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Technical letters,

Refinery-Petrochemical Operations Developments

Abbas A. Ezzat

Petrochemicals Engineering Department, Faculty of Engineering, Pharos University in Alexandria (PUA), Egypt

Abstract:
The global refinery and petrochemical sectors are currently facing unprecedented challenges stemming from fluctuating feedstock prices, rapid energy transitions, market volatility, and increasingly stringent environmental regulations. These factors have forced industry stakeholders to rethink conventional operational strategies and adopt innovative digital solutions to ensure competitiveness and sustainability. Among these emerging solutions, digital twin technologies (DTTs) have gained significant attention as transformative tools for the sector. Digital twin models (DTMs) create dynamic virtual representations of physical assets and processes by integrating real-time plant data, advanced simulations, and machine learning algorithms. This integration enables enhanced monitoring, predictive maintenance, and optimization of refinery and petrochemical operations. The present study investigates the practical applications of DTMs within integrated refinery–petrochemical complexes, emphasizing their role in key performance indicator (KPI) tracking, production accounting, supply chain optimization, and real-time process control. By enabling operators to anticipate disruptions, improve decision-making, and enhance safety, DTMs not only improve efficiency but also contribute to decarbonization and sustainability goals. A case study focusing on suspension polyvinyl chloride (S-PVC) polymerization highlights the tangible benefits of DTMs in improving product quality, output consistency, and operational safety. The findings demonstrate that the adoption of digital twins can significantly advance both economic performance and environmental responsibility, positioning them as essential enablers in the transition toward smarter, more resilient, and sustainable petrochemical industries.

Keywords: Digital Twin Modeling, Suspension, Polyvinyl Chloride, Initiators,

I. Introduction

Refinery-petrochemical complexes today are navigating a rapidly evolving landscape characterized by feedstock price volatility, increased energy efficiency demands, intensified process operations, and evolving regulatory environments.

These challenges have compelled companies to adopt advanced technological solutions to ensure resilience and competitiveness.

The proliferation of data across large-scale processes has further intensified the need for digital transformation.

Managing this influx of complex data necessitates intelligent systems capable of integrating, analyzing, and acting on real-time information to support optimal plant performance and compliance.

As a matter of fact, Digital twin models have emerged as a critical tool in this transformation.

II. Digital Twin Modeling, DTM [1, 2]

i. The applications of DTM enable continuous process optimization by simulating asset behavior and adjusting operational parameters to maintain safe, efficient, and environmentally compliant operations [3, 4].

The adoption of these models will help overcoming the operational challenges such as:

- Limited value chain integration.
- Complex machine learning implementations with high-dimensional data and latency issues.
- Insufficient predictive maintenance frameworks.
- Ongoing development and upgrade requirements.
- Stringent environmental regulations.

Therefore, by integrating digital twins with real-time analytics, machine learning algorithms, and intelligent control systems, refinery-petrochemical operations can significantly enhance plant productivity, reliability, and sustainability.

ii. Also, the Implementation of DTM systems provide a virtual mirror of physical assets, interfacing directly with real-time data streams from equipment and processes. These models are calibrated using historical and test data to maintain accuracy in energy and mass balances.

Their application spans across the full project lifecycle—from engineering and procurement to construction management, logistics, and marketing. Key outcomes from digital twin implementation including:

- Visualization of KPIs based on operational data.
- Enhanced production accounting through detailed mass and elemental balance analysis.
- Improved supply chain planning via optimized parameters.
- Real-time optimization to adjust set points and maximize margins.

By inputting operating parameters and feedstock characteristics into digital twin models, operators can better understand and influence process outcomes.

Figure 1 illustrates a typical digital twin system configuration used in petrochemical plants.

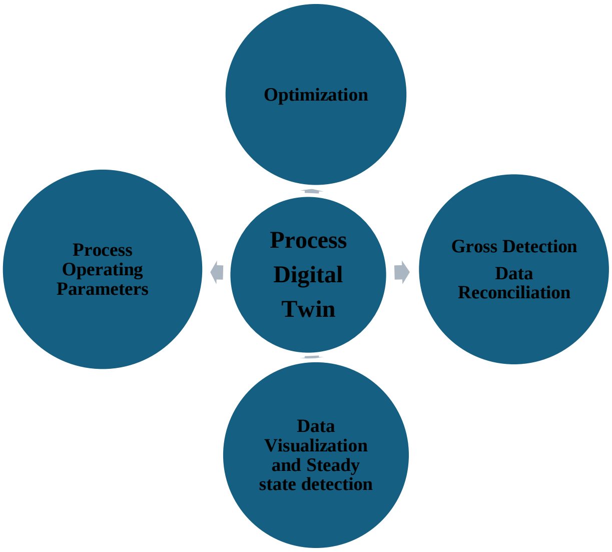

Figure 1: A digital twin model application.

III. The Main Applications of DTM

A. KPI Monitoring and Management

DTM enable continuous tracking of critical performance indicators, offering a comprehensive view of asset and process efficiency.

Historically, the separation of Information Technology (IT) and Operational Technology (OT) limited data utilization. The convergence of these domains—enabled by the Industrial Internet of Things (IIoT), machine learning, and feedback loop integration—now provides comprehensive insights into plant operations.

Digital twins compute intrinsic parameters such as yield, energy use, feedstock performance, equipment status, and emissions in real time.

This supports dynamic benchmarking, enabling continuous improvement and alignment with strategic goals. Organizations can thus enhance overall asset utilization and productivity.

B. Production Accounting

Accurate production accounting is vital for managing raw material inputs and controlling operational losses. DTM support detailed reconciliation of mass imbalances across process streams. These reconciliations help refine stream measurements and balance discrepancies, improving operational precision.

Also, DTM supports elemental balancing and facilitate more accurate and transparent loss attribution, contributing to better financial tracking and operational efficiency.

C. Supply Chain Optimization

DTM enhances planning and scheduling in integrated refinery-petrochemical complexes. They enable dynamic optimization of feedstock selection, product yields, and economic performance.

Advanced features include kinetic model calibration& validation, AI-based workflow automation, equipment health monitoring, and intelligent recalibration recommendations.

These tools will support the following parameters:

- Operational Target Optimization.
- Inventory Management.
- Maintenance Scheduling.
- Environmental Compliance.

As a result, organizations can reduce costs, improve responsiveness, and increase profitability across the value chain.

D. Real-Time Process Optimization

Real-Time Optimization (RTO) identifies gaps between actual and ideal performance. Digital twins analyze these gaps and suggest corrective measures such as:

- Process debottlenecking.
- Equipment tuning.
- Molecular-level feedstock adjustments.
- Margin enhancement.

Advanced Process Control (APC), when integrated with digital twin models, maintains dynamic stability in operations. Unlike traditional Distributed Control Systems (DCS), APC systems use RTO setpoints to maintain optimal conditions in a closed-loop framework.

Two model types are essential:

- Economic models for cost-effective operation.
- Steady-state models for identifying safe process limits.

This real-time synchronization bridges the gap between operational plans and actual performance, enhancing productivity and reducing energy and data losses.

IV. Case Study

In suspension Poly-vinychloride polymerization process, S-PVC, digital twin modeling has been applied to optimize production capacity under the following constraints [3]:

- Initiator selection.
- Reaction runaway prevention.
- Safety requirements.
- Reactor Cooling system limitations.
- Conversion efficiency.
- Product specifications.

The key operating parameters include chemical dosing, temperature and pressure profiles, reactor loading, and agitator dynamics. Initiator selection plays a pivotal role in balancing reaction kinetics and safety.

A. Reaction Kinetics and Control [5]

The polymerization process design of S-PVC is considered isothermal.

On the other hand, as the polymerization conversion increases, the heat generation rate rises, leading to tail-end temperature spikes. Temperature is controlled by different types of cooling jackets. Based on reactor design limitations, cooling limitations are considered.

For optimizing reactor cooling limitations, the strategy involves generating more heat during early conversion stages and less during later stages—achieved by selecting initiators that linearize the reaction rate. This enhances control and safety while improving productivity.

Figure 2 depicts the relation between Vinyl Chloride monomer conversion and the polymerization time

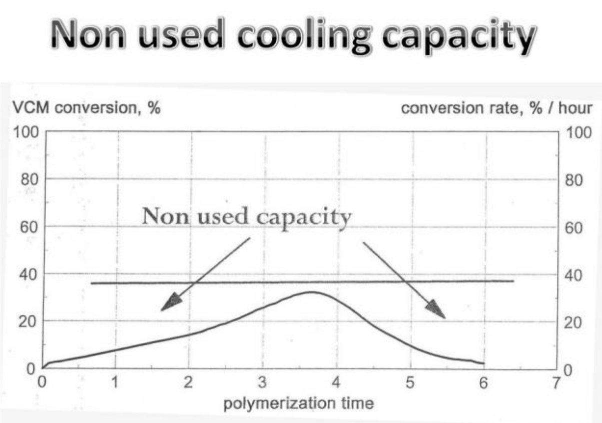

Figure 2: The relation between VCM monomer conversion, and polymerization time.

B. Initiator Selection Strategy

i. Normally, S-PVC processes operate between 45°C and 70°C, requiring optimum half-life initiators. The desired attributes include:
   - Optimum polymerization duration.
   - Stable handling and storage.
   - High efficiency per unit active oxygen.
   - Compatibility with heat exchange capacity.
   - Product specifications

   The dissociation rate of initiators is governed by:

$$K_d = A \cdot e^{\left(\frac{-E_a}{RT}\right)}$$

ii. Applying a single short half-life initiator often requires trade-offs between conversion rate and reactor safety to get on-spec products.

However, to attain maximum reactor yield, mixed initiators could be applied with varying half-lives to optimize plant operability.

C. Study outcomes

i) Mixed Initiator Application approach has been applied, with a combination of Ethyl Hexyl Peroxy Dicarbonate (EHP, 1h half-life @ 64°C) and Cumyl Peroxy Neodecanoate (CPN, 1h half-life @ 53°C).

   This study considered the following constraints [6]:
   - Initiator decay kinetics.
   - Phase-specific efficiency.
   - Post-pressure-drop behavior.
   - Conversion targets.

Figure 3 depicts a comparison between half-life initiator curves and high active peroxides.

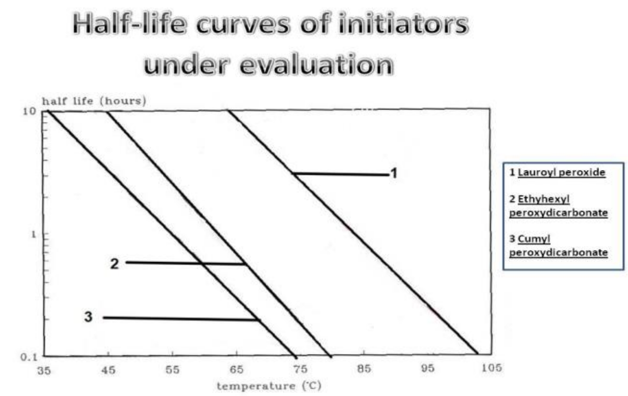

Figure 3: A comparison between half-life curves of applied initiators and the high active peroxides.

ii) DTM has enabled optimization evaluation for attaining fine-tuning of process parameters, including:
   - Reaction rate monitoring.
   - Agitator load.
   - Temperature and pressure profiling.
   - Reactor volume tracking.
   - Resin molecular weight control.
   - Production control variables included cycle times, rate constants, water injection, and volumetric loading.

iii) The evaluation of the Experimental Outcomes using EHP/CPN at 168/375 mg/kg resin and 53°C has conducted. Fig. 4 shows a comparison between a single EHP initiator and mixed EHP/CPN initiators.

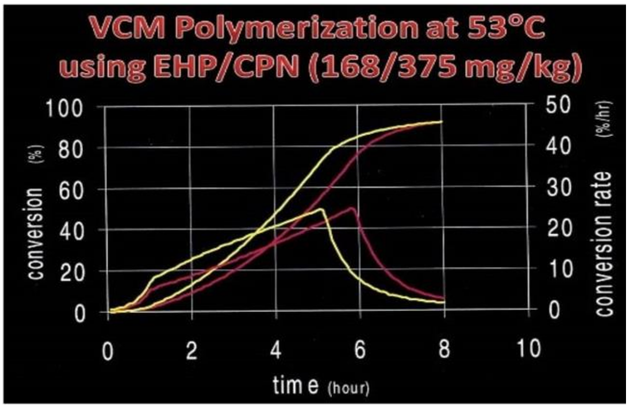

Figure 4: A comparison between single EHP initator and mixed EHP/CPN initiators 168/375 mg/kg resin.

The optimized approach of the study has revealed the following outcomes:

- 50-minute reduction in reactor cycle time per batch.
- 15% increase in specific productivity.
- Enhanced product quality (e.g., reduced fisheye formation).
- Stabilized reactor heat profile with reduced fouling.
- Improved pressure drop rate, minimizing carryover issues.

V. Takeaway

Digital twin technologies are becoming essential tools in refinery and petrochemical operations. Their ability to integrate real-time data, simulate performance, and drive continuous optimization positions them as critical enablers of sustainability and profitability.

The present study on S-PVC reactor optimization demonstrates how digital twin models can significantly improve output, reduce operational risks, and maintain product quality.

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