The role of digital twins in driving sustainability

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As the pharmaceutical sector endeavours to become more sustainable, we hear how digital twins – virtual replicas of systems or products that can help predict performance – are supporting the industry in its efforts

The manufacturing sector is facing growing pressure from consumers, regulators, and investors to reduce its environmental impact. The shift towards more sustainable pathways is not only driven by regulatory compliance but also by future-proofing businesses in a world where resources are finite.

This shift is clear in the pharmaceutical industry, which is striving to enhance the economic and environmental efficiency of its manufacturing processes while maintaining the highest quality standards.

Through new processes such as continuous manufacturing (CM) and the digitalisation of the manufacturing process, a real change is happening in the pharma industry. CM offers significant advantages in manufacturing agility, flexibility, process development, product quality control and overall cost reduction. The digitalisation of pharmaceutical processes and product design has been implemented using digital twins. Digital twins are a series of mathematical equations that describe the performance of the process. They also encompass material and equipment property databases related to the performance of the system.

Digital twins and simulation technologies will be crucial in bolstering the Fifth Industrial Revolution (Industry 5.0 or 5IR). Industry 5.0 places sustainability (and human-robot collaboration) at the core of industrial processes, aiming to maintain productivity while resolving environmental problems.

Impacts of digital twins on sustainability

Digital twins allow manufacturers to model, simulate, and investigate their manufacturing process in a virtual environment. For example, in continuous drug substance manufacturing, modelling can help in optimizing reaction conditions to maximize yield while minimizing energy consumption and material waste.

Computational modelling can virtually investigate new prototypes and equipment changes and simulate the outcome of integrating a new manufacturing module into the production line. This process de-risks capital expenditure.

Digital twins can also play a key role in sustainable product design. For example, discrete element modelling (DEM) and optimization algorithms can inform how a particular product is manufactured. Digital twins have the potential to simulate how different design choices could improve performance and reduce energy consumption.

Organizations can use physics-based models such as finite element analysis (FEA), computational fluid dynamics (CFD), or particle-based methods to simulate and investigate the material on various equipment. This approach can synthesize data for building lightweight Machine-Learning models and parametrize first-principle models. For example, residence time distribution (RTD) models of Continuous Direct Compression (CDC) units (blender and tablet press feed frame) can be completed using process parameters obtained from the discrete element method (DEM).

Using virtual experiment design, additional sustainable benefits can be achieved. These benefits include reduction of material and resource consumption, elimination of drug process development inefficiencies, and enhancement of scale. [(1)]

Models can also be used to maintain equipment to ensure optimal performance levels. Predicting potential failures before they occur will reduce the impact on production and thus reduce waste generation.

The development of carbon monitoring programs is on the increase. These data dashboards create a visual representation detailing all the emissions from the plant. This tool will contribute directly towards net-zero goals, forcing accountability through the visibility of the company's carbon emissions. Advanced dashboards that will use predictive analytics to forecast future emissions are also being discussed.

Digital twin architecture

Digital twin architecture has core components that work together to facilitate simulation, real-time monitoring, and analysis, leading to improved decision-making and optimization of the physical process.

The physical system is equipped with sensors and Internet of Things (IoT) devices that collect real-time data on various process parameters. Data from different units is aggregated and stored in a centralized or distributed data storage system (a cloud platform, an on-premises server, or a combination of both). Visualisation tools, advanced analytics, and Machine-Learning algorithms process the data to derive insights, detect anomalies, and predict future states. This processing can be done in real-time or offline mode, depending on the requirements.

Digital twins include the integration of hybrid models such as data-driven models, flowsheet models, thermodynamic and fluid dynamics models, DEM and kinematic models. Data-driven models include Machine Learning and statistical approaches and are used to predict outcomes, optimize processes, and identify patterns or anomalies based on historical data. Environmental and sustainability models (e.g. energy consumption models) and emission models can be used to track and predict the energy usage of manufacturing processes and calculate and predict emissions and waste generation.

Real-time synchronisation continuously updates a digital twin with real-time manufacturing data, optimising the model and, in turn, providing more accurate analysis and monitoring. This would allow dynamic adjustments to be made during processing, also referred to as advanced process control, which ensures the product is kept within specification at all points during production. The use of digital tools and data in this manner will support real-time release strategies, preventing lengthy quality control analyses only to realise the product does not meet the final release specifications.

Drawbacks of digital twins

Digital twins offer substantial benefits in manufacturing. However, they come with several challenges that need to be carefully considered and managed. First, as a vast amount of data flows between the digital twins and physical systems, this can lead to increased cybersecurity and data privacy concerns. Manufacturers should implement strategies (e.g., data encryption) to secure digital twins from potential security threats.

Cloud-based systems provide several services (e.g., scalability, built-in security, resource optimisation, etc.), as well as best practices that can help enhance security and reduce the initial investment requirements of the digital twin architecture.

Digital solutions are critical to driving sustainability within the pharmaceutical industry. As an industry, we have collated vast amounts of data, and it is now time to use this information to transform how we manufacture medicines. Digital platforms will facilitate valuable collaborations across the industry and are the future of driving change toward more sustainable practices.

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