LUMMUS DIGITAL

From Molecules to Metrics

Physics-Informed AI/ML Hybrid Models to Achieve Operational Excellence in Refinery & Petrochemicals Complex

Contact us: contact@lummusdigital.com

Visit us: www.lummusigital.com

The Operator's Dilemma

Every day, operators face a gap between what models predict and what the plant actually does — and that gap costs margins, energy, and uptime.

First-Principles Models

Miss the long tail of real-world phenomena — fouling, feed variability, aging catalysts

Data-Driven AI

Breaks under physical constraints — predicts impossible temperatures, violates mass balance

THE GAP

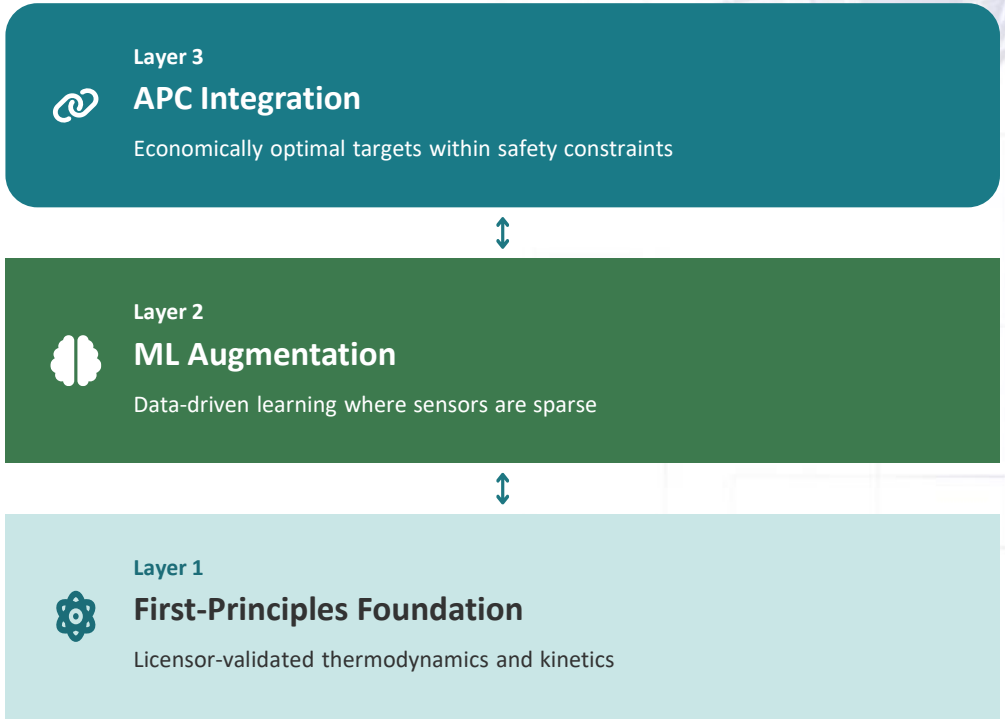
Operators compensate with **conservative setpoints** , leaving margin on the table

The industry needs models that **respect physics AND learn from live plant data**

What If Your Models Understood Your Process?

Lummus Digital bridges the gap with physics-informed AI/ML hybrid models that combine licensor-level first-principles with data-driven learning.

- Validated hybrid models reflecting technology-specific thermodynamics and first-principle kinetics by licensor
- Physics-consistent ML for inferencing where sensors are sparse or noisy
- Integration with APC toward economically optimal targets while maintaining safety and physical constraints

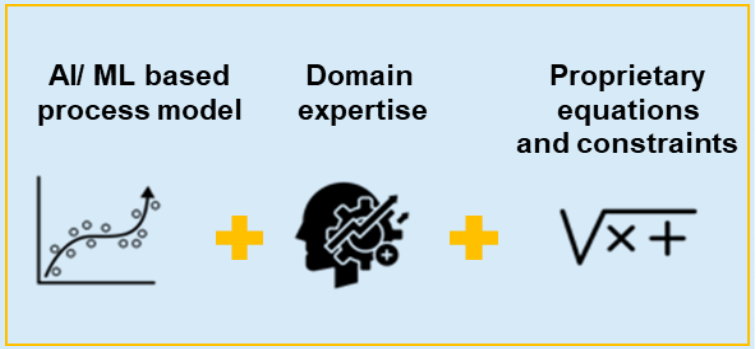


The Hybrid Approach — Three Model Types

Not one-size-fits-all: the right hybrid architecture depends on your unit and data maturity.

AI-Dominant Hybrid

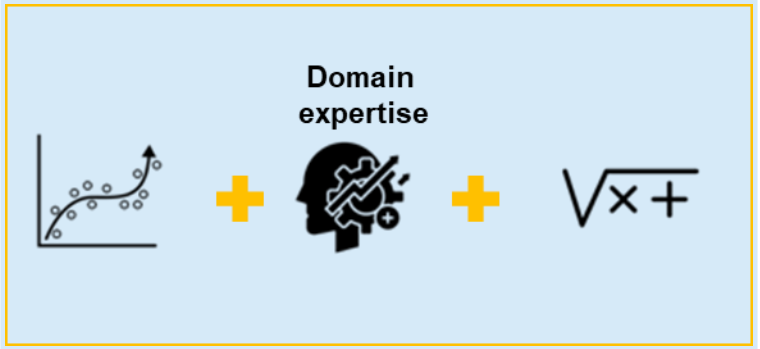
ML models built from plant data, augmented with first principles, process constraints, and domain knowledge



Best fit: **Complex reaction units**

Simulated AI Hybrid

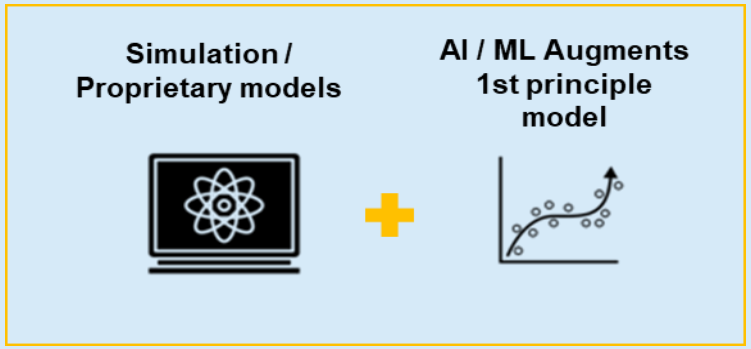
High-fidelity, purpose-fit solutions trained on simulation data for value-chain-wide intelligence from crude input to finished chemical



Best fit: **Full value-chain optimization**

First-Principles Dominant Hybrid

Augments existing first-principles model with AI using operations data to calculate unknown variables



Best fit: **Brownfield deployments**

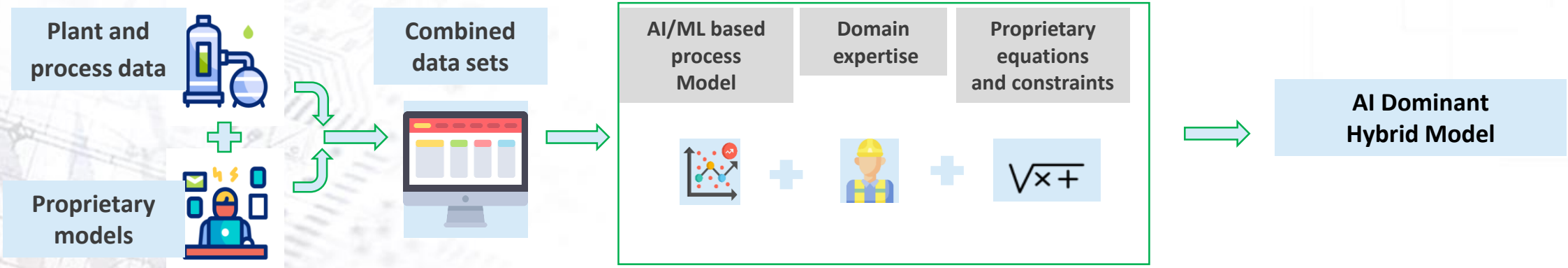
Advocating the Hybrid Approach

Process Knowledge (Domain Expertise):

- 60+ years of chemical engineering, thermodynamics, and kinetics codified in control systems
- Proven safety boundaries, constraint hierarchies, and shutdown logic validated through operational history
- Human understanding of cause-effect relationships: temperature → pressure → flow → yield

AI Learning (Data-Driven approach):

- Detects non-linear patterns invisible to linear physics models
- Adapts continuously to feedstock variability, market shifts, and equipment degradation
- Discovers optimization opportunities beyond original design assumptions



Why Lummus Digital Is Different

The edge is not just AI — it is 110+ years of licensor IP embedded directly into the models.

Deep Process IP

Equipment know-how embedded in high-fidelity models for furnaces, columns, compressors, and reactors

Modular Integration Stack

APC, emissions accounting, asset health, and digital twin integrated in one platform

Built for Real-World Variability

Designed for feed variability, utility constraints, and brownfield realities

Enterprise Governance

Links plant KPIs to enterprise ESG targets, ensuring benefits persist beyond pilot phases

Powered by mcube™ — The Intelligence Backbone

mcube is the enterprise AI platform that securely ingests, contextualizes, and analyzes complex plant data at scale.

Data Ingestion › **Contextualization** › **Analytics** › **Actionable Intelligence**

- Real-time plant data ingestion and streaming
- Secure contextualization of complex operational data
- Advanced analytics and predictive intelligence enablement
- Economic performance visualization across revenue, cost, and margins
- Energy and carbon data monitoring aligned with ESG priorities
- Scalable Enterprise AI foundation with 830+ AI algorithms

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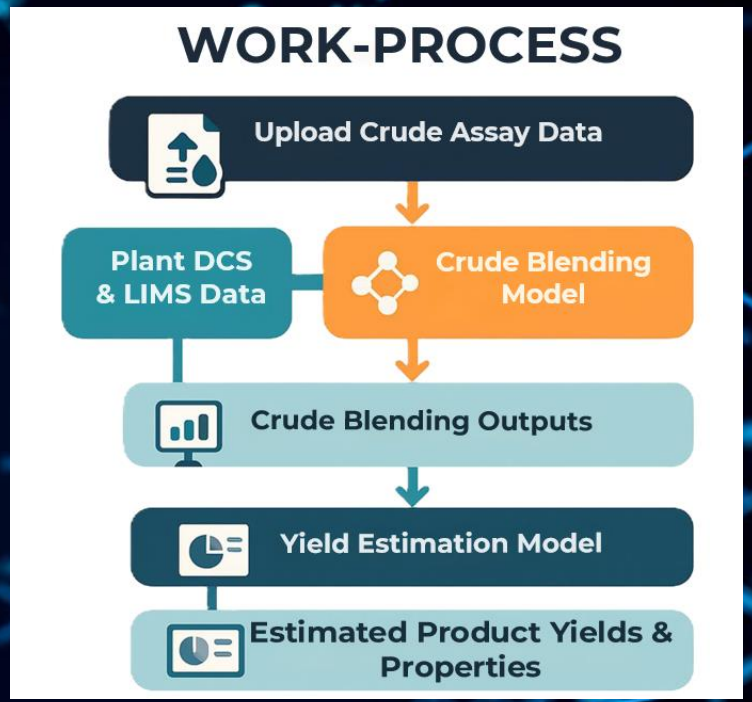
Use Case 1 — LC-MAX Digital Suite for Resid Hydrocracking

The LC-MAX Digital Suite turns one of the most complex refining units into a digitally optimized operation from day one.

- **Hybrid reactor-fractionation** models with hydrogen network optimization
- **Catalyst** activity tracking and fouling prediction
- ML-based soft **sensors for product quality** and delta-coke indicators
- Constraint-aware **severity optimization balancing conversion and yield** against catalyst utilization
- Improved **hydrogen management** and heat-integration tuning

Crude Blend Variability & Yield Estimation Model



Challenges

- **Frequent Feed Changes and Processing Opportunity Crudes**
- **Multiple Parameters to be controlled simultaneously**
- **Reliability Issues**

ACTIONABLE OUTPUTS

Accurate product yield predictions
Wt% and vol% for light ends and liquid products like Naphtha, VGO and pitch

Detailed feed blend properties across all temperature cuts

Reactor temperature and conversion recommendations for optimal efficiency

H2 consumption tracking and impurity removal insights
(Sulfur, Nitrogen, CCR, Nickel, Vanadium)

Accurate predictions help optimize blending, reducing off-spec production and improving profitability.

Catalyst Performance & Inventory Management

Challenges:

- Inefficient catalyst usage
- Uncertain catalyst life
- Poor visibility into catalyst performance

Predicting Catalyst Life

Predictive analytics help estimate remaining catalyst life to optimize replenishment schedules and reduce costs

Monitoring Catalyst Usage

Tracking catalyst performance and metals-on-catalyst levels ensures optimal usage and prevents premature replacement.

Optimizing Operations

Accurate tracking and management support stable operations with high conversion rates and efficient catalyst performance

Catalyst Inventory Management

Effective inventory management helps optimized catalyst addition and most optimal operating conditions

Hydrotreating, Hydrocracking, FCC, LC-Fining, LC-MAX, Polypropylene etc.

Use Case 2 — Ethylene Digital Suite for Naphtha Cracker

For ethylene producers, the suite combines proprietary furnace kinetics (PYPS+) with ML to optimize yields and extend run lengths across the entire cold section.

- **Furnace coil and proprietary kinetics models** with ML-based feed-dependent yield prediction
- **Coking rate and run length predictions** for optimized decoke scheduling
- **Dynamic COT targeting** and coordinated furnace-to-cold-section operation under utility limits
- **Anti-surge-aware compressor control** and fractionation tuning within purity and delta-T constraints
- **APC linkages** through compression, refrigeration, and C2/C3 fractionation

Challenges & Opportunities

Ethylene Heater Optimization Benefits:

0.5 – 1%	Increase in P + E (Propylene + Ethylene) yield
3 – 5%	Increase in unit gross margin
$2 – $5/MT	Increase in unit profitability per ton of ethylene capacity
5000 tons/yr	Reduction of CO_2 by reducing Fuel Gas Consumption

Ethylene Recovery Optimization Benefits:

2%	Increase in Ethylene Recovery
90%	Ethylene Slippage Reduction
40%	Energy Reduction
8000 tons/yr	Reduction of CO_2 emissions

Challenges

“Feed variability & delayed lab results leads to suboptimal outcome”

“Downtime is the silent profit killer. Maintenance is reactive”

“Ethylene Slippage Issues”

“Workforce challenges”

Benchmarking reveals the performance gap - closing this gap is worth millions

Your Next Step

Start the conversation — from a focused diagnostic on one unit to a full complex-wide transformation roadmap.

1

Talk to Us

Visit the Lummus Digital booth at TNChE Asia 2026 to discuss your specific unit challenges

2

Diagnostic

Begin with a digital maturity diagnostic — no commitment, just clarity on where you stand

3

Roadmap

Strategy that knows your process: asset-specific scenarios, transformation roadmaps, and RFP shaping [2]

Thank You

Get started today: **lummusdigital.com**