# Hybrid Modeling:

AI and Domain Expertise Combine to Deliver Economic Value

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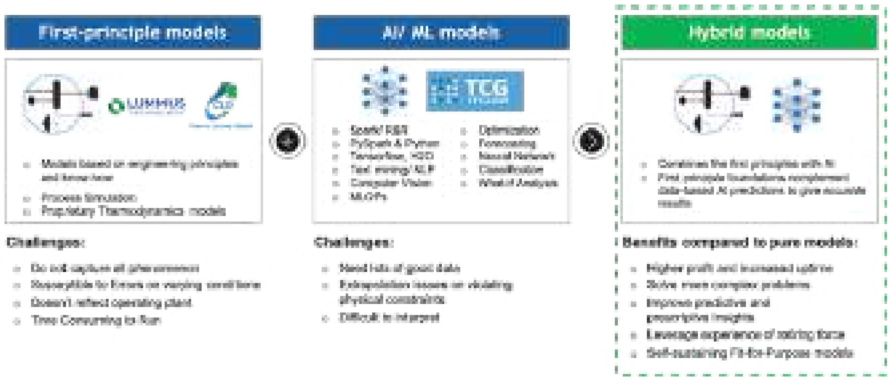
## Executive Summary

This paper summarizes the business challenges the hybrid modeling approach solves, along with Lummus Digital's three hybrid models that bring to the market several immediate avenues for creating value and our unique capability to lead this new wave in technology, to assist and augment the process industry to perceive & deliver economic value.

## Hybrid Modeling

Lummus Digital has developed a method for merging AI and analytics algorithms with domain expertise and first principles-based process simulation models. The resultant approach is a hybrid modeling system, whose achievements stack more than either first principles modeling or AI in on itself.




First principles models are widely recognized for their precise simulation of chemical and hydrocarbon processes. The proprietary first principle/kinetic models/engines have an accuracy and predictive capability validated, relied on, and improved on over several decades of use by industry, researchers, and scientists – these models and first principles relationships are founded on centuries of expertise from the world's top process engineers and operators, incorporating knowledge from Lummus Technologies' R&D teams and clients who have contributed with their inputs and feedback.

With hybrid models, users can model processes and assets that cannot easily be modeled with first principles alone, such as :

- Batch processes, which can be too varied to systematically model
- Fluidized bed processes with complex chemical and fluid behavior
- Susceptible to errors on changing condition
- Complex refining units
- Capturing all phenomenon
- Reflect operating plant condition

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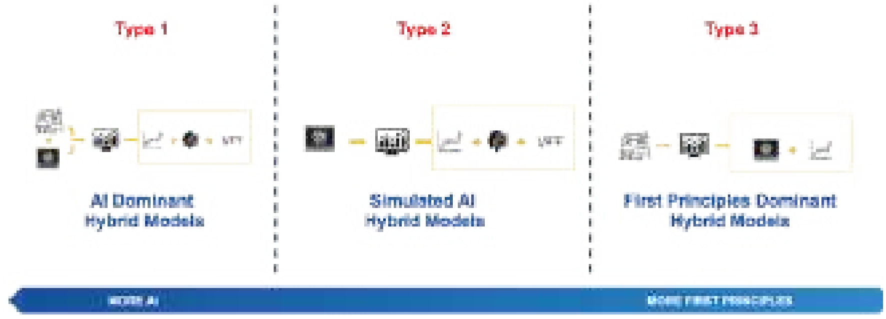
Achieving the ultimate level of precision from these models involves utilizing plant data to fine-tune the first principles models according to actual plant conditions and performance. Skilled expertise and experience are crucial for effective model calibration. Nowadays, AI and machine learning are quickly becoming useful tools to accelerate the utilization of plant data. They can be used to calibrate first principles models and swiftly create data-based models of phenomena and processes.

AI has the potential to decrease the level of expertise needed for modeling process systems. However, practical guardrails that enable its implementation must be established by combining AI with domain expertise safely, reliably, and intuitively.

## Different Types of Hybrid Models

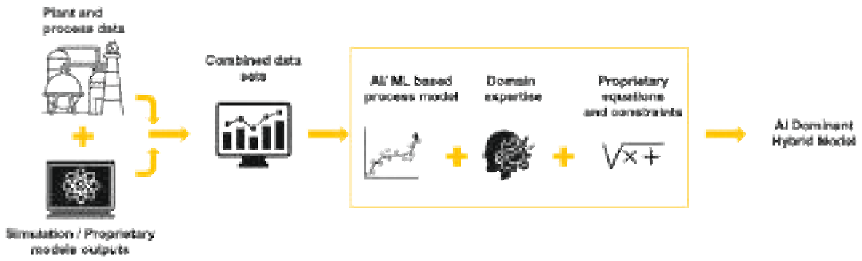



By combining AI, first principles, and domain expertise, hybrid models can rapidly provide a comprehensive and accurate model without the need for extensive expertise. The process of developing an enriched model using machine learning involves utilizing simulated or actual plant or pilot plant data, combined with domain knowledge that includes engineering constraints and first principles. This approach enables the creation of a model without requiring the user to possess extensive process expertise or AI proficiency.

The upcoming generation of solutions offers greater accessibility to the implementation of AI within hybrid models, resulting in enhanced asset design, operation, and maintenance capabilities. These solutions can be deployed online as well as at the edge. By utilizing AI and machine learning, it is possible to construct a model that analyzes a wider range of data, leveraging advanced data science techniques to enhance its predictive abilities. Furthermore, by incorporating engineering principles and domain expertise, such models can be created and maintained more efficiently than traditional methods, without the need for extensive user expertise.

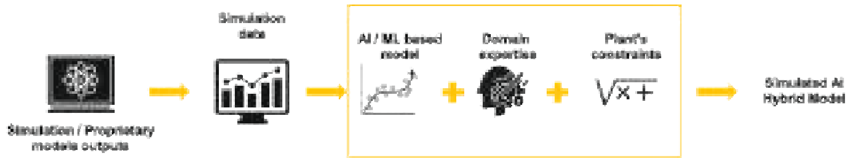
## Type 1: AI Dominant Hybrid Models

- In this approach, we create an AI/ML model based on plant and/or experimental data, augmented by first principles (e.g., thermodynamic properties, etc.), constraints (e.g. mass balance), and domain knowledge.
- Ability to generate completely new predictive, precise models, fully scaling the use of AI in the plant.
- Processes and assets are modeled better, which cannot be easily modeled with first principles alone.
- Examples include complex reaction unit operations, new materi-al processes, and new technology processes such as the Hydroc-racker reactor model.




## Type 2: Simulated AI Hybrid Models

- In this approach, we create an AI / ML model based on data from numerous simulations runs, augmented by domain expertise, first principles, and constraints to build a fit-for-purpose, high fidelity, performant model, which is accurate within the range of the trained model, fully democratizing the application of AI.
- With such models, users can easily extend the scale of modeling from units to the entire site and synchronize the model across design, operations, and maintenance.
- Examples include building value chain-wide models from crude oil input to finished chemical output and building rapidly deploy-able and compact models online at the edge.



### Type 3: First Principles Dominant Hybrid Models

- The approach involves enhancing an existing first principles model by incorporating AI techniques, utilizing operational data to determine previously unknown variables and relationships that were not included in the original model. AI / ML determines the unknown value and its relationships to continuously calibrate the model as conditions change.

- This approach provides a seamless extension to existing first principles models in brownfield deployments, as it can be easily and swiftly implemented, resulting in a significant improvement in accuracy.


## Addressing the Current Business Challenges

The process industry is currently confronting a range of unprecedented uncertainties and macro-economic threats, resulting in an unparalleled level of volatility across all aspects of their operations. With factors such as fluctuating hydrocarbon prices, remote working requirements, and supply chain disruptions, process manufacturers of all sizes are being forced to adapt to change. In order to address challenges such as shifts in feedstock demand and pricing, as well as the societal push for greater sustainability, organizations must navigate complex trade-offs. Many view software technology, particularly AI, as one of the key tools that can enable organizations to not just survive but thrive in the face of these challenges.

**Globally, energy and chemical companies are facing ongoing volatility and turbulence as a result of three external forces. This trio consists of:**

- The worldwide supply and demand shock in the market, as well as the economic recovery we are currently undergoing.

- The increasing push towards energy transition and the goal of achieving carbon-zero industry on a global scale.

- The social contract prioritizing the elimination of casualties and environmental incidents to achieve a safer and more sustainable future.

The combined effect of these factors significantly influences the thought process of industry executives.

Companies in the process industry are focused on achieving flexibility and implementing resilient strategies to produce at an unpredictable utilization factor, while maintaining extended maintenance intervals, yields, and operating margins. Speedy models that can swiftly solve key economic units or entire sites, while being closely tuned to the plant operating conditions, are better equipped to provide answers to the vital questions required to achieve set objectives. Hybrid modeling facilitates fast modeling and deployment, even in remote settings, to tackle dynamic market forces and asset conditions. These models serve as essential c omponents in revolutionizing operations through the implementation of future self-optimizing plants.

By combining the accuracy of empirical models with the robustness of first principles models, users can leverage the power of AI and domain expertise to develop more predictive models at a faster rate, with less expertise required than ever before. Hybrid models offer a more comprehensive representation of the plant, ensuring that the model remains relevant for a more extended period. This reduces the entry barrier for leveraging modeling to optimize assets, as less effort and expertise are required. Once the models are established, connected workers are free to engage in more strategic and high-value-added work.

# Conclusion: Summarizing the Hybrid Modeling's Benefits and Business Value

**Expanding Modeling's Scope and Impact –** Complex units often pose yield, performance, and quality issues. Process engineers can leverage hybrid models to simulate equipment types that are complex or even beyond the scope of traditional first-principle models, including specialty chemical reactors. These models broaden the modeling scope from process to encompass entire sites, employing reduced order hybrid models to enable the resolution of complex problems that were previously unfeasible.

**Democratizing Modeling –** Nowadays, many organizations have a larger percentage of newly graduated engineers, all of whom require access to identical information to work collaboratively Hybrid models empower process engineers without expert modeling skills to develop models for equipment and assets using operational data and built-in data science techniques to create reliable and fit-for-purpose models.

**Generating Precise, Fit-For-Purpose Models –** In the past, distinct fit-for-purpose models were employed in various functional areas, hindering the process of closing the loop. However, with the emergence of reduced-order hybrid unit models, which can accurately depict complex behaviors in a straightforward manner, it is now feasible to generate planning, dynamic optimization, and utilizing the same operating data set and simulation model, it is possible to develop online equipment monitoring models for a given refining unit. This results in closed-loop production optimization.

**Better Sustaining Modeling Benefits –** Hybrid models, consisting of both data-driven and first principles components, are strongly linked to plant data and can remain closely aligned with asset operations even as they evolve. This allows them to sustain the advantages of modeling over pure first principles modeling.

**Expediting Interdisciplinary Collaboration –** Reduced order modeling accelerates collaboration across disciplines by enabling model integration. For instance, hybrid models that incorporate data from rigorous reactor models in refining can enhance information sharing and collaboration, thereby improving planning models.

**Higher profit and increased uptime**

**Improve predictive & prescriptive insights**

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