Tecnología analítica de procesos en la industria 4.0: revisión de aspectos de importación

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RESUMEN

Process Analytical Technology (PAT) es un sistema que surgió proactivamente por la "Food and Frug Administration" (FDA) hace algunas décadas para mejorar la forma tradicional de controlar los procesos analíticos en las industrias. Su directriz fue declarada un sistema para diseñar, analizar y controlar mediciones divergentes de "Critical Process Parameter" (CPP) y "Critical Quality Attributes" (CQA). Su enfoque se ha mejorado utilizando nuevas herramientas como "Quality by Design" (QbD) para establecer una comprensión profunda del proceso de fabricación. Debido a sus aplicaciones multidimensionales, uno de los análisis de procesos analíticos químicos que más se ha crecido en los últimos siglos son las técnicas de espectroscopia (infrarrojo cercano, biosensores, Raman, espectroscopia de fibra óptica) que se han desarrollado con sistemas online o offline utilizando técnicas para potenciar y mejorar la cuantificación industrial de herramientas de control como Cp ("Process Capacity"), CpK ("Process Capacity Index"). Esta combinación de PAT con QbD ha sido muy beneficiosa para impulsar a las industrias hacia una cuarta revolución industrial, donde las tecnologías físicas y digitales se entrelazan con sistemas informáticos como la nube y el Internet de las cosas industrial (IIoT). La adopción de este nuevo sistema en la industria en general ha hecho evolucionar la calidad de los productos ofrecidos, brindando mejor calidad, costo y satisfacción para el cliente final. Esta visión es posible a través del desarrollo de técnicas y software quimiométricos que tienen una mejor interpretación matemática de los datos y problemas químicos, correlacionando a través de la regresión lineal multivariada una mejor comprensión de los parámetros de fabricación. A diferencia de los métodos tradicionales existentes debido a su rapidez, además de ser considerada tecnología "verde" al medio ambiente y los seres humanos, la utilización de reactivos químicos no son necesarios para su análisis. En los tiempos actuales estás técnicas son muy usuales, pues proporcionan un enfoque más dinámico y continuo con datos viables, reproducibles y asertivo en cualquier etapa de la producción en la que se instale. Por lo tanto, esta es una revisión de aspectos importantes que se deben considerar y su conceptualización general, brindando una relación sobre cómo se integra la química analítica con las matemáticas, las tecnologías de la información y especialmente la manufactura.

Palabras Claves: tecnología analítica de procesos; control de procesos; monitoreo en tiempo real, Tecnología de Infrarrojo Cercano, Quimiometría, FDA, Industria 4.0, Calidad por Diseño, Internet industrial de las Cosas, Sistemas Ciberfísicos y Sistemas de Localización en Tiempo Real

Process Analytical Technology in Industry 4.0: Import aspects review

ABSTRACT

The Food and Drug Administration (FDA) proactively developed Process Analytical Technology (PAT) a few decades ago to enhance the old manner of managing analytical processes in industry. Its policy was defined as a method for developing, assessing and regulating diverging measurements of "Critical Process Parameters" (CPP) and "Critical Quality Attributes" (CQA) (CQA). Their approach has been enhanced using new tools such as "Quality by Design" (QbD) to get a thorough understanding of the production process. The spectroscopy techniques, such as near infrared spectroscopy, biosensors, Raman, fiber optic spectroscopy, and others, which have been developed with online and offline techniques to boost and improve industrial quantification of control tools such as Cp ("Process Capacity"), CpK ("Process Capacity Index"). This combination of PAT and QbD has shown to be quite effective in propelling companies into the fourth industrial revolution, in which physical and digital technologies are integrated with computer systems such as cloud and industrial internet of things (IIoT). The implementation of this new approach throughout the industry has improved the quality of the products available, resulting in higher quality, cost, and customer happiness. This vision is made feasible by the development of chemometric techniques and software that provide a better mathematical interpretation for chemical data and issues, as well as a better knowledge of production factors through multivariate linear regression. Unlike existing traditional methods, which are time-consuming and often unhealthy for the environment and humans because they use chemical reagents in their analyses, these "green" techniques take a dynamic and continuous approach, providing reliable data that is repeatable and assertive at any stage of production in which they are installed. As a result, this is a review of significant factors to consider and their general conceptualization, as well as a link between analytical chemistry, mathematics, information technologies, and manufacturing

Keywords: process analytical technology; process control; real-time monitoring, Near Infrared Tecnology, Chemometrics, FDA, Industry 4.0, Quality by Design, industrial Internet of Things, Cyber Physical Systems and Real-Time Location Systems.

Tecnologia Analítica de Processos na Indústria 4.0: Revisão de aspectos de importação

RESUMO

A Process Analytical Technology (PAT) é um sistema que surgiu de forma proativa da "Food and Frug Administration" (FDA) há algumas décadas para aprimorar a forma tradicional de controle de processos analíticos nas indústrias. Sua diretriz foi declarada um sistema para projetar, analisar e controlar medições divergentes de "Parâmetro Crítico de Processo" (CPP) e "Atributos Críticos de Qualidade" (CQA). Sua abordagem foi aprimorada usando novas ferramentas como "Quality by Design" (QbD) para estabelecer uma compreensão profunda do processo de fabricação. Devido às suas aplicações multidimensionais, uma das análises de processos analíticos químicos que mais cresceu nos últimos séculos são as técnicas de espectroscopia (infravermelho próximo, biossensores, Raman, espectroscopia de fibra óptica) que foram desenvolvidas com sistemas online ou offline. aprimorar e aprimorar a quantificação industrial de ferramentas de controle como Cp ("Capacidade de Processo"), CpK ("Índice de Capacidade de Processo"). Essa combinação de PAT com QbD tem sido altamente benéfica para impulsionar as indústrias em direção a uma quarta revolução industrial, onde as tecnologias físicas e digitais estão entrelaçadas com sistemas de computação como a nuvem e a Internet Industrial das Coisas (IIoT). A adoção deste novo sistema na indústria em geral fez evoluir a qualidade dos produtos oferecidos, proporcionando melhor qualidade, custo e satisfação para o cliente final. Essa visão é possível através do desenvolvimento de técnicas quimiométricas e softwares que tenham uma melhor interpretação matemática de dados e problemas químicos, correlacionando através de regressão linear multivariada um melhor entendimento dos parâmetros de fabricação. Ao contrário dos métodos tradicionais existentes devido à sua rapidez, além de ser considerada tecnologia "verde" para o meio ambiente e o ser humano, não é necessário o uso de reagentes químicos para sua análise. Nos tempos atuais essas técnicas são muito comuns, pois proporcionam uma abordagem mais dinâmica e contínua com dados viáveis, reprodutíveis e assertivos em qualquer etapa da produção em que está instalada. Portanto, esta é uma revisão de aspectos importantes a serem considerados e sua conceituação geral, fornecendo uma relação sobre como a química analítica se integra com a matemática, tecnologias da informação e principalmente manufatura.

Palavras chave: tecnologia analítica de processos; controle do processo; Monitoramento em tempo real, Tecnologia de Infravermelho Próximo, Quimiometria, FDA, Indústria 4.0, Qualidade por Design, Internet das Coisas industrial, Sistemas Ciberfísicos e Sistemas de Localização em Tempo Real.

1. INTRODUCTION

Process Analytical Technology (PAT) can be defined as a system for analyzing, controlling, and planning manufacturing processes using real-time measurements for all critical quality parameters in supply chains (raw materials, intermediate products, and final products) [1].

Due to technological advances in the industries, exchange, and improvement of material control monitoring systems, both in environmental aspects (temperature, pressure, volume, etc.) and critical process control parameters (physical, chemical, and microbiological properties, etc.) in real time, occur in a variety of industrial sectors such as: food, pharmaceutical, chemical, etc. [1].

Its definition and concepts were developed in the twentieth century with the combination of chemical applications and mathematical algorithms, using visualization tools to solve manufacturing processes. These application concepts only gained industrial relevance when, in the twenty-first century, the FDA (Food in Drug Administration) expanded the process approach with the formation of directives and PAT definitions in the pharmaceutical industries. Delineating manufacturing mechanisms using critical process parameters (CPP) that directly affect "Critical Quality Attributes" (CQA) dubbed "Quality by Design" (QbD). [2].

The QbD focuses on improving monitoring precision, which allows for a more comprehensive understanding of the products and processes to be controlled, as well as continuous learning of results obtained from process dynamics [1]. Their data, together with PAT and Industry 4.0 advances, are becoming significant components for industrial paradigm shifts.

The mechanism has the ability to make decisions during the manufacturing stages of a product, resulting in a control strategy that includes adjustments and corrections to critical control parameters that show deviations from an ideal specification established by research and development teams, i.e., continuous manufacturing improvement that reduces variations in its operation.

Overall, its application is based on all the components and processes that affect the final product's quality, and it adjusts it using spectroscopy-controlled process control instruments, known as offline and online, respectively, that have their data linked to an exclusive real-time network of a Design of Experiments (DoE) system built during the manufacturing process. [3].

This is consistent with the core principle that quality does not have to be determined through trial and error, but rather by the system's data bases. As a result, considering the entire PAT principle and its application components, we must evaluate the following points:

1. Process analytical chemistry tools: developed for each product matrix and critical control parameter.

2. Acquisition and analysis of multivariate data: initially defined as chemometric tools for the development of better calibration curves for the matrix and critical parameter predefined in the previous stage.

3. Process monitoring and control: used to calibrate, validate, and provide enough data to generate an opportunity evaluation later on.

4. Continuous process and improvement optimization via integrated management: at this final stage, information is collected in the manufacturing floor and transferred in an asynchronous

manner, with the goal of sending it to the cloud and providing real-time feedback on manufacturing parameters.

In this regard, industries in general use these technologies to improve the quality of final product quantification while maintaining environmental and economic responsibility. Consequently, using linear regression algorithms derived from chemometrics models, we can predict control-critical parameters vs international models. The goal of this study is to evaluate the mechanisms required for real-time product release and process controls required for the generation of spectrum data using analytical instruments used in PAT systems that will allow for assertive and precise data prediction for process control.

2. PAT Components

The primary notion of PAT may be defined as a quality attribute tool that identifies and integrates potential measurements, ensuring the high quality of products analyzed by mathematical, physical, microbiological, and mostly analytical studies. In this case, for example, the interaction of the process with the generated data might include a feedback stream that changes the process conditions in real time, benefiting all involved media [4]. According to Bakeev (2010) [5], the PAT system's approach may be divided into three major components:

1 – Process analysis.

2 –Multivariate data analysis (Chemometrics).

3 – Process control.

These stages, together with their respective measurement instruments, are critical for monitoring critical parameters or quality attributes in production lines or even quality laboratories. Its quantification tools are given by multivariate data that are developed to quantify these analyzed parameters and/or attributes, or to identify patterns in data sets using groups, trends, or even outliers. It serves as the foundation for control tools such as Cp ("Process Capacity"), CpK ("Process Capacity Index"), statistical process performance, and so on, for process execution and control. [5].

For a successful implementation of this system, defining and knowing its acceptable range of quality variation (specification limits) are the bases for defining which is the best measurement technology, since they establish theoretical goals of critical sets that will determine financial, organizational and organizational aspects. , operating to have a demand that meets a product design, specification of the best instrument according to its limits of detection and quantification that meets the needs of the end customer [6].

The financial investment in these instruments must be considered when purchasing these technologies, because the models known as "intelligent negotiations" that are currently being managed in the industry 4.0 have classifications of proposals that tend to add value to the company or add value to the flow process, always creating benefits that will benefit their final client indirectly (consumer) [7].

In other words, they are actions ranging from infrastructure investments to operational mindset shifts, using data that helps to understand process-quality relationships in analysis. Their inclusion in an operation has the primary goal of not replacing understanding of the processes and their operational dynamics; nonetheless, they must significantly supplement the on-site operation in terms of sampling principles, response times, and data storage [4].

In conclusion, based on a literary review of the advances in the implementation of PAT systems over the decades, it is still clear that its implementation has some aspects that need to be improved in manufacturing processes. Indicators indicate that many spectroscopy suppliers and developers are introducing advanced equipment to reduce long and slow laboratory analysis activities [6].

3. PAT IN INDUSTRY 4.0

In general, for the implementation of these new processes, such as in the industry 4.0, these new models must add value to the company, that is, they must have a significant impact on business success, where a combination of numerous physical and digital technologies, such as sensors, embedded systems, cloud computing, and Internet of Things (IIoT), is used. All these values will drive a service's (product's) productivity to become more competitive in a technological and information-rich world, making it a relatively difficult, dynamic, and multidisciplinary task whose complexity will increase on an industrial scale.

Fundamentally, the industrial revolution that has resulted from the implementation of PAT and QbD is based on business models whose flow values may provide profitable and sustainable income (by spending less and operating more). In other words, satisfying the needs of customers and the company to achieve business model success that results in profitable growth for businesses through information integration management with the unification of human resources, time, technology, and the entire supply chain, as shown in Figure 1 [7].

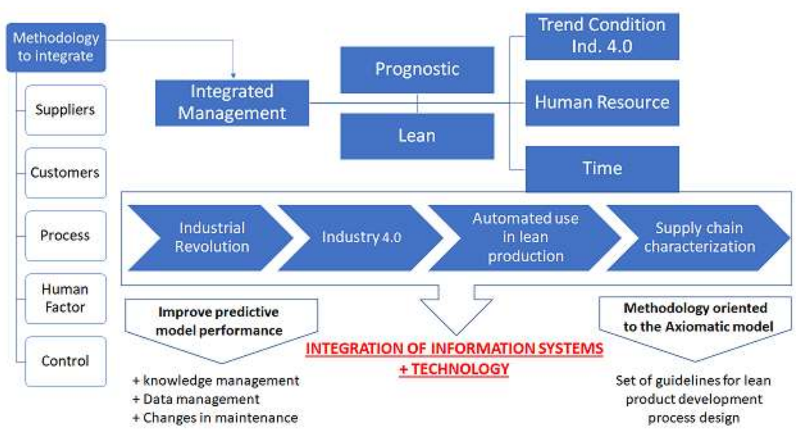

Figure 1: Simulation of an integrated management system in the Industry 4.0. Source: Original creation.

According to Vann et al. (2017) [8], industries have increased their use of sensors that use optical methods such as spectroscopy technology as real-time control devices in recent decades. Their methodologies are integrated into the information systems (integrated management) that drive Industry 4.0 through forecasting, as well as Lean Manufacturing systems that make the characterization of the supply chain axiomatic. As shown in Figure 2, the integrated PAT management system may be found throughout the manufacturing process, beginning with material receipt (raw materials) and ending with the ultimate consumer (finished product), with retro feeding and data adjustments occurring throughout the process [7].

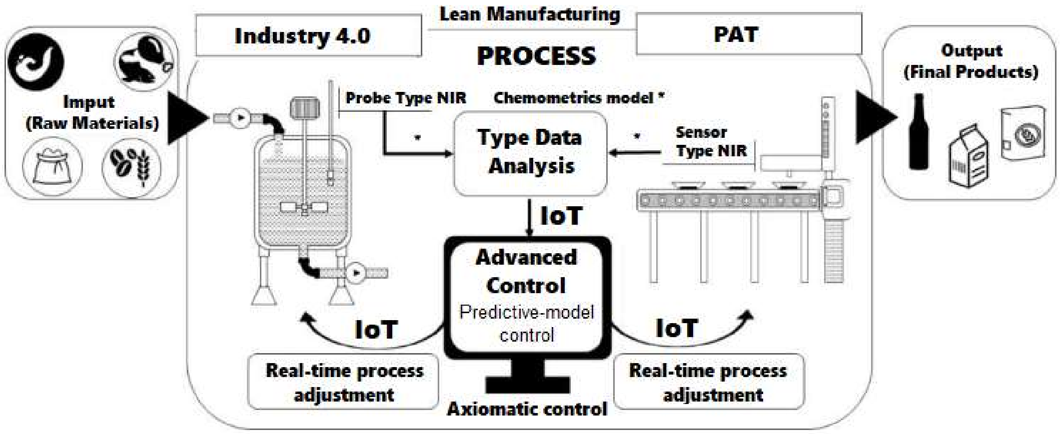

Figure 2: Integrated management system between PAT-Industry 4.0 and Lean Manufacturing. Source: Adapted from Grassi and Alamprese, 2018.

Specifically, NIR spectroscopy is a sensor analysis technique used primarily in PAT business models, where its ability to determine multiple components simultaneously through physical properties, chemical compositions, and microstructure makes it one of the most appropriate, cost-effective, and environmentally friendly processes for material characterization [9].

Their measurement capabilities will be determined specifically by their spectral intervals; that is, in the market, the spectral region will determine the range of reading for the absorption of bands by spectral selectivity of chemical compounds using quantum methods simultaneously [10]. The most common are instruments for near-infrared spectroscopy (2500 a 780 nm / 12800 a 4000 cm-1) and near-infrared spectroscopy (50000 a 2500 nm / 4000 a 200 cm-1) with the advantage of being low-cost operational equipment using non-destructive techniques without the need of chemical reactivators [11].

The PAT is a crucial tool in the industrial quality control revolution being driven by Industry 4.0. Its real-time monitoring resources with the Internet of Industrial Things included (IIoT), through analytical instruments such as spectroscopic sensors integrated in Internet networks and multivariate data from chemometric analysis of continuous learning and information construction, which is gradually moving the monitoring and control to another continuous and quality level.

Its development and implementation are heavily focused on improving control, evaluating, and making quick decisions, maintaining the quality of the final product, increasing productivity, and achieving satisfactory results despite the complexity of the innovations, and increasing industrial competitiveness [12].

Because of the significant changes that have occurred in industries and information technology, the changes brought about by Industry 4.0 are likely to increase productivity in manufacturing processes.

The challenges posed by technology, such as the need for network coordination, connectivity, and communication, have resulted in the development of integrated and flexible systems that connect various decentralized devices known as "Cyber Physical Systems" (CPS), which, through data analysis such as Big Data and artificial intelligence, are in sync with plant communication technologies.

According to Cevikcan and Ustundag, [7], it can be said that this growth has been driven by cloud technologies and the trends of the "Real-Time Location System" (RTLS) of real-time technologies, which results in a real-time production monitoring, which improve the efficiency of the product life cycle, reducing costs, based on the accuracy, precision of data and resource utilization that drives end customer satisfaction.

One of the most common arguments for this is the Toyota system philosophy and key industry 4.0 parameters, which serve as the foundation for PAT manufacturing control systems. Essentially, it is a feedback process, in which a finished product is analyzed, and its process is adjusted according to the problems or predictive process of the control model, by means of readings and adjustments originating from the chemometric models. This is a benefit obtained because it allows for optimal management and use of raw materials, reducing data variation outside of specifications and reducing production cycle errors (continuous improvement).

According to Cevikcan and Ustundag [7], even though PAT models provide benefits such as quality, flexibility, and efficiency, their processes have limitations due to the excessive use of information, the use of unqualified people to interpret them, or financial investment, which causes the company to invest in a costly technology for implementation when compared to other simpler measurement techniques.

4. IMPLEMENTATION CHALLENGES

A series of actions must be considered for proper PAT application. The first step is to specify a required or implementable unit action or process. Alternatively, do a comprehensive evaluation of the feasibility of analytical methods at the laboratory scale to determine which techniques have appropriate sensitivity and selectivity. Frequently, in this system, an exhaustive cost-benefit analysis is performed to determine which technique will arrive at the meeting with the best price, meeting all the client's and company's needs. Second, an appropriate approach must be taken, whether on the process line or in the laboratory, to allow for the measurement of the "Critical Process Parameter" (CPP). The online tests are the first step in moving away from laboratory tests, which can often have external interference or human errors due to their manual nature [4].

On the other hand, these processes can be carried out in two ways: manual tests that take samples and monitor them on a regular basis in accordance with a robust and appropriate protocol for the desired needs; and online tests that keep the instrument connected to the internet automatically, using the company's network and server. Both analyses will provide an instantaneous outcome of the procedure, as data from instruments whose goal is to blind a greater control. As previously said, near-infrared spectroscopy (NIR) is one of the most widely used and accepted methods. This technology is said to be fast and non-destructive, allowing for real-time monitoring and eliminating the need for pre-production sample preparation, with the result that its results are delayed, which may result in undesirable outcomes [13].

4.1 PAT Interaction with Process

In the chemical industry in general, process analysis can be performed using either rapid secondary techniques such as spectroscopy or traditional international reference techniques such as chromatography, air oven, titration, and so on. Its information is obtained by laboratory analysis, usually with trained personnel and a variety of chemical reactions, where obtaining results requires a certain amount of time, from sample preparation through instrument adjustment, analysis, data collection, and result dissemination [11].

Putting these considerations into practice, the way PAT systems interact with processes in most businesses must consider the Toyota JIT ("Just in Time") philosophy, in which long operational times become unviable for processes, especially when high demand and production lines have deadlines to meet. Therefore, having high-tech instruments capable of connecting to process networks, whether via a network or optical fiber connections, is the first step in making changes and improving parameter quality. In other words, they are systems that, if implemented, will be able to meet high demand within predetermined time frames while reducing waste due to non-specified parameters with high precision for industries such as raw materials, semi-finished products, and finished products [11].

This type of technology has certain economic characteristics, such as the ability to replace traditional primary methods in operations with faster and more flexible results. For the most part, they are techniques that expose their analysts less to the use of toxic chemical reagents, owing to the lack of the need for prior treatment in the preparation of the specimens, as well as the ability to analyze several parameters at the same time. Its location can be implemented online, in real-time process lines with network-connected systems, or in offline systems located within a controlled laboratory environment [4].

Both online and offline systems have advantages and disadvantages. Online instruments, in general, need more complex installation systems, ranging from engineering to operational data counting configuration. However, its automation eliminates the expense of managing exhibits as well as the time / man required to get and process data. On the other hand, despite the need for human intervention in their operation, offline instruments have lower implementation and operation costs when compared to online instruments. Alternatively, they might gain advantages over traditional methods by increasing data acquisition speed for process control.

As a result, for these types of technologies to be implemented, PAT systems require that the spectrum data generated by the implemented instruments have a correlation to values obtained by traditional methods. This is typically the case with NIR spectral data when connected to laboratory data from reference instruments in a variety of circumstances. One example of this is the homogeneity of online content, which allows for the development of a precise and comprehensive model [4].

These operations are carried out using mathematical software, which makes use of both spectrum data and reference data as a comparison to create a linear spectral regression model. To summarize the PAT focuses, and generated models are required for their maintenance plans of updating, verifying, and validating at certain times, which necessitates specific hardware for the process, data processing programs that are certified and verified by the instrument's developer [14].

As a result, you might conclude that there will be a variety of ways to execute it, such as manufacturing techniques or installation operations. In other words, its technological limitations in relation to the presented needs and existing models [12].

5. CONCLUSIONS

The goal of this work was to offer the most relevant aspects that must be reviewed in chemical technology processes. A brief overview of how PAT emerged in its technological environment, its relationship with the product cycle via tools like as QbD, and its significance in the generation of IIoT and industry 4.0 concepts. Relevant points include which instruments are now used in various industrial sectors, as well as an explanation of the benefits and drawbacks of these technologies in the quantification of certain properties of a material. The topics covered reflect a small portion of the knowledge gained and the strong relationship that it has with the age of real-time measurement systems (RTLS) and the interfaces that cyberphysical systems (CPS) can have with the research and applications that have already been completed. However, there are still many studies to be done, both in Big Data Analytics research and in the analytic automation of business processes, as well as in the analysis of data for use in various applications.

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