LUMMUS DIGITAL

WHITEPAPER

Digital Twin of a Hydrocracker

Harnessing Hybrid Intelligence for Operational Excellence

Transforming Hydrocracker Operations Through Advanced AI,

First-Principles Process Modeling, and Real-Time Optimization

A Joint Venture of Lummus Technology and TCG Digital
www.lummusdigital.com

Executive Summary

The global refining industry faces unprecedented challenges: tightening environmental regulations, volatile crude slates, fluctuating product demands, and the imperative to maximize operational efficiency while minimizing carbon footprint. Hydrocrackers, as critical units for converting heavy feedstocks into high-value middle distillates and petrochemical feedstocks, represent both significant capital investment and operational complexity.

Lummus Digital, a joint venture between Lummus Technology and TCG Digital, introduces a transformative approach to hydrocracker optimization through its Digital Twin solution. By integrating decades of process engineering expertise from Chevron Lummus Global (CLG) with cutting-edge artificial intelligence and machine learning capabilities, our HCU Reactor Performance Optimizer delivers measurable improvements in yield optimization, catalyst life management, and operational stability.

This whitepaper presents our comprehensive methodology for building and deploying digital twins for hydrocracking units, demonstrating how the fusion of first-principles process models with advanced data science creates unprecedented visibility into reactor performance and enables proactive, profit-maximizing operational decisions.

1. Introduction: The Imperative for Digital Transformation

1.1 The Strategic Role of Hydrocracking

Hydrocracking has emerged as the cornerstone technology for refineries seeking to maximize value from increasingly heavy and challenging crude slates. The ISOCRACKING® technology, offered by Chevron Lummus Global, represents the industry benchmark with more than 65 new units licensed since 2000. These units enable refiners to produce high-quality jet and diesel fuels, heavy naphtha for catalytic reforming, and premium feedstocks for FCC units and ethylene crackers.

The flexibility of modern hydrocrackers to selectively maximize naphtha, jet, or diesel products makes them invaluable assets. However, this flexibility also introduces operational complexity that demands sophisticated decision support systems.

1.2 Operational Challenges Driving Digital Innovation

Refiners today face a constellation of challenges that traditional control systems struggle to address:

- Feed Quality Variability: Unconventional crudes characterized by high residue content, elevated aromatics, and significant impurities require real-time adaptation of operating strategies.
- Catalyst Life Optimization: Balancing conversion severity against catalyst deactivation requires predictive capabilities that account for feed history, operating conditions, and economic trade-offs.
- Product Slate Flexibility: Rapidly shifting market demands for jet fuel, diesel, and petrochemical feedstocks necessitate agile operational responses.
- Energy and Emissions Management: Meeting decarbonization targets while maintaining profitability demands precise optimization of hydrogen consumption and energy integration.
- Equipment Reliability: Preventing unplanned downtime through early detection of fouling, corrosion, and equipment degradation protects both production and safety.

2. The Lummus Digital Advantage: Hybrid Process Modeling

2.1 Foundational Expertise from Chevron Lummus Global

The digital twin for hydrocracking builds upon more than six decades of hydroprocessing expertise from Chevron Lummus Global. This heritage includes operation of more than 100 high-pressure hydroprocessing reactors in Chevron refineries and the development of industry-leading technologies including ISOCRACKING®, LC-FINING™, LC-MAX®, and ISODEWAXING® processes.

2.2 The Four Pillars of Hybrid Intelligence

Lummus Digital's hybrid process modeling approach rests on four integrated pillars that combine to create unparalleled predictive capability:

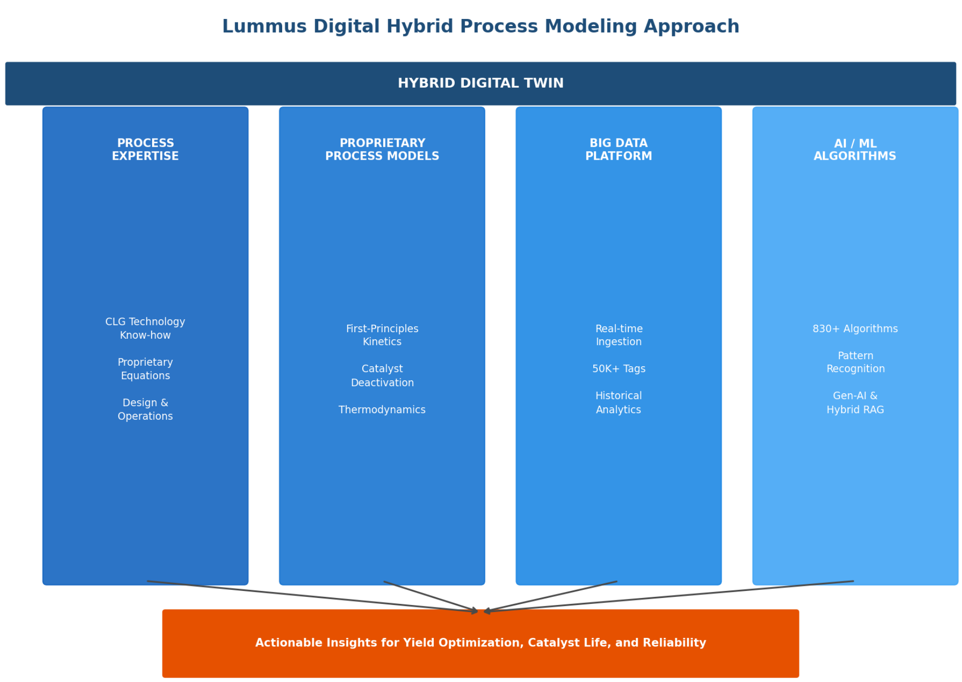

Figure 1: Lummus Digital Four Pillars of Hybrid Process Modeling

- Process Expertise: Rich technical know-how accumulated through licensing relationships with refiners worldwide, proprietary equations validated against commercial data, and deep understanding of operational boundaries.
- Proprietary Process Models: First-principles kinetic models developed over years of refinement capture the fundamental chemistry of hydrocracking reactions.

- Big Data Infrastructure: The mcube™ platform provides precise contextualization of high-volume, high-velocity data streams from DCS systems and process historians.
- AI and Machine Learning: A library of over 830 artificial intelligence algorithms enables pattern recognition and discovery of previously unexplored variable dependencies.

3. Technical Architecture of the HCU Digital Twin

3.1 Digital Twin Architecture Overview

The Hydrocracker Digital Twin integrates real-time plant data with sophisticated process models to deliver actionable insights for operations optimization:

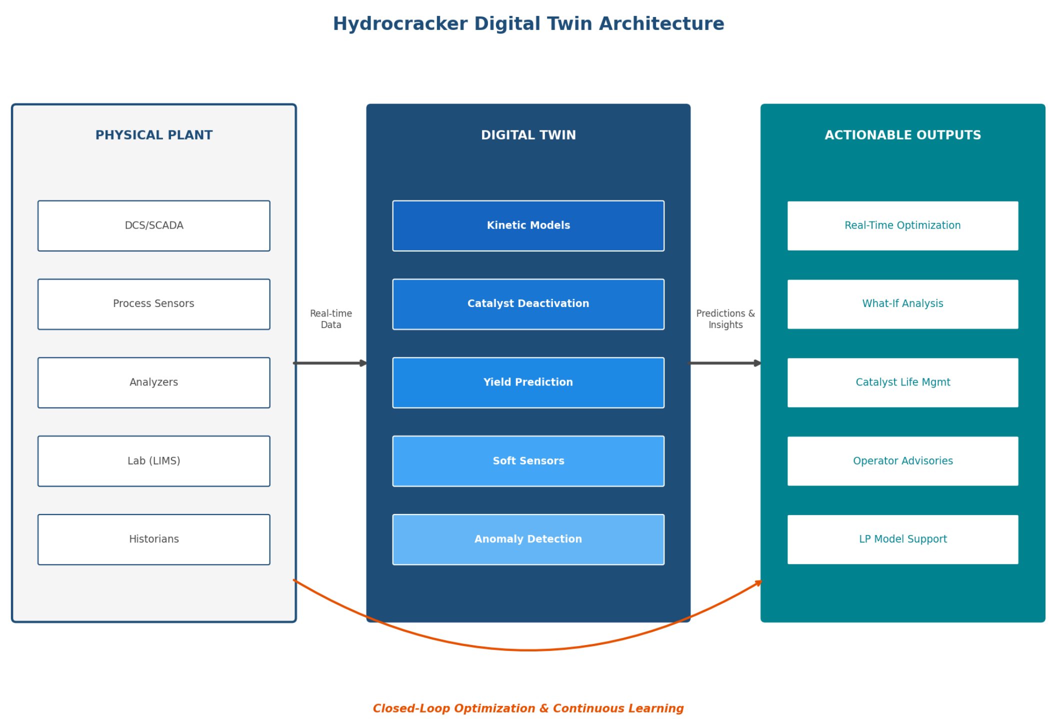

Figure 2: Hydrocracker Digital Twin Architecture

The architecture seamlessly connects the physical plant through real-time data acquisition, processes information through hybrid models, and delivers actionable outputs for optimization, analysis, and planning—all within a closed-loop continuous improvement framework.

3.2 Reactor Modeling Architecture

The core of the digital twin is a rigorous reactor model that captures the complex reaction network occurring within the hydrocracking system:

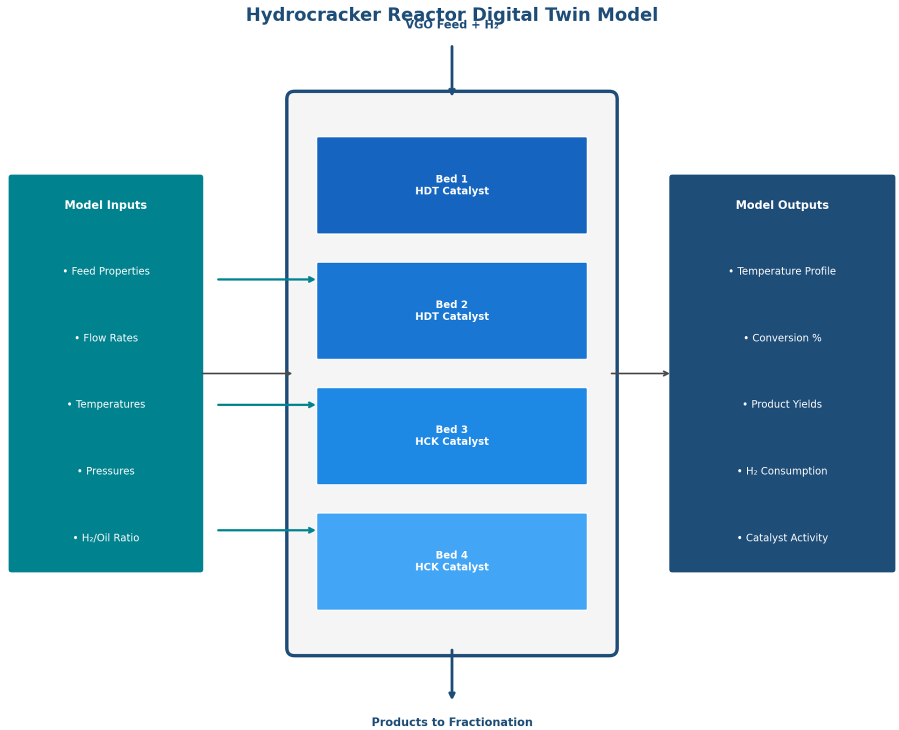

Figure 3: Hydrocracker Reactor Digital Twin Model

The model encompasses multiple catalyst beds with distinct functions—hydrotreating catalyst for impurity removal and hydrocracking catalyst for conversion—along with inter-bed quench systems for temperature control. Model inputs include feed properties, flow rates, temperatures, and pressures, while outputs provide temperature profiles, conversion levels, product yields, and hydrogen consumption.

3.3 Reaction Lumping Strategy

Petroleum fractions contain thousands of individual molecular species. Our approach employs discrete lumping methodology, grouping compounds by boiling range and chemical class while maintaining sufficient resolution to predict key product properties:

- Heavy VGO, Light VGO, Heavy Diesel, Light Diesel, Heavy Naphtha, Light Naphtha, and Gas lumps for yield prediction
- Sulfur, nitrogen, and aromatic subspecies tracking for product quality prediction
- Hydrogen consumption modeling linked to saturation and cracking severity

4. Catalyst Lifecycle Management

4.1 Predictive Catalyst Deactivation Model

Catalyst activity evolution is modeled based on fundamental deactivation mechanisms. The hybrid model combines first-principles understanding of coke formation with machine learning pattern recognition to deliver accurate remaining life predictions:

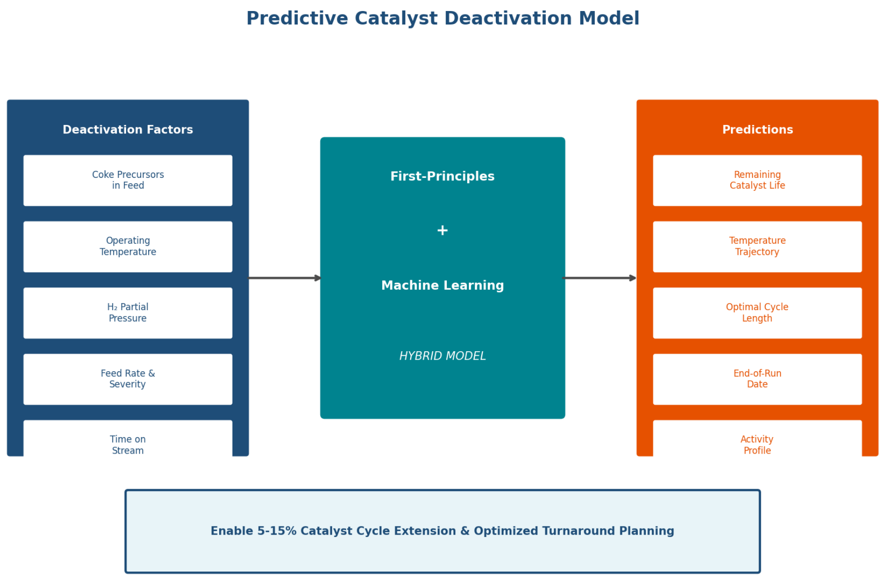

Figure 4: Predictive Catalyst Deactivation Model

The model tracks coke precursor concentrations in the feed, hydrogen partial pressure effects, and temperature history to predict remaining catalyst life. This predictive capability enables:

- Accurate projection of temperature trajectory required to maintain target conversion
- Optimal cycle length determination balancing conversion benefits against catalyst replacement costs
- Feed blending recommendations that protect catalyst while maximizing margin
- Proactive turnaround planning with optimized catalyst ordering

4.2 Value from Catalyst Life Extension

The predictive deactivation model transforms catalyst management from reactive to proactive, typically delivering 5-15% cycle length increases. For a large hydrocracker, this translates to millions of dollars in avoided catalyst costs and deferred turnaround expenses.

5. Functional Capabilities and Use Cases

5.1 Real-Time Performance Monitoring

The digital twin provides operators with continuous visibility into hydrocracker health:

- Comparison of actual yields against model predictions to detect performance gaps
- Catalyst activity tracking with remaining life projections
- Heat exchanger fouling indices derived from temperature approach deviations
- Compressor performance monitoring for recycle gas systems

5.2 What-If Analysis and Scenario Planning

Process engineers leverage the digital twin for strategic planning:

- Feed quality impact assessment: Evaluate yield and quality implications of processing different crude blends before committing crude purchases
- Severity optimization: Determine optimal conversion level balancing product value against catalyst life consumption
- Product slate transitions: Plan operating moves for shifting from maximum diesel to maximum jet production
- Turnaround planning: Project catalyst condition at future dates to optimize shutdown timing

5.3 Real-Time Optimization

When integrated with advanced process control systems, the digital twin enables closed-loop optimization:

- Dynamic adjustment of reactor temperatures to maximize margin while respecting catalyst life constraints
- Recycle ratio optimization balancing conversion benefits against compression costs
- Fractionator cutpoint optimization for product quality giveaway minimization

6. Implementation Methodology

6.1 Project Phases

Lummus Digital employs a structured implementation approach ensuring successful deployment:

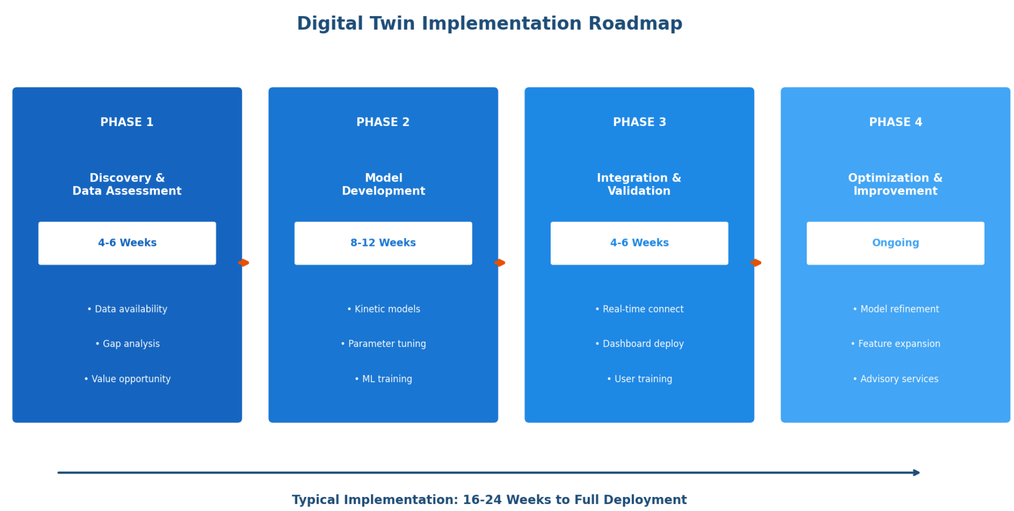

Figure 5: Digital Twin Implementation Roadmap

The phased approach ensures systematic progression from initial discovery through full operational deployment, with clear deliverables and value milestones at each stage.

6.2 Success Factors

Experience across multiple implementations has identified critical success factors:

- Strong sponsorship from operations management ensuring user adoption
- Data quality remediation addressing sensor calibration and LIMS integration
- Collaborative model development engaging site process engineers
- Clear KPI definition enabling ROI tracking

7. Return on Investment and Business Value

7.1 Value Drivers

Digital twin implementations for hydrocrackers deliver value across multiple dimensions:

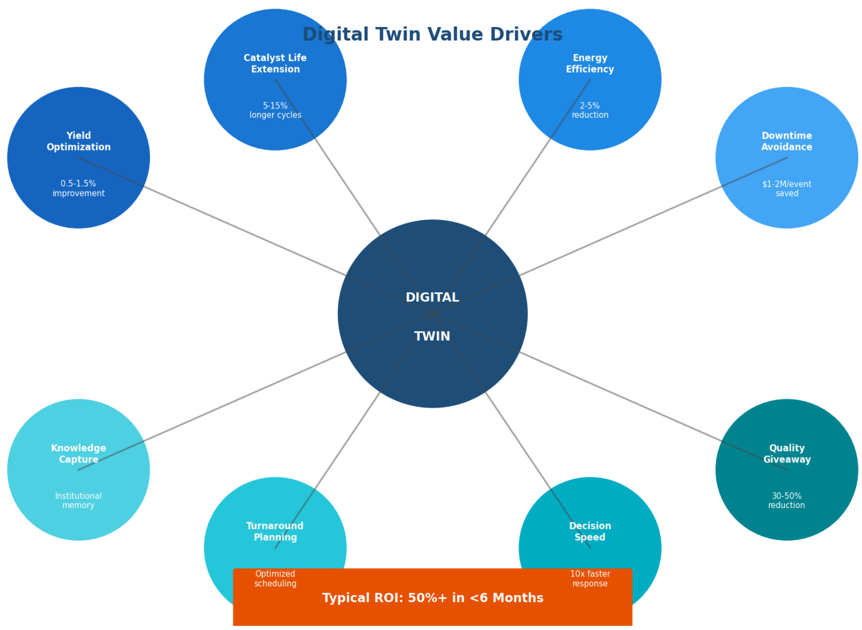

Figure 6: Digital Twin Value Drivers

Value Lever	Typical Impact
Yield Optimization	0.5-1.5% improvement in high-value product yield
Catalyst Life Extension	5-15% cycle length increase
Energy Efficiency	2-5% reduction in energy consumption
Unplanned Downtime Avoidance	$1-2M annually per avoided event
Quality Giveaway Reduction	30-50% reduction in specification margin

Digital twin implementations typically deliver ROI exceeding 50% within six months through these combined value streams.

8. Case Study: LC-MAX® Digital Suite at HPCL Visakh Refinery

Lummus Digital recently achieved a significant milestone with the deployment of India's first LC-MAX® Digital Suite at Hindustan Petroleum Corporation Limited's Visakh Refinery. This implementation demonstrates the practical value of digital twin technology in residue conversion operations.

8.1 Project Scope

The LC-MAX® unit represents a significant advancement in residue conversion, upgrading bottom-of-the-barrel streams into high-value distillates. The digital suite encompasses:

- Real-time reactor performance monitoring across multiple ebullated bed reactors
- Catalyst addition rate optimization balancing conversion and operating costs
- Sediment prediction preventing downstream fouling issues
- Yield optimization across the full product slate

8.2 Value Delivered

The digital twin implementation delivered measurable improvements:

- Enhanced conversion efficiency through optimized reactor temperatures
- Extended catalyst life through proactive activity management
- Reduced unplanned downtime through early anomaly detection
- Improved product quality consistency through soft sensor implementation

9. Conclusion

The digital twin represents a transformative capability for hydrocracker operations. By fusing Lummus Technology's unparalleled process expertise with TCG Digital's advanced AI capabilities, Lummus Digital delivers solutions that address the full spectrum of operational challenges facing modern refiners.

Our hybrid approach—grounded in first-principles chemistry while leveraging the pattern recognition power of machine learning—creates digital twins that are both scientifically rigorous and operationally practical. The result is measurable improvement in yield, catalyst utilization, energy efficiency, and reliability.

As the refining industry navigates the energy transition, digital twins will become essential tools for maintaining competitiveness while meeting sustainability commitments. Lummus Digital stands ready to partner with refiners worldwide in this transformation, bringing more than a century of process innovation together with cutting-edge digital capabilities.

Ready to Transform Your Hydrocracker Operations?

Contact Lummus Digital to discuss your digital twin journey.

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