

Industrial Agentic AI and generative modeling in complex systems

Mohammad Reza Boskabadi¹, Yudong Cao^{2,3},
 Behnam Khadem⁴, William Clements⁵, Z. Nevin Gerek⁶,
 Eric Reuthe^{2,7}, Abhishek Sivaram¹, Christopher J Savoie^{2,7} and
 Seyed Soheil Mansouri¹



Manufacturing, consumer, transportation, and supply chain processes present significant challenges in monitoring, control, and design due to their inherently nonlinear nature and the difficulty of measuring critical variables in real time. The convergence of major innovations from the computer science field has the potential to revolutionize the engineering and control of complex industrial systems. Digital twinning and process simulation have been a staple of computers in process engineering for decades now. However, the advent of advanced sensor systems and big data integration, combined with generative AI and agentified AI (classic and quantum) systems, allows for much more granular and autonomous process control and real-time optimization of complex systems. Advanced process modeling, Agentic AI, and generative AI models have emerged as powerful tools to address the challenges of complex nonlinear systems. We propose here an integrated systems feedback and control architecture (SIC: Sense, Infer, Control) that leverages complementary process knowledge for enhanced real-time monitoring and decision-making, fully integrated into control system functions and the accompanying sensors. In this paper, we explore this integration of generative models in agentic AI ensembles into industrial processes through the lens of four recent industrial case studies: (1) the real-time optimization of motorsports strategy, (2) the development of indirect (soft) sensors for sustainable large-scale manufacturing operations, (3) the creation of sensor data-driven personalized health and cosmetic chemical formulations, and (4) the design of biomanufacturing systems using quantum and classic Agentic AI. These examples demonstrate how agentic and generative models, combined with full-scale process simulation and digital twinning, effectively augment process control, enabling advanced solutions for process optimization, quality improvement, and sustainable operations. The proposed SIC systems architecture serves to enhance process control automation by capturing complex nonlinear patterns and leveraging easily measurable variables. Generative models bridge gaps in process understanding, sensor technologies, control, and monitoring, offering actionable insights for efficient and informed decision-making across diverse industrial applications.

Addresses

¹ Department of Chemical and Biochemical Engineering, Technical

University of Denmark, Kgs. Lyngby, Denmark

² Zapata Computing Inc., Boston, MA, USA

³ Boston Consulting Group, Boston, MA, USA

⁴ Henkel AG, Düsseldorf, Germany

⁵ ORCA Computing, London, UK

⁶ Novo Nordisk, Lexington, MA, USA

⁷ SiC Systems Inc., Providence, RI, USA

Corresponding authors: Savoie, Christopher J (cjs@si-c.io),
 Mansouri, Seyed Soheil (seso@kt.dtu.dk)

Current Opinion in Chemical Engineering 2025, **48**:101150

This review comes from a themed issue on **Innovations in Chemical Engineering**

Edited by **Gerardo J Ruiz-Mercado, Heriberto Cabezas and Csaba Deák**

For complete overview of the section, please refer to the article collection, "[Innovations in Chemical Engineering](#)"

Available online 5 June 2025

<https://doi.org/10.1016/j.coche.2025.101150>

2211–3398/© 2025 The Author(s). Published by Elsevier Ltd. This is an open access article under the CC BY license (<http://creativecommons.org/licenses/by/4.0/>).

Introduction

In industrial processes, the primary goals of ensuring safety, enhancing efficiency, reducing costs, and maintaining high-quality standards all motivate the pursuit of improved operations [1–4]. Traditional process control and optimization rely heavily on direct measurements and deterministic models [4]. However, complex systems often involve latent variables that are challenging to measure directly. This limitation necessitates the use of ‘soft sensors’ [5] that estimate unobservable variables from measured process data and statistical models, including agentified and generative models that can infer missing information and optimize control strategies. These soft sensors are surrogates that can be used to estimate the quality indicator variables (QIVs) of process systems, as will be discussed in the individual case studies. These soft sensors and inference models can be implanted in ensembles of semiautonomous granular

inference agents responsible for different areas of inference and control decision-making. Ensembles of multiagent inference control architectures have been used since 1990s, and distributed systems of AI agents have been used for complex systems control applications since Adaptive Agent-Oriented Software Architectures (AOSA) was first demonstrated [6], forming the basis for developing the original versions of Apple's Siri invented by Hodjat, Savoie, and Amamiya [7••]. This architectural approach enables the generation of real-time estimates essential for process monitoring, providing actionable insights and real-time data for effective process management and ultimately for control actuation.

These modeling architectures utilize multiple sources of both real-time and historical data to identify and represent complex, nonlinear relationships between critical variables and more easily measurable or detectable proxy variables that are strongly correlated with them [8]. By doing so, such inferences enable the generation of real-time estimates that are a proxy for a direct measurement where direct measurements are not always possible, which is essential for process monitoring and tuning [9•].

Generative models are a class of machine learning algorithms designed to generate information and replicate complex data distributions [10,11]. The rapid advancement of generative AI has reshaped various technological sectors [12,13], yet much of the focus has been on large language models (LLMs) such as ChatGPT (OpenAI), Gemini (Google), and CoPilot (Microsoft). However, the true potential of generative AI extends far beyond text generation. By capturing intricate nonlinear relationships and leveraging readily available sensor data, statistically driven generative models can fill critical gaps in process understanding, offering predictive insights and enhanced real-time optimization capabilities. Their integration into industrial workflows enhances decision-making in areas such as predictive maintenance, process optimization, and quality control [14,15]. It is, hence, imperative that sufficient process knowledge, in the form of causal connections or dynamical system functionals, be integrated to enable a better understanding of the process [16].

Recent efforts have heavily focused on the use of generative adversarial networks (GANs) aided by recurrent neural networks, long- and short-term memory, and several other models such as diffusive models and similar approaches. However, it is important to note that data distributions can also be driven by mechanistic models, capturing the system's mean behavior and variance based on underlying measurements [17•]. Despite this potential, challenges remain in ensuring the explainability, interpretability, and robustness of generative models in industrial settings. The integration of domain knowledge, such as mechanistic models and causal relationships, remains critical for building reliable AI-driven decision-

support systems [16]. Thus, a hybrid approach that combines generative AI with process expertise or mechanistic models is necessary to unlock its full potential [17], for example, in biotechnology and chemistry, where the process of producing complex biological products such as enzymes, vaccines, and cell therapies is critical [18–20]. With the increasing demand for precision, scalability, and cost-effectiveness in these fields, advanced computational tools have become indispensable. Generative modeling has been found to offer innovative solutions to design and optimize biological [21–23•] and chemical systems [24•].

This paper explores how generative models and agentified systems, in conjunction with indirect measurement methods, can enhance process efficiency, minimize operational risks, and support adaptive control mechanisms. We propose an original, three-stage systematic architecture — drawing on our collective expertise in industrial generative modeling — that uniquely unifies process instrumentation workflows, agentified mechanistic/AI modeling, and Agentic AI-driven control, distinguishing it from prior hybrid and agent-based approaches. The integration of AI models into Supervisory Control and Data Acquisition (SCADA) systems and distributed control systems (DCS) is discussed, along with industrial applications demonstrating the benefits of AI-driven soft sensing.

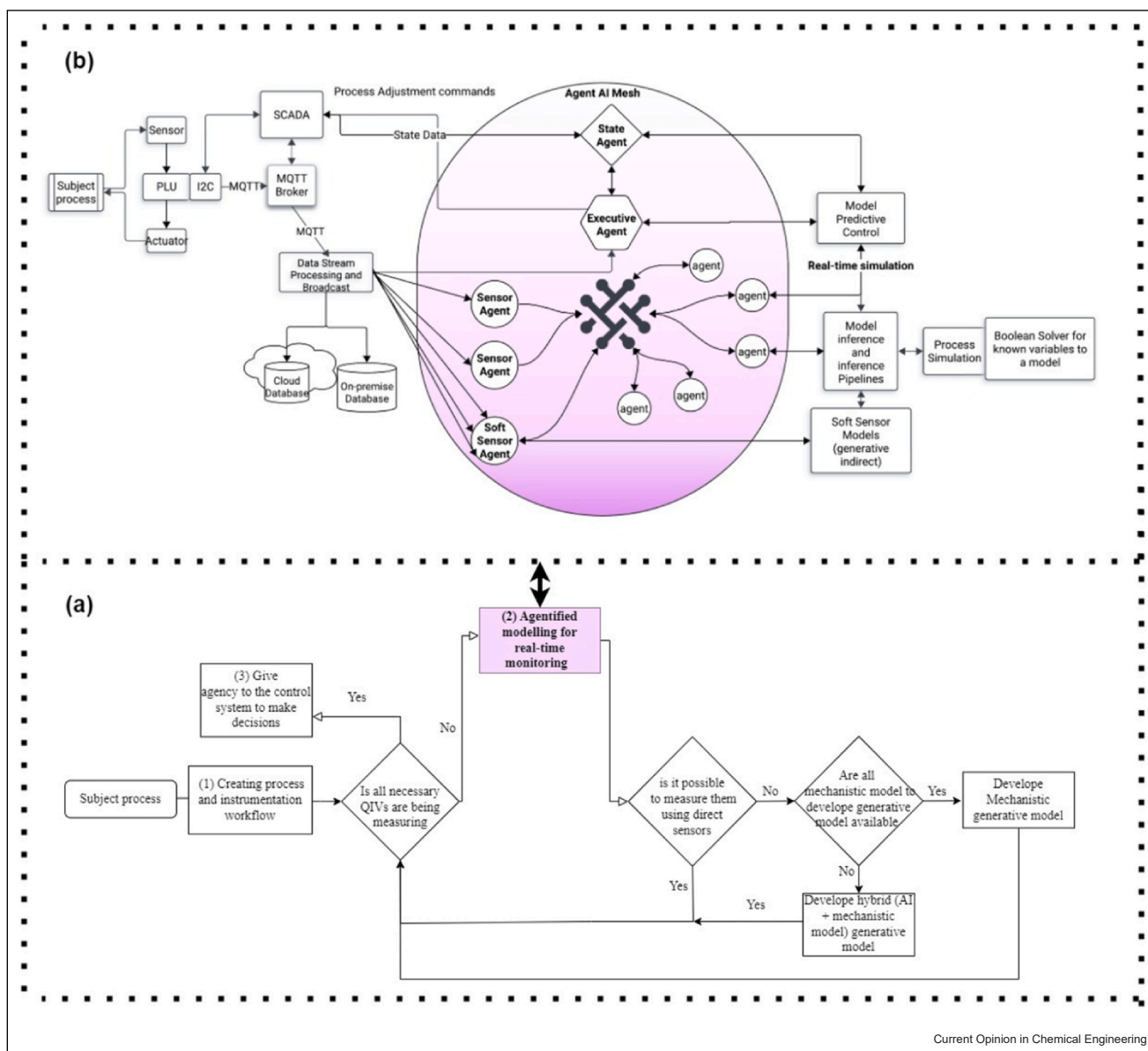
Systematic architecture for industrial Agentic AI and generative modeling

We present a systematic approach addressing complex system challenges in process monitoring and control, as illustrated in Figure 1. This approach consists of three key stages: (1) creating a process and instrumentation workflow to identify critical QIVs for measurement and monitoring, (2) implementing agentified modeling — combining mechanistic modeling and artificial intelligence — to monitor these QIVs through direct measurement or predictive modeling, and (3) integrating this data into the control system, granting it agency to make real-time decisions for process control.

This systematic approach begins with a comprehensive process and instrumentation workflow that defines the process task and maps out all relevant variables — including process characteristics, dynamic states, process conditions, and critical QIVs — into a structured knowledge base. This base comprises mechanistic models, parametric data, solvers, and both physical and soft sensors. To facilitate data collection and storage, this knowledge base is often maintained in an on-premises database, as shown in Figure 1b, ensuring secure and rapid access to process data for real-time monitoring.

When the initial stage fails to capture all necessary QIVs for effective monitoring, the approach pivots to the

Figure 1



(a) The systematic approach for generative modeling, including 1) creating a process and instrumentation workflow, 2) agentified modeling for real-time monitoring, and 3) give agency to the control system. **(b)** Agent models and their connection to SCADA and control system.

second stage, which is agentified modeling, combining mechanistic process models with artificial intelligence. Here, we distinguish between traditional 'AI agents' that perform specialized data processing and predictive tasks, and 'Agentic AI' that imparts autonomous, decision-making capabilities to the system. The system leverages industrial communication protocols such as MQTT (Message Queuing Telemetry Transport), a lightweight messaging protocol for efficient data streaming and processing, and I2C (Inter-Integrated Circuit), a serial

communication protocol used for connecting sensors and actuators to the control system, as depicted in Figure 1b. If sufficient process knowledge is available, the system leverages this to 'close the loop' with targeted generative models; if not, hybrid modeling techniques are employed to develop generative agents (or soft sensors) that predict or measure the desired process parameters. The integrated network of agents feeds directly into the control system, enabling it to make informed, real-time decisions.

In the third stage, the accumulated data — whether directly measured or generated via predictive modeling — are seamlessly integrated into the control system, endowing it with the agency to make real-time decisions. This control system often includes components like SCADA for high-level process supervision and PLC (Programmable Logic Controller) for managing actuators and executing control commands, as illustrated in Figure 1b. In this stage, the control system not only utilizes outputs from traditional AI agents (as established in stage 2) but is also empowered by Agentic AI to autonomously execute decision-making and adapt to changing process conditions in real time. This integration transforms the control system into an adaptive, autonomous entity that continuously monitors process variables and adjusts operational parameters to maintain optimal performance. By merging direct measurements from sensor agents with predictive outputs from traditional AI agents and then empowering the system with Agentic AI, the control system operates on a robust, closed-loop feedback mechanism. By merging direct measurements from sensor agents with predictive outputs from AI agents and insights from model agents, the control system operates on a robust, closed-loop feedback mechanism.

To demonstrate the versatility and effectiveness of our systematic approach, we selected four case studies across diverse domains: auto racing, plant-wide manufacturing, consumer products, and biomanufacturing scale-up. The auto racing example highlights generative models' value in low-inertia systems, underscoring their applicability to chemical processes. The plant-wide manufacturing case exemplifies all three stages in an already-implemented industrial setting. The consumer products example broadens relevance by tackling inherently chemical production processes, and the biomanufacturing study addresses scale-up challenges in complex biological systems. As summarized in Table 1, each case maps its process and instrumentation workflows (Stage 1), agentified modeling components (Stage 2), and Agentic AI-driven control integration (Stage 3) onto real-world operations.

Case 1: A motivating example of generative modeling as a soft sensor in motor sports

Motorsport is a high-stakes environment where split-second decisions can define the difference between victory and defeat. In such a setting, real-time analytics are not just beneficial — they are essential. Motorsports teams like Andretti Autosport rely on real-time data to make immediate adjustments during a race, from tire pressure and degradation monitoring to optimizing fuel consumption and adjusting race strategy based on evolving track conditions and weather.

The literature on motorsports analytics has highlighted several key algorithmic and data-driven approaches aimed at improving performance and strategic decision-making during races. One major area of focus is optimal trajectory planning, where machine learning models are developed to determine the fastest possible racing lines, enabling real-time adjustments in response to changing track conditions [25]. Energy management strategies represent another significant domain of research, especially for hybrid vehicles. Optimization algorithms in this area consider not only vehicle dynamics but also competitors' behavior to minimize lap times while staying within energy constraints [26]. Predictive modeling is also a prominent focus, with data-driven approaches being used to identify key factors that influence race outcomes, such as yellow flag probability, vehicle dynamics, tire performance, and environmental conditions. These models support more effective strategic planning and race execution [27].

These studies underscore the critical importance of real-time data processing and predictive analytics in motorsports. The integration of advanced generative AI models extends this body of research by providing instantaneous, predictive insights that complement existing analytical techniques. Specifically, generative models can create synthetic data that closely mirrors actual sensor measurements, enabling deeper insights into vehicle behavior and the wear of critical components. This approach addresses several gaps identified in the literature, pushing the application of data analytics in motorsports further into real-time, decision-support contexts.

The generative AI solution developed by Zapata AI for Andretti Autosport [28] complements the existing literature by integrating advanced predictive analytics and real-time synthetic data generation into an edge-to-cloud architecture tailored for high-performance environments like racing. This approach effectively addresses the critical need for low-latency, high-reliability decision support that traditional algorithmic methods in the literature often overlook.

The system architecture (Figure 2) is designed to handle the intense computational demands of motorsport analytics through a combination of edge and cloud-based processing:

- *Transportable edge deployment.* The core of the solution is a transportable edge computing unit equipped with high-performance GPUs (Graphics Processing Units). This hardware is deployed trackside, enabling the immediate ingestion and processing of telemetry data directly from the cars. By processing data at the edge, the system minimizes latency, providing real-time feedback on critical metrics like tire degradation, fuel

Table 1

Case studies mapped to the three-stage systematic architecture (see Figure 1).

Case	Stage (1)	Stage (2)	Stage (3)
1	- Define QIVs: tire degradation, fuel consumption, engine temperature, track conditions - Deploy pressure, temperature, accelerometer sensors - Establish real-time telemetry pipelines	- Fuse mechanistic vehicle-dynamics models with AI agents for slip-angle, degradation & yellow-flag prediction - Edge-deploy generative models to synthesize “virtual” sensor streams when measurements are missing	- Control-room Agentic AI autonomously interprets combined real + synthetic data to adjust pit-stop timing, tire pressures & fuel strategy - Continuously updates tactics without human prompts
2	- Map sugar-beet process (unloading → washing → extraction → crystallization → drying) - Identify QIVs: Brix index, temperature, pressure - Install & calibrate sensors + sampling routines	- Build hybrid soft sensor by fusing mechanistic nucleation/crystal-growth models with AI agents to predict Brix index in real time - Apply data normalization and deep-learning denoising on time series	- Integrate soft-sensor outputs into the SCADA/DCS system - Agentic AI autonomously adjusts crystallization residence time & operating parameters - Optimize energy use, CO₂ emissions & throughput
3	- Deploy NIR & visible-light sensors in SalonLab device to measure cysteic acid, “bulk effect” & color - Capture scalp/hair traits and consumer preferences via app - Structure all inputs into a unified decision matrix	- Train chemometric ML agents on spectral data to predict hair metrics (cysteic acid, bulk effect) - Deploy LLM-based agents to translate textual consumer preferences into formulation parameters - Use generative modeling agents to propose novel molecular formulations	- SalonLab control interface empowered by Agentic AI to select and refine personalized shampoo formulations - Continuously update recommendations in real time as new sensor data and feedback arrive
4	- Map micro → macro scales (metabolic pathways → reactor hydrodynamics → mixing) - Identify QIVs: O₂/CO₂, nutrients, pH, temperature, light irradiance, tracer profiles - Deploy imaging, spectroscopy & capacitance probes; define MicroTUBE & MacroTUBE protocols	- MicroTUBE agents: mechanistic calibration with imaging/spectroscopy to train generative models - MacroTUBE agents: AI-driven tracer distribution modeling + compressed-sensing inference of reactor states - Hybrid quantum/classical agents: Deploy QUBO/SDP solvers for metabolic pathway optimization and generative diffusive models for counterfactual state estimation.	- Integrate MicroTUBE & MacroTUBE outputs into the QΨ-TUBE pipeline - Agentic AI autonomously selects scale-up strategies, adjusts aeration/agitation, and runs counterfactual simulations - Continuously reconcile live sensor data, mechanistic priors & synthetic predictions to refine process parameters

efficiency, and component wear. This contrasts with cloud-only solutions in the literature, which often introduce delays due to data transmission. Internet connectivity at some tracks is often unpredictable in terms of reliability and latency.

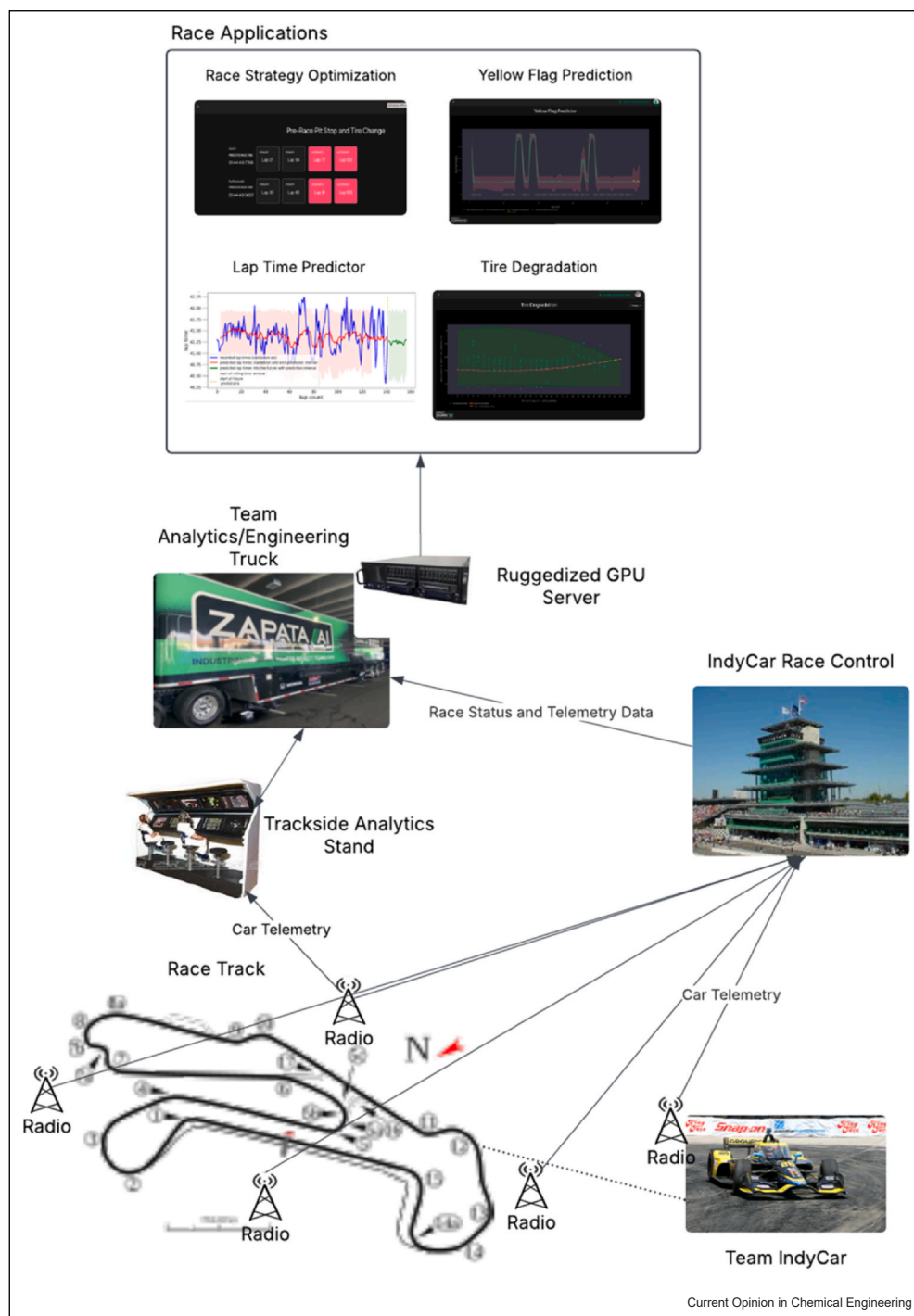
- *Cloud-based model training and synchronization.* The cloud infrastructure serves as a scalable environment for training generative models on large datasets, including historical telemetry and synthetic data generated during prior races. These models are periodically synchronized with the edge deployment to ensure that the latest predictive insights are available trackside. The hybrid approach leverages the cloud for computationally intensive tasks while maintaining low-latency decision support at the edge, aligning with best practices discussed in academic research for handling high-frequency data streams in dynamic environments.
- *Generative AI for real-time inference.* The solution features advanced generative models that create synthetic ‘virtual sensor’ data streams, filling in gaps where direct measurements may be unavailable or unreliable. For example, the models can infer

parameters such as the slip angle of the tires that are critical for understanding tire degradation. This capability aligns with state-of-the-art techniques in predictive analytics but extends them by leveraging generative AI to provide a more comprehensive and accurate representation of vehicle behavior in real time.

This generative AI solution builds on the strengths of existing algorithmic and predictive modeling frameworks while addressing critical gaps identified in academic research. By integrating real-time synthetic data generation and deploying it at the edge, the solution overcomes the latency issues associated with cloud-only approaches. Furthermore, the hybrid architecture supports a continuous feedback loop, where new data inform model updates, ensuring that predictions remain accurate and relevant throughout the race.

Ensembles of multiple models for Lap Time/Gap Prediction, Yellow Flag Probability, Tire Degradation, and Race Strategy Optimizations are built using 10+ years of historical data collected from telemetry on the cars as

Figure 2

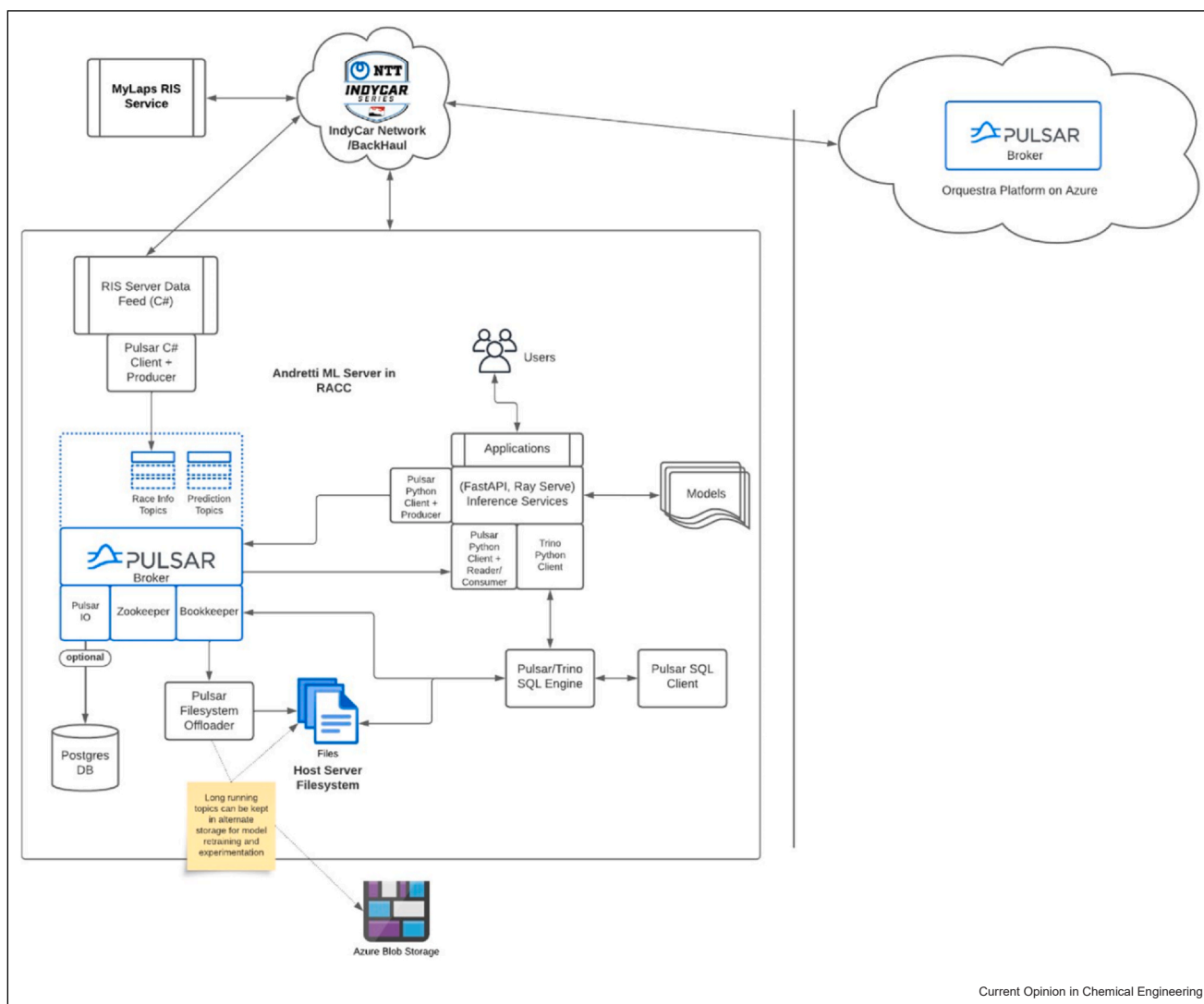


Operational architecture for real-time decision-making in motorsport, featuring transportable edge computing for immediate analytics and cloud-based infrastructure for enhanced model training and predictive insights. AI capabilities are deployed.

well as IndyCar Series data. Simulation data from a Driver-in-the-Loop IndyCar simulator are used as well. All models utilize multiple data pipelines for generating training data and receive real-time data during the race. In

the cases of Yellow Flag prediction and Lap Time prediction, two or more models are used for each of the cars on the track, and those models feed a group prediction model. During the course of a race, close to one hundred

Figure 3



Technical implementation Race Strategy services.

models could be running inference at the same time. Each model performing inference is capable of processing up to 200 messages per millisecond (Figure 3).

The objective of motorsport analytics should be to enhance real-time decision support and maximize race performance in high-stakes environments. Three issues and challenges related to this application are listed below:

- Ensuring low-latency data processing (the system must leverage transportable edge computing units with high-performance GPUs to deliver immediate insights, despite unpredictable internet connectivity and rapidly changing race conditions).
- Integrating edge and cloud architectures effectively (synchronizing cloud-based model training with

trackside edge deployments is crucial for providing up-to-date predictive analytics, yet remains challenging due to high data volumes and the need for continuous, real-time updates).

- Maintaining the accuracy and reliability of synthetic sensor data (generative AI models must accurately infer critical vehicle parameters — such as tire slip angles and degradation rates — to support split-second decision-making, addressing potential gaps where direct measurements are unreliable or unavailable).

Case 2: Plant-wide manufacturing process monitoring

The production of sugar from sugar beets is a highly intricate and multistage process carried out within specialized sugar factories. This journey begins with trucks

delivering sugar beets to the factory, where they are initially assessed at the weighbridge. The process then proceeds through several critical steps, including sampling, unloading, washing, slicing, and extraction in the extraction tower. The extracted juice is purified in a dedicated purification unit before undergoing evaporation, crystallization, centrifugation, and drying. The resulting sugar is subsequently stored in silos until it is dispatched from the service center. Among all these stages, crystallization is particularly significant, as it has a profound impact on the final specifications of the sugar crystals, energy consumption, and the factory's overall carbon footprint. When the crystal size distribution falls outside the desired range, the material must be recycled for remelting and recrystallization, adding complexity to the operation.

The crystallization of sugar from sugar beet syrup is a complex and dynamic process involving the transformation of syrup into massecuite. This process is inherently nonlinear and nonstationary, shaped by intricate mechanisms of nucleation, crystal growth, and aggregation [29]. Despite its critical importance, there is no comprehensive mechanistic model available to accurately describe the interplay between crystallization dynamics and operating conditions. As a result, current control strategies largely rely on the online monitoring of key process parameters. However, in industrial batch crystallizers, accurately measuring the crystal size distribution, a key QIV, remains a significant challenge [30].

This case study highlights collaborative research conducted by Nordzucker and the Technical University of Denmark, which aimed to address this challenge. The research utilized process knowledge and artificial intelligence to model the complex dynamics and nonlinearities in the original dataset. The focus was on generating the Brix index, a critical measure of dissolved solids in a liquid, as a key QIV representing crystal size distribution.

The study adopted a hybrid approach, combining process control expertise with machine learning techniques. By leveraging easily measurable variables, such as temperature and pressure, the model successfully generated the Brix index for real-time process monitoring. This information supported decision-making and complemented batch-processing operations. Further information regarding performance and validation of the developed soft sensor for sugar crystallization has been reported by Boskabadi et al. [31].

The results demonstrated that the soft sensor developed in this study effectively predicted the Brix index, capturing the process's dynamic and nonlinear characteristics. This aligns with steps 2 and 3 of the systematic approach presented in Figure 1, where generative modeling enables real-time monitoring and decision-making. By implementing this monitoring system and granting agency to the control system,

batch residence time during crystallization was significantly reduced. Consequently, this leads to lower energy consumption and CO₂ emissions while increasing production capacity.

The objective of deploying a soft sensor in plant-wide manufacturing should be to enhance process monitoring reliability and ensure alignment with Industry 4.0 goals. Three issues and challenges related to this deployment are listed below:

- Data variability and measurement noise must be addressed effectively (inconsistent sampling rates, sensor drift, and noisy measurements require data normalization and deep learning techniques to capture key time-series patterns).
- Feature imbalances need careful management (leveraging process knowledge and data-driven insights for feature reduction is crucial to maintain computational efficiency and ensure seamless integration into control systems).
- Scalability and model adaptability remain critical challenges (the need for retraining under varying operational conditions calls for the development of self-adaptive algorithms for real-time calibration, ensuring robust performance across diverse industrial settings).

Case 3: Predictive consumer product modeling

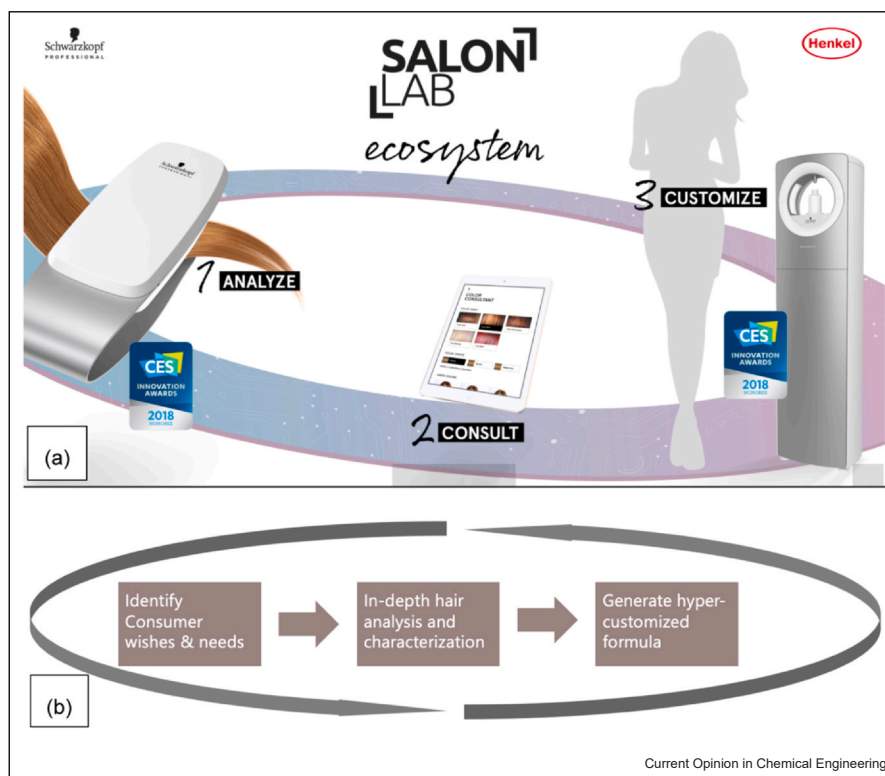
The structure and chemical composition of hair fibers have been well-understood for many years. However, due to the vast diversity in hair types, the cosmetic industry faces challenges in meeting the unique needs of each consumer [32]. This has led to a rapid shift toward product customization and the integration of digitally connected beauty tools [33,34]. In response to these trends, Henkel Consumer Brands introduced the SalonLab Ecosystem in 2018 (Figure 4). This innovative approach is built upon three key elements: (a) advanced hair analysis, (b) understanding consumer needs and preferences, and (c) personalized product formulation.

Step 1: Advanced hair analysis

The process begins with a smart device equipped with a near-infrared (NIR) sensor and a visible light sensor to analyze the hair fiber. NIR spectroscopy is a well-established, highly effective analytical method for non-destructive examination of hair characteristics. Recent advancements in sensor technology and miniaturization have enabled the application of this technique outside traditional laboratory settings. This allows for precise identification of the hair cortex's chemical composition and the effect of hair care products.

Through NIR analysis, much information about the hair can be obtained, including two critical metrics: cysteine

Figure 4



(a) SalonLab ecosystem, including hair analysis, consultation with customers, and personalized products. (b) Generative AI hyper-customization for customized products, including considering customer needs, hair analysis, and generating hyper-customized formula.

acid concentration (a degradation product of cystine) and the 'bulk effect' of care products on the hair. The resulting spectral data show excellent correlation with sensory assessments, enabling a rational and systematic classification of both the hair and hair-plus-product based on their current condition. To achieve a comprehensive hair diagnosis, the actual color of the hair fiber is also measured using a visible light sensor.

The quantification of cysteic acid, prediction of the 'bulk effect,' and detection of hair color are all achieved through the development of chemometric machine learning models. These models are trained on a diverse database containing hair samples from various origins, colors, and conditions, ensuring robust and accurate analysis.

Step 2: Visual assessment and consumer consultation

In the next phase, a visual evaluation is conducted to assess factors such as scalp condition, previous treatments, hair length, thickness, etc. In addition, user expectations regarding desired outcomes (e.g. volume, shine, smoothness, strength) are gathered through a consultation application. This dual approach ensures a comprehensive understanding of the consumer's specific needs and hair health.

Step 3: Customized shampoo formulation

All collected data — from both the scientific analysis and the consumer consultation — are integrated into a decision matrix. This matrix guides the creation of a customized shampoo formulation tailored to the individual's unique hair profile and desired results. The SalonLab concept has been introduced in professional hair salons worldwide, providing personalized solutions for a diverse range of hair types.

Expanding with generative AI

Building on this success, Henkel Consumer Brands is now leveraging Generative AI algorithms to scale the concept further. By analyzing consumer preferences on a mass scale, inputs in textual format can be fed into customized LLMs. These models accurately interpret specific consumer desires and seamlessly integrate them with the formula generation system, enabling even more precise and personalized hair care solutions (Figure 4). Employing Generative AI would not be limited to only understanding consumer sentiment, but it can also be used for innovation and discovery at the chemical and molecular level. Combining these two mentioned capabilities of Generative AI, new chemical formulas tailored

to the specific hair types and conditions, meeting consumer needs and expectations can be generated.

This innovative approach not only enhances the consumer experience but also represents a significant step forward in the digital transformation of the beauty industry, making hyper-customized hair products accessible on a global scale.

The objective of hyper-customized hair product formulation should be to seamlessly merge scientific analysis with personalized consumer needs while ensuring robust performance and safety. Three issues and challenges related to this innovation are listed below:

- Ensuring robust and consistent hair analysis (advanced NIR and visible light sensor techniques must reliably capture diverse hair types outside of controlled laboratory conditions, addressing potential issues like sensor calibration and measurement variability).
- Integrating multimodal data effectively (combining chemometric machine learning outputs with visual assessments and consumer consultation data into a cohesive decision matrix requires sophisticated data fusion strategies to accurately reflect individual hair profiles and desired outcomes).
- Scaling customization with generative AI (leveraging LLMs to interpret consumer preferences and generate new chemical formulations introduces challenges in maintaining the validity and safety of synthetic data, as well as ensuring seamless integration between textual insights and molecular innovation).

Case 4: Biomanufacturing process scale-up with quantum and classical agents

Bioprocess engineering requires information at various levels of granularity across scales like metabolic pathways, reaction kinetics, reactor specifications, and interaction of the micro to the macroscale and vice versa [35,36]. While many of these phenomena can be modeled mechanistically, engineering towards the goal of maximizing process throughput and other constraints satisfaction requires tools from artificial intelligence (AI) such as search, optimization, sampling, and machine learning to model process correlations [37,38,39]. The complexity is further enhanced due to the unavailability of data from many critical microscale states such as metabolic fluxes, cell morphology, viability, and so on, not disregarding the stochasticity in the dynamics of the individual cells and observability limitations of the process. Developing systematic algorithms validated by experiments forms the foundation for developing pipelines for the accelerated scale-up of manufacturing biomolecules. Some of the measurables that affect the growth of the cell are O₂ level, CO₂ level, nutrient concentration, pH, and temperature [40–42]. In the

context of certain species, like microalgae, light irradiance also plays a key role [43,44].

Currently, there is a lack of transferability of measurement technologies and scale-up strategies. It is also computationally intensive to estimate the state of a cell in a bioreactor given *just* the operating conditions of the bioreactor. Some aspects seen during experiments are to estimate the state of a bioreactor from macroscopic measurements and process causations obtained from *controlled experiments*. Another explored alternative is to use process information to trigger metabolic pathways to aid in manufacturing desirable compounds, avoiding byproducts and inhibitors.

Advanced monitoring from imaging, spectroscopy, and capacitance probes has made it possible to have at-line/on-line monitors. While great instrumental advancements, sporadic measurements, and transferability of results post-calibration are a hindrance. However, some online instrumentation and *independent experiments* aided by mechanistic knowledge can be leveraged to generate explainable monitoring solutions. Generative models are a class of machine learning algorithms designed to understand and replicate complex data distributions. By leveraging these models, researchers and practitioners in biomanufacturing can unlock several critical capabilities:

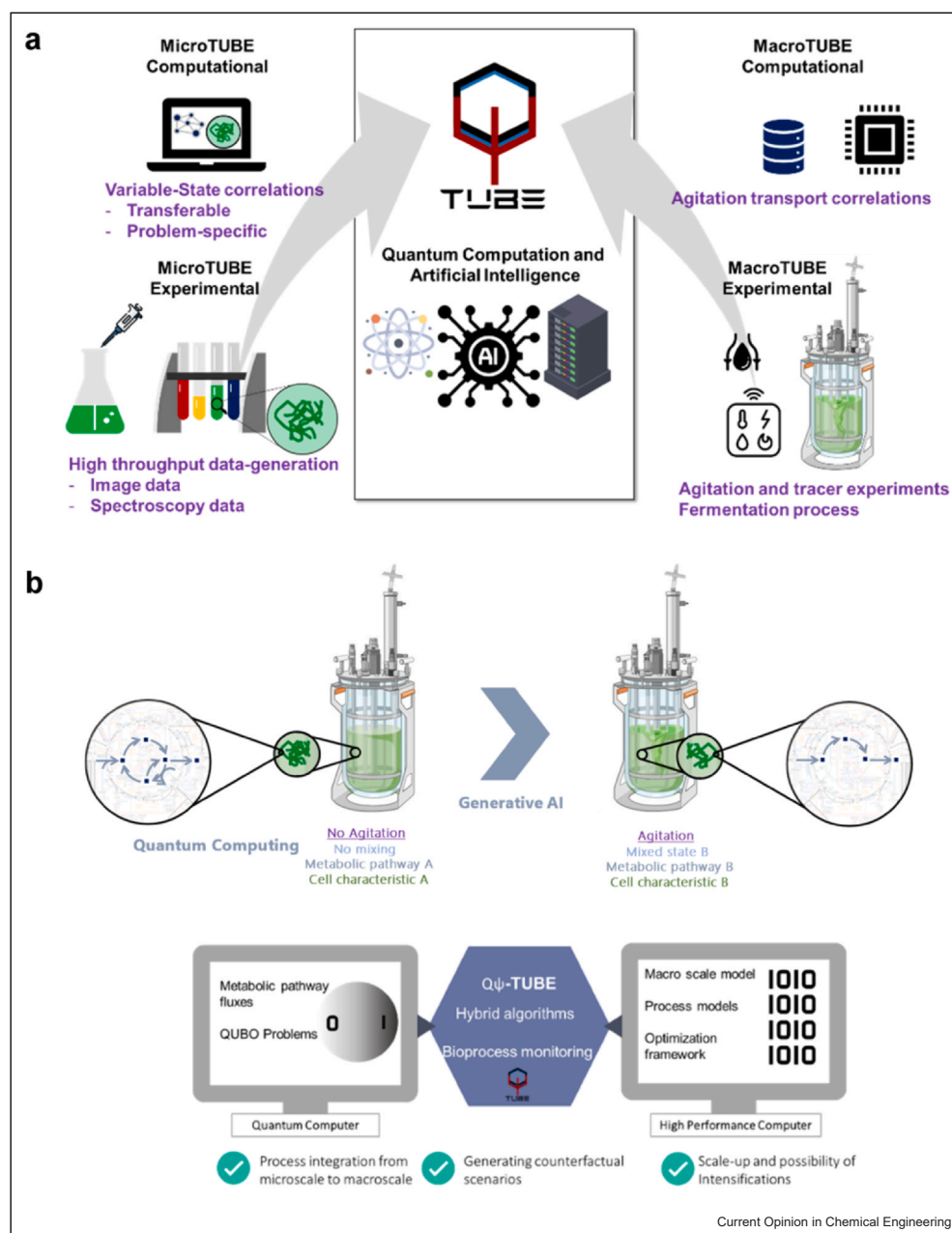
1. De Novo Design: Generative models can create entirely new biological sequences, such as proteins or DNA/RNA sequences, tailored for specific functions or properties. For instance, designing enzymes with higher stability or therapeutic proteins with improved efficacy.
2. Optimization of Bioprocesses: These models enable the fine-tuning of fermentation conditions, media formulations, and process parameters to maximize yield and quality.
3. Predictive Insight: By learning from existing datasets, generative models can predict the outcomes of genetic modifications, aiding in the development of engineered organisms for bioproduction.
4. Personalization: In the context of personalized medicine, generative models can assist in crafting patient-specific biologics, such as tailored vaccines or cell therapies.

This example aims to create a transferable real-time data-agnostic monitoring system, with process knowledge gained from micro and macroscale experiments by integrating a diverse range of offline sensors that can help in generating fast scale-up solutions. With inclusion of hydrodynamics, it is important to look at variations in the reactor to account for different environments experienced by the organism. A route to modeling this is using generative modeling to capture the distribution of substrate concentrations.

Quantum-inspired algorithms for search, optimization, and sampling are important for a domain like bioprocess engineering, where the dimensionality of the search space is very high [45]. They also aid in the representation of complex data structures more naturally and compactly than classical systems, which can make certain machine-learning tasks easier. However, quantum algorithms often have high computational and hardware requirements [46]. On the flip side, a completely classical route requires tremendous compute for large-scale monitoring. This would specifically

be challenging when the compute is *also* used for counterfactual simulations. We hence propose a hybrid strategy combining hard multifaceted data with soft sensing using quantum computing, generative modeling, and predictions using inline sensors. In this paradigm, some problems are solved using quantum computing and others use classical computing (Figure 5). Some speed-ups we envision with this hybrid approach are in metabolic pathway estimation using quantum semidefinite programming and quadratic unconstrained binary optimization (QUBO), mechanism

Figure 5



(a) QΨ-TUBE combines MicroTUBE and MacroTUBE. (b) Quantum computing and AI in QΨ-TUBE.

identification and compressed sensing, and estimation of process variables and cell state via generative models, like diffusive models. This entire workflow can be envisioned to be a part of a QCAI-TUBE (Q Ψ -TUBE) pipeline for the quantum and classical artificial intelligence for technology upgradation in bioprocess engineering.

Q Ψ -TUBE combines two modules, MicroTUBE for microscale calibration and MacroTUBE for macroscale estimation and optimization, each with experimental and computational parts (Figure 5a). Microscale imaging and spectroscopy are conducted based on known factors/variables that affect cell growth dynamics, like O₂ level, CO₂ level, pH, and temperature, to model a variable's effect on the metabolic pathway and cell states. These factors are used as seed values to inform generative models to predict cell morphology and viability. Proteomic analysis is used for quantum search and optimization to identify the metabolic pathway leading to the formation of desirable proteins (Figure 5b).

In MacroTUBE, tracer variability experiments are conducted (Figure 5a) in see-through reactors. Reactors are run at different agitation speeds, aeration velocity, and viscosity media to understand the effects of these inputs on mixing. Generative AI creates dynamic tracer profiles with operating conditions as input. The independently optimized modules are integrated into Q Ψ -TUBE for monitoring and counterfactual simulations.

The theoretical and practical possibility of this architecture is aided by sufficient advancement in quantum and classical artificial intelligence. With advancements such as quantum generative networks (Q-GANS) for estimation of prior distributions with quantum circuits and the generator model with generative adversarial neural networks [47], we envision similar work with the scale-up strategy to model an end-to-end pipeline for the estimation of novel-protein production.

Conclusions and perspectives

Generative models have demonstrated significant potential in addressing diverse industrial challenges. This study presents a systematic approach to generative modeling and agentic AI for process system engineering. This systematic approach consists of three different steps, including creating the process and instrumentation process diagram for the desired process. Then, the measuring process variables are determined using direct measurement. In this step, if measuring the process variable is not directly possible, generative modeling considering both process knowledge and artificial intelligence plays a crucial role in monitoring variables. Finally, this information

could be used for different purposes, including process control, optimization, and scale-up.

To investigate this systematic approach, four case studies showcasing the application of generative modeling in real-time motorsport optimization, customer-focused product design, the development of soft sensors for sustainable food manufacturing, and decision-making tools for biomanufacturing scale-up were investigated. These examples highlight the versatility of generative models in understanding and replicating complex data distributions, enabling their application in varied industrial domains.

While the promise of industrial Agentic AI and generative modeling is vast, several key limitations must be addressed before they can be more widely adopted in chemical engineering. High-quality, representative datasets remain scarce or costly to obtain, constraining model training and generalization. Seamless integration with wet-lab experiments is often hindered by mismatched data formats and timescales, complicating validation and calibration efforts. The inherently 'black-box' nature of many generative architectures also raises concerns around interpretability and trust, especially in safety-critical applications. Moreover, real-time, agentic decision-making at scale demands significant computational resources and robust edge-to-cloud infrastructure, which may not be available in all industrial settings. Finally, purely data-driven models can produce misleading or unsafe recommendations if not grounded in mechanistic process knowledge, highlighting the necessity of hybrid approaches that blend domain expertise with agentic AI.

By acknowledging these challenges alongside the demonstrated benefits, we underscore the importance of ongoing research into explainable generative methods, self-adaptive calibration algorithms, and cost-effective data acquisition strategies. As these elements mature, the synergy between generative modeling and complex industrial systems will continue to drive innovation, efficiency, and sustainability across chemical and bioprocess engineering.

CRedit authorship contribution statement

Mohammad Reza Boskabadi: Writing – original draft, Visualization, Investigation. **Yudong Cao:** Writing – original draft, Investigation. **Behnam Khadem:** Writing – original draft, Investigation. **William Clements:** Writing – review & editing. **Z. Nevin Gerek:** Writing – review & editing, Investigation. **Abhishek Sivaram:** Writing – review & editing, Investigation. **Eric Reuthe:**

Writing – review & editing, Investigation. **Christopher J Savoie**: Conceptualization, Writing – review & editing. **Seyed Soheil Mansouri**: Writing – original draft, Methodology, Conceptualization, Supervision, Project administration, Funding acquisition.

Data Availability

Data will be made available on request.

Declaration of Competing Interest

The authors declare the following financial interests/ personal relationships which may be considered as potential competing interests: Seyed Soheil Mansouri reports financial support was provided by Technical University of Denmark. If there are other authors, they declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

References and recommended reading

Papers of particular interest, published within the period of review, have been highlighted as:

- of special interest
- of outstanding interest

1. Destro F, Inguva PK, Srisuma P, Braatz RD: **Advanced methodologies for model-based optimization and control of pharmaceutical processes**. *Curr Opin Chem Eng* 2024, **45**:101035, <https://doi.org/10.1016/j.coche.2024.101035>
2. Zhang X, Song C, Zhao J, Xu Z: **Deep Gaussian mixture adaptive network for robust soft sensor modeling with a closed-loop calibration mechanism**. *Eng Appl Artif Intell* 2023, **122**:106124.
3. Sun Y-N, Qin W, Hu J-H, Xu H-W, Sun PZH: **A causal model-inspired automatic feature-selection method for developing data-driven soft sensors in complex industrial processes**. *Engineering* 2023, **22**:82-93.
4. Gani R, et al.: **A multi-layered view of chemical and biochemical engineering**. *Chem Eng Res Des* 2020, **155**:A133-A145. Provides a detailed overview of a multilayered approach to problem within chemical and biochemical engineering.
5. Loo JY, Ding ZY, Baskaran VM, Nurzaman SG, Tan CP: **Robust multimodal indirect sensing for soft robots via neural network-aided filter-based estimation**. *Soft Robot* 2022, **9**:591-612.
6. Hodjat B, Savoie CJ, Amamiya M: **Adaptive interaction using an adaptive agent-oriented software architecture**. *US Patent* 6594684; Jul. 15, 2003.
7. Hodjat B, Savoie CJ, Amamiya M: **Adaptive agent-oriented software architecture**. *US Patent* 6144989; Nov. 07, 2000.. This patent provides the details on the original technology behind Apple's Siri and its agent-oriented architecture.
8. Qiu K, Wang J, Wang R, Guo Y, Zhao L: **Soft sensor development based on kernel dynamic time warping and a relevant vector machine for unequal-length batch processes**. *Expert Syst Appl* 2021, **182**:115223.
9. Anstine DM, Isayev O: **Generative models as an emerging paradigm in the chemical sciences**. *J Am Chem Soc* 2023, **145**:8736-8750. This paper reviews generative models like GANs, VAEs, and diffusion models for chemical inverse design, emphasizing their ability to generate novel compounds with desired properties and addressing key challenges in their application.
10. De S, Bermudez-Edo M, Xu H, Cai Z: **Deep generative models in the industrial internet of things: a survey**. *IEEE Trans Ind Inform* 2022, **18**:5728-5737.
11. Harshvardhan GM, Gourisaria MK, Pandey M, Rautaray SS: **A comprehensive survey and analysis of generative models in machine learning**. *Comput Sci Rev* 2020, **38**:100285.
12. Zhang EY, Cheek AD, Pan Z, Cai J, Yan Y: **From turing to transformers: a comprehensive review and tutorial on the evolution and applications of generative transformer models**. *Sci* 2023, **5**:46.
13. Sengar SS, Hasan AB, Kumar S, Carroll F: **Generative artificial intelligence: a systematic review and applications**. *Multimed Tools Appl* 2024, **1-40** <https://link.springer.com/article/10.1007/s11042-024-20016-1>.
14. Perkins M, Roe J, Postma D, McGaughan J, Hickerson D: **Detection of GPT-4 generated text in higher education: combining academic judgement and software to identify generative AI tool misuse**. *J Acad Ethics* 2024, **22**:89-113.
15. He L, Hausman H, Pajonk F: **Generative artificial intelligence: a new frontier of scientific misconduct?** *Int J Radiat Oncol Biol Phys* 2024, **120**:1210-1213.
16. Nielsen RF, Nazemzadeh N, Sillesen LW, Andersson MP, Gernaey KV, Mansouri SS: **Hybrid machine learning assisted modelling framework for particle processes**. *Comput Chem Eng* 2020, **140**:106916.
17. Stillman NR, Mayor R: **Generative models of morphogenesis in developmental biology**. *Semin Cell Dev Biol* 2023, **147**:83-90. This study showcases GPT-4's ability to extract data from synthetic biology literature, enabling accurate fermentation predictions and advancing biomanufacturing through AI-driven insights.
18. Ghazi Vakili M, et al.: **Quantum-computing-enhanced algorithm unveils potential KRAS inhibitors**. *Nat Biotechnol* 2025, **1-6** Jan 22.
19. Kapoore RV, Padmaperuma G, Maneein S, Vaidyanathan S: **Coculturing microbial consortia: approaches for applications in biomanufacturing and bioprocessing**. *Crit Rev Biotechnol* 2022, **42**:46-72.
20. Boskabadi MR, Ramin P, Kager J, Sin G, Mansouri SS: **KT-Biologics I (KTB1): a dynamic simulation model for continuous biologics manufacturing**. *Comput Chem Eng* 2024, **188**:108770.
21. Rafieyan S, Ansari E, Vasheghani-Farahani E: **A practical machine learning approach for predicting the quality of 3D (bio) printed scaffolds**. *Biofabrication* 2024, **16**:45014.
22. Mock M, Langmead CJ, Grandsard P, Edavettal S, Russell A: **Recent advances in generative biology for biotherapeutic discovery**. *Trends Pharmacol Sci* 2024 **45**:255-267.
23. Xiao Z, Li W, Moon H, Roell GW, Chen Y, Tang YJ: **Generative artificial intelligence GPT-4 accelerates knowledge mining and machine learning for synthetic biology**. *ACS Synth Biol* 2023, **12**:2973-2982. This study showcases GPT-4's ability to extract data from synthetic biology literature, enabling accurate fermentation predictions and advancing biomanufacturing through AI-driven insights.
24. Mansouri SS, Sivaram A, Savoie CJ, Gani R: **Models, modeling and model-based systems in the era of computers, machine learning and AI**. *Comput Chem Eng* 2024, **194**:108957. This paper highlights modeling techniques and model-based tools for chemical and process engineering, addressing challenges in system representation and offering insights into advancing design and analysis workflows.
25. Garlick S, Bradley A: **Real-time optimal trajectory planning for autonomous vehicles and lap time simulation using machine learning**. *Veh Syst Dyn* 2022, **60**:4269-4289.
26. Paparusso L, Riani M, Ruggeri F, Braghin F: **Competitors-aware stochastic lap strategy optimisation for race hybrid vehicles**. *IEEE Trans Veh Technol* 2022, **72**:3074-3089.
27. Patil A, Jain N, Agrahari R, Hossari M, Orlandi F, Dev S: **A data-driven analysis of Formula 1 car races outcome**. In *Proceedings of the Irish Conference on Artificial Intelligence and Cognitive Science*. Springer; 2022:134-146.
28. Zapata AI and Andretti INDYCAR Gear Up to Apply Industrial Generative AI to Race Day Strategy and Analytics; 2024 [Online].

Available from: (<https://zapata.ai/news/zapata-ai-andretti-industrial-generative-ai-race-day-strategy-analytics-2024/>).

29. Meng Y, et al.: **Hybrid modeling based on mechanistic and data-driven approaches for cane sugar crystallization.** *J Food Eng* 2019, **257**:44-55.
30. Boskabadi MR, Sivaram A, Sin G, Mansouri SS: **Machine learning-based soft sensor for a sugar factory's batch crystallizer.** *Computer Aided Chemical Engineering Elsevier*; 2024:1693-1698.
31. Boskabadi MR, Murugaiah M, Nielsen TR, Sivaram A, Sin G, Mansouri SS: **Virtual sensor for sustainable large-scale process monitoring.** *Ind Eng Chem Res* 2025 **64**, https://pubs.acs.org/doi/full/10.1021/acs.iecr.4c03342?casa_token=c8RU3w6S1kAAAAAA%3AmTBj4sTS4fZd9zDnxVucjyHrG8GSRGZQL8DJ3psRHoI3HeuhMGptFBaquizbdC37Z_w9FCTas3EjqeQ.
32. Park YW, Hong P: **Beauty reimaged: navigating the cosmetic industry's digital transformation.** *Cosmetics Marketing Strategy in the Era of the Digital Ecosystem: Revolutionizing Beauty in the New Market Frontier.* Springer; 2024:47-74.
33. Coelho MCCD, Imamović I: **AI-driven personalization in beauty retail: exploring how AI-based applications influence customer satisfaction and brand loyalty.** *Leveraging AI for Effective Digital Relationship Marketing.* IGI Global; 2025:131-162.
34. Tzou H, Tseng J, CTO P: **How AI and AR can help beauty industry.** *IEEE Consum Technol Soc* 2022, **1**:7-14.
35. Coolbaugh MJ, et al.: **Pilot-scale demonstration of an end-to-end integrated and continuous biomanufacturing process.** *Biotechnol Bioeng* 2021, **118**:3287-3301.
36. Fasim A, More VS, More SS: **Large-scale production of enzymes for biotechnology uses.** *Curr Opin Biotechnol* 2021, **69**:68-76.
37. Rathore AS, Nikita S, Thakur G, Mishra S: **Artificial intelligence and machine learning applications in biopharmaceutical manufacturing.** *Trends Biotechnol* 2023, **41**:497-510.
38. Mehta A, Niaz M, Adetoro A, Nwagwu U: **Advancements in manufacturing technology for the biotechnology industry: the role of artificial intelligence and emerging trends.** *Int J Chem Math Phys* 2024, **8**:12-18.
39. Isoko K, Cordiner JL, Kis Z, Moghadam PZ: **Bioprocessing 4.0: a pragmatic review and future perspectives.** *Digit Discov* 2024, **3**:1662-1681.
40. Ruff SE, et al.: **Hydrogen and dark oxygen drive microbial productivity in diverse groundwater ecosystems.** *Nat Commun* 2023, **14**:3194.
41. Lage S, Toffolo A, Gentili FG: **Microalgal growth, nitrogen uptake and storage, and dissolved oxygen production in a polyculture based-open pond fed with municipal wastewater in northern Sweden.** *Chemosphere* 2021, **276**:130122.
42. Lu T, Jin M, Yang M, Huang D: **Deep learning-based prediction of critical parameters in CHO cell culture process and its application in monoclonal antibody production.** *Int J Adv Appl Sci Res* 2024, **3**:108-123.
43. Wang K, et al.: **How does the Internet of Things (IoT) help in microalgae biorefinery?** *Biotechnol Adv* 2022, **54**:107819.
44. Bakshi S, Leoncini E, Baker C, Cañas-Duarte SJ, Okumus B, Paulsson J: **Tracking bacterial lineages in complex and dynamic environments with applications for growth control and persistence.** *Nat Microbiol* 2021, **6**:783-791.
45. Li Y, et al.: **Efficient molecular conformation generation with quantum-inspired algorithm.** *J Mol Model* 2024, **30**:228.
46. Andersson MP, Jones MN, Mikkelsen KV, You F, Mansouri SS: **Quantum computing for chemical and biomolecular product design.** *Curr Opin Chem Eng* 2022, **36**:100754.
47. Rudolph MS, Toussaint NB, Katabarwa A, Johri S, Peropadre B, Perdomo-Ortiz A: **Generation of high-resolution handwritten digits with an ion-trap quantum computer.** *Phys Rev X* 2022, **12**:31010.