Development of a Conceptual Framework for Evaluating the Flexibility of Future Chemical Processes

Luo, Jisiwei; Moncada, Jonathan; Ramirez, Andrea

DOI
10.1021/acs.iecr.1c03874

Publication date
2021

Document Version
Final published version

Published in
Industrial and Engineering Chemistry Research

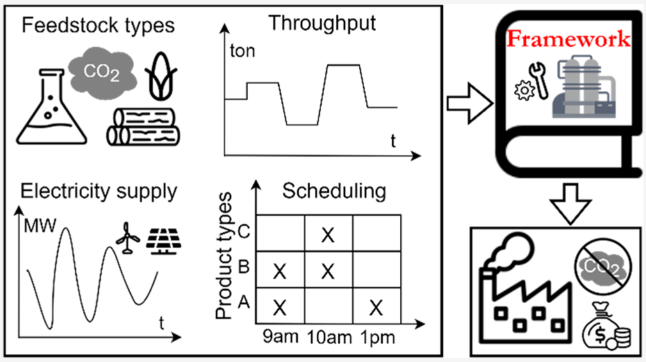
I&EC research
Industrial & Engineering Chemistry Research
pubs.acs.org/IECR
Review

Development of a Conceptual Framework for Evaluating the Flexibility of Future Chemical Processes

Jisiwei Luo,* Jonathan Moncada, and Andrea Ramirez

Cite This: *Ind. Eng. Chem. Res.* 2022, 61, 3219−3232
Read Online

ABSTRACT: Incorporating (operational) flexibility into process design has been a key approach to cope with uncertainties. The increasing penetration of renewables and the need for developing new low-carbon technologies will increase the demand for flexibility in chemical processes. This paper presents a state-of-the-art review focusing on the origin, definition, and elements of flexibility in the chemical engineering context. The article points out a significant overlap in terminology and concepts, making it difficult to understand and compare flexibility potential and constraints among studies. Further, the paper identifies a lack of available metrics for assessing specific types of flexibility and the need for developing indicators for exploring the potential flexibility of novel chemical processes. The paper proposes a classification of flexibility types and provides an overview of design strategies that have been adopted so far to enable different types of flexibility. Finally, it offers a conceptual framework that can support designers to evaluate specific types of flexibility in early-stage assessments of novel chemical processes.



1. INTRODUCTION

Chemical companies adopt emerging technologies or adapt existing technologies to maintain or improve their competitiveness. However, external factors such as volatile market conditions or changing environmental policies introduce uncertainties affecting process or company performance. Trade-offs can arise in terms of effort, time, cost, or technical performance when a company fails to adopt novel technologies or adapt existing technologies to respond to emergent uncertainties. Introducing flexibility into a plant or a process design is one of the most opted responses to cushion the potential effects of uncertainties.[1]

Flexibility in chemical processes is not a new or unfamiliar topic. Back in 1962, Thomas[2] suggested increasing attention to batch processing plants. They had the flexibility for easy expansion to respond to local steadily increasing market demand and the flexibility for multipurpose applications to accommodate variations in process conditions and change product types. More importantly, they were more economically feasible.[2] During the 1980s and 1990s, researchers investigated the optimal design of flexible chemical processes or plants under uncertainties, focusing on applying mathematical approaches.[3−9] The research was based on the premise that a flexible plant is expected to guarantee a feasible region of process operating parameters that are manageable via manipulating control variables.[6,10] With the advent of the 21st century, the potential for producing multiple products, namely polygeneration, gained attention in the literature. For instance, Yamashita and Barreto[11] studied integrated energy systems that could be designed with output flexibility. The system was amenable to diverse feedstocks and capable of flexibly producing various products, including electricity. Meerman et al.[12] explored flexible operation of an integrated gasification polygeneration (IG-PG) plant that had both feedstock (i.e., coal and different types of biomass) and output flexibility (electricity at peak hours and biofuels during off-peak hours) as a way to respond to changes in market conditions.

Results of a bibliometric analysis focusing on flexibility in the chemical industry over the past three decades are shown in Figure 1. The figure illustrates the changes in research scope in flexibility in the chemical industry. (The size of the circles reflects the frequency with which the keyword appears in the literature inventory. The distance between the two circles reflects the closeness of their connection (see Methodology for more information).) In the 1990s, as it can be seen in Figure 1a, the most common keywords were mathematical models, optimization, process control, computer simulation, scheduling, algorithms, and flexible manufacturing system. Approaches were

Received: September 27, 2021
Revised: February 16, 2022
Accepted: February 17, 2022
Published: February 25, 2022

https://doi.org/10.1021/acs.iecr.1c03874
Ind. Eng. Chem. Res. 2022, 61, 3219−3232

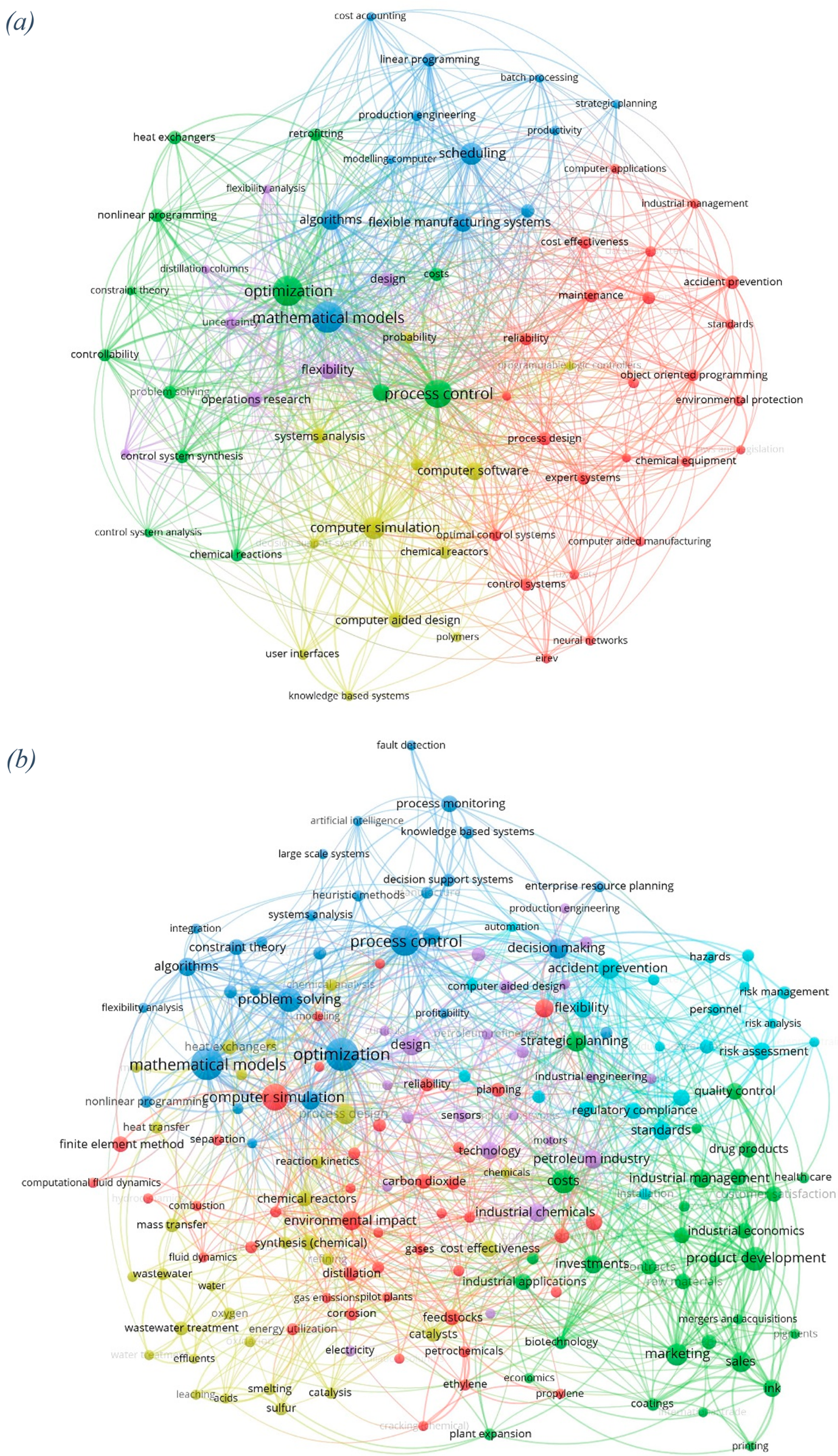


Figure 1. continued

https://doi.org/10.1021/acs.iecr.1c03874
Ind. Eng. Chem. Res. 2022, 61, 3219−3232

(c)

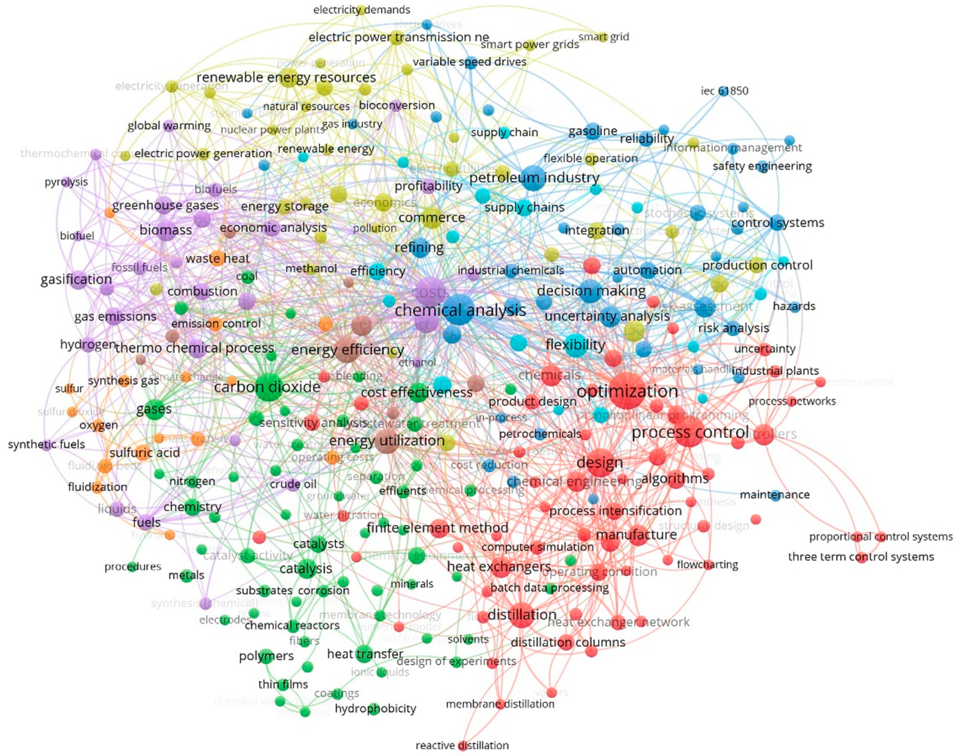


Figure 1. Bibliometric analysis network maps of flexibility-related keywords in the chemical industry, in (a) 1990−1999, (b) 2000−2009, and (c) 2010-July 2020.

developed mostly related to numerical analysis, often used to identify trade-offs between capital cost and flexible processes design in terms of, among others, operating conditions and equipment selection.[8,13,14] Studies made use of mathematical models such as mixed-integer linear programming (MILP) or mixed-integer nonlinear programming (MINLP) to determine, for instance, optimal scheduling patterns of flexible batch operation processes to minimize the changeover time between different operations, maximizing the production time and manufacturing flexibility to meet volatile market demands.[15−17] Computer simulation has been a valuable tool since then, and it is not surprising that it appeared prominently in the research at the time.

During the first decade of the 21st century (Figure 1b), flexibility included more frequently business, safety, and environmental aspects. However, some of these elements had already emerged in the previous decade. As the oil crisis that occurred in the 1990s ended and a further takeoff in the chemical industry happened, an increasing number of studies were published on how to manage a chemical company flexibly in terms of, for instance, investment and marketing.[18−21] Meanwhile, costs and environmental impacts started to be used not only to monitor performance but often also as indicators of the feasibility to invest in (flexible) chemical plants.[22−25] Regarding the technical design of a chemical plant, driven by safety concerns, equipment was required to be designed with flexibility in mind so that variations in operating conditions could be accommodated to avoid severe equipment failure and, hence, entire process failure.[22,26]

With the growth of environmental awareness in the past decade, a more comprehensive range of environment-related topics appeared in flexibility studies (see upper left quadrant in Figure 1c), exemplified by issues such as energy efficiency, energy utilization, carbon dioxide, renewable energy sources, and biomass. Of particular interest for the design of flexible chemical processes is the variable supply of energy from renewable sources. For instance, the seasonality of biomass and its variability in origin and type[27] have resulted in studies focusing on the design of chemical plants with feedstock flexibility at its core.[28,29] Similarly, "smart power grids", a topic that at first sight seems irrelevant to the chemical industry, has emerged in flexibility studies. It is often used in conjunction with terms referring to significant deployment of renewable energy sources (RES) such as solar and wind energy,[30,31] illustrating a current trend on further coupling the chemical and the power sectors. The increasing penetration of intermittent RES in the power grid has brought up technical challenges for the chemical industry as it is now expected that the chemical industry will conduct flexible operations within a range of loads and help balance fluctuations in electricity supply.[32]

The overview above points out a change in the attributes and goals through which flexibility has been defined over time. This is not always obvious as the same terminology is often used, but its meaning changes. For example, while the *flexible operation* is described in some studies as the ability to operate over a range of operating conditions,[7,13] others define it as the ability to easily switch between operations.[16,33] The term is the same, but the implications are different. Other terms that are used to mean the same or overlapping concepts are, for instance, feedstock flexibility,[28,29,34] fuel flexibility,[12] volume flexibility,[35,36] and operational flexibility.[7,37] Using similar terminology to refer to different concepts, some of them overlapping, creates confusion in the field, making it difficult to compare studies and assess the types of flexibility and their potential. The conflating terminology is also difficult for selecting indicators to evaluate and monitor flexibility. Several metrics for quantifying flexibility

https://doi.org/10.1021/acs.iecr.1c03874
Ind. Eng. Chem. Res. 2022, 61, 3219−3232

are available in the literature, such as flexibility index,[7] stochastic flexibility index,[8,9,38,39] and dynamic flexibility index.[40] The metrics involve three kinds of variables (i.e., control, design, and state) and uncertain parameters. They have their origin in the field of process systems engineering. They aim to analyze the overall flexibility of chemical processes and help designers identify optimal designs, which balance the degree of flexibility and cost. It is however unclear how to apply these metrics to assess designs of future concepts, that is, theoretical designs of technologies that are not yet at commercial scale. In these cases, uncertain parameters, the three kinds of variables described previously, and the relations among them are not well understood. Therefore, for such designs, there should be simplified and explorative metrics that allow evaluating and comparing the flexibility of different plant designs or plant configurations.

Given the importance of flexibility in the coming decades, there is a need to harmonize flexibility-related terminology, concepts, and indicators to decrease confusion for researchers new to the topic. Moreover, it is essential to propose a framework that can suffice the assessments of and the comparisons among novel designs. Such a framework can support designers and decision-makers in the chemical industry to better understand the types of flexibility they are designing toward, how different types of flexibility interact with each other, and how to assess the level of specific flexibility types a design has. However, such a systematic framework is currently lacking, though a few studies have already worked on harmonizing the definitions of several flexibility types and reviewing known strategies to enhance feedstock flexibility.[34,41] This paper aims to fill this gap by examining how flexibility has been studied and proposing a conceptual framework for evaluating specific flexibility types of novel chemical processes. The framework encloses definitions, elements, types, and indicators of different flexibility types in the chemical (including biochemical) engineering context. In the light of the future coupling between the chemical industry and the energy system, we are particularly interested in the demand for flexibility of chemical processes.

2. METHODOLOGY

This work departs from definitions, taxonomies, and other relevant concepts of flexibility presented in the literature of chemical engineering. First, a systematic literature search was performed to retrieve information needed for constructing the framework. Then a framework was developed that combines definitions, elements, types, and indicators of flexibility.

The literature review focused on journal papers studying flexibility from 1990 to July 2020 collected via Scopus. The goal was to make an inventory of (i) the definitions used, (ii) existing taxonomies, and (iii) indicators used to assess flexibility. Furthermore, to make certain that biochemical technologies were also included, as they are expected to play a role in flexibility in the future chemical industry, searching criteria relating to biochemical technologies were added. The searching criteria are given in Table S2 in the Supporting Information (SI).

In total, 1521 studies were identified on Scopus. Studies that look into the flexibility of materials and do not focus on the chemical industry or study flexibility at the molecular or laboratory scales were excluded. This resulted in 1249 that were further analyzed. Both author and indexed keywords of the 1249 studies were mapped by decade using VOSviewer. VOSviewer is a software tool for creating bibliometric maps based on the correlation among a set of data. It allows the generation of network maps and the identification of correlations. For further information on this tool, we refer to https://www.vosviewer.com/. The results of this analysis have been discussed in the Introduction section. To prepare the literature inventory, a sample of 106 papers was selected and further analyzed to develop a conceptual framework for evaluating the flexibility of novel chemical processes.

For each study, the goal was first summarized, and the terms used for different kinds of flexibility were documented along with their implicit or explicit definition. However, if a term was mentioned without a definition and the definition could not be derived from the study, the term was not further considered in the review. In addition, the design strategies used to enable each kind of flexibility were also documented, if any. Flexibility types (i.e., some of the flexibility terminologies) without design strategies were excluded from the framework. Second, when possible, the relation among different flexibility types was captured. Finally, indicators used to measure or evaluate flexibility were noted, if any.

3. STATE-OF-THE-ART

3.1. Definition of Flexibility. In chemical engineering, one of the most common uses of flexibility is as a component of operability, this is often named *operational flexibility*[7,28,36,42−51] or *process flexibility*.[38,52−56] Flexibility is usually defined as the ready capability of a plant to *operate* over a range of conditions feasibly.[57] Walsh and Perkins[58] considered operability as the ability of a system to tackle uncertainty, accommodate disturbances, and resolve concerns for reliability and maintenance. Bahri et al.[59] indicated that operability is a process that is easy to operate and control. Grossmann and Morari[60] defined operability as the ability of a chemical plant to perform satisfactorily under conditions different from the nominal design conditions. Operating condition is an umbrella term that can refer to process operating parameters (e.g., temperature, flow rates, and pressure), product specifications, feed quality, and so on.[60,61] "Ready" implies the ability to accommodate expected (e.g., stochastic process operating parameters[38]) or wanted uncertainties in some conditions (e.g., intermittent renewable energy supply). Flexibility is incorporated in the design of the physical process line(s), where related unit operations and equipment are specified. It is also denoted as process[50,53,62] or processing route.[52] In this article, it is addressed as process line.

Other components of operability refer to controllability, reliability, and resiliency.[4,7,60,63,64] *Controllability* addresses the quality and stability a process presents when responding to short-term perturbations and transitions from one operating point to another.[7,64] Controllability thus relies on designing and implementing a control system that directs and regulates equipment behavior.[22,64,65] *Reliability* is associated with the probability of mechanical or electrical failure during normal operation.[7] *Resiliency* is sometimes defined as the ability of the plant to move fast and smoothly from one operating condition to another,[61] or as the dynamic capability to quickly recover from process disturbances in a fast and smooth manner.[60] Resiliency has the ultimate goal of determining a system's inherent dynamic characteristic (e.g., deadtime[66]) without selecting a particular controller.[57] In recent years, resilience engineering[67,68] has become a popular topic in system engineering. The perception of resilience in this context is different from the one used in the chemical engineering context. The discussion on resilience engineering is outside the scope of this article.

https://doi.org/10.1021/acs.iecr.1c03874
Ind. Eng. Chem. Res. 2022, 61, 3219−3232

Finally, it is important to note that while most studies examine flexibility as a characteristic of steady systems,[15,58] some studies have studied flexibility in the context of dynamic systems.[38,57,64,65] Steady-state flexibility is the flexibility as discussed in the two previous paragraphs. Among the papers studied in this review, only Grossmann et al.[57] explicitly explained that realizing dynamic flexibility in a plant involves identifying manipulated variables that guarantee feasible operation in the worst case of time-varying uncertain parameters. The authors suggest that "dynamic flexibility" is not designed for a particular transient disturbance but for the overall dynamic performance of a plant. This review article focuses on steady-state flexibility, which is shortly referred to as flexibility.

3.2. Types of Flexibility. Different terms of flexibility can be identified (see Table 1). A problem, however, is that the definitions used for the different terminologies overlap in the literature (see Table 2). In this section, the definitions used in each case are further discussed. It should be noted that flexibility terminologies "operational flexibility" and "process flexibility" are also found in the literature, and they have already been identified as the synonyms of "flexibility" in section 3.1. Therefore, though they are listed below, they are not discussed in detail in this section.

Table 1. Flexibility Terminologies Identified in Literature

terms	ref
operational	7, 28, 34, 36, 37, 42−51, 60, and 69−71
process	22, 29, 38, 52−56, 72, and 73
feedstock	12, 28, 34, 41, 42, 53−55, and 74−77
raw material	55 and 78
fuel	11 and 12
plant	12, 27, 32, 43, 46, 73, and 79−82
volume	21, 35, 36, 52, 53, 83, and 84
product	28, 34, 42, 52, 53, 55, 74, 78, 80, 84, and 85
production	12, and 86−89
expansion	1 and 36
scheduling	87 and 90
recipe	53 and 91
capacity	34, 36, 42, 85, and 92
location	42 and 92
innovation	42
load	93 and 94
electrical	95 and 96
others (without any term)	2−6, 8−10, 13, 15−20, 23, 24, 30, 31, 33, 40, 57−59, 61−66, and 97−106

3.2.1. Same Concepts—Different Terminologies. 3.2.1.1. The Ability to Handle Changes in Quantities and/or Qualities of Inflow Materials. *Feedstock flexibility*, *fuel flexibility*, *raw material flexibility*, *electrical flexibility*, and *load flexibility* are terms used in the literature to indicate the ability of a piece of equipment, a process line, or a plant to handle changes in quantities and/or qualities of inflow materials. Quality refers to the chemical compositions or physical properties (e.g., boiling point, density, state of matter, and size). Raw material flexibility or feedstock flexibility is often studied as an option to maximize flexibility of a complex processing network and minimize the net present value of its operations.[55,100] For instance, in the petrochemical industry, pipelines were designed early on to handle crudes with different qualities to avoid the high capital cost of installing dedicated pipelines as well as to accommodate fluctuations in crude flow rate.[5] Another design strategy to enable raw material flexibility is to produce the main product from different raw materials by using different production schemes.[52] A production scheme, also called production pathway,[29,47,52] specifies the requirements for the raw material, the product qualities and the synthetic pathway (including unit operations, and hence their corresponding process operating parameters as well as utilities) to complete the conversion. In this case, process line design (e.g., equipment selection and sizing) plays a major role in enabling raw material flexibility.

With the development of biotechnology, and the need to reduce CO_2 emissions, the use of non-fossil feedstocks has gained relevance in the chemical industry. Due to the uncertainties in the long-term availability of, for example, lignocellulosic feedstocks and the need to minimize the dependence on a given type of feedstock, designing processes that can deal with the use of multiple types of feedstocks has gained relevance. Common strategies are to (i) select and/or design equipment that can deal with variations in types of feedstocks,[12,28] (ii) blend different types of feedstocks,[101] and (iii) install buffer unit(s) to regulate fluctuations in, for example, chemical composition. Kou and Zhao,[28] for instance, proposed a plant design based on a gasifier that was capable of converting multiple types of feedstocks into syngas. Their design contains an extra process unit to regulate the fluctuating ratio of components in the syngas stream before the syngas is sent to the following conversion unit. Similar examples are published in other works.[27,29,53,75]

Renewable energy resources are, however, not only renewable carbon feedstocks but also renewable electricity feedstock. In recent years, the introduction of RES with an intermittent nature has resulted in challenges in balancing the power grid. With the potential of using electrified chemical processes in the industrial sector as a demand-side management (DSM) strategy or as an

Table 2. Overview of Overlap between Flexibility Terminologies

	flexibility terminology	concept/definition
same or similar concepts, different terminologies	feedstock, fuel, raw material, electrical, load	ability to handle changes in quantities and/or qualities of inflow materials
	product, recipe	ability to change the quality of outflow materials
	production, product	ability to switch to a different production scheme
	volume, capacity, production, expansion	ability to vary throughput
concepts matched with a unique terminology	scheduling	ability to adjust resource allocation to different production cycles
	location	ability to move a plant from one place to another
	innovation	ability to adapt to try out innovative products and processes
same terminology applied to different concepts	operational	ability to operate over a range of conditions feasibly
	plant	ability of a plant to operate over a range of conditions

https://doi.org/10.1021/acs.iecr.1c03874
Ind. Eng. Chem. Res. 2022, 61, 3219−3232

energy storage strategy, requirements for electrical flexibility or load flexibility are emerging. This kind of flexibility is then defined as the ability of a machine, process line, or plant to cope with uncertainties in the electricity supply. There are three general design strategies explored in the literature:[50,70,71,93−95,102] (i) selecting and/or designing equipment (function-wise) so that it can be dynamically operated; (ii) selecting and/or oversizing equipment (capacity-wise) that meet wide load requirements; and (iii) installing buffer units (e.g., batteries for buffering electricity supply fluctuations or storage tanks for decoupling units with flow rate fluctuations from steadily operated units and hence buffering changing flow rates) to cope with the uncertainties in qualities and quantities of flows caused by fluctuating electricity supply. To lower operating costs, the ability to adjust electricity consumption subject to changing electricity prices is also studied in, for instance, flexible operations of air separation plants.[104]

3.2.1.2. The Ability to Change the Qualities of Outflow Materials. The ability to produce outflow products with different qualities is referred to in the literature as *product flexibility* or *recipe flexibility*. This type of flexibility may be required when reactions inherently result in multiple products[55] or when a company aims to maximize the flexibility of a process network containing multiple process lines and to minimize its operating costs or diversify revenues.[27,53] Mansoornejad et al.[52] pointed out that *recipe flexibility* is basically a strategy to enable product flexibility, where different production schemes are exercised on either the same process line or different process lines, but certainly with different operating conditions. Note that though some facilities can produce a set of products with different qualities, they are not considered flexible with regard to the outflow materials if the products can only be produced in fixed proportions at all times.[55] Two strategies are frequently employed to realize this type of flexibility:[27,28,52] (i) select synthetic pathways that inherently result in multiple products; (ii) implement different production schemes. Uria-Martínez et al.[77] and Norton and Grossmann[55] pointed out that different production schemes can be completed in the same process line by sharing part of the same process line or in corresponding dedicated process lines.

3.2.1.3. The Ability to Vary Throughput. The need to vary throughput over time is driven by uncertainties in product demand or feedstock availability. Several terms such as *volume flexibility*, *production flexibility*, *capacity flexibility*, and *expansion flexibility* are used in the literature to describe this type of flexibility. Despite the different terms, three common design strategies can be identified to enable this type of flexibility, namely,[53,72,78,88] (i) designing equipment to handle peaks in flow rates, (ii) installing parallel same units or even entire process lines so that some equipment can be switched on/off to adjust the overall production level, and (iii) robust scheduling. Note that the ability to adjust the production level via expanding or contracting is denoted as capacity flexibility by Wörsdörfer et al.[92] as well as expansion flexibility by others,[1,36] who are particularly interested in designing modular plants.

3.2.1.4. The Ability to Switch to Another Production Scheme. Another type of flexibility is the ability of a plant to switch to another production scheme. This is usually required for plants where part (or all) of production resources are shared among different production schemes. Mansoornejad et al.[52] described *product flexibility* (denoted as *production flexibility* by Meerman et al.[12]) as the ability to economically changeover to produce a new (set of) product(s), which is different from the definition of product flexibility in section 3.2.1.2. Polygeneration facilities are a typical example of plants that are designed around the idea of production flexibility (see, for instance, Meerman et al.[12]). The design strategies in literature[12,52] to address this type of flexibility are (i) select and/or design equipment that is able to handle inflow materials with different qualities and/or produce outflow materials with different qualities, and (ii) select or design production schemes and equipment that can be switched on/off at request.

3.2.2. Concepts with Agreement on Terminologies. *Scheduling flexibility* is the ability to adjust the allocation of production resources for different production cycles over time. It is a type of flexibility that is historically present in batch or semicontinuous processes, where part of or the entire production resources could be shared among more than one production scheme over time. A set of production resources refers here to a process line and all relevant materials that could be processed (e.g., raw materials) or consumed (e.g., utilities and labor) on a line for a production cycle. A production cycle includes all the time spent on making a product, from the preparation of production resources until the product is packed up and ready for delivery. The realization of scheduling flexibility considers the process design and the effort of supply chain planning. However, in this article, only design strategies related to process design are addressed. In the literature,[5,15,103] flexibility has been also studied regarding scheduling multipurpose plants, though the term was not explicitly used. Nowadays, some electrochemical plants, in which electricity acts mainly as a feedstock type, are expected to be designed with scheduling flexibility, so production cycles can be scheduled easily upon request, responding to DSM.[95] Scheduling flexibility is often embedded into the plant design via (i) equipment sizing, or (ii) installing multiple same units or process lines.[5]

A summary of the different terminologies and concepts and the overlap between them is provided in Table 2. Note that *location flexibility* and *innovation flexibility* were seldom the focus of studies dealing with flexibility and the respective design strategies were hardly found in the literature. Therefore, they are not discussed further in this article. The term *operational flexibility* and *process flexibility* are identical to flexibility, as explained in section 3.1. Hence, they are also not further elaborated in this section. Moreover, *plant flexibility* is an umbrella term for all types of flexibility that a plant has, and thus it is not a specific type of flexibility that can be enabled via specific design strategies.

3.3. Hierarchical Levels of Flexibility. In the literature, there are three hierarchical levels often considered during plant design: plant, process line, and equipment. The plant level involves all process lines and their corresponding production schemes in a plant. A process line was previously defined in section 3.1. The process line level further incorporates the production schemes that can be exercised on it. The equipment level indicates a single piece of equipment and everything related to it (e.g., dimensions, functions, or utilities usage). In some multipurpose plants, changes in, for example, feedstock type, product type, or throughput, are tackled by installing dedicated process lines or by modifying the process line that will be used by multiple production schemes.[52,55,77] Modifying a process line requires installing or removing extra equipment or modifying single pieces of equipment. For instance, if a gasifier does not have the ability to handle inflow syngas with a fluctuating CO/H_2 ratio, extra equipment can be installed to adjust the ratio ahead of the gasifier.[12] Examples for design details at the

Table 3. Classification of Flexibility Types and Their Respective Concept and Design Strategies

type	concept	design strategies
feedstock	the ability to handle changes in quantities and/or qualities of inflow materials	(i) implement different production schemes to produce different product types (ii) blend different types of feedstocks (iii) select and/or design the equipment that can deal with variations in feedstock quality (iv) install buffer unit(s) to regulate fluctuations in feedstock quality.
product	the ability to change the qualities of outflow materials	(i) select synthetic pathways that inherently produce multiple products (ii) implement different production schemes
volume	the ability to vary throughput	(i) select and/or design (function-wise) equipment that can deal with variations in throughput (ii) select and/or design equipment (capacity-wise) that meet wide load requirements (iii) install buffer units to decouple units with variations in throughput from steadily operated units (iv) install parallel units or process lines (v) robust scheduling
scheduling	the ability to adjust resources allocation for different production cycles	(i) oversize equipment (ii) install parallel same units or process lines
production	the ability to switch to exercise another production scheme	(i) select and/or design equipment that can handle inflow materials with different qualities and/or produce outflow materials with different qualities (ii) select and/or design production schemes and equipment that can be switched on/off at request

equipment level can be also seen in electrochemical plants, where electrolyzers must be selected or designed with the ability to cope with fluctuations in electricity supply,[50,93,95] and in multifeedstock and multiproduct biobased plants where different biomass feedstock types are handled through the same set of pretreatment and conversion units, while following upgrading and purification units are dedicated to each product.[12,27,28,77] It should be noted that often more than one level has to be considered simultaneously to enable flexibility.

3.4. Indicators for Evaluating Flexibility. To understand flexibility is important to not only define the concept but also to develop indicators that allow it to be assessed and monitored. Most indicators in the literature originate from the field of process control. The most known is the flexibility index (FI) developed by Swaney and Grossmann[7] followed by other metrics developed upon it (e.g., stochastic flexibility index,[8,9,38,39] dynamic flexibility index[40]). They are used for characterizing and quantifying the overall operational flexibility of high-TRL technologies with all the involved variables (i.e., design, state, and control) and uncertain parameters known. The flexibility index calculates the size of the space of uncertain parameters (e.g., throughput, temperature, pressure) over which steady-state operation of chemical processes could be feasibly managed through adjusting the control variables (e.g., flow rates, valve coefficient).[7,60,73,84] It is, however, difficult to apply it when the values of the variables (i.e., design, state, and control) and the relations among them are not fully understood, which is the case in ex ante assessments of low-TRL technologies. Such designs are not technologically ready to be assessed using the flexibility index. A similar metric to the flexibility index is the operability index (also known as output controllability index), proposed by Vinson and Georgakis.[105] A comprehensive study on the similarities and differences between the flexibility index and the operability index was done by Lima et al.[73] Different to the flexibility index, which measures the space of parameters that can be manipulated by control variables, the operability index calculates the extent to which the desired output variables (e.g., purity of products, product quantity) can be achieved using available input variables (e.g., purity of feedstock, inflow rates) with the presence of known disturbances.[73] A variant of the operability index is the servo operability index (also noted as servo output controllability index), also developed by Vinson and Georgakis.[105] In contrast to the operability index, the desired output variables are translated into corresponding desired input variables. Therefore, these two metrics focus on the input and output variables and, hence, can be incorporated into designs at the process synthesis phase, where the process control structure is unknown while the control objectives are known.[73,105,106] These metrics reflect the overall operability of designs on different hierarchical levels to achieve desired results. It should be noted that the metrics are not intended for quantifying specific flexibility types, and therefore require (minor) adaptions.

It is, however, surprising that there is a lack of a standardized set of indicators that allow evaluating specific flexibility types in the literature. Also in many studies, explicit indicators are lacking altogether. Flexibility is often used as part of the scoping of the studies rather than a goal that needs to be evaluated. In the studies that attempted to evaluate specific flexibility types, two categories of indicators were used to compare the degree of flexibility between design options. One category measures the range of available options. The other focuses on impacts (also noted as trade-offs by some researchers). For the first category, for instance, the number or type of feedstocks that can be processed is used as an indicator of flexibility to select equipment.[12,28] In the articles studying the ability to deal with fluctuating electricity, normalized maximum ramping rates, maximum turndown ratios, response time, the range of operable current density, peak-to-base load ratio, or load range are often used as indicators of flexibility.[50,70,93−95,102]

For the second category, in order to compare alternative flexible designs, researchers have also considered impacts in economic, technical, or environmental performances as indicators of flexibility. Impacts are case-specific, and hence the acceptability of impacts is subjective, which in many studies is simply described as "without violating the design specifications or constraints".[22,60,69] However, there are studies where specific indicators are used to evaluate impacts. The overall economic performance of a plant has widely been applied as an indicator because economics is one of the most important drivers for enabling all kinds of flexibility. Huesman[50] quantified the impact of flexibility in economic performance by comparing the profits of two electrochemical plants powered by electricity with different levels of intermittency. Energy efficiency is seen as

https://doi.org/10.1021/acs.iecr.1c03874
Ind. Eng. Chem. Res. 2022, 61, 3219−3232

an indicator in which flexibility in handling uncertainties in production rate,[93] feedstock, and product qualities is studied.[12,95] Downtime has also been used as an indicator where the changeover between production schemes is frequently required,[87,95] because it affects the production time and hence the overall production level.

4. FRAMEWORK FOR COMPARING AND ASSESSING FLEXIBILITY

In this section, we present a framework developed to support the identification, comparison, and evaluation of flexibility in the early-stage design and the ex ante assessments of novel chemical processes.

4.1. Step 1: Define Uncertainties. As discussed in section 3.1, flexibility is implemented to respond to uncertainties, either stochastic process operating parameters or expected uncertainties. Therefore, the first step is to identify the uncertainties to which the design needs to respond. Answering the following questions can help designers in this task:

- What are the potential sources of uncertainties (e.g., feedstock qualities/quantities, product qualities/quantities)?
- What are the boundaries of uncertainties (e.g., highest or lowest possible flow rates)?
- What is the expected frequency of changes in operating parameters, over a given time horizon (e.g., flow rate fluctuates at all times or only once between two production cycles)?

4.2. Step 2: Define Flexibility. After the uncertainties are identified, the needs for flexibility have to be defined. Table 3 depicts five types of flexibility identified from the literature review: *feedstock flexibility*, *product flexibility*, *volume flexibility*, *scheduling flexibility*, and *production flexibility*. As discussed in section 3.2, they are directly derived from the sources of uncertainties introduced to processes. The identification of the needs is case-specific. Therefore, the flexibility types should be adapted when needed as explained in section 4.2.1. Moreover, it should be stressed that when dealing with changes in quantities of the inflow materials (i.e., part of feedstock flexibility), this type of flexibility is essentially analogous to volume flexibility. Therefore, accordingly, the design strategies and indicators of volume flexibility can be applied.

4.2.1. Define Flexibility by Specifying the Elements of Flexibility. On the basis of the literature review, we identify five elements that need to be considered when defining flexibility: (i) target, (ii) range, (iii) hierarchical level, (iv) time scale, and (v) impact. Such a definition can therefore be the ability of [a plant/process line/equipment] to operate over [a range of operating conditions] on [a certain time scale basis] to cope with [a target] with acceptable [impact]. The contents of the brackets need to be specified in each case.

- **Target**. A target is derived from the sources of uncertainties and elaborates the content of a flexibility type, which narrows down the design scope. For instance, if the general concept of feedstock flexibility is defined as "the ability to handle changes in quantities and/or qualities of inflow materials", then it is necessary to explicitly describe the flexibility type, for example, "the ability to cope with fluctuating electricity supply". The target here is fluctuating electricity supply.
- **Range.** Flexibility is designed to handle deviations from nominal operating conditions. A range indicates how many options are available once the operating conditions deviate from the nominal ones. A range is derived from the boundaries of uncertainties. They can be a series of continuous values (e.g., 30−50 kg/h) or a set of discrete criteria (e.g., product types such as biofuel or hydrogen). Continuing with the example above, the range can be expressed, for instance, as "the ability to operate over 20−110% of the nominal electricity load to cope with fluctuating electricity supply".
- **Hierarchical level.** The hierarchical level reflects the degree of detail a design needs to reach in order to meet the design requirements derived from the flexibility needs. The hierarchical levels also reflect at which level the flexibility needs to be assessed for a given purpose. The amount of data and requirements decrease with the level of aggregation. For instance, Wang et al.[93] used peak-to-base load ratio to evaluate a plant's flexibility with regard to operations powered by intermittent renewable electricity, while Buttler and Spliethoff[94] used the range of load ratio to compare the flexibility among different electrolyzers in relation to operation under fluctuating electricity supply. Continuing with the example above, if only the electrolyzer requires flexibility, then the definition becomes "the ability of the electrolyzer to operate over 20−110% of the nominal electricity load to cope with fluctuating electricity supply".
- **Time scale.** Uncertainties are time-dependent. A unit time period can be a second, an hour, a day, a season, a production cycle, or others. Selecting the unit of time will depend on the goal of the assessment. For example, some biorefineries have to change feedstock type every season, while some multiproduct batch plants may need to change over to another production scheme after every production cycle. Adding the time scale to the above example, the definition can be elaborated as "the ability of an electrolyzer to operate over 20−110% of its nominal electricity load to cope with fluctuating electricity supply at all times".
- **Impact.** Designing for flexibility often results in impacts when compared to a reference design. Such impacts concern, for example, technical performance (e.g., conversion efficiency, product purity), economic performance (e.g., net present value, payback time), human resources (e.g., time, effort) and/or environmental performance (e.g., global warming potential, acidification). Impacts can be either positive or negative (i.e., penalties). Impacts are often quantified by comparing the performance of the (relatively more) flexible design to the performance of a reference design. Specifying in advance impacts or limits to impacts can help narrow down the number of design options. For instance, adding the requirements related to impacts to the above example, the flexibility can be then finally specified as "the ability of an electrolyzer to operate over 20−110% of its nominal load to cope with fluctuating electricity supply at all times while keeping the overall conversion efficiency above 80% at minimum cost, effort or downtime".

4.2.2. Pay Attention to Possible Relations among Different Types of Flexibility. When designing novel chemical processes, it should be noted that a need for a given type of flexibility might trigger needs for other types of flexibility. For example, production flexibility will be needed when feedstock and or

https://doi.org/10.1021/acs.iecr.1c03874
Ind. Eng. Chem. Res. 2022, 61, 3219−3232

product flexibility is enabled at the equipment and or process line level. Production flexibility might, in turn, trigger the need for scheduling flexibility. Another example at a different level is the expectation from power companies for (electro)chemical plants to have enough scheduling flexibility to operate at request, which would trigger the need for the plants to have feedstock flexibility.[95] However, interactions among different flexibility types are case-specific and often only detectable during the design procedure, leading to iterative work.

4.3. Step 3: Apply Design Strategies for Flexibility. Once the needs for flexibility are defined, the following step is to identify and select strategies to address flexibility. Table 3 summarizes design strategies identified in the literature for the five general flexibility types. Note that the strategies can be considered in any order depending on the purpose of the study. Furthermore, note that if changes in the quantities of inflow materials are expected (i.e., part of feedstock flexibility), the design strategies are similar to those of volume flexibility.

4.4. Step 4: Evaluate Flexibility. As discussed in section 3.4, indicators for evaluating specific flexibility types are scarce in the literature and, if available, they often focus on one type of flexibility. This section provides illustrative examples of standardized indicators per type and hierarchical level (see Table 4). The list is not exhaustive and can be further expanded or adapted over time. Some of the indicators were based on the literature (i.e., No. 1 and 8). Others are proposed to make the assessment of different types of flexibility more comprehensive. Note that flexibility is in fact a relative value (flexible compared to), and hence the value of an indicator should be compared between a (relatively more or less) flexible design and a reference design.

Flexibility can impact a plant at different hierarchical levels, as discussed in section 3.3. Whether such impact is considered acceptable is case-specific, and it is up to the evaluator to decide whether a given impact is acceptable, for instance, increasing flexibility at the cost of environmental or economic performance. Therefore, in the table, a desired direction for the impacts is not specified. Furthermore, note that when there is only one process line in a plant, the indicators at the process line level can also be applied to the plant level. In addition, the assessment can concern theoretical designs, for instance, designs of novel plants that are not commercial. In this case, some of the indicators in the table are not applicable. Examples of how to implement some of the indicators in Table 4 are briefly illustrated below.

Feedstock Flexibility. One indicator (no. 2 in Table 4) that can be used to characterize this type of flexibility is "the ability to use varying feedstock types while producing the same product type in a given period of time". Its math expression quantifies the maximum number of feedstock types that can be used to produce a given product and is reported as an absolute value. For instance, a process line uses a feedstock type to produce a product. Due to the unavailability of the feedstock in winter, the designers introduce another feedstock type to keep the operation ongoing. As a result, feedstock flexibility is increased at the process line level. However, using the second feedstock type would result in twice more energy being used at the same production rate. Not using the second type of feedstock would increase the risk of having to close up the plant for periods of time (and thus, result in economic losses). The indicators can hence provide insights into the trade-offs. Nevertheless, they do not suggest any acceptability. Stakeholders have to determine the trade-offs between the feedstock flexibility increasing revenue and utility usage leading to cost penalties.

There is also a more complex indicator (no. 1) that characterizes "the ability to handle expected changes in feedstock qualities while satisfying the product specifications in a given period of time". It is an indicator adapted from the operability index introduced by other works,[73,105,106] where more detailed explanations and illustrations are available. It sheds light on the extent to which the potential changes in input variables (e.g., concentration, moisture content, and temperature) are within the design range. The design range is based on the equipment design and output specifications. Equipment design determines the range in the input variables that a given piece of equipment can handle, which is referred to in the operability index as available input space (AIS).[105] In the case of concentration, for instance, this would mean the range between the lowest and highest concentrations specified in the equipment design. The output specifications determine the range of values of input variables that lead to desired output variables, which is referred to in the operability index as desired input space (DIS).[105] The range in potential changes in the input variables is referred to in this article as expected input space (EIS). All the input variables here only characterize feedstock qualities. In this context, the indicator reflects the extent to which a design can accommodate the uncertainties in the feedstock qualities. The maximum possible value of its math expression is 1. If it is below 1, it implies that the design still has room for improvement from a technical perspective.

Product Flexibility. Similar to the feedstock flexibility indicator, an indicator (no. 5) that gives an absolute value is proposed. This indicator is defined as "the ability to produce a variety of product types while using the same feedstock type in a given period of time". It provides information about the maximum number of product types that can be produced by a given feedstock type, for instance, at the plant level. Note that the value of the indicator can differ between hierarchical levels. The total number of products may be higher at the plant level than at the process line or even at the equipment level, indicating that the measure of flexibility is highly dependent on the level at which it is evaluated. As was discussed before, flexibility is evaluated to explore potential impacts, for instance, in terms of additional costs or even additional profit.

Volume Flexibility. An indicator (No. 8) that can be used to assess volume flexibility is "the ability to cope with changes in throughput rates without violating the equipment design in a given period". Throughput rate can be characterized by either the mass or volumetric flow rate. Its math expression elucidates a range of throughput rates allowing to meet product specifications, which are normalized to the designed throughput rate. For instance, the nominal load of a given commercial electrolysis stack that uses renewable electricity is 20 kW. However, it also produces the product as long as the load of the stack is between 5 kW and 22 kW. According to the indicator, the volume flexibility is 25% ~ 110% at the equipment level. However, when the load is between 25% and 50%, though the product specifications are satisfied, the product yield (impact in this example) drops by 15% calculated using the math expression of the no. 10 indicator.

Scheduling Flexibility. Scheduling flexibility is only applicable when the design is physically available. The indicator (no. 12) characterizes "the ability to start a production cycle without wasting much time in preparation in a given period of time". Its math expression can be used to calculate the ratio between time spent on preparation and time of the whole production cycle. The lower it is, the higher scheduling flexibility the design has. The indicator (no. 15) provides insight into the reduction in

https://doi.org/10.1021/acs.iecr.1c03874
Ind. Eng. Chem. Res. 2022, 61, 3219−3232

Table 4. Examples of Indicators for Evaluating Flexibility

type	no.		definition	math expression	description	more flexible when[a]	object[b]	levels[c]	notes
feedstock	1	range	The ability to handle expected changes in feedstock qualities while satisfying the product specifications in a given period of time	$\frac{\mu(\text{DIS} \cap \text{AIS} \cap \text{EIS})}{\mu\text{EIS}}$ (adapted from ref 105)	To what extent the potential changes in input variables are within the design range based on the equipment design and output specifications	↑	existent new	1,2	DIS, desired input space AIS, available input space EIS, expected input space μ, a measure function calculating the size of the corresponding space All the input variables here only characterize feedstock qualities
	2	range	The ability to use varying feedstock types while producing the same product type in a given period of time	$max(N_{fp})$	Maximum number of feedstock types that can be used to produce a given product type	↑	existent new	1,2,3	N_{fp}, number of feedstock types that produce a given product type p.
	3	impacts (technical)	Changes in the amount of product as a consequence of changes in feedstock types in a given period of time	$m_p - m_p^{\text{design}}$[d]	The deviation in the quantity of a given product type compared to the designed value		new	2, 3	m_p, quantity of a given product type p produced. m_p^{design}, m_p under the designed scenario
	4	impacts (technical)	Changes in the use of utilities as a consequence of changes in feedstock types in a given period of time	$m_U - m_U^{\text{design}}$[e]	The deviation in utility usage compared to the designed value		new	1, 2, 3	m_U, quantity of utility usage m_U^{design}, m_U under the designed scenario
product	5	range	The ability to produce a variety of product types while using the same feedstock type in a given period of time	$\max(N_{pf})$	Maximum number of product types that can be produced from a given feedstock type	↑	existent new	1, 2, 3	N_{pf}, number of product types that are produced from a given feedstock type f.
	6	impacts (technical)	Changes in the amount of feedstocks use as a result of changes in the product types in a given period of time	$m_f - m_f^{\text{design}}$	The deviation in the total quantity of a given feedstock type compared to the designed value		new	2, 3	m_f, quantity of a given feedstock type f. m_f^{design}, m_f under the designed scenario
	7	impacts (technical)	Changes in the use of utilities as a consequence of changes in product types in a given period of time	$m_U - m_U^{\text{design}}$	The deviation in utility usage compared to the designed value		existent new	1, 2, 3	
volume	8	range	The ability to cope with changes in throughput rates without violating the equipment design in a given period of time	$\frac{\dot{m}_{\text{in/out}}^{max}}{\dot{m}_{\text{in/out}}^{\text{design}}} \sim \frac{\dot{m}_{in/out}^{min}}{\dot{m}_{in/out}^{design}}$ [f] (adapted from ref 94)	Throughput rate range that allows to meet product specifications, normalized to the designed throughput rate	↑	existent new	1, 2, 3	$m_{\text{in/out}}^{\text{min}}$, minimally throughput rate leading to meet product specifications, either inlet or outlet flow rate. $m_{\text{in/out}}^{\text{design}}$, designed throughput rate.
	9	range	The ability to cope with expected changes in throughput rates without unwanted results in a given period of time	$\frac{\mu((\text{DIS} \cap \text{AIS} \cap \text{EIS})}{\mu\text{EIS}}$ (adapted from ref 105)	To what extent the potential changes in input variables are within the design range based on the equipment design and output specifications	↑	existent new	1, 2, 3	All the input variables here only characterize volume (or throughput rate)
	10	impacts (technical)	Changes in the product quantity as a consequence of changes in the throughput rates in a given period of time	$\frac{m_p}{m_f} - \frac{m_p^{\text{design}}}{m_f^{\text{design}}}$	The deviation in product yield compared to the designed value		new	2, 3	
	11	impacts (technical)	Changes in the use of utilities as a consequence of changes in throughput rates in a given period of time	$m_U - m_U^{\text{design}} \times \frac{\dot{m}_{\text{in/out}}}{\dot{m}_{\text{in/out}}^{\text{design}}}$	The deviation in utility usage compared to the designed value multiplied by the load ratio		new	1, 2, 3	$\dot{m}_{\text{in/out}}$, a given throughput rate
scheduling	12	range	The ability to start a production cycle without wasting much time in preparation in a given period of time	$\frac{t_{\text{preparation}}}{t_{\text{productioncycle}}}$	The ratio of the time spent on preparation to the time duration of a complete production cycle	↓	existent	1, 2, 3	$t_{\text{preparation}}$, the time between the moment the production order is received and when the production actually starts $t_{\text{preparation cycle}}$, time spent on a complete production cycle.
	13	impacts (technical)	Changes in the amount of product as a consequence of changes in production cycles in a given period of time	$m_p - m_p^{\text{design}}$	The deviation in the quantity of a given product type compared to the designed value		existent	1, 2, 3	

https://doi.org/10.1021/acs.iecr.1c03874
Ind. Eng. Chem. Res. 2022, 61, 3219−3232

Table 4. continued

type	no.		definition	math expression	description	more flexible when[a]	object[b]	levels[c]	notes
production	14	range	The ability to alternate production schemes on the same process line in a given period of time	$\max(N_{sl})$	Maximum number production schemes on a given process line	↑	existent new	2	N_{sb} number of production schemes that can be exercised on a given process line *l*.
	15	impacts (technical)	The quantity of utilities spent for switching between production schemes in a given period of time	$m_U^{\mathrm{switching}}$	Utility usage for switching between production schemes		existent	1, 2, 3	

[a]The arrows indicate the desired direction of flexibility compared to an alternative (e.g., the higher the value the more flexible the design or the lower the value the more flexible the design). [b]Object indicates whether the indicators are applicable to an existent or a new design. [c]Levels 1, 2, and 3 correspond to equipment, process line, and plant level, respectively. [d]Whenever there is a m_p in the expression, m_p should be adjusted when needed to fit in each hierarchical level. [e]Whenever there is a m_U in the expression, m_U should be adjusted when needed to fit in each hierarchical level. [f]Whenever there is a $\dot{m}$ in the expression, $\dot{m}$ should be adjusted when needed to fit in each hierarchical level.

production quantity due to time spent in preparation, compared to the scenario when fewer production cycles (can be 1 by design) are required to be executed in a given period of time. Stakeholders then need to decide the extent to which the scheduling flexibility of the design should be that it responds faster to the supply chain planning. However, they also have to balance it with certain impacts in terms of, for instance, the economic performance.

Production Flexibility. If production flexibility is defined as "the ability to alternate production schemes on the same process line in a given period of time", the indicator (no. 14) can cast light on it. Its math expression counts the maximum production schemes that can be exercised on a given process line, which is an absolute value. The higher the value is, the more flexible the process line is. However, switching between different production schemes on the same process line usually does not sacrifice nothing at all times. The math expression of the no. 15 indicator quantifies for example, how much utility water is used to clean the process line for the switch. Stakeholders should weigh the importance between production flexibility that might, for instance, lower the capital cost and the extra utility usage that could for instance increase the operating cost.

5. CONCLUSION

This paper aimed to develop a conceptual framework of flexibility that can serve as a guideline for the design and assessment of novel flexible chemical processes. The article identified how flexibility-related topics have evolved in the past three decades, shifting from focusing on the optimization of, mostly, well-understood high TRL processes to the design of novel chemical processes that employ renewable energies such as biomass, intermittent renewable electricity, and others, which inherently carry additional uncertainties. We identified significant overlaps in terminology and concepts, resulting in confusion when comparing different studies dealing with flexibility. On the basis of the literature, we proposed a definition and identified five types of flexibility: feedstock flexibility, product flexibility, volume flexibility, scheduling flexibility, and production flexibility. Furthermore, the article identified design strategies that are adopted to enable these types of flexibility, from which process designers could draw lessons when designing for similar flexibility needs.

To support the design and assessment of different flexibility types, we identified five elements of flexibility: target, range, hierarchical level (i.e., equipment, process line or plant), time scale, and impact. Further, as standardized indicators to evaluate the specific flexibility types of processes are largely lacking, the article proposed a first set of indicators for evaluating specific flexibility types independent of a control structure. In further work, the indicators should be tested and further refined and economic as well as environmental perspectives should be further incorporated. In this article utilities are considered part of the production scheme; however, since utilities and their related equipment also gained attention in the context of flexibility (e.g., heat exchange network), utilities should be incorporated as a separate factor into the framework.

Finally, it is important to stress that coupling of the energy sector, with increasing penetration of renewable energy, and the chemical industry will remain a key challenge in the coming decades. The need and requirement for flexibility will gain increasing importance for both sectors and will play a key role in the way novel chemical processes are designed and implemented. The development of methodologies that support the

https://doi.org/10.1021/acs.iecr.1c03874
Ind. Eng. Chem. Res. 2022, 61, 3219−3232

assessment of flexibility options early on requires further work and attention from the academic and industrial communities.

■ ASSOCIATED CONTENT

Supporting Information

The Supporting Information is available free of charge at https://pubs.acs.org/doi/10.1021/acs.iecr.1c03874.

Details on mapping parameters of the bibliometric graphs in VOSviewer and the searching criteria for the literature search performed on Scopus (PDF)

■ AUTHOR INFORMATION

Corresponding Author

Jisiwei Luo − *Department of Engineering Systems and Services, Faculty of Technology, Policy and Management, Delft University of Technology, Delft 2628 BX, The Netherlands;* orcid.org/0000-0003-0935-3315; Email: J.Luo-1@tudelft.nl

Authors

Jonathan Moncada − *Department of Engineering Systems and Services, Faculty of Technology, Policy and Management, Delft University of Technology, Delft 2628 BX, The Netherlands; TNO, Energy Transition Studies, Amsterdam 1043 NT, The Netherlands*

Andrea Ramirez − *Department of Engineering Systems and Services, Faculty of Technology, Policy and Management, Delft University of Technology, Delft 2628 BX, The Netherlands*

Complete contact information is available at: https://pubs.acs.org/10.1021/acs.iecr.1c03874

Notes

The authors declare no competing financial interest.

■ ACKNOWLEDGMENTS

This work was supported by Shell and a PPP-allowance from Top Consortia for Knowledge and Innovation (TKI's) of the Dutch Ministry of Economic Affairs and Climate Policy in the context of the TU Delft e-Refinery Institute. The authors would like to express their gratitude to Prof.dr.ir. Paulien Herder at Delft University of Technology for her insights into the chemical industry.

■ REFERENCES

(1) Ajah, A. N.; Herder, P. M. Addressing flexibility during process and infrastructure systems conceptual design: Real options perspective. *Ieee Sys. Man Cybern.* **2005**, 3711−3716.

(2) Thomas, L. R. Batch processing plants. *Can. J. Chem. Eng.* **1962**, *40*, 179−182.

(3) Grossmann, I. E.; Halemane, K. P. Decomposition Strategy for Designing Flexible Chemical-Plants. *AlChE J.* **1982**, *28*, 686−694.

(4) Grossmann, I. E.; Halemane, K. P.; Swaney, R. E. Optimization Strategies for Flexible Chemical Processes. *Comput. Chem. Eng.* **1983**, *7*, 439−462.

(5) Grossmann, I. E.; Sargent, R. W. H. Optimum Design of Multipurpose Chemical Plants. *Ind. Eng. Chem. Proc. Dd.* **1979**, *18*, 343−348.

(6) Grossmann, I. E.; Sargent, R. W. H. Optimum Design of Chemical-Plants with Uncertain Parameters. *AlChE J.* **1978**, *24*, 1021−1028.

(7) Swaney, R. E.; Grossmann, I. E. An index for operational flexibility in chemical process design. Part I: Formulation and theory. *AlChE J.* **1985**, *31*, 621−630.

(8) Straub, D. A.; Grossmann, I. E. Evaluation and Optimization of Stochastic Flexibility in Multiproduct Batch Plants. *Comput. Chem. Eng.* **1992**, *16*, 69−87.

(9) Straub, D. A.; Grossmann, I. E. Integrated Stochastic Metric of Flexibility for Systems with Discrete State and Continuous Parameter Uncertainties. *Comput. Chem. Eng.* **1990**, *14*, 967−985.

(10) Halemane, K. P.; Grossmann, I. E. Optimal Process Design under Uncertainty. *AlChE J.* **1983**, *29*, 425−433.

(11) Yamashita, K.; Barreto, L. Energyplexes for the 21st century: Coal gasification for co-producing hydrogen, electricity and liquid fuels. *Energy.* **2005**, *30*, 2453−2473.

(12) Meerman, J. C.; Ramirez, A.; Turkenburg, W. C.; Faaij, A. P. C. Performance of simulated flexible integrated gasification polygeneration facilities. Part A: A technical-energetic assessment. *Renew. Sust. Energy Rev.* **2011**, *15*, 2563−2587.

(13) Fichtner, G.; Reinhart, H. J.; Rippin, D. W. T. The Design of Flexible Chemical-Plants by the Application of Interval Mathematics. *Comput. Chem. Eng.* **1990**, *14*, 1311−1316.

(14) Varvarezos, D. K.; Grossmann, I. E.; Biegler, L. T. A Sensitivity Based Approach for Flexibility Analysis and Design of Linear Process Systems. *Comput. Chem. Eng.* **1995**, *19*, 1301−1316.

(15) Kondili, E.; Pantelides, C. C.; Sargent, R. W. H. A general algorithm for short-term scheduling of batch operations—I. MILP formulation. *Comput. Chem. Eng.* **1993**, *17*, 211−227.

(16) Mockus, L.; Reklaitis, G. V. Mathematical programming formulation for scheduling of batch operations based on nonuniform time discretization. *Comput. Chem. Eng.* **1997**, *21*, 1147−1156.

(17) Verwater-Lukszo, Z.; Keesman, K. J. Computer-aided development of flexible batch production recipes. *Prod. Plan. Control.* **1995**, *6*, 320−330.

(18) de Bakker, F. G. A.; Fisscher, O. A. M.; Brack, A. J. P. Organizing product-oriented environmental management from a firm's perspective. *J. Clean. Prod.* **2002**, *10*, 455−464.

(19) Karuppiah, R.; Grossmann, I. E. Global optimization for the synthesis of integrated water systems in chemical processes. *Comput. Chem. Eng.* **2006**, *30*, 650−673.

(20) Ayers, J. Demand-Driven Supply Chain Implementation. *Chem. Eng. Prog.* **2006**, *102*, 21−23.

(21) Ferdows, K.; Carabetta, C. The effect of inter-factory linkage flexibility on inventories and backlogs in integrated process industries. *Int. J. Prod. Res.* **2006**, *44*, 237−255.

(22) Malcolm, A.; Polan, J.; Zhang, L.; Ogunnaike, B. A.; Linninger, A. A. Integrating systems design and control using dynamic flexibility analysis. *AlChE J.* **2007**, *53*, 2048−2061.

(23) Capello, C.; Hellweg, S.; Badertscher, B.; Betschart, H.; Hungerbuhler, K. Part 1: The ecosolvent tool - Environmental assessment of waste-solvent treatment options. *J. Ind. Ecol.* **2007**, *11*, 26−38.

(24) Villegas, J. D.; Gnansounou, E. Techno-economic and environmental evaluation of lignocellulosic biochemical refineries: need for a modular platform for integrated assessment (MPIA). *J. Sci. Ind. Res. India.* **2008**, *67*, 927−940.

(25) Petrie, J.; Alexander, B. Considerations of process flexibility in design of chemical processes for satisfaction of economic and environmental objectives. *Second International Symposium on Environmentally Conscious Design and Inverse Manufacturing, Proceedings* **2001**, 1012−1017.

(26) Dvoretskii, D. S.; Dvoretskii, S. I.; Ostrovskii, G. M. Integrated design of power- and resource-saving chemical processes and process control systems: Strategy, methods, and application. *Theor. Found. Chem. Eng.* **2008**, *42*, 26−36.

(27) Giuliano, A.; Poletto, M.; Barletta, D. Process optimization of a multi-product biorefinery: The effect of biomass seasonality. *Chem. Eng. Res. Des.* **2016**, *107*, 236−252.

(28) Kou, N. N.; Zhao, F. Techno-economical analysis of a thermochemical biofuel plant with feedstock and product flexibility under external disturbances. *Energy.* **2011**, *36*, 6745−6752.

(29) Ng, K. S.; Hernandez, E. M. A systematic framework for energetic, environmental and economic (3E) assessment and design of polygeneration systems. *Chem. Eng. Res. Des.* **2016**, *106*, 1−25.
(30) Abate, S.; Lanzafame, P.; Perathoner, S.; Centi, G. New Sustainable Model of Biorefineries: Biofactories and Challenges of Integrating Bio- and Solar Refineries. *ChemSusChem.* **2015**, *8*, 2854−66.
(31) Yang, S.; Chen, Q. Q.; Liu, Z. Q.; Wang, Y. F.; Tang, Z. Y.; Sun, Y. H. Performance analysis of the wind energy integrated with a natural-gas-to-methanol process. *Energy Convers. Manage.* **2018**, *173*, 735−742.
(32) Bui, M.; Flo, N. E.; de Cazenove, T.; Mac Dowell, N. Demonstrating flexible operation of the Technology Centre Mongstad (TCM) CO2 capture plant. *Int. J. Greenh. Gas. Con.* **2020**, *93*, 102879.
(33) Tousain, R. L.; Bosgra, O. H. Market-oriented scheduling and economic optimization of continuous multi-grade chemical processes. *J. Process Contr.* **2006**, *16*, 291−302.
(34) Bruns, B.; Herrmann, F.; Polyakova, M.; Grünewald, M.; Riese, J. A systematic approach to define flexibility in chemical engineering. *J. Adv. Manuf. Process.* **2020**, *2*, No. e10063.
(35) Heitmann, M.; Schembecker, G.; Bramsiepe, C. Framework to decide for a volume flexible chemical plant during early phases of plant design. *Chem. Eng. Res. Des.* **2017**, *128*, 85−94.
(36) Seifert, T.; Lesniak, A. K.; Sievers, S.; Schembecker, G.; Bramsiepe, C. Capacity Flexibility of Chemical Plants. *Chem. Eng. Technol.* **2014**, *37*, 332−342.
(37) Kou, N.; Zhao, F. Operational flexibility: A key factor in the development of biofuel technologies. *Sustain. Energy Techn.* **2013**, *1*, 28−33.
(38) Pistikopoulos, E. N.; Mazzuchi, T. A. A Novel Flexibility Analysis Approach for Processes with Stochastic Parameters. *Comput. Chem. Eng.* **1990**, *14*, 991−1000.
(39) Straub, D. A.; Grossmann, I. E. Design Optimization of Stochastic Flexibility. *Comput. Chem. Eng.* **1993**, *17*, 339−354.
(40) Dimitriadis, V. D.; Pistikopoulos, E. N. Flexibility Analysis of Dynamic-Systems. *Ind. Eng. Chem. Res.* **1995**, *34*, 4451−4462.
(41) Riese, J.; Grunewald, M. Challenges and Opportunities to Enhance Flexibility in Design and Operation of Chemical Processes. *Chem. Ing. Technol.* **2020**, *92*, 1887−1897.
(42) van Kranenburg, K. J.; Sofra, S.; Verdoes, D.; de Graaff, M. *Small-scale flexible plants - Towards a more agile and competitive EU chemical industry*; TNO: Delft, 2015. http://resolver.tudelft.nl/uuid:639798ee-c8ca-4949-9acf-24ac4c5eef25 (accessed 2020−11−02).
(43) Lai, S.; Hui, C. Measurement of plant flexibility. *Comput.-Aided Chem. Eng.* **2007**, *24*, 189−194.
(44) Hossiso, K. W.; Ripplinger, D. The Value of Switching Production Options in a Flexible Biorefinery. *Agric. Resour. Econ. Re.* **2017**, *46*, 146−173.
(45) Kuo, Y. C.; Chang, C. T. On Heuristic Computation and Application of Flexibility Indices for Unsteady Process Design. *Ind. Eng. Chem. Res.* **2016**, *55*, 670−682.
(46) Kasivisvanathan, H.; Ng, D. K. S.; Poplewski, G.; Tan, R. R. Flexibility Optimization for a Palm Oil-Based Integrated Biorefinery with Demand Uncertainties. *Ind. Eng. Chem. Res.* **2016**, *55*, 4035−4044.
(47) Martinez-Hernandez, E.; Sadhukhan, J.; Campbell, G. M. Integration of bioethanol as an in-process material in biorefineries using mass pinch analysis. *Appl. Energy.* **2013**, *104*, 517−526.
(48) Adi, V. S. K.; Chang, C. T. A mathematical programming formulation for temporal flexibility analysis. *Comput. Chem. Eng.* **2013**, *57*, 151−158.
(49) Zhang, Q.; Grossmann, I. E. Planning and Scheduling for Industrial Demand Side Management: Advances and Challenges. In *Alternative Energy Sources and Technologies*; Springer: Switzerland, 2016; pp 383−414.
(50) Huesman, A. Integration of operation and design of solar fuel plants: A carbon dioxide to methanol case study. *Comput. Chem. Eng.* **2020**, *140*, 106836.
(51) Svensson, E.; Berntsson, T.; Stromberg, A. B. The value of flexibility for pulp mills investing in energy efficiency and future biorefinery concepts. *Int. J. Energy Res.* **2014**, *38*, 1864−1878.
(52) Mansoornejad, B.; Chambost, V.; Stuart, P. Integrating product portfolio design and supply chain design for the forest biorefinery. *Comput. Chem. Eng.* **2010**, *34*, 1497−1506.
(53) Dansereau, L. P.; El-Halwagi, M.; Mansoornejad, B.; Stuart, P. Framework for margins-based planning: Forest biorefinery case study. *Comput. Chem. Eng.* **2014**, *63*, 34−50.
(54) Silva-Fernandes, T.; Marques, S.; Rodrigues, R. C. L. B.; Loureiro-Dias, M. C.; Fonseca, C.; Girio, F. Enzymatic hydrolyses of pretreated eucalyptus residues, wheat straw or olive tree pruning, and their mixtures towards flexible sugar-based biorefineries. *Biomass Convers Bior.* **2016**, *6*, 385−396.
(55) Norton, L. C.; Grossmann, I. E. Strategic planning model for complete process flexibility. *Ind. Eng. Chem. Res.* **1994**, *33*, 69−76.
(56) Thomaidis, T. V.; Pistikopoulos, E. N. Optimal-Design of Flexible and Reliable Process Systems. *Ieee T. Reliab.* **1995**, *44*, 243−250.
(57) Grossmann, I. E.; Calfa, B. A.; Garcia-Herreros, P. Evolution of concepts and models for quantifying resiliency and flexibility of chemical processes. *Comput. Chem. Eng.* **2014**, *70*, 22−34.
(58) Walsh, S.; Perkins, J. Operability and Control in Process Synthesis and Design. In *Advances in Chemical Engineering*; Academic Press: New York, 1996; Vol. *23*, pp 301−402.
(59) Bahri, P. A.; Bandoni, A.; Romagnoli, J. Operability assessment in chemical plants. *Comput. Chem. Eng.* **1996**, *20*, S787−S792.
(60) Grossmann, I. E.; Morari, M., *Operability, Resiliency, and Flexibility: process design objectives for a changing world*; Carnegie Mellon University: 2018.
(61) Morari, M. Flexibility and Resiliency of Process Systems. *Comput. Chem. Eng.* **1983**, *7*, 423−437.
(62) Chen, Q.; Grossmann, I. E. Effective Generalized Disjunctive Programming Models for Modular Process Synthesis. *Ind. Eng. Chem. Res.* **2019**, *58*, 5873−5886.
(63) Pistikopoulos, E. N. Uncertainty in-Process Design and Operations. *Comput. Chem. Eng.* **1995**, *19*, S553−S563.
(64) Svensson, E.; Eriksson, K.; Wik, T. Reasons to apply operability analysis in the design of integrated biorefineries. *Biofuel Bioprod Bior.* **2015**, *9*, 147−157.
(65) Bahri, P. A.; Bandoni, J. A.; Romagnoli, J. A. Integrated flexibility and controllability analysis in design of chemical processes. *AlChE J.* **1997**, *43*, 997−1015.
(66) Holt, B. R.; Morari, M. Design of resilient processing plants—V. *Chem. Eng. Sci.* **1985**, *40*, 1229−1237.
(67) Hollnagel, E.; Woods, D. D.; Leveson, N. *Resilience engineering: Concepts and precepts*; Ashgate, 2006.
(68) Hollnagel, E. *Resilience engineering in practice: A guidebook*; Ashgate, 2013.
(69) Zheng, C. L.; Zhao, F.; Zhu, L. Y.; Chen, X. Operational Flexibility Analysis of High-Dimensional Systems via Cylindrical Algebraic Decomposition. *Ind. Eng. Chem. Res.* **2020**, *59*, 4670−4687.
(70) Teichgraeber, H.; Brandt, A. R. Optimal design of an electricity-intensive industrial facility subject to electricity price uncertainty: Stochastic optimization and scenario reduction. *Chem. Eng. Res. Des.* **2020**, *163*, 204−216.
(71) Chen, C.; Yang, A. D. Power-to-methanol: The role of process flexibility in the integration of variable renewable energy into chemical production. *Energy Convers. Manage.* **2021**, *228*, 113673.
(72) Arora, A.; Li, J.; Zantye, M. S.; Hasan, M. M. F. Process Design Frameworks for Economic Utilization of Small-Scale and Unconventional Feedstocks. In *Proceedings of the 9th International Conference on Foundations of Computer-Aided Process Design*; Elsevier: Amsterdam, 2019; Vol. *50*, pp 83−88.
(73) Lima, F. V.; Jia, Z.; Ierapetritou, M.; Georgakis, C. Similarities and differences between the concepts of operability and flexibility: The steady-state case. *AlChE J.* **2009**, *56*, 702−716.
(74) Dahmen, N.; Henrich, E.; Henrich, T. Synthesis Gas Biorefinery. In *Advances in Biochemical Engineering/Biotechnology*; 2017/03/24 ed.; Springer: Switzerland, 2019; Vol. *166*, pp 217−245.

(75) Dou, C.; Bura, R.; Ewanick, S.; Morales-Vera, R. Blending short rotation coppice poplar with wheat straw as a biorefinery feedstock in the State of Washington. *Ind. Crop. Prod.* **2019**, *132*, 407−412.
(76) Jiang, J. C.; Xu, J. M.; Song, Z. Q. Review of the direct thermochemical conversion of lignocellulosic biomass for liquid fuels. *Front. Agric. Sci. Eng.* **2015**, *2*, 13−27.
(77) Uría-Martínez, R.; Leiby, P. N.; Brown, M. L. Cost of Oil and Biomass Supply Shocks under Different Biofuel Supply Chain Configurations. *Transp. Res. Rec.* **2018**, *2672*, 31−40.
(78) Yue, D. J.; You, F. Q. Planning and Scheduling of Flexible Process Networks Under Uncertainty with Stochastic Inventory: MINLP Models and Algorithm. *AlChE J.* **2013**, *59*, 1511−1532.
(79) Hanak, D. P.; Biliyok, C.; Manovic, V. Calcium looping with inherent energy storage for decarbonisation of coal-fired power plant. *Energy Environ. Sci.* **2016**, *9*, 971−983.
(80) Stitt, E. H. Alternative multiphase reactors for fine chemicals. *Chem. Eng. J.* **2002**, *90*, 47−60.
(81) Dias, M. O.S.; Junqueira, T. L.; Cavalett, O.; Pavanello, L. G.; Cunha, M. P.; Jesus, C. D.F.; Maciel Filho, R.; Bonomi, A. Biorefineries for the production of first and second generation ethanol and electricity from sugarcane. *Appl. Energy.* **2013**, *109*, 72−78.
(82) Bensaid, S.; Conti, R.; Fino, D. Direct liquefaction of lignocellulosic residues for liquid fuel production. *Fuel.* **2012**, *94*, 324−332.
(83) Becker, T.; Lier, S.; Werners, B. Value of modular production concepts in future chemical industry production networks. *Eur. J. Oper. Res.* **2019**, *276*, 957−970.
(84) Mansoornejad, B.; Pistikopoulos, E. N.; Stuart, P. Metrics for evaluating the forest biorefinery supply chain performance. *Comput. Chem. Eng.* **2013**, *54*, 125−139.
(85) Fürer, S.; Rauch, J.; Sanden, F. J. Definitions of Multiproduct Plants and Flexibility Demands. In *Multiproduct Plants*; Wiley-VCH: Weinheim, 2003; pp 787−792.
(86) Mansoornejad, B.; Pistikopoulos, E. N.; Stuart, P. Incorporating Flexibility Design into Supply Chain Design for Forest Biorefinery. *J. Sci. Technol. Forest Prod. Process.* **2011**, *1*, 54−66.
(87) Capón-García, E.; Ferrer-Nadal, S.; Graells, M.; Puigjaner, L. An Extended Formulation for the Flexible Short-Term Scheduling of Multiproduct Semicontinuous Plants. *Ind. Eng. Chem. Res.* **2009**, *48*, 2009−2019.
(88) Sievers, S.; Seifert, T.; Schembecker, G.; Bramsiepe, C. Methodology for evaluating modular production concepts. *Chem. Eng. Sci.* **2016**, *155*, 153−166.
(89) Al-Qahtani, K.; Elkamel, A. Multisite facility network integration design and coordination: An application to the refining industry. *Comput. Chem. Eng.* **2008**, *32*, 2189−2202.
(90) Stefansdottir, B.; Grunow, M.; Akkerman, R. Classifying and modeling setups and cleanings in lot sizing and scheduling. *Eur. J. Oper. Res.* **2017**, *261*, 849−865.
(91) Ferrer-Nadal, S.; Puigjaner, L.; Guillen-Gosalbez, G. Managing risk through a flexible recipe framework. *AlChE J.* **2008**, *54*, 728−740.
(92) Wörsdörfer, D.; Lier, S.; Crasselt, N. Real options-based evaluation model for transformable plant designs in the process industry. *J. Manuf. Syst.* **2017**, *42*, 29−43.
(93) Wang, G. H.; Mitsos, A.; Marquardt, W. Renewable production of ammonia and nitric acid. *AlChE J.* **2020**, *66*, No. e16947.
(94) Buttler, A.; Spliethoff, H. Current status of water electrolysis for energy storage, grid balancing and sector coupling via power-to-gas and power-to-liquids: A review. *Renew. Sust. Energy Rev.* **2018**, *82*, 2440−2454.
(95) Brée, L. C.; Bulan, A.; Herding, R.; Kuhlmann, J.; Mitsos, A.; Perrey, K.; Roh, K. Techno-Economic Comparison of Flexibility Options in Chlorine Production. *Ind. Eng. Chem. Res.* **2020**, *59*, 12186−12196.
(96) Baetens, J.; Zwaenepoel, B.; De Kooning, J. D. M.; Van Eetvelde, G.; Vandevelde, L. Thermal systems in process industry as a source for electrical flexibility. *2017 52nd Int. Univ. Power Eng. Conf. (UPEC)* **2017**, 1−6, DOI: 10.1109/upec.2017.8231869.
(97) Sammons, N.; Eden, M.; Yuan, W.; Cullinan, H.; Aksoy, B. A flexible framework for optimal biorefinery product allocation. *Environ. Prog.* **2007**, *26*, 349−354.
(98) Di Pretoro, A.; Montastruc, L.; Manenti, F.; Joulia, X. Flexibility analysis of a distillation column: Indexes comparison and economic assessment. *Comput. Chem. Eng.* **2019**, *124*, 93−108.
(99) Di Pretoro, A.; Montastruc, L.; Manenti, F.; Joulia, X. Flexibility Assessment of a Distillation Train: Nominal vs Perturbated Conditions Optimal Design. In *29th European Symposium on Computer Aided Process Engineering*; Elsevier: Amsterdam, 2019; pp 667−672.
(100) Sahinidis, N. V.; Grossmann, I. E. Multiperiod investment model for processing networks with dedicated and flexible plants. *Ind. Eng. Chem. Res.* **1991**, *30*, 1165−1171.
(101) Bello, S.; Feijoo, G.; Moreira, M. T. Energy Footprint of Biorefinery Schemes. In *Energy Footprints of the Bio-refinery, Hotel, and Building Sectors*; Springer: Singapore, 2019; pp 1−45.
(102) Osman, O.; Sgouridis, S.; Sleptchenko, A. Scaling the production of renewable ammonia: A techno-economic optimization applied in regions with high insolation. *J. Clean. Prod.* **2020**, *271*, 121627.
(103) Adamides, E. D.; Yamalidou, E. C.; Bonvin, D. A systemic framework for the recovery of flexible production systems. *Int. J. Prod. Res.* **1996**, *34*, 1875−1893.
(104) Pattison, R. C.; Baldea, M. Optimal Design of Air Separation Plants with Variable Electricity Pricing. In *Proceedings of the 8th International Conference on Foundations of Computer-Aided Process Design*; Elsevier: The Netherlands, 2014; pp 393−398.
(105) Vinson, D. R.; Georgakis, C. A new measure of process output controllability. *J. Process Contr.* **2000**, *10*, 185−194.
(106) Gazzaneo, V.; Carrasco, J. C.; Vinson, D. R.; Lima, F. V. Process Operability Algorithms: Past, Present, and Future Developments. *Ind. Eng. Chem. Res.* **2020**, *59*, 2457−2470.

https://doi.org/10.1021/acs.iecr.1c03874
Ind. Eng. Chem. Res. 2022, 61, 3219−3232