A systematic approach to define flexibility in chemical engineering

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Abstract
Increasing economic and environmental challenges leads to the need for changes in the chemical industry. In this context, a promising approach is utilizing flexible apparatuses and flexible plants to react to changing boundary conditions. However, the concept of flexibility in chemical engineering, which originated in manufacturing, still lacks a comprehensive organization and categorization of different types of flexibility. Thus, in this work, the origin of flexibility in manufacturing is traced, and a literature overview on flexibility in chemical engineering is provided. Based on a subsequent cluster analysis, four types of flexibility are identified and defined. Furthermore, this work enables research on flexibility to be integrated into a general and consistent definition of flexibility. The definitions are applied to examples from literature to achieve comparability. While enabling the qualitative assessment of flexibility, this work identifies open research gaps regarding the quantification of flexibility.

KEYWORDS
capacity flexibility, definition of flexibility, feedstock flexibility, flexibility types, operating window, operational flexibility, plant operation, product flexibility

1 | INTRODUCTION

The term flexibility is gaining more importance in research literature (see Figure 1), indicating its significance in chemical engineering. Furthermore, flexibility is seen as a key concept in the current Strategic and Innovation Research Agenda of the European Technology Platform SusChem.[1] However, literature shows general inconsistency when it comes to the definition and application of the term flexibility. While the research of a coherent definition for the term flexibility has received a clear interest over the last decades in manufacturing, definitions for chemical engineering are not as widely discussed. In manufacturing, flexibility is considered crucial to achieve competitive advantage.[2] Authors from manufacturing agree that flexibility is needed in order to handle uncertainty in the system environment.[3] With regard to chemical engineering, boundary conditions concerning raw material, as well as product diversity and energy supply, are changing. This has led to an increased research interest in the field of flexibility in chemical engineering. Originating from process systems optimization, various methods to quantify flexibility in chemical engineering systems are available. Based on the
formulation of the steady-state flexibility index,[4,5] further methods were developed. In the context of this contribution the dynamic flexibility index,[6] the temporal flexibility index,[7] and the stochastic flexibility index[8,9] should be highlighted. Those methods were applied to chemical engineering systems along various time and length scales, from single unit operations,[6,10] to heat exchanger networks[11,12] and processes[13-17] as well as supply chain and logistics.[18] With these methods, it is possible to predict the operational flexibility of a chemical engineering system under uncertain parameters. However, it can be found that in current literature various other types of flexibility not directly related to mathematical optimization but rather focused on desired flexibility options are discussed. The majority of these studies is driven by changing boundary conditions within the chemical industry, which are highlighted in Sections 1.1 and 1.2.

1.1 | Changing raw material supply and time to market

The European chemical industry is on the verge of change. The globalization of available markets creates not only the new opportunities, but also the need for shorter product lifecycles, highly individualized and/or specialized products to outperform competitors.[19] In addition, the chemical industry is confronted with a transformation in supplied raw materials and energy. The chemical industry needs to adapt to these challenges in the future. To limit anticipated losses, new strategies for plant operation and design are needed.[9]

According to a study conducted by the German Association of the Chemical Industry, the proportion of pharmaceutical and specialty chemical products, requiring highly specialized production processes, is increasing.[20] This increasing product variety requires highly flexible chemical plants.[21] Conventionally, batch-wise operated multipurpose plants are used for that case. However, batch-wise processing does not comply with the requirements of resource-efficient production in terms of energy and raw material consumption, since options for process integration and optimization are limited.[22] Therefore, a continuously producing multipurpose plant that can adapt its capacity to the market developments[23] and produce different products can be of strategic advantage.[24] Another strategy could be to enable a fast time to market by utilizing and modifying an already designed plant.[25]

On the other hand, world-scale plants in bulk and basic chemicals are dominant. This type of plant is designed to operate at minimum cost, for a fixed capacity and the highest possible efficiency.[26] In particular, this type of plant does not fulfill the requirements for the challenges of the chemical industry, so that new approaches have to be developed. Therefore, the overall flexibility of production plants in the chemical industry has to be increased. Future tasks comprise increasing resource efficiency, diversifying the raw material base and compensating for geographical disadvantages through know-how and innovation.[20]
1.2 | Changes in energy supply

The reduction of greenhouse gas emissions is vital to limit global climate change and global temperature increase below 2°C. Hence, the European Union is transforming its energy system from fossil fuels to renewable energies. A significant number of studies and research work demonstrates the theoretical feasibility of a German or European energy system, which is largely or entirely based on renewable energies. The transition to this new energy system will lead to an altered generation structure in the power sector. This leads to changing boundary conditions for the chemical industry.

New requirements for the components of the energy system arise due to the volatile power generation from renewable energies. Technologies for the storage of energy will be needed to supply energy in times of low electricity production and to store energy during times of high electricity production. However, the adaptation of power consuming components to the actual power availability reduces the necessity for energy storage and increases the usage of renewable power during peak production. Hence, flexibility requirements concerning the dynamic plant operation of power consuming components of the energy system are rising.

Important processes in the chemical industry are directly or indirectly linked to the power grid and are hence subject to flexibility requirements. Electrochemical apparatuses directly couple the power grid and chemical production. Most prominently, this concerns the production and usage of hydrogen produced via water electrolysis, which is supposed to substitute hydrogen from steam reforming of natural gas. Another significant electrochemical process is the chlorine-alkali-electrolysis for the production of chlorine as a basic chemical.

The changing production pattern of the feedstock may impose the need for flexibility indirectly to the respective downstream units. Renewable hydrogen may be used in the Haber-Bosch-Process to generate ammonia. It is also the feedstock for all so-called Power-to-X technologies, which enable chemical energy storage and are able to produce a variety of products, for example, methane, methanol, or synthetic fuel.

Until now, the term flexibility has been broadly used with different or overlapping interpretations in chemical engineering. A categorization of the various existing types of flexibility is still missing. Therefore, a cluster analysis is performed to provide a comprehensive overview and identify the requirements necessary for coherent definitions. Further, existing definitions lack comparability due to mismatching scope and application area. As laid out, changing boundary conditions give rise to an increased research interest in flexibility issues.

To highlight the historical development, the transfer of concepts for flexibility from manufacturing to chemical engineering is highlighted in Section 2. Following these considerations, an approach to harmonize existing definitions within the field of chemical engineering is presented in Section 3. The proposed definitions seek to establish a common understanding in chemical engineering by linking the types of flexibility to state variables and clarifying application domains. The relevance is further illustrated in Section 4, where examples from literature focusing on flexibility are discussed. This work concludes with a discussion of the main findings and presents perspectives for future research in Section 5.

2 | ORIGIN AND DEFINITIONS OF FLEXIBILITY IN CHEMICAL ENGINEERING

In order to achieve a more explicit understanding of the development of the concept of flexibility in chemical engineering, it is important to give a brief overview of its origin and adaptation. Furthermore, pointing out approaches that have been proposed to define flexibility in the past is crucial to harmonize the term.

2.1 | Flexibility in manufacturing

Already at the beginning of the 20th century, the term flexibility was commonly used in the field of manufacturing. Highly dynamic markets and rapidly changing environments lead to efforts to overcome borders of fixed company structures. The questions arose how flexible production facilities are and how flexible they should be. Flexibility was considered as one of the major strategic factors. Even though it was certain that an increase in flexibility of a production line leads to a beneficial situation, it would also come with an increase in costs. Especially in the case of fluctuating demand in the market, flexibility would provide major benefits. Over time, flexibility has become one of the main objectives in the area of manufacturing and a critical point in measuring overall production performance of a manufacturing system. In addition, flexibility can be used as a measure of a manufacturing plants' ability to respond to changing environmental conditions. High flexibility may lead to better competitiveness and long-term success.

Numerous authors dealt with the concept of flexibility in manufacturing, which gave rise to many different definitions. Alone in technical English literature, several different definitions of flexibility exist. There are multiple reviews that can be found which try to condense...
the amount of information regarding flexibility in manufacturing. Examples are Toni et al., Wiendahl et al., Gupta and Goyal, Seebacher et al., and Kaluza et al. The reason for this amount of information is mainly due to the inconsistent terminologies and the complexity of flexibility. A definition widely used in manufacturing describes flexibility as follows: flexibility of a system is its adaptability to a wide range of possible environments that it may encounter.

Another common definition was presented by Ropohl. Ropohl considers manufacturing flexibility as the property of the system elements that are integrally designed and linked to each other in order to allow the adaptation of production equipment to various production tasks. Flexibility can not only be applied to the production system as a whole but also to structures within the system, thus reducing the complexity of the system. This results in different types of flexibility. Examples for the different flexibility types are machine flexibility, process flexibility, product flexibility, and volume flexibility. Most of these types provided in the literature are based on the work of Browne et al. Sethi and Sethi conducted a review in which multiple types of flexibility that have been adapted from Browne et al. are discussed.

2.2 Flexibility in chemical engineering

The concept of flexibility has also been adopted for chemical engineering; however, missing a specific definition for an extended period of time. The justification for the necessity of considering flexibility in chemical engineering corresponded to a great degree to the necessity in manufacturing. The driving forces here are, among others, the highly volatile market of the chemical industry, the long phases of creating new production systems, the sources of raw materials that are uncertain in the long term, and the high difficulty in the control of process engineering systems. In particular, the market for the chemical industry, which is characterized by a wide range of products, some with low production volumes, offers the possibility of increasing competition through the use of flexibility. Figure 2 gives an overview of the definitions that have been proposed in the literature in the course of time for chemical engineering.

In 1983, Grossman et al. were one of the first to see the importance in flexibility for chemical engineering. It was known that in order to safely operate a chemical plant, the plant must be capable of dealing with variations in parameter values that can occur during operation while satisfying specifications and constraints. These variations include but are not limited to changes in ambient temperature, deactivation of catalysts and wear out of mechanical equipment. In order to design chemical processes that are able to deal with these uncertainties, they presented a method to determine the optimal design of a chemical process under the uncertainty of changing parameter values. A flexibility test and flexibility index were introduced to measure the feasible region of a chemical system under the influence of uncertain parameters, giving tools to quantify flexibility. However, no unambiguous definition of flexibility was proposed. The term flexibility is discussed by Grossmann in connection with the operation of a chemical plant, describing operational flexibility as “the problem of ensuring feasible regions of operations”. The concept of the flexibility index has been adapted and applied to several different
application cases throughout the years. Reviews of some of the work that has been conducted can be found in Lim et al.,[54] Zhang et al.,[55] and Grossmann et al.[56]

Based on the definition of flexibility from the area of manufacturing, in 1988, Gruhn and Fichtner[51] were first to define flexibility universally for process engineering systems in the literature. The necessity for flexibility was seen due to three different aspects. First, during the long phase of creating new production plants, undergoing development, design, planning, and operation of a production process, many conditions and objectives in the functionality of the production plant change drastically. Second, in specific areas of the chemical industry, the demand for new products changes in short periods of time. A wide range of products in connection with low production volume is characteristic. Third, the variables required to control a chemical production process cannot be measured very accurately during operation. Production processes are subject to stochastic influences from system input parameters, internal process parameters, and the environment. This influence has to be compensated by the flexibility of the process. Therefore, flexibility of a process engineering system was defined as the ability to adapt quantitative changes of the functional objectives and functional conditions within technically defined limits to achieve new functional qualities of the system without substantially changing the nature and number of its elements.

Consequently, Gruhn and Fichtner adapted five types of flexibility from the manufacturing to investigate the flexibility of process engineering systems from different perspectives. The flexibility types respectively being product flexibility, capacity flexibility, parameter flexibility, structure flexibility, and location flexibility. The types of flexibility are defined as follows. Product flexibility is seen by the authors as the ability to change the produced products within a reasonable time period, without changing the main structure of the production system. Capacity flexibility is seen as the ability to satisfy changing demands in capacity, while using reserves and structural changes within the production system. Parameter flexibility is considered as the ability to compensate stochastic and dynamic changes. Structure flexibility is seen as the ability to change the material, energetic or informational connection within the system to achieve different conditions of operation. Lastly, location flexibility is considered as the degree of dependency of the production system toward a production site.

In addition to the types of flexibility, Gruhn and Fichtner[51] stated that there is a temporal dependency of flexibility. Dynamics of the process engineering system thereby depend on its characteristics. If the system is capable of dealing with different products and different states in process parameters, transitions might occur during operation. This leads to the question of the dynamic behavior at the state transitions. Furthermore, start-up and shutdown of chemical processes play a major role during operation. It is therefore important to understand how quickly a system can be switched on and off. In general, the stability of the system is essential during operation so that a stable process can be maintained while dynamic changes occur.

If the market situation and customer demands change substantially, chemical plants have to be capable of producing different products and amounts. This is particularly the case in the area of specialty chemicals. Due to the incapability of continuous mono production plants to meet these requirements, multiproduct plants are utilized. This type of plant enables different flexibility options. In 2006, Rauch[57] stated that three of the five types of flexibility defined by Gruhn and Fichtner are especially relevant for multiproduct plants: structural flexibility, product-assortment flexibility, and flexibility in capacity. Grossmann as well as Gruhn and Fichtner did not specify for which type of chemical production system their approach of flexibility is applicable. Moreover, they assumed that their approach is generally applicable to every production system. In contrast, Rauch investigated various multiproduct plant concepts with regard to the three different types of flexibility. The purpose was to determine which type of flexibility is particularly represented in each multiproduct plant concept.

In 2014, Seifert et al.[58] addressed different types of flexibility for chemical plants in a similar way as Rauch 2006 for situations with highly changing demands. However, modular production plants were considered in this context. The authors pointed out the necessity of plant concepts that include cost-efficient operation while simultaneously fulfilling various demand scenarios. They proposed a general definition for flexibility and capacity flexibility. However, the proposed definitions originate from manufacturing[41] and do not refer specifically to process engineering. Similar to the definitions in manufacturing, capacity flexibility was divided into two subgroups, volume and expansion flexibility. The authors stated that it is necessary to divide capacity flexibility, depending on the expected market situation. Volume flexibility was hereby described as a parameter range under which a plant can be operated by maintaining specifications. The authors relate volume flexibility to the previously defined operational flexibility from Grossman et al.,[52] and state that volume flexibility depends on the operating window of a plant. Therefore, manipulating volume flexibility of a plant means affecting the operating window. In contrast, expansion flexibility changes the capacity of a production plant by installing additional
apparatuses or production lines to meet the market demand. In this case, methods from the manufacturing were adapted to evaluate the flexibility in a case study. The methods were applied to select cost-efficient and flexible modular plant setup and attempt to give values for each flexibility while including costs to evaluate the advantages and disadvantages in costs with or without flexibility.

In 2015, van Kranenburg et al. presented an overview on different flexibility types. According to the authors, a future ideal production plant should possess all presented types of flexibility. Van Kranenburg highlighted several market trends that could make flexibility relevant for the chemical industry. Thus, investigating what motivation the different flexibilities built up on and the time span required to become relevant. As seen by the authors the most common types of flexibility are capacity, product, innovation, location, and feedstock flexibility. These types of flexibility were applied on a specific type of production plant, in this case small-scale modular production plants.

In 2016, Krasberg et al. analysed the methodological and technical requirements for process development, process design, and construction to overcome the hurdle that prevents the implementation of continuous-operated small scale production facilities. One of the significant hurdles, that was identified, is the limited flexibility of small-scale facilities in comparison to batch operation. Flexibility of small-scale facilities allows for reuse of equipment and lower investment costs. Different flexibility mechanisms have been analyzed. Three main flexibility concepts were found that are relevant for continuous production: parameter flexibility, time flexibility, and structure flexibility. Parameter flexibility is defined as a representation of achievable operating windows (e.g., pressure, temperature, throughput, heat flow, media, operating environment). The author states that with increasing degree of process intensification, the operational flexibility decreases. Time flexibility is defined as the ability of a production plant to separate process time from process operating parameters. While for batch-wise plants, the length of process steps is largely independent of the apparatus and is easy adjustable to process requirements, for continuous plants, time behavior of the apparatus is determined by the sizing. A change of the process requirements is possible by changing the mass flow. Additionally, structure flexibility is defined as the ability of a production plant to decouple the sequence of process steps. While batch apparatuses are applicable for different unit operations, the continuous apparatuses show limited flexibility regarding the operation of the whole plant.

When considering modular production, fully transformable plants, and standardization, flexibility rises as one of the key factors for success. In this context, Wörsdörfer pointed out three types of flexibility that are particularly important for transformable plants. The concept of a transformable plant hereby relates to the idea of small-scale production plants that were mentioned earlier. The technical implementation of transformable plants includes standardized container modules. These modules are compatible with each other and the equipment for the corresponding unit operations and the necessary peripherals, including the measurement and control technology. The equipment within the container modules must meet special requirements for this type of production plant. These include good scalability, continuous operation, and changed process conditions due to the compact design. Thus, the flexibility types being as follows: Capacity flexibility to adjust the limits of the plant to an increasing demand. Process flexibility given by the ability of the transformable plant to exchange apparatuses within the production process or whole container to form new production lines. Relocation flexibility due to the implementation of the processes in standard container. Thus, enabling the option to transport plants. The flexibility was assessed for the chemical industry by developing a catalog of criteria and determining the significance of these criteria for a production concept using Analytic Hierarchy Process and Analytic Network Process.

As pointed out by Gruhn and Fichtner, transitions and the dynamic behavior of a process engineering system is of importance when it comes to achieving a flexible system. Matthischke et al. addressed this dependency giving a definition for a type of flexibility to handle transient operation between different steady states. Hence defining load flexibility. Four aspects are mentioned that are subjugated to load flexibility. Respective being the range of the operating window, the time for start-up and shutdown, the velocity with which the transition occurs, and limitations the changes undergo.

Table 1 summarizes the discussed types of flexibilities and links them to the associated plant type they are defined for originally.

The authors compared in Table 1 do not only give definitions of different flexibility types for the plant type under investigation (mono plants, multipurpose plants or modular plants), they also present strategies to enhance flexibility. Taking a closer look at those strategies, one can conclude that there are three main strategies to enhance flexibility: (optimal) design and operation of apparatuses and processes as well as a more general transformability along all scales. Not all strategies are applicable to all combinations of plant and flexibility type. In contrast, some combinations are more promising than others. Transformability, meaning the ability to adapt to
changing boundary conditions on processes and process environment level easily, is applicable to modular and multipurpose plants rather than to mono plants. On the other hand, on apparatus level, new or flexibility-optimal design and operation strategies are of major interest, independently of plant type. The same applies on process level, whereas continuously operated mono plants are of highest interest for those strategies. The strategies discussed for the application of presented flexibility types in general are revived to some extent in the examples discussed in Section 4.

3 | SYSTEMATIC APPROACH TO DEFINE FLEXIBILITY

As is evident from historical considerations and the current state of literature, the concept of flexibility is not uniformly applied to the field of chemical engineering or considered in sufficient detail. Multiple interpretations of the same term exist. Different dimensions of flexibility are stated with overlapping meanings. This is partly due to the fact that the last comprehensive review dates back to Gruhn and Fichtner published in German in the year 1988.[51]

The discrepancy in the literature regarding the usage of flexibility can be seen by the example of capacity flexibility. Definitions of capacity flexibility are given by Rauch,[57] van Kranenburg et al.,[59] Seifert et al.,[58] Gruhn and Fichtner,[51] and Wörsdörfer et al.[61] In general, applicable definitions are provided by the first three aforementioned authors, essentially describing it as the ability of a plant to adapt to changing capacity demands. However, depending on the specific research perspective, other dimensions, such as expansion flexibility or structural flexibility, are named. The definition of Gruhn and Fichtner[51] specifies that structural changes within the plant are allowed as well as oversizing, to achieve a higher capacity. Furthermore, Wörsdörfer et al.[61] base their considerations on the modularization of chemical plants. Capacity flexibility is hereby described as the addition of highly standardized small-scale plants to achieve a higher production rate.[61] While the concept of capacity flexibility by Seifert et al. provides a general definition, it is divided into two subcategories: expansion flexibility and volume flexibility. This concept was applied in the context of modular plants.[58] While it is uniformly agreed that capacity flexibility entails that a plant possesses the ability to change its production output, the definitions differ in detail.

Another important characteristic in the consideration of flexibility is the dynamic behavior of an apparatus or process. The dynamic behavior is a sequence of changes
in state variables, caused for example, by a certain load profile, and may result in spatial gradients of temperature, pressure or concentration. Furthermore, start-up and shutdown operations are inherently dynamic. Hence, flexibility comprises the ability of the apparatus, process and process level to handle dynamic behavior, for example, load changes or a fast start-up. However, no general statement can be made, since the gradient tolerance is highly specific and uniquely dependent on the respective process level. Until now, this aspect rarely appears in literature.

It can be seen that significant ambiguity in the usage of the term “flexibility” exists and hence leads to a lack of comparability. However, chemical processes are complex highly nonlinear systems with a multiplicity of possible states, interdependent variables and strong boundary conditions. For in depth investigations, an accurate problem description is required.

3.1 Methodical approach

This work is based on extensive literature research of past and current studies focusing on flexibility. On the one hand, the development of the concept of flexibility was retraced to its origins in literature. On the other hand, studies on flexibility in chemical engineering were classified by cluster analysis. For this analysis, the following conditions were set:

- Does the definition differ or is it applicable to different process levels, such as apparatus, process or plant?
- Is the definition concise, unambiguous and does it allow a direct relation to physical process quantities?
- To enable a high level of comparability, does the definition relate to a fixed plant setup?
- Does the definition relate to steady-state operation?

To the best of our knowledge, Figure 3 provides the results of the cluster analysis for the most significant types of flexibility in the literature and their respective authors. It appears to be useful to distinguish two different layers of flexibility for the aforementioned flexibility types in order to provide coherent definitions. The first layer is the types of flexibility that are intended. The term intended here refers to the variables to be considered for the respective flexibility type. If changes in these variables are desired, the type of flexibility can be described as intended. Therefore, capacity flexibility, product flexibility, and feedstock flexibility as well as intended operational flexibility can be assigned to the intended flexibility layer. The second layer being the types of flexibility, where changes in the considered variables are uncertain. This layer describes uncertain, stochastic changes in state variables of the process and can also be connected to the term robustness of a system. This includes the area of operational flexibility under uncertainty and the intersections of operational flexibility under uncertainty and capacity, feedstock, and product flexibility (see Figure 3). These intersections contain no definite assignment. For example, if changes occur in the feed flowrate of a chemical process, the assignment depends on the reason of its change. If the changes occur in a desired way, which is controlled for example, by the plant operator, then the flexibility can be considered as intended capacity flexibility. However, if the changes occur in an undesired or stochastic way, then the flexibility can be either considered as uncertain operational flexibility or uncertain capacity flexibility. In conclusion, it was shown that capacity, feedstock, and product flexibility can be seen as special cases of operational flexibility. However, it is helpful to distinguish between an intended and an uncertain cause leading to an increased need of flexibility.

The differentiation between an intended or uncertain cause of change in the flexibility parameter helps to improve distinguishability between the types of flexibility. Additionally, it simplifies the application of the correct definition for the specific case. The applicability is demonstrated for the examples that are given in Section 4. Building up on the existing definitions, a unifying approach is presented in the following section.

3.2 Harmonizing the definition of flexibility

To facilitate research in the context of flexibility, it is proposed to break chemical processes down into three levels of consideration. This is often done in chemical engineering and also resembles the actual organizational structure of a plant. Flexibility is found on each stage. Hence, the apparatus level, the process level, and the process environment are distinguished. A single apparatus, for example, a reactor, may offer significant flexibility in handling different feedstocks qualities and quantities. However, the process may be limited by its separation unit in achieving sufficient qualities in composition. Flexibility restrictions may apply due to the process environment, for example, in supply of additional hot or cold streams or waste stream management. The three process levels are defined here as follows:

- Apparatus: Material conversion and separation in chemical engineering is achieved by unit operations. An apparatus is defined as the technical realization and constructional implementation of a unit operation.
For the purpose of considering flexibility this includes the essential peripheral equipment of the apparatus along the main process path.

- Process: A process is defined as the interconnection of apparatuses by means of a process flow sheet to accomplish a defined end. This may be for example, a specified amount of a certain product with a fixed composition.

- Process environment: A process is surrounded by a certain process environment and touches upon system boundaries. This comprises the interaction with for example, utility systems, safety and legal restrictions, location-specific physical boundary conditions, or supply limitations.

Furthermore, chemical engineering relies on thermodynamics to describe chemical processes. Any system is uniquely defined by its state variables temperature, pressure, composition, and the number of mols. Adding flow rates completes the necessary description for processes, depicted in Figure 4. From this it is deduced, that any flexibility must origin in the ability to change one or more state variables of the process streams or of the process itself. This approach is used to harmonize and update existing definitions of flexibility into a coherent and applicable concept for chemical engineering. The aforementioned definitions relate to the intended or uncertain change of one variable under consideration for flexibility. Thereby, the dependent variables (eg, product specifications and feedstock) are subject to boundary conditions that are imposed above all by safety, environmental or legal restrictions.

From Figure 4, it becomes obvious that, regardless of the described process levels, only a limited number of state variables are available for flexibility considerations. Those state variables are inherently connected with the derived flexibility types and can thus be considered as flexibility parameters. Building on that, one can give straightforward definitions of the flexibility types regarding intended flexibility of a chemical engineering system. Therefore, looking at the feed stream of those systems, flexibility parameters are the relative composition of the feed $x_{\text{in},i}$ and the total amount of feed per time $F_{\text{in}}$. Thus, the relative composition is associated with the flexibility type feedstock flexibility that can be defined as follows:

"Feedstock flexibility is the ability to handle changing feedstock without violating product specifications or capacity."

As a result, a chemical engineering system, which can be described as flexible regarding feedstock, is able to handle varying relative compositions $x_{\text{in},i}$ without the need to change apparatus or process design.

If a chemical engineering system is flexible regarding capacity, the system can handle changing feed flow rates. This results in need of large operating windows for the apparatus and the overall process, respectively. This boundary condition, with respect to the flexibility parameter $F_{\text{in}}$, results in the following definition:
Capacity flexibility is the ability to handle changing feed quantities, more specifically feed flow rates, without violating product specifications.

Considering the products of a chemical engineering system, the available flexibility parameter is the product quality $x_{out,i}$ or in a more elaborated system the actual product itself. To have the product as a flexibility parameter originates in multiproduct plants and was transferred to the concept of modular process engineering. Within this framework, it is intended to produce varying products using either batch equipment or only a limited number of equipment modules. The goal is to realize quick product changeovers resulting in short time to markets to produce reasonable amounts of a new molecule. This requirement can be transferred to continuously operated mono-plants as well, resulting in the following definition:

Product flexibility is the ability to produce changing products or product qualities within certain specifications and capacity boundaries.

Lastly, a chemical engineering system is defined by a vector of operational parameters $\Phi(t)$, like for example, the temperature $T_{sys}$ or pressure $p_{sys}$ of the system or the feed. These operational parameters also include model parameters, such as for example, reaction rates or heat transfer coefficients. As derived in Section 3.1, this vector, or single elements of this vector, can also be seen as a parameter for intended flexibility:

Operational flexibility is the ability to handle changes regarding input or operational parameters without compromising feedstock, capacity or product specifications.

Table 2 gives an overview on flexibility types and parameters and exemplifies the impact on apparatus and process, respectively. These types of flexibility are encountered at every process level. However, they are not mutually exclusive. Two or more types of flexibility may appear simultaneously. A process can be flexible in capacity as well as in the ability to handle a wide range of feedstock compositions. Furthermore, a change in one state variable almost necessarily leads to a certain variance in other process variables. However, for the sake of defining and classifying flexibility, the intended change of the variable and the prevailing effect on the process is to be considered.

The proposed definitions of flexibility offer the advantage of a uniform structure and are based on a thorough evaluation of the available literature. Additionally, they are related to a mathematical description of chemical engineering systems. Therefore, they are applicable in various fields of chemical engineering such as process and systems optimization. Furthermore, they provide an update under current developments and evolved boundary conditions. This is a step further to the generic evaluation of research and business cases. The relevance of this classification shall be further demonstrated with examples from current literature in the following section.

4 | APPLICABILITY OF DERIVED DEFINITIONS

The following section exemplifies the scope and application of the derived definitions of flexibility. An increasing number of publications is focusing on aspects of flexibility (see Figure 1). However, various research exists that does not explicitly label the results as flexibility, but may be interpreted as such. By applying the derived definitions, a qualitative assessment is possible. In the following, a multitude of examples from literature is classified. This classification follows the definitions presented in Section 3 and includes various applications from chemical engineering. Hereby, the following areas of application were identified dealing with the proposed flexibility types: Power-to-X, air-separation, modular production, process intensification, and stationary and dynamic system analysis. The aim of the categorization is to enable a high level of comparability between different research works that deal either directly or indirectly with the different types of flexibility. Therefore, Section 4 is structured according to the different types of flexibility. In the discussion of each flexibility type, first concepts regarding single unit operations are discussed followed by work dealing with complete processes.

4.1 | Capacity flexibility

Research subsumed under capacity flexibility is generally dealing with strategies to allow for a change of throughput or feed capacity. Oftentimes, the mere physical dimensions of the apparatus are not the limiting factor.
As the following examples show, main challenges are process and temperature control, fluid dynamics, and maintaining composition specifications.

Power-to-X processes, such as the methanation of CO₂ for the production of synthetic natural gas, are currently being investigated in respect to their flexibility due to the likeliness of fluctuating input quantities from volatile power supply. While the production of hydrogen via electrolysis usually offers a broad operating window, the bottleneck in terms of the flexibility is often considered to be the hydrogen conversion. This has led to numerous works focusing on key aspects of the operability and dynamic behavior of exothermic catalysis reactors to increase capacity flexibility.

To enable the demand-oriented production of synthetic natural gas from renewable sources, Rönsch et al. qualitatively investigated the influence of load changes on a methanation plant. The simulated plant setup consists of three adiabatic methanation reactors with a recycle stream. Temperature control to prevent catalyst deactivation was found to be a key factor in the capacity flexible operation of the methanation reactors. Subsequently, the following investigations focused in detail on specific reactor types. Rönsch et al. studied the start and stop operation of an adiabatic methanation reactor. The goal was to identify the maximum standby time to allow for a warm and thus instantaneous restart of the reactor and hence for intermittent production patterns.

Matthischke et al. compared the startup behavior and the influence of the recycle ratio on different volume flows for different reactor types, namely an adiabatic and a cooled fixed-bed reactor. The ability of methanation reactors to operate under different feed volume flows and compositions was proven via modeling studies.

Bremer et al. conducted further research to allow for dynamic hot spot control during reactor startup through adjustment of the coolant temperature. Furthermore, the time to reach steady-state operation was minimized. The developed model is able to analyze the impact of fluctuations or disturbances in the feed and thus allows for investigations of operational flexibility. This investigation was extended to studies of operation range extension through control of the reaction hot spot and stabilization of unstable operation points consequently resulting in a higher capacity flexibility of the reactor.

Biegger et al. proposed a new layout for an adiabatic methanation reactor. The main feature of the new reactor is its division into four compartments, instead of

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**TABLE 2** The four flexibility types with their respective definitions and the characteristic physical process quantities are shown. Notes: The impact of a change in the respective process quantity on apparatus or process, here having the educts A and B and the products P, is visualized by characteristic diagrams over time. Ideal and instantaneous changes of state are assumed.
one single vessel. The new design offers the possibility to operate the compartments individually. Thus, it provides the ability to handle a wide range of volume flows and hence increases capacity flexibility.

Brée et al.\cite{69} and Roh et al.\cite{70} respectively, discuss the flexible operation of chlor-alkali electrolysis. The authors investigate a switchable membrane-based chlor-alkali process that is operated capacity flexible with respect to electricity prices. Here, switchable means the possibility to switch between standard cathodes and oxygen depolarized cathodes using a bi-functional electrode. Both modes differ in specific electricity demand as well as hydrogen production and oxygen consumption, respectively. Flexibilization of chlor-alkali process is achieved by two main strategies: switching between the named modes to decrease chlorine production when electricity prices are high and increasing chlorine production when electricity prices are low.\cite{69} The second primary measure investigated to increase flexibility is potential oversizing of the process.\cite{70} Both studies show that a cost-efficient operation of the chlor-alkali processes is possible by simultaneous increase in flexibility.

Radatz et al.\cite{71} present an approach to design equipment with high capacity flexibility by means of a wide operation window. The approach was developed using modular equipment with a fixed design. The approach is based on sampling and global sensitivity analyses, which was applied in Radatz et al.\cite{71} to a shell and tube heat exchanger. The operating constraints like pressure drop and velocity boundaries on tube and shell side were considered to ensure operability. Performing sensitivity analysis, the design parameters having highest impact on capacity flexibility were found (e.g., tube and shell diameter). In contrast, tube length and tube pitch ratio had a low impact on the capacity flexibility. Comparing the flexible design to the conventional design led to a 4-fold increase in operational window, but only 14% higher annual costs. In Radatz et al.\cite{25} the method was extended using an evolutionary algorithm and resulted in 11-fold enlarged operating window for 50% higher investment cost.

Cryogenic air separation is investigated for flexibility options due to its high energy demand, with capacity flexibility in focus. As it holds true for electrolysis, fluctuating energy prices may be exploited or grid services such as demand side management may be offered, if the throughput of the cryogenic air separation plant may be varied.\cite{72,73} A detailed dynamic model of an air separation column has been recently developed to understand the flexible plant operation of air separation units. Thus, a comprehensive analysis of dynamic operations such as warm start, cold start, load change, and sudden plant halt was conducted. Multiple conclusions for a modified plant design and control strategies were drawn.\cite{72} Furthermore, Caspari et al.\cite{74} showed that the main power consumption in a cryogenic air separation column is caused by the recycle compressor of the liquefaction cycle. Capacity flexibility to follow electricity prices during operation may be achieved by deactivating the liquefier and providing the internal column reflux from the liquid nitrogen tank instead until a critical liquid level is reached.

Riese et al.\cite{75} discuss different measures to enhance the capacity flexibility of absorption and distillation columns. For absorption columns, capacity flexibility is shown by a modular approach. Therefore, results for an experimental investigation of a modular absorption system are discussed. The authors show that capacity scales linearly with the number of modules operated in parallel. While the hydrodynamic measures pressure drop and liquid hold-up show consistent results, it is stated that separation efficiency is critical due to non-unique phase distribution in a rectangular set-up. Additionally, the authors present a concept to enhance capacity flexibility of conventional columns by means of column and tray design. The approach is investigated using a steady-state simulation study for a large-scale separation task. Results show high potential to enhance capacity flexibility by column and tray design. Nevertheless, experimental proof still has to be provided.

Huang et al.\cite{76} present a new approach to solve large scale optimization problems occurring during large-range transition of operation variables in continuous chemical processes. The authors discuss this approach considering an uncertain throughput-fluctuating and, therefore, according to the definitions presented in Section 3.2, a capacity flexible ethylene column. The presented approach is based on dynamic optimization procedures. Results show that for large transition ranges, as needed in a capacity flexible operation, conventional control strategies are not sufficient and new dynamic optimization strategies are needed.

### 4.2 Feedstock flexibility

Research that is related to feedstock flexible processes and apparatuses can be summarized as dealing either with changes in compositions within the feed of a chemical system or with completely different feedstocks. Noteworthy is the relevance of feedstock flexibility for biorefineries. Biomass as a feedstock yields a lot of uncertainty when it comes to its composition and specification depending on geographical region and harvesting time. Thus, leading to a need for flexible processes.
To name one example, Kenney et al.\cite{77} pointed out three important attributes for the processing of biomass feedstock. These attributes are the amount of ash, sugars, and the morphology of the biomass particles. In order to achieve a feedstock flexible biorefinery, the variation of those attributes has to be compensated. The authors give a brief example of how to handle different amounts of carbohydrates within the biomass. Thus, implementing a step of formulation or blending as preprocessing. The carbohydrate content of the feedstock is upgraded with the goal to reduce the variability. Exemplarily, corn stover could be blended with sugarcane bagasse leading to a mixture of higher sugar content.

However, feedstock flexibility is also present when dealing with the processing of fossil-based feedstock. Maußner et al.\cite{78} use a multilevel reactor design methodology to address feedstock flexibility of chemical reactors. As an example, they study the synthesis of maleic anhydride derived from different feedstock containing varying ratios of \textit{n}-butene and \textit{n}-butane. The aim of the proposed design methodology is to identify a reactor set-up that is able to cope with varying feedstock compositions by adjusting operating parameters according to the scenarios. An introduction to the methodology can be found in Freund and Sundmacher\cite{79} and an overview to further developments and applications is given in Freund et al.\cite{80}. The authors consider three feedstock scenarios (pure \textit{n}-butene, pure \textit{n}-butane, and a mixture of \textit{n}-butene and \textit{n}-butane, respectively) using literature based kinetic approaches to model the reaction in more detail. The problem results in a bi-objective optimization with two main objective variables. The derived reactor concept is able to handle all considered feedstock with maximized selectivity to maleic anhydride and minimized variance in selectivity. The latter is particularly important to ensure high product qualities in all scenarios studied. Thus, the authors are able to determine a reactor design that ensures above-mentioned objectives independently of feedstock composition. Additionally, due to the multilevel design approach the proposed technical solution also satisfies other performance criteria like conversion or pressure drop.

Sudhoff et al.\cite{81} evaluate the flexibility of the rotating packed bed for distillation. A spider web diagram was used to evaluate the design parameters with regard to feedstock and capacity flexibility. Sudhoff et al.\cite{81} developed a model to investigate the flexibility of the apparatus. Hence, the influence of the design parameters on the feedstock and capacity flexibility is evaluated. The model consists of known equations and correlations for hydrodynamics as well as new correlations for mass transfer with a new concept of equiareal discretization and integrated centrifugal acceleration. To evaluate flexibility for a given problem, first the design parameters are calculated and then the process is analyzed. The result of the process analysis and evaluation of flexibility is a region in which the design and operating variables can be manipulated without losing the required product specifications.

\subsection*{4.3 Product flexibility}

The concept of product flexibility becomes especially relevant when considering increasing market volatility. In the majority of the literature considered, product flexibility is seen as particularly important when the market is forcing the product portfolio to change quickly. Most of the examples can be found in the production of specialty products.

Rauch\cite{57} gives multiple examples for plants that are capable of producing different products, especially specialty chemicals. Multiproduct plants can be differentiated into different classes, with the standard batchwise operated multiproduct plants being most common. A prominent example for the use of standard multiproduct plants with product flexibility is the production of azo dyes. Azo dyes are usually produced in agitated vessels. In the process first a diazonium ion is created by mixing a primary aromatic amine with a hydrochloric acidic nitrite solution at a temperature around 0°C. In a second agitated vessel more, aromatic compounds that are used for the azo coupling are pre-processed. The actual reaction (azo coupling) takes place by mixing the components in a third agitated vessel. By altering the aromatic compounds for the coupling reaction, the color of the azo dye can be manipulated. Due to the fact that all of the process steps are unaffiliated from the technical implementation, product flexibility is gained.

Pereira et al.\cite{24} conduct a study in which they analyze the application of flexible biomass based ethanol-butanol plants. Two ethanol and butanol dedicated plants are compared to one flexible plant that has the ability to produce both products depending on the demand. The driving factor for the approach to consider a flexible plant is the shortage of ethanol feedstock during sugarcane off-season in Brazil. The authors present a concept of using eucalyptus pulp for the production of ethanol and butanol to increase competitiveness. Ethanol is produced during off-season and butanol while sugarcane is widely available. Monte Carlo simulations are performed to evaluate the economic benefit that a plant with product flexibility has compared to dedicated plants. Results show that the Net Present Value of the resilient plants is higher in relation to the dedicated plants. However, the technology for the pretreatment of the biomass needs to be considered in order to maximize competitiveness. This leads to
the conclusion that a plant that can produce more than one product, thus is product flexible and can provide a benefit under volatile and changing demands.

De Lucas-Consuegra et al. \cite{82} developed a new configuration for a solid electrolyte membrane reactor to convert an ethanol-water feed stream to synthesis gas. The new reactor setup allows for synthesis gas to be produced with an adjustable $\text{H}_2/\text{CO}$-ratio from 1.5 to 12. The resulting product gas ratio depends on the process parameters temperature and electric current. External feeding of $\text{O}_2$, as is typical for partial catalytic oxidation processes, can be avoided. Usually, the composition of synthesis gas must be tailored for its specific application. While for example, the production of electricity in a fuel cell from synthesis gas requires a high $\text{H}_2/\text{CO}$-ratio, typical synthesis applications such as ammonia or methanol synthesis require a low value. Hence, the newly developed reactor may be classified as product flexible, since its product composition can be adjusted to supply syngas for different applications.

Staak et al. \cite{83} discuss the applicability of divided-wall columns in multipurpose production environments. One described case deals with varying concentration of single components in the feed of the divided-wall column, which can be interpreted as either a feedstock or a product flexible operation according to presented definitions. An additional feature of the presented column layout is the possibility to adjust to different separation tasks by using multiple feed streams and side draws at different stages.

### 4.4 Operational flexibility

The quantification of operational flexibility is often achieved throughout the literature by solving either the mathematical optimization problem that was defined by Grossmann et al. in 1985 or by solving a modified version of the formulations based on the concept of Grossmann et al. An overview of recent developments can be found in Grossmann et al. \cite{56} Operational flexibility is therefore directly connected, but not limited, to the solution of an optimization problem under uncertainty. \cite{55}

Yuan et al. \cite{84} present a membrane based flexible carbon capture system. Using optimization methods, the aim of the study is to identify a system design with minimized costs operable under intended time variable operation of the upstream natural gas power plant according to electricity prices. According to the presented results, the ratio between carbon and electricity prize affects scheduling of the flexible carbon capture system the most.

Huang et al. \cite{85} also investigated operational flexibility in a batch reaction system. Two different reaction systems are considered. First, the chlorination of benzene and second, a more general consecutive reaction system. The uncertain parameter assumed here is the reaction rate constant. The authors introduced a new method based on the dynamic flexibility index from Dimitriadis and Pistikopoulos \cite{6} called the operation feasibility index. The developed method is seen by the authors as an effective tool to evaluate the feasible region of a batch reaction system. Results show that by altering the temperature of the batch system, a point of optimal flexibility could be found while satisfying the given constraints.

Pretoro et al. \cite{10} compared different approaches derived from the optimization problem by Grossmann et al. \cite{4} to evaluate flexibility with a case study. The case is the separation of pentane from butane, propane, and propylene (debutanizer) in a distillation column. The following uncertainties in process parameters were considered: Changing butane and pentane flowrates, due to the nature of the upstream process, changing performance of the heat exchanger, due to fouling, changing cooling water temperature, due to seasonality, and changing vapor velocities, due to weeping and flooding. To maintain the product quality, reflux, and distillate flowrates can be manipulated.

Zhou et al. \cite{86} proposed a framework in which the degree of operational flexibility is determined by the application of the dynamic analysis of the flexibility index proposed by Dimitriadis and Pistikopoulos. \cite{6} Two different cases of two different reactions in batch reactors are analyzed. The aim is to assess the influence of the initial reactor temperature on the reaction toward flexibility to optimize the dynamic performance of the system. It is assumed that the reactor has to satisfy multiple requirements, such as a minimum conversion of the reactants and maximum temperatures. The uncertainty in these examples is due to changes in the heat of reaction. An initial temperature is determined to maximize the operational flexibility of the system. It could be shown that by determining the dynamic flexibility index, a system can be manipulated so that best conditions for flexibility are achieved.

### 4.5 Intended flexibility vs flexibility under uncertainty

In the following section, the difference between intended flexibility and flexibility under uncertainty is highlighted. According to chapter Section 3, the flexibility type depends on the altered state variable and its prevailing effect. In a second step, the cause for the alteration must be questioned. If the change is intended, it is explicitly desired and controllable by, for example, the plant.
operator. This is classified as intended flexibility. In contrast, flexibility under uncertainty refers to stochastic changes in state variables, which apparatuses, processes, or the process environment are able to handle while fulfilling their target specifications. The assignment is shown for selected examples from the previous sections in Figure 5.

Taking the example of methanation from the previous Section 4.1 into account, the hydrogen production, and hence the feed for the methanation, may be produced as surplus electricity is available from the grid. This represents a stochastic feed input since the exact production pattern is not known. Although the methanation plant is likely designed to cope with varying capacities, in this case, the flexibility type would be labeled as operational flexibility under uncertainty. It could be shown that the definitions are applicable to many areas of chemical engineering. However, the areas of application might be extended as long as the criteria of the definitions are complied with.

5 | CONCLUSION AND FUTURE PERSPECTIVES

The interest in flexibility has been significantly growing in the last decade in chemical engineering. While in other areas the flexibility of production systems was already considered a key feature, interest in chemical engineering was relatively low. Research regarding flexibility was mostly related to stability and operability of a production system. Yet, it has not been of central interest in the development of processes. Recent developments in the environment of chemical industry, however, have provided the required motivation for more flexible production systems. Although the term flexibility is easy to grasp, it becomes difficult when applied in a consistent manner, which leads to a typical problem with flexibility: While the basic concept of flexibility is easily relatable and understandable, flexibility becomes complex and hard to capture in detail. Furthermore, definitions that have been proposed throughout the literature vary in their precision and some even differ in their meaning while using identical terms. Therefore, the aim of the presented research is to give a more comprehensive and clearer understanding of the concept of flexibility in chemical engineering by providing definitions that harmonize and extend the different concepts from literature. The proposed definitions are set out to enable a standardized and comparable concept. The application to examples from literature shows that the proposed definitions allow for classification and comparability. Additionally, the application of the definitions has emphasized two major aspects. First, there already is a lot of ongoing research toward the topic of flexibility. Second, many authors deal with different problems that include the idea of flexibility even though it might not be mentioned or conceived in that way.

**FIGURE 5** Selected examples from the literature applied to the proposed definitions
Looking upon the changing boundary conditions for
the chemical industry, the trend of an increasing need for
flexibility is likely to continue.

However, the integration of flexibility needs to be
connected to its intention. This will also enlarge transpar-
ency for the reader of future work. As of now, a transfer
of practical conclusions from highly theorized and meth-
odological studies to more applied research questions
remains challenging across disciplines. Therefore, the
proposed classification into intended and uncertain flexi-
bility aims to facilitate the identification of objectives
within future research, including optimization-based
approaches.

In addition, to enable the targeted development of
flexible processes in the future, a comprehensive evalua-
tion of flexibility in chemical engineering in all design
stages is required. The already developed optimization-
based methods provide useful tools to quantify flexibility
and have proven feasibility. Nevertheless, one major
downside of these methods is the requirement for all
boundary conditions to be known a priori to shape the
domain in order to determine flexibility. For future chal-
lenges in chemical production, it might be beneficial to
incorporate intended flexibility in earlier design stages
where not all boundary conditions are finally set. Never-
theless, the methods developed primarily for operational
flexibility under uncertainty also provide tools to quantify
flexibility for new problems originating from intended
flexibility. This transfer of methods is already performed
for some special cases.

Although there is enormous progress in developing
both steady-state and dynamic optimization-based
methods, literature is still missing the application of these
methods to complex and more realistic problem formul-
ations. Most systems analyzed have linear constraints or
quasi-convex feasibility domains, which often disagrees
with a description of phenomena and processes close to
reality. Problem formulations and constraints usually
need to be simplified to ensure the identification of a
global optimum. Therefore, critically addressing the
usability of these methods for realistic problem formul-
ations is essential. A synergistic approach combining heu-
ristic or simulation-based methods with optimization-
based methods could be a promising approach in order to
reduce computational effort and thus enhance usability.
A proficient combination allows identifying the necessary
level of detail to describe the problem sufficiently and
additionally helps to exclude insignificant phenomena.

Lastly, flexibility, especially intended flexibility, is
always associated with dynamic operation of unit opera-
tions and plants. Taking the example of a coupling
between fluctuating energy generation and chemical pro-
cesses (eg, Power-to-X concepts) or scheduling problems
for demand side management into account, one can con-
clude that the accuracy for time dependencies has to be
very high. This holds above all true if large gradients are
necessary. Therefore, a correct and validated description
of dynamic transitions and phenomena is needed. This is
only possible if all occurring phenomena are profoundly
understood. For this purpose, in many unit operations
experimental work using advanced measuring techniques
is helpful. In addition, even if phenomena are profoundly
understood, a correct description of those needs to be
incorporated in models that are used to predict dynamic
behavior. Additionally, addressing delay terms, which
can for example be a function of material characteristics
like in catalyzed reactions, in a correct and validated
manner, is an important challenge.

CONFLICT OF INTEREST
The authors declare no potential conflict of interest.

NOTATIONS
Latin letters
F mol/s molar flow rate
n mol number of mols
p bar pressure
t — time
T K temperature
x — molar fraction

Greek letters
Φ — vector of operational parameters

Indices
i — component
in — input
out — output
sys — system

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