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Simulating Process-Product Interdependencies in Battery Production Systems

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Abstract

Battery production requires a highly complex manufacturing process chain consisting of different process steps. Both product and process parameters deviate throughout the whole process chain. Shape and scale of those distributions heavily affect subsequent process steps and final battery quality. Multi-level Simulation can be used to predict the impact of different distributions. In the paper, a concept is presented describing how process parameters and its distributions influence structure of intermediate products, which in turn affect battery performance. The former transition is realized through an agent-based process chain model approach while the latter uses an extended pseudo-2-dimensional battery model.

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Keywords: Simulation, Statistical process control, Manufacturing system

1. Introduction

The outcome of production processes is subject to fluctuations within defined tolerances [1]. Depending on process parameter setting and machine accuracy, characteristics of produced goods can differ considerably. In product and process development, the impact of process parameters and previous intermediate product characteristics are varied systematically in order to effectively control the outcome. Unnecessarily high demands in terms of product properties and its quality features promote narrow tolerances, making the design of processes and plants complex and cost-intensive [2]. Due to necessary cost reduction in cell production, an optimization of the production processes regarding a targeted and appropriate definition of production tolerances is of great importance.

Battery production is highly complex due to a large number of process steps with various converging and diverging material streams (Figure 1). Each process step is capable of influencing (intermediate) product characteristics with many process-product interdependencies still being unknown due to a high number of influencing process parameters and product characteristics. However, battery technology is a cornerstone of future energy systems, as it influences market success of electric vehicles as well as stationary energy storage systems. Understanding battery productions and subsequently increasing battery quality requires a holistic method to cover all interdependencies in the manufacturing system and their effects on the battery cell.

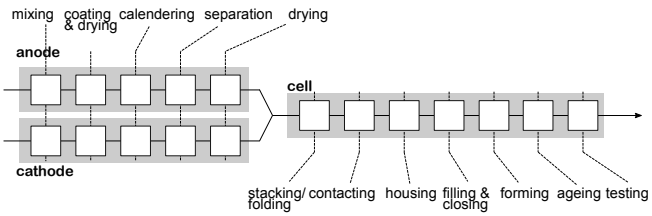

Fig. 1. Process chain of lithium-ion battery cells for stacking or folding cell assembly [3].

Up to now, there are several statistical methods (e.g. statistical process control, Design of Experiments, Six Sigma), which are used primarily in industrial production, in order to increase product quality. The application of these statistical procedures is required for the establishment and operation of a quality management system according to ISO 9001. Areas of application include manufacturing technology, usually containing discrete production steps and process engineering, which exhibits continuous and discontinuous production steps [4,5]. While all these approaches consider statistical methods in quality assurance, none of them uses a

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simulation-based approach, which addresses interdependencies of quality parameters along the process chain, characterization of the final product, and predictively considers investment and operational costs. Therefore, there is a need for a methodology that makes it possible to investigate the effects of fluctuations in individual processes along the entire process chain not only on subsequent processes but also on product properties. This paper presents a methodology, which uses a combined process chain and cell simulation. While process chain simulation allows characterizing the physical properties of electrodes, e.g. composition and geometric features, battery cell simulation is used to describe effects on the final product, i.e. battery performance.

2. Background

Simulation is a widely used method in order to describe time-dependent effects on a real world system. It is based on models, which are trying to imitate system behavior. Results generated by the simulation are transferred to the real world system and thus can be used to draw conclusions and support decisions. There are different model types (static vs. dynamic, deterministic vs. stochastic, continuous vs. discontinuous) and techniques (discrete event (DE), dynamic system (DS), system dynamics (SD), agent based (AB)) which can be individually costumed to the underlying system [6,7]. Furthermore, it is possible to combine different techniques (DE, DS, SD, AB) in a single simulation in order to address various aspects of a system. This enables the user to choose a fitted model approach.

Process chain and battery cell simulation differ in that the former addresses multiple spatial and temporal scales of a manufacturing system, while the latter focusses on the effect of electrode structure and its characteristics and the performance of the cells [3]. Hence, both systems require different model approaches. In order to determine the effects of process tolerances on battery performance, the results of the process chain simulation function as input for the battery cell simulation.

2.1. Simulation of manufacturing systems

Manufacturing systems include different spatial scales from processes, machines, and process chains. Each scale requires unique aspects to be considered. At process scale, a DS simulation approach is used to describe how different processes affect the value stream. Machines and equipment simulation is based on DS, but benefit additionally from a DE approach since it allows characterizing different machine states. Process chain simulation typically utilizes DE and AB modeling. Both simulation approaches enable the user to represent the different process steps as individual states or agents. Moreover, AB can display product units as agents allowing them to interact dynamically with machines from the process chain [3,7].

In the literature, only few approaches exist that address the effects of different process steps in the manufacturing of battery cells on the final product quality. In most cases, not all spatial scales are considered. One of the few examples is the simulation of different formulation strategies during mixing by Liu et al. [8]. They assessed whether temperature increasing rather than temperature constant conditions are more practicable to process a better electrode structure. Forouzan et al. developed a mesoscale particle-based simulation technique which predicts the microstructure of lithium-ion electrodes [9]. Furthermore, numerical flow simulations have been used by Kaiser et al. for the dimensioning and design of coating modules [10]. Schönemann proposed a multiscale simulation approach for battery production systems, which considers the relevant characteristics and elements of a battery production system [3]. His framework covers products, processes, machines, process chain, technical building services and the building scale each being addressed utilizing the best-suited modeling approach in order to represent specific production system details.

However, these approaches do not consider the effects of fluctuations on the subsequent process steps and are mostly limited to individual process steps. In contrast, the present work provides a holistic method to combine multilevel simulation with the field of statistical process control for analyzing effects of parameter fluctuations on quality parameters along the process chain.

2.2. Physical battery modeling

Battery quality highly depends on the electrode structure formed during the manufacturing process. This structure directly affects the physical processes inside a battery cell. A meaningful model-based quantification of fluctuating battery properties requires a model that is based on knowledge of the structure-properties relationship.

Battery modelling is an extensive research field and numerous different models are available. These models vary in terms of complexity, computational cost and reliability. In general, most common battery models can be classified by the following categories: Equivalent circuit models [11], data driven models [12], and physical models. Physical models thereby strongly deviate in complexity, ranging from computational efficient electrochemical engineering models [13] to highly complex multiphysical [14] or multiscale models [15]. Common electrochemical engineering models include electrochemical kinetics and transport phenomena and they possess relatively low computational costs [16]. A broadly used electrochemical engineering model is the pseudo-two-dimensional (P2D) model developed by Doyle et al. [13].

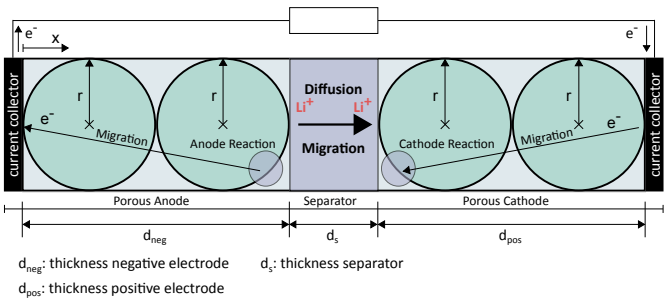


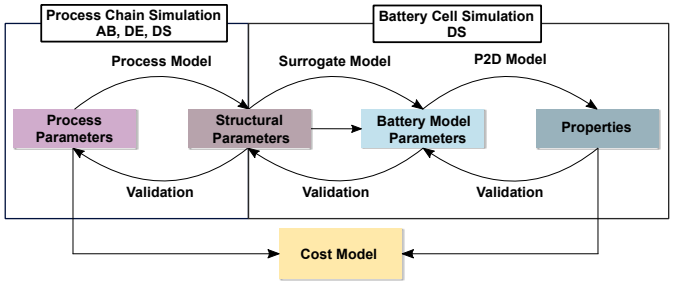
Fig. 2. Concept of P2D Model.

The P2D model evaluates the ongoing processes in the lithium-ion battery related to a homogeneous electrode structure, including the diffusion, migration and the intercalation in the solid particles and the diffusion and

migration in the electrolyte along the axial coordinate x through the cell and the radial coordinate r inside the active material particles. The reaction kinetics are described by the Butler-Volmer kinetics [13]. The simulated battery consists of positive and negative porous electrodes, a separator and current collectors. The model characterizes the electrolyte concentration, electrolyte potential, solid-state concentration and solid-state potential within the porous electrodes as well as the electrolyte concentration and electrolyte potential within the separator [16]. The description of these processes is done by coupled nonlinear partial differential equations (PDEs). The discretization and the main aspects of the model can be seen in Figure 2.

3. Multi-level simulation concept

Battery production is characterized by a highly complex process chain and a large number of interactions between individual process steps. Variation of a single process parameter (PP) can cause a variety of other parameters to change. The proposed method needs to be able to determine the effects of varying process parameters on final battery performance. However, the direct consideration of the effects of process parameters on battery properties neglects physical changes within the electrode leading to an incomplete understanding of interactions [17]. Therefore, the here presented concept is fundamentally based on a process-structure-property correlation, i.e. varying process parameters may cause significant changes in electrode structure, which in turn affect cell properties [13]. Structural parameters (SP) refer to the physical characteristics of electrodes, e.g. viscosity, electrode thickness or porosity. However, these do not take into account the electrochemical characteristics of the battery, e.g. diffusion coefficient of lithium in the solid matrix or electrical conductivity. Consequently, the process-structure-property correlation is extended by battery model parameters (BMP), which include both physical and electrochemical characteristics and are essential to determine battery performance (Figure 3).



Process Parameter	Structural Parameter	Battery Model Parameter	Properties
Mixing Time [s]	Particle Size [m]	Particle Size [m]	Energy Density [Wh kg^{-1}]
Foil velocity [m s^{-1}]	Coating Thickness [m]	Coating Thickness [m]	Power Density [W kg^{-1}]
Coating volume [m^3 s^{-1}]	Porosity [-]	Porosity [-]	Discharge Capacity [Ah]
Drying Time [s]	Tortousity [-]	Eff. Electr. Conductivity [S m^{-1}]	
Drying Temperature [K]	Density [kg m-3]	Active Surface Area [m²]	
Roller Gap [m]	Adhesion Strength [N m^{-2}]	Eff. Diffusion Coefficient [m² s^{-1}]	
⋮	⋮	⋮	

Fig. 3. Modeling concept to determine effects and examplary PP, SP, BMP and properties in battery production.

Transitions between parameter levels (PP, SP, BMP and properties) can be realized through different model types. Process models are used to describe the relationship between process and structural parameters. There are several structural parameters, such as particle size or electrode surface area, which function directly as battery model parameters. Other battery model parameters, e.g. conductivity, have to be determined using three-dimensional surrogate models based on structural parameters. Afterwards, a P2D cell model is applied to determine different battery performance properties such as energy density. Intensive validating is conducted to achieve reliability of the models and the procedure. Process models are validated on the basis of results from real machine trials while validation of Surrogate and P2D models employ measurements from cell diagnostic data analysis. In order to evaluate the effects of different process settings on battery properties in monetary terms, both components are integrated into a cost model, which considers operating and capital costs for different process parameters and machines.

The proposed method allows determining interdependencies between process and quality parameters. The aim of the method is to examine the effects of product tolerances on subsequent process steps and final battery characteristics in order to predict beneficial tolerance ranges for structural and battery model parameters (Figure 4). These target values can be used to select machines with just the required accuracy (3) since unnecessarily high precision (2) usually causes high acquisition costs without any beneficial effects on final product quality while low precision (1) leads to insufficient accuracy or quality during production. Target tolerances can be selected with regard to both qualitative and economic aspects. Consequently, this method contributes to further reduce battery production costs and improve battery quality.

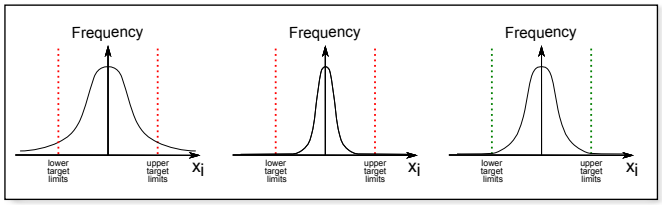


Fig. 4. Normal parameter distributions of (1) insufficient accuracy of SP/BMP (2) unnecessary high accuracy of SP/BMP and (3) beneficial accuracy of SP/BMP.

3.1. Process chain simulation

3.1.1. Process chain infrastructure

In order to describe the general material flow in battery production, a process chain infrastructure is established. The infrastructure is based on a combined AB und DE simulation approach implemented in Anylogic® and serves as a carrier model in which different process models can be implemented. Anylogic is a simulation software, which supports various model techniques (DE, DS, SD, AB) and thus is predestined for process chain simulation. Both the processes and the product units are displayed as agents allowing them to interact in the battery production environment (Figure 5).

In the simulation, product unit agents move along an underlying process chain. In the end, a single product unit

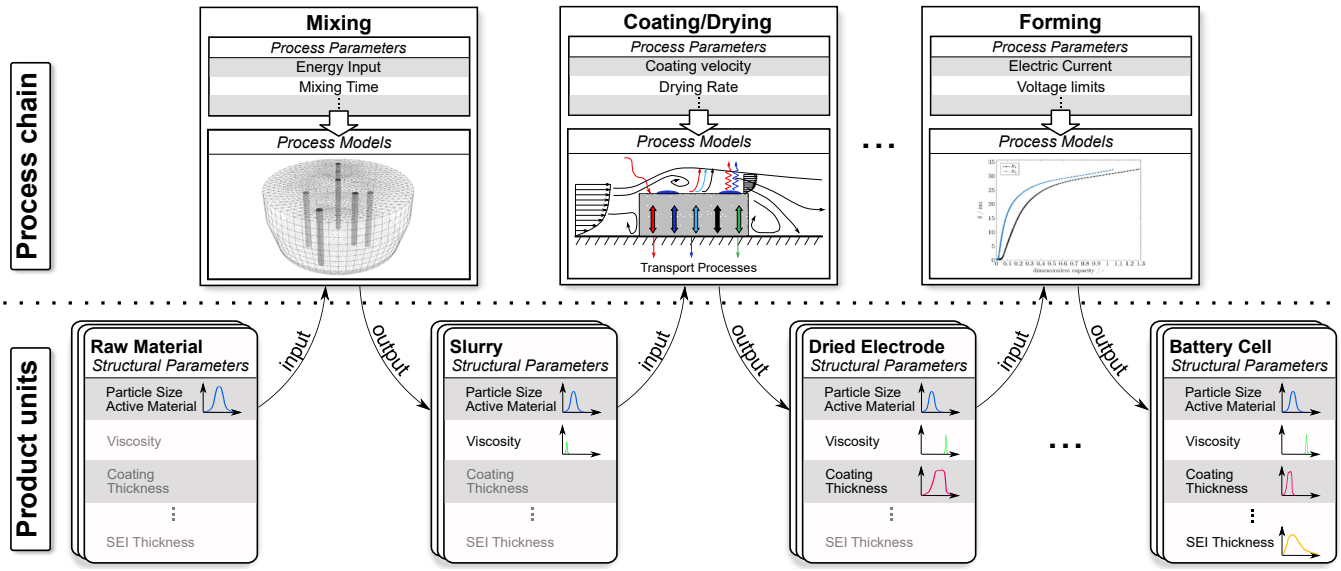


Fig. 5. Concept of process chain simulation showing exemplary interactions of product units and processes and possible evolving parameter distributions. Mixing: CFD simulation of planetary pin mixer [18]; Coating/Drying: Exchange processes model for drying [19]; Forming: SEI thickness during first charge of forming process [15].

reflects one battery cell, which will serve as input for battery cell simulation. Accordingly, previous intermediate products function as the equivalent amount/length of *raw material, slurry, coated* and *dried foil*.

Initially, raw material product units are characterized by structural parameter distributions, e.g. particle size of active material. In the first process step, raw material undergoes various transformations leading to a new intermediate product. Similarly, each following process step may either add new structural parameters such as *viscosity* during *mixing* or alter existing ones, e.g. *electrode thickness* during *calendering*. Product unit agents are not bound to the physical form of the intermediate product but merely reflect its properties. Thus, they go through different stages, such as *slurry, dried electrode* and eventually end up as *battery cells*. Transformations are described by process models (see 3.2).

The behavior of machine and product unit agents is based on discrete events allowing machines to consider different machine states (Off, Ramp Up, Idle and Processing) and product units to move along the process chain individually. Their structure ensures that product agents can only be processed when the machine agent is in *Idle* mode. Machine agents are able to deal with different process flows in battery production. During mixing, material is commonly processed in batch processes. Coating, drying and calendering is generally continuous, while cell manufacturing is mostly discrete [20]. Machine agents are able to contain multiple product unit agents during batch processes. The combination of product unit and machine agent represents the core of the process chain simulation. It provides necessary logistics, e.g. considering process time, batch sizes for the transport and transformation of product units along the process chain. The process chain simulation serves as a platform, which has to be filled with process models, in order to describe the effects of specific process steps on intermediate product characteristics.

3.1.2. *Process models*

Process models, either deterministic or stochastic, quantitatively describe the change in properties of processes to (intermediate) products. Deterministic models rely on physical laws while stochastic models are based on previous observations and contain probability distributions. Its system behavior is affected by random events. Compared to deterministic models, they are not universally valid and can therefore only be applied to systems that have already been investigated [6]. Thus, the proposed multiscale simulation will focus on the use of deterministically generated models, which in turn are able to describe statistical phenomenon, such as distributed process and structural parameters.

Process models describe the change and emergence of structural parameters during processing. Process parameters and structural parameters of previous intermediate products usually affect physical process models. The former are set mostly as discrete values, e.g. drying temperature in coating/drying, but may indeed cause fluctuating effects on intermediate products due to machine inaccuracy. The latter appear solely in the form distributions due to naturally occurring and unavoidable inaccuracies during production. Figure 6 exemplary shows a calendering process model by Meyer et al. [21], which is implemented in the process chain carrier model. The process model allows predicting electrode porosity depending on line load and structural parameters of the incoming dried electrode. Common distributions in production systems are Normal and Weibull distributions and can be described by characteristic parameters (e.g. mean and variance) [4]. Quality management enforces lower and upper target limits in which structural parameters have to deviate. Exceeding these limits would cause negative effects in the following process steps and final product quality.

Measured structural parameter distributions of raw material suffice to determine distributions of subsequent structural parameters. During process chain simulation, the deterministically generated process model equation is

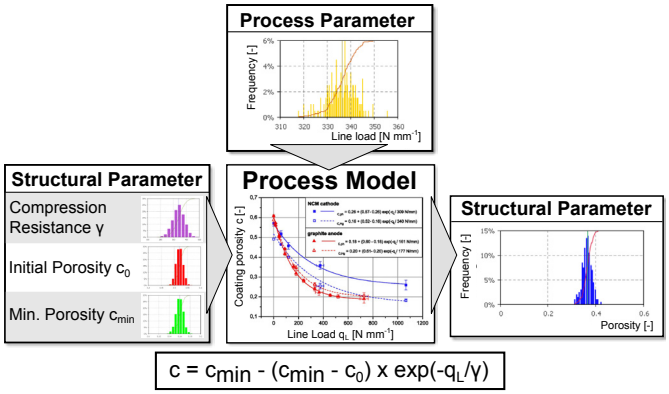


Fig. 6. Exemplary deterministic process model by Meyer et al. [21] (see equation) determining porosity after calendering.

repeatedly applied to randomly selected values from the input parameter distributions. This operation is carried out over a certain number of process time-dependent intervals, generating discrete structural parameter distributions for the ensuing process step (Figure 6). Due to the apposition of process models along the process chain, different distribution forms overlap creating unique distribution patterns. Analyzing the development of those patterns along the process chain, helps identifying key parameters and possibly detects compensating effects along the process chain. These decisive findings can be used to systematically improve battery production. However, due to a large number of parameters, there are different interactions within the production process. Many of these interactions are currently only known qualitatively but due to the key role of battery technology within electromobility, they represent the focus of current research projects. The process chain model serves as a platform in which existing and future process models can gradually be integrated. The final product of the process chain simulation is a fully characterized battery cell, based on which effective parameters can be determined that are required for its electrochemical characterization.

3.2. Battery cell simulation

In this section the concept of the battery cell simulation, which is illustrated in Figure 2 is discussed. The aim of the battery cell simulation is to set up a platform that is able to evaluate the effect of the electrode structure on battery properties, e.g. discharge capacity and energy density. This enables to describe interactions and evaluate fluctuations of structural parameters. The model includes three types of parameters: structural parameters, battery model parameters and performance properties of the battery. The correlation between these types of parameters is determined with two mechanistic models, the battery model and the surrogate model.

The battery model represents the core of the battery cell simulation. It is used to simulate the effect of battery model parameters on performance properties based on mass, charge and energy balances and constitutive equations containing laws of physics. As the classic P2D model is based on homogenized structures, it is extended to consider the fluctuations of structural parameters. Two types of fluctuations are considered: long-range fluctuations, between different electrode sheets, called electrode-to-electrode deviation and short-range fluctuations, within a single sheet, called sub-electrode deviation. The two types are treated as follows: For the first one, the properties are determined based on the averaged structural parameters over the whole electrode area. For the second type, the area of the electrode is divided into a finite number of sub-electrodes. The structural parameters of each sub-electrode differ to another. This is illustrated in Figure 7. Each of the sub-electrodes is described with a single battery model. The single models are connected in parallel to each other. This enables the model to represent the influence of fluctuations on sub-electrode level.

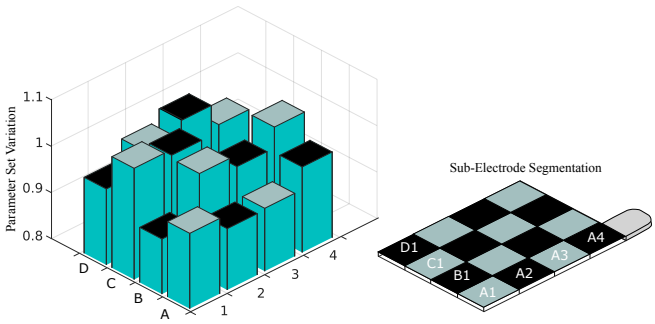


Fig. 7. Principle of segmentation and allocation of sub-electrode deviations.

The transformation of some structural parameters to battery model parameters is realized using a surrogate model, as the battery model does not directly contain structural information, but partly lumped parameters. The additional transformation step in between the two parameter types from structural to battery model parameters increases the evaluated structural information and thus the value of the overall simulation. This enables a better understanding of the complex interactions between the structural parameters and the battery properties.

The presented approach enables to evaluate the battery performance property and its sensitivity to electrode structure, and assesses the quality of the final product. Further, this knowledge-based understanding of the interactions between structure and performance properties and the propagation of fluctuations can be used for a directed optimization process of structural parameters and the production process. Finally, simulated properties of the battery are the base for the economic evaluation of the production process within a cost model.

4. Conclusion

A multi-level simulation concept is presented which determines effects of varying process parameters on structural parameter distributions, battery model parameter distributions and battery performance properties. The simulation consists of a linked process chain and battery cell simulation. The process chain simulation is based on a combined agent-based and discrete event simulation approach, in which deterministic process models determine structural parameters of individual process steps. Special focus is placed on the propagation of different parameter distributions along the process chain. This novel simulation approach attempts to combine two simulation approaches, which were previously considered separately, in order to predict the effects of the manufacturing process of batteries on their later properties. Results may

be used to determine key process parameters and necessary accuracies during production process. The output of process chain simulation is an electrode, which is characterized by the structural parameters. This serves as an input for the battery cell simulation. In the first step of the battery cell simulation, the selected structural parameters are transformed via a surrogate model into battery model parameters. This enables the model approach to use more structural information for the determination of the performance properties, improving the analysis of the influence of the structural parameter on cell properties. In the second step, the estimated battery model parameters serve as input for an extended pseudo two-dimensional model that takes into account electrode-to-electrode and sub-electrode deviations. Finally, the combined approach allows predicting battery performance deterministically based on initial raw material characterization and process parameters. Furthermore, the results of the battery cell simulation can be fed back to determine beneficial process parameter settings by conducting process parameter analyses. Using multi-level simulation, the different levels (battery cell, machine, process chain) can be addressed individually with a suitable modelling approach. A cost model is implemented in the simulation concept to evaluate different process parameter settings financially. While this simulation approach has been applied to battery production, it is also applicable for other production systems with complex process chains and high demands on final quality, e.g. pharamceutical industry.

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