Supply Chain Digital Transformation for Profitability and Sustainable Operations: Industry Needs and Recent Achievements

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Hydrocarbon processing industries face many pressures in maintaining their social licenses to operate in affordable and ultimately profitable ways. Climate change and the coming energy transition will lead to a world of rapidly changing supply and demand patterns that will cause difficulties for organizations trying to adapt to the changing world order. This paper examines how digital technologies can build on current operations planning, scheduling, and control practices to help organizations meet these demands. This paper goes beyond conventional digitization and procedural automation to look at the bigger picture, using examples drawn from KBC's history of yield- and energy-based profit improvement, translated through Yokogawa's digital technologies to our fast-moving world of continuous change and improvement. It explains our current activities and how we are using data sciences to build on our first-principles, physics-based modeling tradition.

INTRODUCTION

The hydrocarbon processing industry (HPI) has enjoyed many years of sustained growth, generating significant economic prosperity for developed nations and offering a path to growth for developing nations. It has seen continual change driven by the invention of new process technologies that boost yields, as well as regulations that change product specifications, improve safety, and reduce environmental impact.

The way refineries and petrochemical facilities are planned and operated has evolved along with the technological changes in chemical processes and advances in computing power and applied mathematics, although the fundamentals have remained consistent.

These many years of sustained growth are now threatened by climate change and societal pressures to adapt and reduce the carbon footprint of the HPI. The rise of the electric car along with ongoing improvements in battery technology will change (and often lower) demand patterns for transport fuels, which in some markets will be reformulated to include renewable feedstock sources. Reducing carbon footprints will drive operations toward lower or net-zero carbon emissions, thereby reducing energy consumption and increasing the use of renewables while also cutting costs. This change is occurring at a time when much of the human capital in the industry is retiring, leaving knowledge gaps to be filled by technology as part of a broader trend toward unmanned and largely autonomous operations.

All in all, planning and operations systems will need to become much more flexible and agile for refineries to survive.

CURRENT TECHNIQUES AND CHALLENGES

The approach to supply chain and operations planning and scheduling typically follows the pattern shown in Figure 1.



Figure 1 Supply chain and operations planning and scheduling

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Explanation of each box:

- The planning function typically comprises two primary tasks: creating the supply plan for the next one to three months, which is principally concerned with crude selection, and the production or operations plan, which is principally concerned with breaking the supply plan down into operating blocks or campaigns over the current month. Supply plans can take multiple facilities into account, whereas production plans typically consider a single facility from feedstock to finished product.
- The scheduling function considers how to translate plans into short-term operating instructions that respect logistics constraints imposed by tankage, feedstock arrivals, and product shipments as well as equipment lineups needed for different operations.
- Operating instructions feed into process and offsite control and real-time optimization (RTO), which drive the plant itself.
- Reconciliation and variance analysis involve tracking actuals versus schedules and plans, to identify the reasons for variance and determine corrective actions.
- This analysis feeds into production accounting or the daily reconciliation of production data, thereby realizing official production balances.
- The analysis also feeds into rigorous simulation models of key chemical processes such as fluid catalytic cracking, hydrocracking, hydrotreating, coking, and naphtha reforming plants, which are used to update the simplified (also known as reduced or surrogate) models of those processes used by the planning and scheduling tools.

KBC and Yokogawa Technologies for Integrated Supply Chain

KBC and Yokogawa provide all the core technologies necessary for integrating the supply chain. Key software solutions are:

- Petro-SIM for rigorous simulation of steady state and dynamic operation, scaling from individual equipment to a complete refinery or petrochemical facility.
- VM Production Accounting (VM-PA), which handles every aspect of material balance and inventory composition tracking for process industries, suitable for site-wide balances that match oil movements data with tank level information and process measurements. VM-PA meets all production accounting and engineering balance needs.
- VM Supply Chain Scheduling, which handles the logistics scheduling, translating operating plans into optimal daily instructions that respect the tankage and logistics constraints of the facility.
- RT-OP and VM-ERTO which meet the needs of realtime optimization of process systems (RT-OP) and utility systems (VM-ERTO).
- Planning needs are met by Chevron's PETRO solution supplied by Yokogawa or by other third-party packages.

Today's Challenges

Although individual technological solutions for the functions mentioned above have evolved considerably over the years, integration of functions is often manual, leading to feedback cycles that are reactive. Individual plant representations in the planning and scheduling models are predominantly linear, which limits their validity. Meanwhile, model update cycles can be lengthy and dependent on scarce experts. The separation of optimization considerations from logistics constraints inherent in the planning/scheduling split can lead to suboptimal results where the project is typically behind schedule.

The complexity of the solution, which involves siloed data and manual processes, leads to significant inertia to change. This hinders the production flexibility needed in the current business environment, where production demand patterns can change rapidly and operators face pressures to reduce energy consumption and environmental impacts.

In other words, the rate of change in market demand and the regulatory environment is higher now than in the past. New operating modes must be identified, validated through simulation models and test runs, and then incorporated into planning and scheduling systems quickly, expanding the operating envelopes available. This can only be achieved with sufficient speed to overcome the system inertia through integration and streamlining, and with flexible and accurate simulation models underpinning the system.

This required flexibility and accuracy is becoming the domain of the digital twin model, as explained below.

Delivering greater production flexibility, overcoming inertia through streamlining/integration, and increasing use of models all challenge traditional IT architectures built around expensive fixed server infrastructures.

The Digital Twin

A digital twin is a virtual or digital copy that accurately mimics the actual performance of a human, device, system, or process in real-time and that can be executed and manipulated, thereby facilitating improvements. Digital twins are often based on simulations but are more than the traditional firstprinciples process simulators (Table 1).

Table 1	Traditional	simulator	VS.	digital t	twin
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Traditional simulator	Digital twin		
Accurate representation of a particular operating case	Accurate representation of the asset over its full operating range and life		
Static provision of a snapshot in	Captures the full history and		
time	future of the asset		
Built when needed to answer a question	Automated monitoring of unit health and model performance leading to an always-valid, always- up-to-date digital twin for what-if and unit-optimization analysis		
Owned and used by isolated groups when needed	Centralized single version of the truth, integrated with business systems		

Digital twins of process units that are built from rigorous simulation models operationalized with real-time data are currently used for monitoring and optimizing unit performance. They allow the real asset to accommodate real constraints and physics by providing the ability to forecast, predict, and optimize molecular behavior under different pressures, temperatures, volumes/flows, and catalyst service. Accordingly, these rigorous models handle associated nonlinear relationships and infer information that cannot be directly measured. However, not everything can be explained by physics alone, and it is not possible to provide answers at the speed and cost that businesses can afford.

Digital Twins and the Challenge of Scale

All models need to be maintained so that users can trust the results, but there are existing challenges with update cycles for planning and scheduling models. To develop more detailed models that support operational flexibility, model developers must address how the models can be intelligently updated (e.g., adding functionality to differentiate between a transient data issue causing a mismatch between model and actual versus a real change in the behavior of the plant) without requiring significant increases in human capital and other resources. Maintaining one or two digital twins is much easier than maintaining tens to hundreds of detailed models across the enterprise.

This enterprise scale and the ability to apply consistent techniques and models across multiple refineries are a key challenge also behind realizing more autonomous operations run from central operating centers.

DIGITAL TRANSFORMATION: TOWARD A SOLUTION

The past decade has seen significant growth in digital technologies, realized through cloud computing platforms, the so-called Internet of Things (IoT), maturity in data analysis methods, and the rise of artificial intelligence (AI) and machine learning (ML). These technologies provide opportunities for a step change in how businesses plan and execute their operations beyond simple streamlining of work processes and digitalization of manual tasks. The technologies offer the opportunity to create significant new value through this *digital transformation*, as explained below.

Cloud Computing

Cloud computing allows organizations to move their private data center operations onto servers run by third-party providers, who maintain and provide the necessary hardware. This helps streamline IT operations but provides little new value for the business as a whole. Flexibility comes from the elasticity of computing capacity offered by cloud computing, wherein a computing task can be spread across many tens, hundreds, or even thousands of processors in parallel, reducing the required computational time. These additional resources are dynamically made available by the cloud provider, activated and charged when needed, and deactivated when complete.

For example, computer-intensive tasks such as plan optimization or complex sensitivity studies can take hours or days when run sequentially, but just minutes when run in parallel. Such a reduction changes how engineers and planners use technology, allowing for greater interactivity. If tasks execute faster, more analyses can be attempted, which leads to better and more robust solutions. Operations research problems that were intractable due to the excessive computing time required to reach an answer can now be solved.

Data Lakes and Big Data Analysis

Manufacturing organizations typically record significantly more data than they can analyze, often keeping data within application silos, thereby limiting the crossapplication analysis that can lead to new insights. The latest technologies for massive-scale data storage and analysis allow organizations to break these data silos, making a much wider range of information available for analysis by business intelligence tools and for use by ML algorithms.

To understand the potential causes of issues with machine reliability and equipment fouling, it is important to, for example, look across data silos in order to combine process measurements with equipment performance characteristics, feedstock compositions, vibration information from portable sensors, maintenance records, weather records, and operator event logs. This process might provide insights into causes and facilitate the construction of ML predictors that give early warnings of potential issues.

AI and ML

AI technologies have matured remarkably in the first two decades of this century and now offer considerable power to augment and even replace conventional technologies. AI and the associated class of ML provide techniques for building diagnostic and/or predictive models for situations such as equipment reliability, early event detection, preheat train fouling, and deviation analysis. Larger scale AI models are being built for operator advisory systems and fast energy optimization solutions.

Cloud platforms have enabled substantial growth in AI/ ML adoption, providing the data storage and processing power needed for model creation and maintenance. However, specialist platforms that can handle enterprise scale are increasingly necessary.

Flexible Rules, Workflow, and Orchestration

Cloud computing achieves its elasticity by using different types of computing architecture, ranging from the conventional server to the virtual machine model. Programs written for the desktop world must be restructured, and in some cases significantly rewritten, for the cloud, and so they are able to scale and to run in parallel. Thereafter, they can take advantage of standard cloud technologies for orchestrating calculation engines and services as well as their integration with flexible rule engines for running workflows. Supply Chain Digital Transformation for Profitability and Sustainable Operations: Industry Needs and Recent Achievements

These technologies allow us to build agility into systems, significantly lowering the cost of making changes to established workflows and overcoming inertia.

YOKOGAWA CLOUD – MEETING THE CHALLENGES

Yokogawa and its subsidiary KBC have embarked on the creation of a cloud platform and associated applications that solve the challenges inherent in digitally transformed supply chain planning and optimization solutions. The platform is infrastructure-agnostic and can be run on the major cloud infrastructure services such as Microsoft Azure and Amazon Web Services. Applications can run using a SaaS model or be implemented either within the client's own private cloud or using on-premise servers. The graphic below outlines the platform's capabilities (Figure 2).

The platform allows applications such as KBC's Petro-SIM, Supply Chain Scheduling, Energy Optimization and Production Accounting products to run as cloudnative solutions that take full advantage of its elastic cloud computing, data management and storage, workflow, and orchestration capabilities. It also allows applications to take advantage of common visualization and reporting functions for a consistent user experience.

Moreover, the platform offers rich, enterprise-scale AI/ML capabilities through integration with the C3 AI Suite, allowing solutions to be enhanced with AI and ML functionalities applied across an enterprise. KBC applications are being rewritten to work in these environments, with both the platform and applications undergoing early-stage customer validation.

Yokogawa Cloud Application to Supply Chain Optimization

As shown, the Yokogawa Cloud platform contains the necessary building blocks to support an automated, datadriven, and flexible supply chain optimization solution. AI/ ML capabilities are key to managing the model scale and complexity necessary to deliver operational agility across many areas:

- Use AI to analyze model and key performance indicator (KPI) deviations, detect when models need updating, and then carry out that regeneration. This saves significant time and human resources.
- Use real data augmented with synthetic data from calibrated simulation models to create ML models for planning, scheduling, and optimization. This improves the accuracy of model planning for more realistic plans.
- Use refinery-wide simulation models driven by AI to identify and rank improvement ideas.
- Use ML to create operations advisors that help unit operators, as shown by the case study below.

Case Study

A leading European refinery wanted to maintain maximum energy efficiency of a crude distillation unit (CDU) while achieving its production plan, regardless of disturbances in the process. The unit KPIs did not adequately reflect the unit performance objectives and the advanced process control (APC) did not fully optimize the operation due to limited ability to manipulate all independent variables, with some key operating parameters (such as liquid and vapor rates) not being measured. Historical operating data were also not being analyzed automatically to identify improvements in different



* For simplicity only Azure IOT Hub is used in the diagram. If the platform is deployed on AWS it will be "AWS IOT" and on- premise it is a custom MQTT Broker or Rest API ** In Discussions with DSHQ

Figure 2 Yokogawa DX platform architecture

production situations, for example crude switching, causing a significant impact on the crude unit and downstream units.

The solution combined first-principles Petro-SIM models with ML. The in-built optimizer in the Petro-SIM was used to train the ML model with optimized solutions for many different production scenarios. Based on what the ML model was able to "learn" from multiple automated Petro-SIM runs against multiple different scenarios, faster and more-automated optimization by the ML model was realized.

The Petro-SIM model used was an accurate representation of the CDU and was calibrated using at least two years of historic data. Examples of the data automatically provided to the Petro-SIM are operating and crude data sourced directly via the process historian as well as laboratory and yield accounting data. The ML model was trained on the same historic data as well as additional optimized solutions from the Petro-SIM. The ML model was able to assess the current data and rapidly provide new optimized targets to the APC systems in place (Figure 3).

Unlike alternative solutions, the ML model also progressively learned from experience, taking both fresh plant data and new synthetic data and optima from the Petro-SIM model. This data-driven solution was tested and able to maintain the process unit at maximum energy efficiency while achieving the production plan. The main users were the unit engineer and shift supervisor, and to a lesser degree the APC engineer and panel operators. In the future, the solution might also provide input to the maintenance, planning, and control and instrumentation teams as the ML model continues to learn the unit operations.



Figure 3 Case study

Scaling Up to Enterprise Level

The solution described in this case study applies to a single process unit at a refinery of a major integrated oil company, operating multiple refineries. Each refinery has multiple process units of various types, many of which can deliver benefit through energy demand optimization. Instead of one solution, therefore, the client may require tens to hundreds of such solutions. A complex solution today can take six months or more to build, so the only practical way to deploy tens to hundreds of solutions is to industrialize the creation and maintenance process. In other words, we need to build a model factory that will support running multiple processes in parallel, with consistent methods for creating and executing simulation and machine learning models with realtime data.

This model factory is the role of the C3 AI Suite within the Yokogawa Cloud, providing a proven, enterprise-scale technology alongside the established technologies of KBC and Yokogawa.

CONCLUSION

The oil refining industry is facing an uncertain future due to climate change and the coming energy transition. Refineries need to adapt how they operate in order to meet carbon reduction demands while also remaining profitable. This will require significant upgrades to operations management.

This paper showed how digital technologies can drive the transformation necessary to achieve operational agility while also reducing the burden on refinery personnel of performing mundane manual tasks, and described what Yokogawa is doing to help the industry.

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