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# SMART IT FRAMEWORKS FOR AUTOMATION AND QUALITY CONTROL IN CHEMICAL MANUFACTURING

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**Abstract**

*The Industry 4.0, artificial intelligence (AI), and high regulatory standards of quality and data integrity prompt a structural change in the chemical manufacturing sector. The conventional automation architectures that have been based on remote distributed control systems (DCS), programmable logic controllers (PLCs), and laboratory information systems are no longer needed to provide real-time quality assurance, operational agility, and regulatory-compliant data management. This review is based on advances in the field of smart manufacturing, process analytical technology (PAT), soft sensing, predictive quality analytics, digital twins, and multi- agent/service-oriented control architecture with particular attention to its implementation in a* ***Smart IT framework*** *to perform automation and quality control of chemical manufacturing. The paper reviews the current standards and paradigms including Quality by Design (QbD), GAMP 5, ALCOA(+), and real-time release testing (RTRT) after which it evaluates the* ***current IT and control architectures*** *(pyramidal ISA-95 style, SOA, holonic and multi-agent systems) and AI-based quality technologies (predictive quality, computer vision, soft sensors, digital twins). Contributing to this, it suggests a* ***layered Smart IT*** *model that integrates physical properties, connectivity and edge infrastructure, integration services, AI driven intelligence, and governance and compliance into a coherent and closed loop quality and automation structure. The framework puts importance on modularity, service orientation, human-oriented multi-agent coordination, and regulatory-by-design validation of AI components. Lastly, the paper provides implementation roadmaps, illustrative scenarios, and open research directions which incorporate the unified views of the experts in IT, AI, and chemical engineering.*

## INTRODUCTION

Pharmaceuticals, polymers, agrochemicals, specialty chemicals, and consumer products are manufactured using chemicals, which can be described as difficult to react with, hazardous substances, demanding quality standards, and highly regulated industries[1].

Historically, automation in this industry has been concerned with process and throughput and quality control has to a large extent been done through off-line testing in laboratories and end product inspection[2]. It has led to reactive quality control, late identification of deviations and large scrap and rework in both batch and continuous plants[3].

This landscape is being redefined by the combination of a number of trends:

Industry 4.0 and smart manufacturing includes a combination of industrial internet of things

(IIoT), cloud computing, advanced analytics, and cyber-physical systems[4].

Process Analytical Technology (PAT) and QbD and promoting real-time monitoring of critical process parameters (CPPs) and critical quality attributes (CQAs) and replacing quality-by-testing with quality-by-design and continuing verification[5], [6].

Digital twins, soft sensors, which can be used to create high-fidelity virtual representations of processes to optimize processes, predictive maintenance, and what-if analysis[7].

Predictive quality control, anomaly detection and automated visual inspection using AI and machine learning (ML)[8].

Changing regulatory and data-integrity requirements, such as ALCOA(+), GAMP 5 and RTRT direction[9]. These changes demand Smart IT structures which are beyond single advanced control undertakings.

These frameworks should be able to smoothly combine automation plant-floor (DCS/PLCs), PAT instruments, LIMS, MES, ERP, historians and AI services and must be traceable, cyber secure and validate complex, learning-based elements[10].

This review has the following objectives: To offer an organized review of smart manufacturing technologies in terms of automation and quality control in chemical manufacturing. To evaluate critically the current IT and control architectures and their appropriateness to highly automated AI-enabled quality assurance. To suggest a multi-layer Smart IT structure and concept of multi- agent coordination which suits chemical manufacturing. To map implementation directions and research issues of IT, AI, and chemical engineering views.

**Foundations: Quality, Regulation, and Smart Manufacturing Paradigms**

Quality by Design, PAT, and Real-Time Release Testing

Quality by Design (QbD) redefines the process of pharmaceutical and chemical products development as a structured model of process development beginning with set quality goals and focusing on process knowledge and risk management of quality[11]. Core QbD elements include:

The definition of Quality Target Product Profile (QTPP) and determination of CQAs that define product performance[12].

Quantitatively defining critical material attributes (CMAs) and CPPs and relating them to CQAs[13].

Setting a design space- a multidimensional area of CMAs/CPPs within which CQAs are acceptable[14].

Planning a control strategy and life-cycle management concept of continuous improvement[15].

PAT operationalizes QbD in the production process by integrating real time monitoring of CPPs and CQAs into the process through the deployment of analytical tools (e.g., NIR, Raman, UV- Vis, chromatography, imaging)[16].

In-line/on-line sensors, Chemo metrics and multivariate analysis of data, soft sensors and inferential models, Combined control measures and automatic response[17]. This is the underlying concept of Real-Time Release Testing (RTRT) is the capability to release product on in-process measurements and process data, not just relying on end-product laboratory tests, essentially speeding up manufacturing cycle and mitigating the risk of batch rejection, validated multivariate models that forecast final product quality based on intermediate measurements which have been proven to have accuracy and robustness and regulatory acceptable traceability and documentation to show that full control of product quality is maintained during the entire release process[18].

PAT and RTRT are thus inherent forerunners and allies of AI-driven clever IT frameworks.

**Industry 4.0 and Smart Manufacturing in Chemicals**

Industry 4.0 combines IIoT, cyber-physical systems, cloud/edge computing, big data analytics, and AI and transforms smart factories into connective, transparent, and decentralized intelligence[19]. Smart manufacturing efforts have targeted various strategic aspects in chemical and petrochemical industries. Plant monitoring and proactive maintenance (e.g. of turbines, compressors and extruders), in real-time, allows predicting failures of equipment and preventing them, greatly prolonging the lifecycle of assets and minimizing unexpected downtimes. State-of- the-art yield optimization, energy-saving, and quality optimization analytics use past and real-time data to detect process inefficiencies and offer a remedial course of action, which converts data information into a real-life reduction of costs and performance[20]. Complex unit digital twins and integrated-site virtual labs enable the analysis of scenarios in virtual

laboratories which helps an engineer to explore design-space and make operational decisions prior to implementing modification to actual plants[21]. The integrated IT/OT architecture that connects control systems to Manufacturing Execution Systems (MES), Laboratory Information Management Systems (LIMS), and Enterprise Resource Planning (ERP) platforms in a seamless way breaks organizational silos and allows the organization to operate data-intensive across its sphere of manufacturing[22].

These initiatives show pragmatic productivity, quality and sustainability improvements, which are, however, normally put in place as individual initiatives instead of a cohesive IT platform[23].

**Data Integrity, GAMP 5, and ALCOA(+)**

The chemical manufacturing smart IT systems work under the strict requirements of Good Manufacturing Practice (GMP) and data-integrity requirements[24]. The regulative instructions set high standards in a variety of frameworks. ALCOA and ALCOA+ principles establish primary data governance properties: it has Attributable (traceable to source and owner) and Legible (recorded and can be read) properties, is Contemporaneous (recorded at time it was created) and Original (stored in its native format and change history)[25], it is Accurate (right and complete) and further, in the ALCOA+ model, Complete, Consistent, Enduring (indefinite retention) and Available (readily readable and available to inspection and analysis) attributes are demanded

throughout the data lifecycle. Laboratory and production system data integrity needs thorough execution of secure audit trails to record all access and updates, role based access control which limits system privileges to authorized persons and validated computerized systems which are rigorously qualified prior to usage[26]. GAMP 5 has become the industry-standard best-practice framework of risk-based validation of automated and computerized systems, and offers lifecycle guidance, explicitly covering AI/ML components and open-source software[27]. The FDA data-integrity guidance and associated EMA/WHO expectations define the regulatory interpretation: lack of adequate data-integrity controls are violations without necessarily finding intentional manipulation and subjecting organizations to strict liability to show control[28].

In the specific case of GAMP 5, it offers a lifecycle and V-model of specifying, designing, testing, and maintaining computerized systems, now fully enumerating AI/ML and open-source components[29]. This requires smart IT systems to incorporate these principles in such a way that AI services, layers of integration, and data platforms are fit to be used as intended and provably under control[30].

Existing IT and Control Architectures in Process Industries

Traditional Automation Pyramid and ISA-95 Paradigm

The majority of chemical plants have traditionally been hierarchical, with automation taken in form of a pyramid that isolates the manufacturing functions and separated them into different levels. Level 0-1 involves field devices, that is, sensors, actuators, analyzers, final control elements, and programmable logic controllers (PLCs) and distributed control systems (DCS) that offers real-time regulatory control[31]. Level 2 provides supervisory control, human-machine interfaces (HMI), and SCADA systems that provide human operators with the ability to visualize and modify the state of the plant[32]. Level 3 accommodates Manufacturing Execution Systems (MES) to control the batch management and production scheduling as well as Laboratory Information Management Systems (LIMS) to control the quality testing and the results monitoring[33]. Level 4 is on the enterprise level, which has Enterprise Resource Planning (ERP) systems controlling financial, supply chain and business operations. These layers are defined by conceptual interfaces and roles, or standards like ISA-95, but integration in practice remains typically inflexible, vendor-specific, and project-specific, denying an organization the ability to flex and agile, as well as the ability to integrate data across layers to support advanced quality analytics, machine learning, and digital twins[34].

**Service-Oriented Architectures and Modernized MES**

Service-Oriented Architectures (SOA) are used to break up the functionality of monolithic MES and tightly-coupled integrations into modular services provided through standard interfaces and coordinated through enterprise service buses (ESB) or API gateways[35].

SOA in the manufacturing environment facilitates several transformational capabilities. Loose

Fidelity between MES/LIMS, ERP and specialized applications using clearly-defined service interfaces enables each system to independently develop without necessarily having to rewrite in sync with the technology stack[36]. This is easier to evolve and replace parts as the systems are not tightly integrated but communicate via contract based services and this allows organizations to upgrade or even change vendors in a step by step way[37]. Standardized protocols and data representations make platform-independent connectivity of IIoT devices and analytics possible, allowing the integration of heterogeneous sensors and analytics tools irrespective of their manufacturers. MES modernization models based on SOA explicitly focus on modernizing the
legacy MES through stage-by-stage breakdown into reusable services that are interoperable with the existing operational technology (OT) before switching to microservices or event-driven architectures which in turn are more scalable and responsive[38], [39].

**Holonic and Multi-Agent Manufacturing Control**

Multi-agent systems (MAS) and holonic manufacturing systems (HMS) offer decentralized, autonomous, and cooperative control forms that are in line with dynamic and complex manufacturing systems[40].

The main features of the holonic and agent-based control essentially define their difference against the centralized control[40]. Autonomy of units (holons/agents) gives each agent or holon local decision-making, within predetermined limits, allowing the agent to respond more quickly to local conditions, without having to receive centralized directives.[41] The coordination of production, distribution of resources and conflict resolution among agents is done through cooperation and negotiation mechanisms, defining emergent system behaviors through local interactions. Fault tolerance and self-organization allow the system to dynamically adjust to failure of equipment or change in conditions and redistribute responsibilities among the rest of the agents without forcing the system to replan centralization[42]. The agent-based architectures are especially appropriate to contemporary batch manufacturing and multi-product plants since they can be easily mapped to natural manufacturing structures into reconfigurable and modular manufacturing cells and process units[43].

Recent studies show that MAS architectures are viable to support various chemical engineering tasks including process synthesis, plant-wide optimization, and supply chain coordination, where agents interact with domain specific tools and databases in order to carry out a specific task. Nonetheless, MAS architectures, which use different topologies including linear chains, directed acyclic graphs, cyclic graphs, and centralized hub-and-spoke, are largely at the pilot stage and proof-of-concept stage[44]. Mass implementation in controlled chemical production remains small and mostly experimental, both due to the technical maturity challenges, and the organizational risk aversion inherent in regulated industries of safety of critical concern[45].

**Limitations for Quality-Centric Smart Manufacturing**

These architectures have a good technological basis, but they demonstrate a high level of weakness in terms of enabling integrated, AI enabled quality control on the scale and sophistication required in current chemical manufacturing[46]. These issues are causing compliance failures, audit reports, and a lack of trust and reliability in the system whenever an organization tries to operationalize an AI-driven decision-making decision; quality data is scattered across legacy systems; it is challenging to correlate process-state conditions with quality results. These loopholes drive a more holistic Smart IT structure[47]. AI, Analytics, and Digital Technologies for Automation and Quality

Predictive Quality and Advanced Analytics

Predictive quality control involves using both past and real time data of production to predict deviations in quality and prescribe corrective measures beyond the conventional univariate statistical process control (SPC)[48].

The predictive quality systems in our modern time combine various sources of information and analysis. Multi-source data (process variables such as temperatures, pressures, flow rates, PAT signals, e.g. spectroscopic and imaging data, laboratory outcomes, e.g. assays, impurity levels, physical properties) is fed into these systems and advanced machine learning models (random forests, gradient boosting, deep learning architectures) are trained on past manufacturing data to make predictions of critical quality attributes (CQAs) or probabilities of defects with quantified confidence levels. Interactive dashboards allow quality

engineers and process experts to conduct full root-cause analysis on quality events and pursue ongoing quality enhancement efforts on the basis of foresighted insights and not on the basis of problem-solving action.

The proven advantages of such systems are high: defects decrease due to the early intervention, first-time-through yield due to process operating points optimization, and testing-time decrease due to data-based decision-making shown at all the organizational levels, including operators and management[49].

**Computer Vision for Visual Quality Control**

Visual inspection of chemical and pharmaceutical products and packaging is becoming more popular as computer vision systems, made possible through deep learning (especially convolutional neural networks), are utilized to monitor them[50].

The computer vision use encompasses the entire spectrum of visual quality control. Surface inspection of tablets and capsules unravels the existence of defects in their coatings, chips, imprinting, and discoloration, which may influence bioavailability or patient adherence[51]. Container and bottle inspection ensure integrity through detecting cracks, contamination, deformation, color/opacity anomalies and seal integrity problems that may undermine stability of the product. The packaging line checks on missing caps, misaligned labels, wrong fill level and other packaging flaws systematically to correct any packaging errors that influence the presentation of the product and regulatory standards.

The present-day computer vision systems make use of various technological advances in order to perform better. Multi-angle imaging and in some cases hyperspectral imaging has high-resolution visual data who have been taken under controlled lighting conditions that are ideal in detecting defects[52]. Fine-grained classification with supervised learning models trained on thousands of images of defects with expert-labeled defect categories, and anomaly-detection models that flag any visually abnormal items regardless of whether they accurately match known defect categories make it possible to maintain line speed and at the same time, quality.

These systems have been shown to be better in critical dimensions than human visual inspectors: faster, capable of a continuous inspection rate of line speed, highly consistent, and capable of detecting small defects that human perception cannot detect. Notably, such systems produce abundant data on defect frequencies and patterns that allow quality engineers to lead to the idea of continuous improvement using data-driven root-cause analysis and preventive action.[53]

**Soft Sensors and Chemometrics**

In most chemical factories, important quality variables (e.g., composition, viscosity, polymer properties, impurity levels, etc.) are not measured continuously[54]. Such variables are determined using empirical or hybrid models based on easily measured process data by soft sensors (or virtual sensors).

Soft sensors have a conceptually simple but technically advanced mechanism of operation[55]. They also make use of highly frequency and readily available measurements (temperatures, pressures, flow rates, and spectroscopic data) to approximate the infrequent or delayed measurements, like laboratory assays, product compositions, and quality indices, which would otherwise require wait time of hours[56], [57]. These models, combined with decades of process data and knowledge of chemistry as embedded in model calibration, form quantitative relationships between easy to measure process setpoints and difficult to measure quality variables, which are used in inferential control strategies to adjust process setpoints in real time without waiting until laboratory confirmation[58]. Near-real-time quality estimation gives the feedback to operators and automated controllers through offering quality estimates that can be used to response to drift in a preventive manner instead of being reactive.

Demanding applications have been relatively successful regarding soft sensors. In the pharmaceutical industry, soft sensors have been deployed in a wide range of applications, including distillation columns, debutanizers, crystallization, and polymerization units, with the construction of risk-based control systems and QbD implementations and real-time release-testing programs, using soft sensors to provide quality monitoring and control in terms of the CQAs of concentration, particle size, crystallinity, and polymorphism[59], [60].

**Digital Twins in Chemical Process Industries**

Digital twins are computer-based versions of real objects or procedures that are supported by the ongoing data synchronization process. Digital twins are found in chemical manufacturing at: Equipment level (e.g. compressors, pumps, reactors), Process level (whole units/ flowsheets), Plant/site level (integrated operations, supply chains)[61].

Digital twins contribute to a varied amount of strategic and operational goals. The optimization of processes and what-if simulation are used to investigate the performance of equipment and process configurations to different feed compositions, ambient temperature, and market demand scenarios to identify robust working windows at the time of implementation[62]. Twin Studies Quality forecasting and design-space exploration Twin designs.

Twin designs are used to estimate the behavior of quality across the design space in variability given different process conditions to support regulatory submissions and control strategy documentation[63]. Twin models are useful in regulatory documentation and training of operators as they help to provide evidence based on regulatory inspections and safe simulation of virtual environments where operators can develop skills[64]. Although potentially effective, digital twins are currently being adopted in chemical industries with a growing number of applications, but still encounter significant challenges due to the complexity of data integration, model fidelity and maintenance, and managing organizational change as companies retrain employees and incorporate twins into the decision-making process. Proposed Smart IT Framework for Automation and Quality Control

Architectural Overview

Based on the technologies and paradigms discussed, it is presented in the paper as a layered Smart IT architecture adapted to chemical production, which is a combination of service orientation, multi-agent coordination, and AI-based quality control.

**Figure 1** conceptually illustrates a **multi-agent and service-oriented control framework** where Process Control, Quality, Maintenance, Scheduling, and Safety Agents interact over a service bus, interfacing with plant units and enterprise systems.




**Figure 1: Multi-agent and service-oriented control framework for a smart chemical plant.**

A **layered Smart IT architecture** comprising five conceptual layers: Physical & Control Layer Sensors, actuators, analyzers, PAT, PLC and DCS. Connectivity & Edge Layer OPC UA servers, IIoT gateways, edge compute nodes which combine and pre-process the information. Integration Layer ESB/API gateway; MES, LIMS, historian connections; event streaming and data-virtualization. Intelligence Layer Hosts ML models, soft sensors, optimization engines, and digital twins on AI and analyst platforms. Application & Governance Layer; Quality dashboards, real- time responsibility, electronic batch records, risk management, model and data governance, cybersecurity, and tooling validation[65] as shown in figure 2

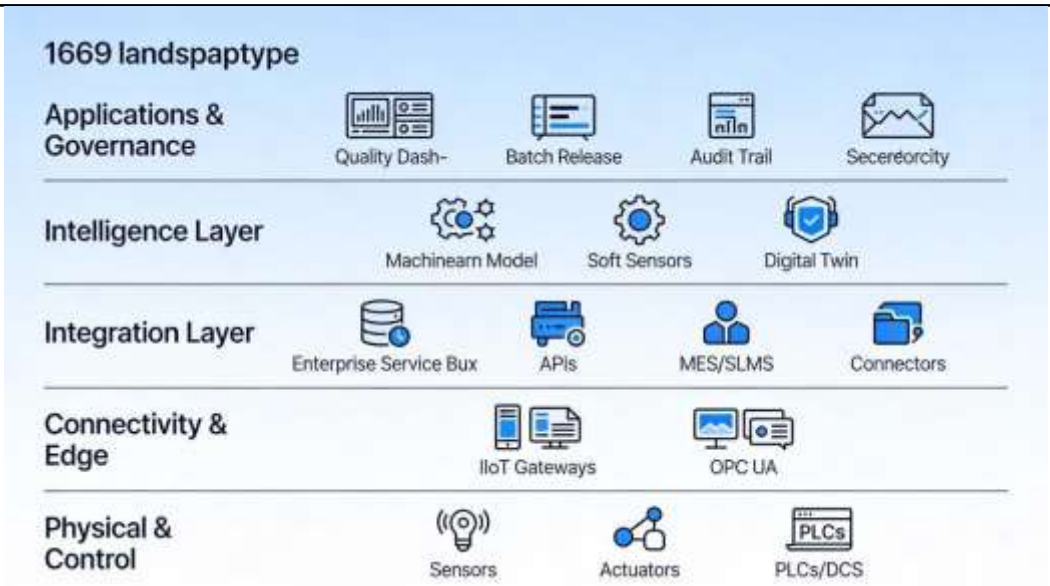


**Figure 2: Layered smart IT architecture for automation and quality control in chemical manufacturing. This layered approach separates concerns (operation vs intelligence vs governance) and supports incremental adoption.**

### Closed-Loop Quality Control Concept

An intrinsic part and parcel of the framework is a closed-loop quality control architecture (as shown in figure 3) that has successfully incorporated PAT instruments, soft sensors, AI prediction models, and classical feedback control into a single quality assurance system. Live data feeds of PAT sensors, process control systems (DCS/PLCs) and lab systems feed into the analytics platform using secure, verified data pipelines with detailed audit history[66]. The continuous prediction of quality risk levels and critical quality attributes (CQAs) is provided by the use of soft sensing and predictive models, which utilizes both statistical and mechanistic relationships to beat delay issues in measurements as encountered in a laboratory[67]. The logic and orchestration services, based on predictive outputs, are decision logic, which is a set of recommendations that consist of suggested setpoint changes to process controllers, alerts to human operators when quality risk reaches excessive levels, and batch-hold or release recommendations, based on the accumulating evidence. RTRT engines combine model forecasts with the acquired design space expertise and validated control policies to either automate or support intelligently the batch and lot release decisions, reducing the release cycle with respect to the strict quality evidence[17]. In this workflow, extensive traceability and regulatory background is ensured by automatically recording model versions, feature values, intermediate computations, and final decisions to meet ALCOA(+) audit trail standards, GAMP 5 change management disciplines and QbD documentation standards[68].

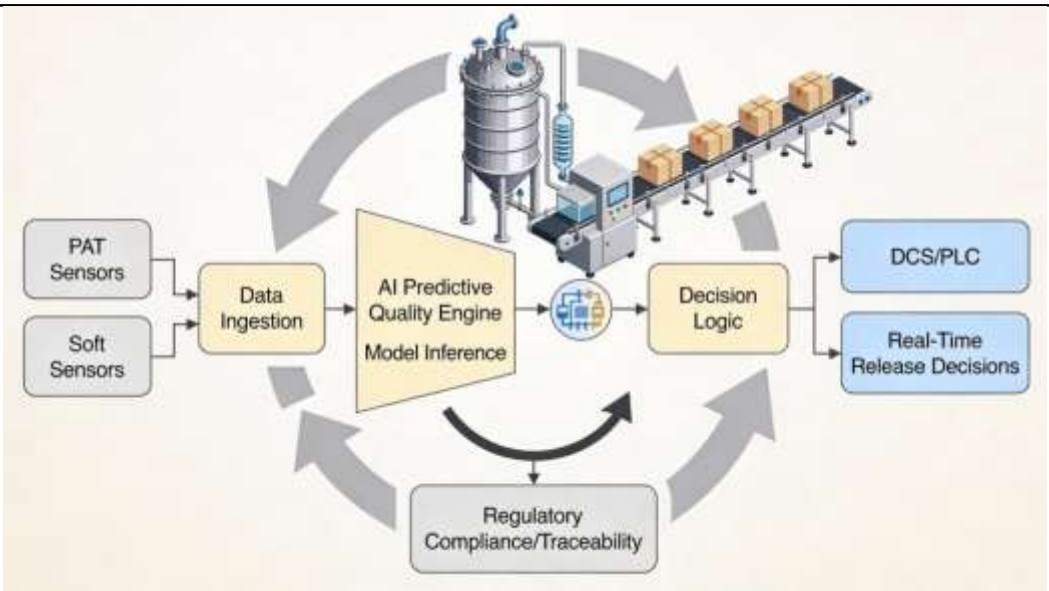


**Figure 3: Closed-loop quality control integrating PAT, soft sensors, and AI in chemical manufacturing.**

**Digital Twin Ecosystem**

The framework has digital twins as a first-class citizen in the Intelligence Layer[69]. Digital twins are used as lifelong counsellors and predictors of key manufacturing units and some product lines. Sensors and historians provide them with real-time data about the processes and they update their internal state estimate and provide optimal operating points in the validated design space considering the current equipment condition and product specifications. They also forecast critical quality attributes (CQAs) and out-of-specification probabilities that have quantified confidence intervals, to make quality decisions before the laboratory confirmation[15]. They are used to predict equipment degradation and maintenance requirements of critical equipment, to support predictive maintenance programs which trade off equipment reliability against the cost of operation in a variety of operating strategies. Framework has been illustrated in figure 4.

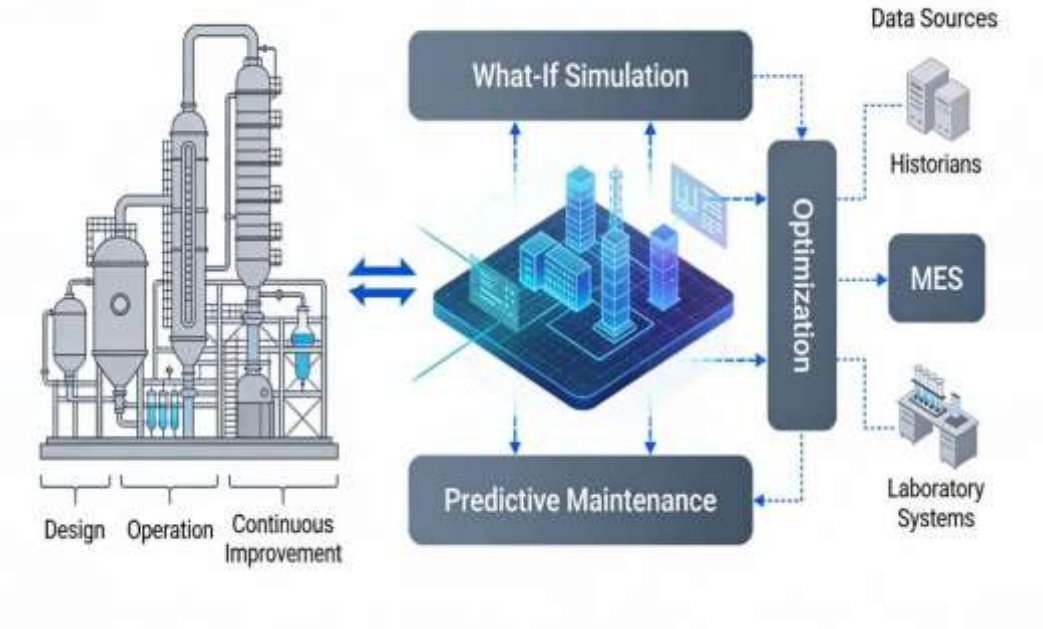


**Figure 4: Digital twin ecosystem for a chemical production unit with analytics and lifecycle integration. Digital twins also act as testbeds for AI and control strategies before deployment, supporting GAMP-style validation and change management.**

**Multi-Agent, Human-Centric Coordination**

In an attempt to operationalize autonomy without loss of human oversight, the framework uses a multi-agent coordination layer that is based on MAS and the holonic systems[70].

The representative agents cover the key functional areas of chemical production. Process Agents are independent of each large manufacturing unit (reactor, distillation train, dryer, crystallizer) and optimize unit operations subject to constraints continuously and seek the help of other agents when deviations are observed. Quality Agents observe real time PAT values, soft sensor values and forecasted quality model values; they recommend set changes to avoid predicted quality variation and escalate quality notifications when systematic problems are identified and they keep a meticulous quality log within them to be used by regulators and analysts[71]. Maintenance Agents process the data on asset health-vibration, temperature, efficiency trends, and plan the predictive maintenance work, which reduces the impact of production and increases the life of the assets. Scheduling Agents optimize the production sequences and change grades in the entire plant under various constraints (equipment availability, energy limits, staffing), collaborating with the other safety-in-depth mechanisms on site (SIS)[72].

The agents communicate by means of the standardized service bus of the Integration Layer and present their services as reusable, discoverable services (e.g., predict CQAs, optimize schedule, schedule maintenance) that may be called upon both by other agents and by human operators[73], [74]. Importantly, human experts, including control engineers, quality scientists and chemical engineers, have the final say, and autonomy is typically configurable, with levels of autonomy ranging from advisory (agent recommends, human decides), to supervised autonomy (agent acts, but human may override), to fully automatic (agent acts and human does not interact to formulate decision). This MAS architecture based on human-factors is especially critical in regulated and safety critical manufacturing systems, in which the preservation of human agency and the transparency of reasoning is an important element in creating trust in the organization and encouraging regulatory compliance by encouraging clear accountability[75].

**Comparative Perspective: Architectures and Quality Technologies**

**Table 1. Comparison of /IT Architectures for Chemical Manufacturing**

| Aspect | Traditional Automation Pyramid | SOA-Enabled Architecture | Holonic/Multi-Agent Architecture |
|---|---|---|---|
| **Integration style** | Point-to-point, hierarchical | ervice bus/APIs, modular | ecentralized, agent-to-agent |
| **Flexibility** | ow; changes require major projects | Medium–high; services can evolve independently | gh; agents can be reconfigured and extended dynamically |
| **pport for AI & analytics** | Add-on, often offline | Natural place for analytics services | Agents can embed analytics, support local intelligence |
| **Data availability** | ragmented by layer/system | Improved via data virtualization & ESB | Potentially rich but requires robust data infrastructure |

| | | | |
|---|---|---|---|
| **Resilience to disturbances** | ntral coordination; limited adaptivity | Depends on design; entralized services may be bottlenecks | igh; local autonomy and self-ganization improve robustness |
| **gulatory validation (GxP)** | Mature practices for DCS/MES | Requires structur l validation of services and integrations | Validation more complex; requires systematic agent behavior verification |
| **uitability for closed-loop quality** | onstrained by data silos and rigid workflows | ood; can orchestrate PAT, soft sensors, and RTRT | Very promising; supports istributed quality agents but calls for strong governance |

**Table 2. Mapping Smart Quality Technologies to Objectives in Chemical Manufacturing**

| Technology | mary Quality Objective | Typical Use Cases | Key Enablers |
|---|---|---|---|
| **PAT tools (spectroscopy, imaging)** | eal-time CQAs/CPPs monitoring | Blend uniformity, drying, crystallization, residual solvents | n-line sensors, mometrics, integration |
| **Soft sensors** | ntinuous estimation of lab-measured properties | Composition in distillation, olymer properties, emissions | Process data historians, /chemometric models, |
| **Predictive quality analytics** | Early detection and prevention of defects | Yield optimization, scrap reduction, process tuning | Integrated data lake, ML ipeline, operator dashboards |
| **Computer vision QC** | utomated visual inspection | Tablet/capsule inspection, bottle/container integrity, packaging checks | gh-res cameras, deep learning |
| **Digital twins** | olistic process optimization and what-if analyses | nt-wide debottlenecking, energy minimization, grade- change optimization | Combined first-inciples and ML models, real-time data streaming |
| **RTRT engines** | Faster, risk-based product release | Continuous and batch drug product release | T & soft sensors, QbD design pace, regulatory acceptance |

**Implementation Roadmap: From Legacy Automation to Smart IT Framework**

Transitioning to the proposed Smart IT framework is best approached via staged maturity levels, especially in brownfield chemical plants.

**Stage 1 – Instrumentation and Data Foundation**

Stage 1 deals with equipping the plant with the contemporary sensing and data capture. Organizations must enhance sensing and PAT functionality by making specific investments in analysis instruments on units with the largest quality contribution (e.g., critical reactors, separation trains, crystallizers) where real-time measurement will be used to create the most critical quality and yield contributions. Create strong data historians which will record high frequency process data (milliseconds to minutes resolution) with full archival capability to form the rich datasets needed to develop models and troubleshoot at a later stage in the project. Introduce extensive data-integrity management controls, including ALCOA(+) concepts, audit trails that cannot be edited, use encryption to store data, and role-based access control, as well as safe administration processes on any new system deployed[76]. Start implementing soft sensors on significant quality variables that would otherwise be determined in the laboratory, and use this step to develop internal capability in inferential modeling and to create expectations on the expected performance.

**Stage 2 – Connectivity and Edge Integration**

Stage 2 is the infrastructure that defines the connectivity and edge computing infrastructure that facilitates distributed analytics in real time. To achieve interoperability, organizations ought to install IoT gateways and OPC UA servers to standardize the protocols used in connecting plant-floor controllers (PLCs/DCS) to analytical instruments and higher-level systems, thus doing away with the proprietary integration that had earlier obstructed interoperability.[77] Install edge computing nodes that are close to production lines to store local analytics and computer vision models to reduce network latency in making time-sensitive decisions and reduce bandwidth usage in high frequency sensor outputs. Centralize data sources at a central point of data platform with defined data models, semantic tagging and metadata management and generate a single source of truth, upon which downstream analytics, AI systems, and reporting systems can be able to rely and count on.

**Stage 3 – Integration and Service-Oriented Architecture**

Stage 3 allows the service-oriented architecture which is used to support the modular and scalable applications. Organizations are requested to make integration middleware consisting of enterprise service bus (ESB), API gateway and/or event streaming platform (e.g., Apache Kafka, Pulsar), the exposures of the Manufacturing Execution Systems (MES), Laboratory Information Management Systems (LIMS), data historians, and PAT instrument outputs, discoverable and consumable services[78]. Break down important MES functions into modular, versioned services,
e.g. lot genealogy and traceability, deviation management and incident tracking, batch execution, state transitions, and recipe/parameter management, to allow these services to be independently evolved and replaced. Possibly provide simple orchestration workflows to simple closed-loop conditions (e.g., PAT measurements leading to automatic alarms or manual review, soft sensor outputs suggesting advisory set point as a control measure to the operators of the control room) that can show value without need to be complexly automated.

**Stage 4 – Intelligence Layer and Closed-Loop Quality**

The 4th stage implements the intelligence layer, which drives AI-based decision support. Organizations must adopt a central AI/analytics system that scales the full model life cycle: data preparation and feature engineering, model training and tuning with verified data, rigorous model validation against holdout test data and cross-validation, production deployment with automatic version management and rollback abilities, and finally continuous monitoring that indicates model deterioration. Pilot computer vision quality control on specific lower risk tasks like the packaging inspection or intermediate product inspection, allow organizational experience and confidence with visual AI, before implementing the same to the final product critical inspection. Make the major manufacturing units digital and start using them out-of-the- box in what-if mode and operator training on virtual equipment and gradually advance to real- time

advisory mode as the accuracy and usefulness improve[79].

**Stage 5 – Multi-Agent Coordination and Autonomy**

Stage 5 realizes the utmost automation and intelligent autonomy using multi-agent co-ordination. Organizations must implement software agents, which are wrapping AI models, decision rules, and domain knowledge and each agent possesses clearly defined roles (Quality Agent, Maintenance Agent, Scheduling Agent, Safety Agent) and responsibilities that allow coordination and accountability[80]. Establish adjustable autonomy levels of the various agent classes and situations- advisory (agent incorporation of PAT tools, soft sensors, and predictive
quality models into proven framework of releases, which will allow a product to be released faster and with more confidence, but without compromising regulatory compliance and product safety[81], [82].

recommends, human is responsible), supervised autonomous (agent takes action, but can be overridden by human), and complete autonomous (agent takes action and does not involve human operators), and create human-machine interfaces that would ensure that operators are informed and involved. Gradually automate more and more closed-loops, and retain strict governance by using a risk based GAMP 5 validation approach, in which agents and models are considered configurable or custom systems with documented requirements, thorough testing and formal change restrictions which must be enforced before and after implementation. Develop Real-Time Release Testing (RTRT) of selected products, step by step

**Key Performance Indicators and Benefits**

The Smart IT framework, when fully implemented, is expected to deliver substantial improvements across critical operational metrics:

**Table 3**: Projected KPI improvements: Traditional Automation vs. Smart IT Framework Implementation

| Key Performance Indicator | Baseline (Traditional) | Target (Smart IT Framework) |
|---|---|---|
| Product Quality Improvement | 0% | 15% |
| Defect Detection Time | 48 hours | 2 hours |
| Production Efficiency | 78% | 92% |
| Data-to-Decision Cycle Time | 24 hours | 1 hour |
| Regulatory Compliance Score | 85% | 98% |
| First-Pass Yield | 82% | 96% |
| Annual Cost Savings | 0% | 12% |

These indicators demonstrate the quality consistency improvement, operation efficiency, rapid decision-making, and compliance stance. The cumulative gains should be anticipated in organizations that practice the implementation of the framework throughout the five-stage roadmap, and the initial stages provide better data integrity and operational transparency, and the subsequent ones will bring substantial quality and cost advantages by providing a closed-loop and optimizing AI-powered automation.

**Interdisciplinary Considerations: Roles of IT, AI, and Chemical Engineering**

The suggested Smart IT system is an interdisciplinary approach by its nature:

IT engineers and architects develop the service-oriented, secure, and scalable integration and data platforms, high availability and cybersecurity, and devops/mlops pipelines that are GxP compliant[83].

The ML models (predictive quality, soft sensors, vision, anomaly detection) are developed and validated and maintained, the features of explainability are designed, and model risk assessment is collaboratively created by AI and data scientists[27].

CQAs/CPPs are defined by the chemical and process engineers, interpreting the model output within the framework of process physics, design control strategy, and making their contribution to the validation and continuous improvement[84].

To balance the pace of innovation with regulatory safety and operational safety, collaborative governance frameworks, such as AI/Analytics Councils, cross-functional validation teams, etc., are needed.

**Challenges and Open Research Directions**

Although it promises pilots and structures, a number of challenges still exist:

1. **Information and model** control in controlled settings. Versioning, monitoring and retiring models require robust practices, such as change control and impact analysis that would be consistent with data-integrity and GAMP 5 guidelines[85].
2. **Transparency and human confidence in AI-based decision-making**. The operators and quality professionals should know why models suggest some things. The study of interpretable ML, surrogate modeling and process engineer-specific visualization methods is of great importance[86].
3. **Standardization and interoperability**; although assisted by OPC UA, ISA-95, and new standards of the digital-twins, standard semantic modeling of CQAs/CPPs, batches, and quality events across vendors and plants are developing. Adaptive systems can be validated on a large scale[87].
4. **Conventional validation** presupposes fixed software but AI models can be retrained or adapt. Hybrid strategies which involve lock-model intervals, regular revaluation and continuous monitoring of performance should be refined further methodologically and harmonized with regulations[88].
5. **Cyber security** in plants of high connections. Attack surfaces are augmented by the growth of IoT and cloud connectivity. Zero-trust principles and integrated security architecture should be incorporated throughout all layers, especially the focus on safety- instrumented systems and critical control loops of the safety-instrumented systems package[32] .
6. **Socio-technical changes management**. It requires training, redefining of roles and developing confidence in systems that work closer to being fully autonomous to be successful in adoption. The suggested human-in-the-loop multi-agent architectures can provide a way forward but require a keen organizational design[89].

The interface between multi-agent systems, digital twins, and the GxP-compliant validation is a young field of research with highly promising opportunities of input on the part of the IT, AI, and chemical engineering communities[90]. Some of the areas that need to be addressed are strong strategies to oversee the model continuously, architectures to validate the learned models to controlled settings, agent behavior verification and failure mode analysis, integration patterns of bridging digital twins to real-world control systems, and strategies of organizational change management that allow maintaining human agency and can bring positive automation[7], [91].

**Conclusion**

The manufacturing of chemicals is set to gain greatly with the adoption of Smart IT systems that integrate the best automation, real-time quality assurance, AI, and strict adherence to regulations. The current paradigms, QbD, PAT, digital twins, predictive quality analytics and holonic/MAS control offer a few essential building blocks yet have frequently been implemented separately. This review has proposed a service oriented, multi-agent and layered Smart IT framework that: Combines physical, connectivity, integration, intelligence and governance layers, Introduces closed-loop, AI-intensified quality management based on PAT, soft sensors, and predictive analytics, Discuss digital twins and agents as the key components of process optimization and decision support, Maintains alignment with ALCOA(+), GAMP 5, and QbD in order to be auditable and reliable.

As an interdisciplinary perspective, these frameworks necessitate the concerted action of IT engineers, AI specialists, and chemical engineers with the assistance of organizational and regulatory ingenuity. The way to go ahead should be strong reference architecture, open-source model and data governance standards, and case studies to prove that this can be done in end-to-end Smart IT deployments in wide chemical industries. The shift towards smart and AI-powered manufacturing is a technological and organizational process. Organizations that manage to make this transition, through investments in the underlying infrastructure of data, by encouraging interdisciplinary cooperation, and integrating quality and governance concerns throughout their automation programs, will achieve significant competitive advantages in product quality, operational flexibility, regulatory compliance and cost savings.

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