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Polyolefins, derived from olefins, are essential materials in various industries due to their versatility, cost-effectiveness, and favourable mechanical properties. The global polyolefin market, particularly polyethylene, is experiencing significant growth, with some forecasts suggesting it could double over the next 20 years. However, the production process faces challenges, including complex polymerisation reactions that require precise control to achieve desired polymer specifications, such as bulk density and melt flow index (MFI).

The following study investigates the challenges in polymer production using process simulation software integrated with advanced kinetic polymerisation models. It focuses on real-time reactor performance, prediction of polymer properties under varying conditions, and strategies to minimise grade transition times and reduce off-grade products. In addition, sensitivity analysis evaluates the impact of different operating conditions on polymer yield and quality, providing actionable insights for optimising the polyolefin manufacturing process. Ultimately, the proposed approach supports more consistent product quality and helps lower production costs.

### Polyolefin market

Polyolefins are pivotal materials in packaging, automotive, construction, and consumer goods due to their versatility, durability, and low cost. Polyethylene accounts for roughly 34% of global plastic demand and continues to drive industry growth, according to recent market analysis.[1]

The polyolefin market is experiencing substantial growth, with the global polyethylene market valued at about $120 billion in 2024 and projected to reach $165 billion by 2030, reflecting a compound annual growth rate (CAGR) of around 5.5%.[1] Global polyethylene production now exceeds 100 million metric tons annually, underscoring its dominance within the broader polyolefin sector. Sustained demand across flexible packaging, construction materials, and advanced manufacturing is expected to drive capacity expansion through the next decade, highlighting the importance of process efficiency, product quality, and innovation in polymer production.

#### Production challenges

However, polyolefin production presents several challenges. The polymerisation process involves complex reactions and operating conditions that must be controlled to prevent reactor temperature runaways and achieve polymer-grade specifications, such as bulk density and MFI.

Lab-scale development and commercial scale-up for new polymer grades and technologies introduce further uncertainty. Variables such as monomer and comonomer composition, solvent modifiers, hydrogen flow rates, reactor conditions, and catalyst activity affect product properties. These factors make it difficult to consistently produce polyolefins with specific properties. Maintaining tight control over molecular weight distribution and MFI during grade transitions while minimising off-grade production remains one of the industry's greatest challenges.

Addressing these challenges is essential to meet market demand for high-quality polyolefin products. Therefore, manufacturers aim to validate process design and enhance performance through advanced monitoring, control, optimisation, and decarbonisation initiatives.

Applying polymerisation modelling software helps reduce scale-up risks, experimental time, and operational issues. It also improves design accuracy, monitoring, and control for specific polymer grades. In addition, polymerisation modelling software calibrates process models to enhance prediction accuracy for reactor performance, polymer yield, and product properties. Sensitivity analysis tools within the simulator identify key process parameters that affect yield and quality. This approach enables engineers to consistently achieve desired specifications.

The integrated platform, combining polymerisation reactor modelling, process digital twins, real-time optimisation (RTO), and advanced process control (APC), provides real-time prediction of polymer properties during grade transitions. This capability helps operators optimise operating conditions while reducing transition time and off-grade production. The result is a more efficient and cost-effective process.

### Methodology

Engineers can apply process simulation and digital twin technologies to monitor plant data, tune simulation models, calibrate them to match actual plant behaviour, and predict polymer properties using the following methodology. In this study, the software's historian and metering functions were used to connect real-time operational data to the polymer

**Generic polymerisation reactor KPIs and key process variables**

| Key performance indicators (KPIs) | Key process variables |
|---|---|
| • Polymer production rate/yield | • Feed flow rate |
| • Conversion | ▪ Monomer/comonomer flow rate |
| • Polymer properties | ▪ Solvent/modifier/hydrogen flow rate |
| ▪ Melt flow index (MFI) | • Utility flow rate/temperature |
| ▪ Polymer density (ρ) | |

Table 1

**Base case operating conditions**

| Base condition | Value |
|---|---|
| Temperature °C | 100 |
| Pressure, bar | 41.22 |
| Feed and catalyst mass flow rate, t/h | |
| Ethylene | 20 |
| 1-Hexene | 0.1 |
| Hydrogen | 0.001 |
| Isobutane | 16 |
| Catalyst A | 0.01 |
| Catalyst B | 0 |

Table 2

model. Integrating plant data with the model, including digital twin capabilities, enabled online calibration of the polymerisation model based on actual plant performance. The automated digital twin increased confidence in the model's accuracy and reliability, with further elaboration as follows:

- **Integrating plant data with simulation software**: The first step in setting up the process digital twin involved defining key performance indicators (KPIs) for polymer modelling and connecting the process simulator with plant data historians. This integration allowed engineers to monitor real-time operating data and plant performance alongside simulation results for continuous comparison and analysis.
- **Sensitivity analysis and strategy development**: The simulation software's sensitivity analysis tools helped engineers identify critical process parameters and operating conditions that influenced polymer yield and properties. Applying sensitivity analysis with optimisation enabled engineers to fine-tune the polymerisation reactor to improve efficiency and product performance.
- **Real-time monitoring and calibrating with process digital twin**: With plant data accessible within the simulation software, engineers monitored deviations between simulated and actual plant behaviour. This iterative process involved tuning reaction kinetic parameters to align simulation results with plant data. Using the calibrated model, engineers can predict key polymer properties, such as MFI, polymer density, and polydispersity index (PDI) to minimise off-grade products.

The process digital twin also supported operator training and decision-making. Engineers simulated grade changes before implementing them, reducing the risks of delays or errors.

The ultimate objective of using simulation software for polymer modelling was to analyse, monitor, predict, and optimise process variables, such as olefin feed, initiator, hydrogen, catalyst rates, temperature, and pressure. The goal was to enhance polymerisation reactor performance, achieve desired polymer properties, and minimise grade changes by reducing transition time and off-grade production. This study examined high-density polyethylene (HDPE), MFI, polymer conversion rate, and yield using comprehensive process modelling.

In the polymer industry, multiple product grades are often produced in a single production line. Switching catalysts is common, as different catalyst types produce polymers with distinct physical properties, such as molecular weight distribution, branching, tensile strength, impact resistance, and MFI.

In this study, catalyst type A was switched to catalyst type B to produce a polymer grade with higher MFI and lower density. By applying the simulation model within the process digital twin model, engineers could monitor real-time polymer MFI and maintain stable feed rates. This minimised off-grade production without delays caused by laboratory testing. The digital twin automatically ran and saved the simulation, enabling sensitivity analysis of how different parameters and operating conditions affected MFI, conversion rate, and yield without extensive reconfiguration.

A high-fidelity digital twin linked with real-time plant historian data enabled plant-wide optimisation and energy integration across the petrochemical, polymer, and plastic recycling plants on a single platform. By simulating the behaviour of both catalysts and resulting polymer properties, the digital twin fine-tuned the process to achieve the desired polymer grade quickly, minimising the off-spec production period during catalyst switches.

It tracked variables such as temperature, pressure, catalyst activity, and polymer properties, providing immediate feedback on process response to the new catalyst changes. This approach reduced trial-and-error and ensured faster transitions. Dynamic simulation helped find the best catalyst injection rate, reactor temperature profile, hydrogen and comonomer feed strategy, within the transition time.

### Sensitivity analysis and strategy development

The sensitivity analysis tools available in the process simulation software were applied to evaluate how key process variables and operating conditions impact KPIs. **Table 1** lists polymerisation KPIs and key process variables, highlighting examples of polymer MFI and density.

This analysis incorporates two KPIs, MFI and density, as polymer property metrics. The MFI is defined as the mass (in grams) of polymer that flows through a capillary of specified diameter and length within 10 minutes under pressure generated by a 2.16 kg load at 190°C.

Sensitivity analyses were conducted under the base operating conditions shown in **Table 2.** The process variables included temperature, pressure, mass flow rate of ethylene, hydrogen, and catalyst flow rate to evaluate their effect on polymer yield and properties, specifically MFI and density.

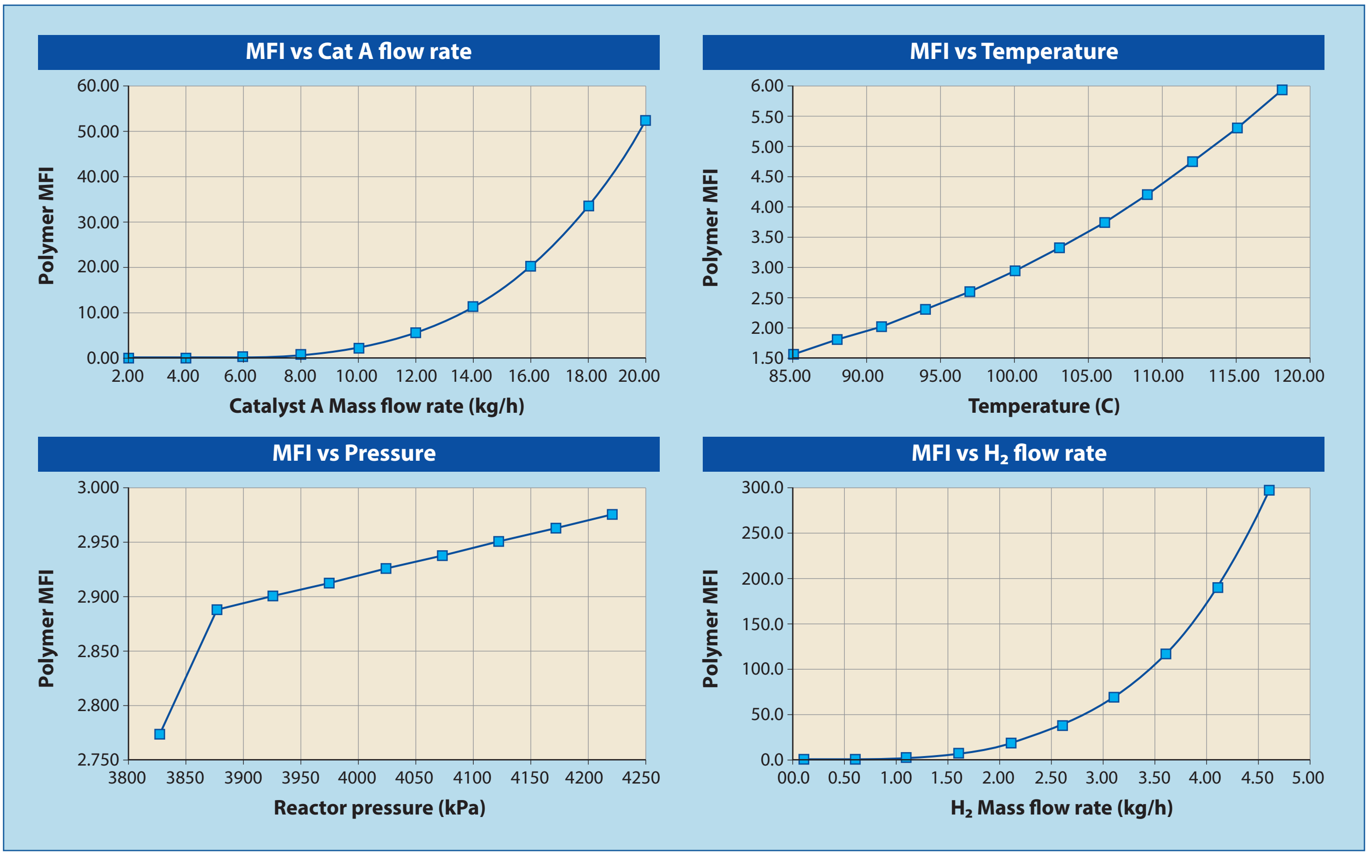


**Figure 1** Effect of operating conditions (catalyst A and B mass flow rates, temperature, pressure, and H2 mass flow rate) on polymer MFI

**Effect of operating conditions on polymer MFI**

As shown in **Figure 1**, increasing the catalyst mass flow rate, temperature, and pressure produces a higher polymer MFI.

- Increasing catalyst type A flow rate from 2 to 20 kg/hr raised MFI from 0.5 to 60 g/10 min.
- Raising temperature by 40% increased MFI from 1.5 to 6 g/10 min.
- Increasing pressure by 15% raised MFI from 2.75 to 3.5 g/10 min.
- Increasing hydrogen flow rate from 1 to 5 kg/hr spiked MFI from 0.5 to 300 g/10 min.

These insights enable engineers to adjust the catalyst mass feed rate, temperature, or pressure to reach the desired polymer MFI. They also support strategies to reduce off-grade product levels in silos. For instance, producing a polymer with a higher MFI that can be blended with an existing lower MFI polymer in off-grade silos to produce on-specification products becomes feasible.

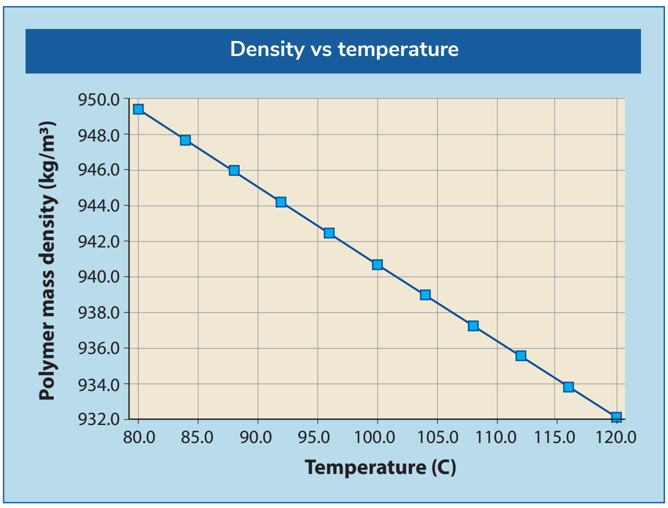


**Figure 2** Effect of temperature on polymer density

**Effect of operating conditions on polymer density**

As shown in **Figure 2**, temperature exerts the strongest influence on polymer density. A 40% temperature increase reduces polymer density from 950 to 932 kg/m³. In contrast,

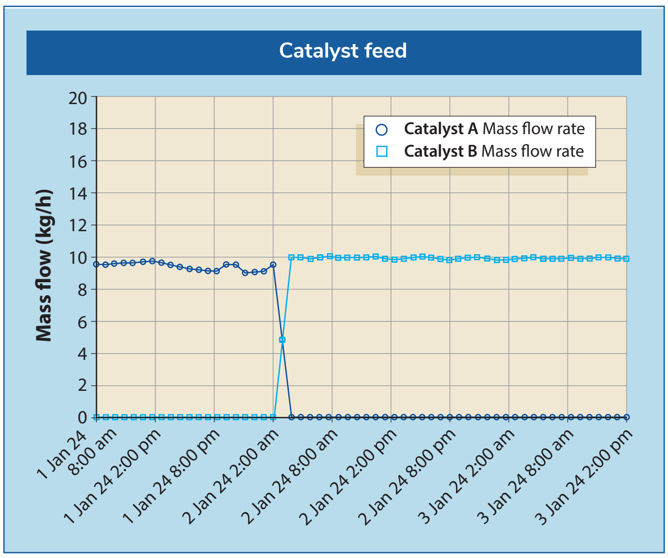


**Figure 3** Monitoring catalyst A and B feed flow rates during grade transition

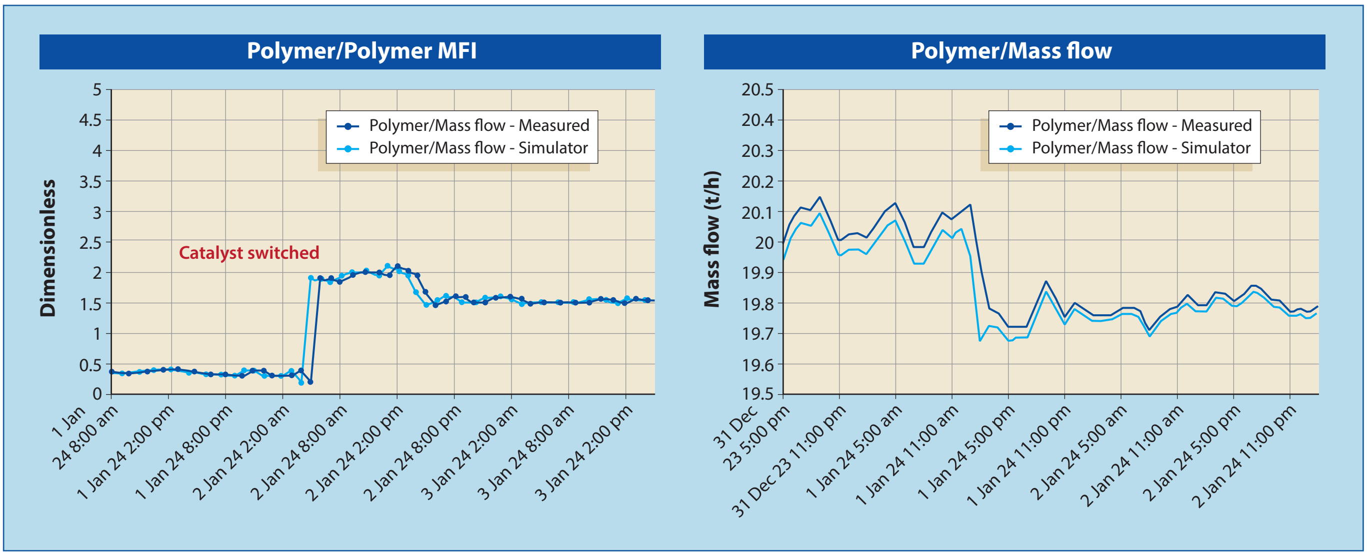


**Figure 4** Monitoring polymer MFI and mass flow rate: measured vs simulated data

variations in 1-hexene and hydrogen flow rates have a negligible impact, while changes in ethylene feed flow rate have a slight impact. These findings underscore the importance of precise temperature control in optimising polymer properties.

**Polymer process digital twin modelling analysis**

Beyond parameter sensitivity, the digital twin solution enables the monitoring and prediction of polymer properties during grade transitions. A dynamic process simulation model was developed to monitor polymer grade changes during catalyst transitions and predict polymer properties. The model was connected to plant historian data, and simulation results were validated against actual measurements to confirm accuracy. Once validated, the model was used to predict the evolution of polymer properties, such as MFI, density, and molecular weight, over time as feed and catalyst conditions changed. This made it possible to estimate the required transition time.

**Figure 3** shows catalyst flow rates over time during the transition from catalyst A to catalyst B. To achieve the polymer grade transition from MFI 0.2-0.4 g/10 min to MFI 1.4–1.6 g/10 min, approximately 12 hours of transition time was required. During this time, the MFI increased from 0.5 to 1.5 g/10 min, corresponding to catalysts A and B, respectively. **Figure 4** compares measured and simulated MFI results during the transition. During that time, the polymer mass flow rate revealed a slight decrease before stabilising.

By running the polymer modelling process digital twin, engineers could predict polymer properties in advance and reduce transition time, thereby reducing the off-grade products per transition. The off-grade production quantity is the product of transition time multiplied by the polymer production rate that is outside the specification range. Collectively, these results demonstrate how sensitivity analysis and digital twin prediction complement each other to optimise polymerisation performance while minimising off-grade production.

## Summary and conclusions

The adoption of a process simulation digital twin offers a promising solution to address polymerisation challenges in polyolefin production. By using advanced modelling and simulation capabilities, engineers can improve product quality and polymer properties while optimising operational conditions. The study showed that increasing catalyst mass flow rate, temperature, and hydrogen feed produced higher polymer MFI, while temperature increases have a negative impact on polymer density. Sensitivity analysis within the polymerisation reactor simulation clearly identified these relationships, allowing operators to fine-tune process parameters such as catalyst flow rate, temperature, and pressure to achieve desired polymer properties like MFI and density.

By enabling real-time monitoring and predictive analysis, the digital twin reduced grade transition time and minimised off-grade products, ultimately lowering cost. Additionally, the integration of polymer modelling with advanced process control (APC) systems and operator training simulators (OTS) enhanced decision-making, allowing users to validate control strategies and train operators in a safe, virtual environment. Dynamic polymer models can be linked with distributed control system (DCS) emulators in OTS. Additionally, these models can be connected to APC to tune proportional-integral-derivative (PID) before applying them.

Together, these capabilities support more efficient, indirectly lower emission polymer production and continue Bringing Decarbonization to Life.



**Reference**

**1** *Polyethylene Market Size* (2025-2030), Virtue Market Research, January 2025, VMR-1463.

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