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Exploring potential diffusion pathways of biorefinery innovations—An agent-based simulation approach for facilitating shared value creation

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Abstract

In many European countries with plentiful forest resources, novel forest-based businesses play a key role in the transition from our current fossil-based economy towards a circular bioeconomy. For example, kraft lignin, a by-product from the pulping industry, is produced in large amounts globally. To date, however, it is still only offered on the market by a small number of pulping companies. The successful innovation diffusion of related new technologies and businesses requires establishing a collective effort among multiple societal actors to motivate the sharing of value creation processes. In this paper, potential innovation diffusion pathways are modeled and simulated by means of an agent-based approach (Biorefinery Products Innovation Diffusion model, BioPID). The paper investigates the conditions needed to encourage the diffusion of kraft lignin innovations as a (partial) replacement for fossil-based feedstock in selected applications. The results reveal the basic mechanisms behind potential innovation diffusion pathways. The major barriers were found to be the high level of uncertainty surrounding the additional costs arising in lignin processing, the small number of lignin providers, and the presence of relatively homogeneous pricing strategies based on opportunity and basic preparation costs. The analysis of two product categories revealed different patterns in terms of innovation diffusion and potential greenhouse gas emissions. A novelty of BioPID is that it allows for iterative technology evaluation and technology foresight analysis of biorefinery projects (e.g., by combining techno-economic, socio-technical, and environmental aspects). This produces knowledge for diverse stakeholders involved in the lignin innovation ecosystem, thus enabling better communication on shared values and furthering innovation diffusion.

Abbreviations: ABM, agent-based model; AP, announced pledges (IEA oil price projection); BioPID, Biorefinery Products Innovation Diffusion; CF, carbon fiber; CT, carbon pricing; EoS, economies of scale; EU, European Union; GP, goods producer (lignin processor); IEA, International Energy Agency; LPF, lignin phenol formaldehyde; MC3, MCx, model scenarios including the "minor-change" lignin producer variant (3: AP oil price projection; x: lignin price development follows the oil price development; cMC3, cMCx:, referring to CFs; rMC3, rMCx, : referring to phenols for LPF resins); NGO, non-governmental organization; NZ, net zero emissions by 2050 (IEA oil price projection); PEX3, PEX7, PEXx, model scenarios including the "price-expectation" lignin producer variant (3: AP oil price projection; 7: AP + CT oil price projection; x: lignin price development follows the oil price development; cPEX3, cPEX7, cPEXx, referring to CFs; rPEX3, rPEX7, rPEXx, referring to phenols for LPF resins); R&D, research and development; SD, sustainable development (IEA oil price projection); SP, stated policies (IEA oil price projection); TEA, techno-economic assessment; TEA7, model scenario including the "individual pricing" lignin producer variant (7: AP + CT oil price projection; cTEA7, referring to CFs; rTEA7, referring to phenols for LPF resins).

KEYWORDS
agent-based model (ABM), business ecosystem management, environmental impact analysis, innovation diffusion pathways, lignin biorefinery, shared value creation, sustainability transition, techno-economic analysis

1 | INTRODUCTION

1.1 | Shared and sustainable value from the forest for circular bioeconomy transition

Companies' business strategies, models, and related production have a significant impact on the transition towards greater sustainability (Loorbach & Wijsman, 2013; Baumgartner & Rauter, 2017; Bidmon & Knab, 2018). However, achieving progress in such a transition requires that the diverse efforts of several societal actors at a variety of socio-technical levels be aligned (Avelino, 2021; Köhler et al., 2019). Business organizations thus need to interact and collaborate with numerous stakeholders in their value creation processes to benefit businesses as well as their stakeholders (Freeman, 2010). This entails the generation of shared values and a joint purpose in order to encourage the value creation process (Breuer & Lüdeke-Freund, 2017; Freudenreich et al., 2020). This process is essential in harmonizing and integrating economic, environmental, and social perspectives when attempting to promote overall sustainability.

It is believed that forest-based resources and related businesses are set to play a key role in the transition from our current fossil-based economy towards a more sustainable circular bioeconomy, in particular in forest-rich countries (e.g., Austrian Federal Ministry for Sustainability and Tourism et al., 2019; Ministry of Agriculture and Forestry, Finland, 2023; Regeringskansliet, 2022; Staffas et al., 2013). New, innovative products based on industry side streams, the cascading use of wood, and higher added value have been highlighted in several public and private policies (e.g., European Commission, 2018). The European Commission, for example, has published several strategy papers on numerous sustainability-related objectives, for example, the European Green Deal (European Commission, 2019a). The European Green Deal aims at intensifying the European Union's (EU's) climate ambitions for 2030 and 2050 and at mobilizing industry in order to achieve a cleaner and more circular economy. Other related EU strategies address issues such as bioeconomy (European Commission, 2018), carbon economy (European Commission, 2021a), and the development of biorefineries (European Commission, 2021b). Biorefining, as stated in the IEA Bioenergy Task 42 (De Jong et al., 2011), is commonly defined as the "*sustainable processing of biomass into a spectrum of marketable products (food, feed, materials, chemicals) and energy (fuels, power, heat)*" (De Jong et al., 2011, p. 10; for further definitions, see also Berntsson et al., 2014, p. 19). The bioeconomy strategy (European Commission, 2018) aims at increasing resource efficiency, circularity, and value creation, and places particular emphasis on the importance of biorefineries in using wastes or residues.

However, developing novel products is rarely possible unless a collaborative effort is made by companies with other firms and societal actors, such as citizens, non-governmental organizations (NGOs), and governments (Jonker & Faber, 2019; Pedersen et al., 2021; Planko & Cramer, 2021). The importance of establishing shared value creation, inter-organizational networks, and collaborative business models in the development and diffusion of new products in rapidly changing business environments has been highlighted by numerous studies, in particular by sustainability-focused business model, value creation, and network management studies (e.g., Aarikka-Stenroos et al., 2014; DiVito et al., 2021; Evans et al., 2017; Freudenreich et al., 2020; Hörisch et al., 2014; Jonker & Faber, 2019; Melander & Wallström, 2022; Möller & Svahn, 2009). In addition, open innovation approaches, based on the idea that collaboration and the sharing of knowledge among diverse stakeholders is advantageous for all actors involved (Chesbrough, 2003), have been found to support shared value creation and the promotion of sustainability (Camilleri et al., 2023, see also Del Rıo et al., 2015; Melander & Pazirandeh, 2019). Chistov et al. (2021, p. 11) introduce the open eco-innovation concept "*as an umbrella term for all the activities of an organization that strategically utilize access to external resources to potentialize internal eco-innovation development or to commercialize internally developed technologies and intellectual property*." The role of a supportive multi-actor business ecosystem is seen to be particularly important in the case of radical sustainability innovations (Planko et al., 2016). Hence, business management scholars have come to the same conclusion as transition scholars, that is, that the successful (wide-scale) innovation diffusion of sustainability technologies requires the aligned and collective effort of multiple societal actors. Planko et al. (2016) point out that transition scholars call this collaborative process between firms and their stakeholders as "collective system building" and further define collective system building as the "*processes and activities that firms can conduct in networks to collectively create a favorable environment for their innovative sustainability technology*" (Planko et al., 2016, p. 2329).

Despite the recognition of the significance of forest-based businesses and related new products in a circular bioeconomy, the unsustainable use of forest resources and lack of forest protection remain key challenges from the perspective of many societal actors (Edwards et al., 2022; Nousiainen & Mola-Yudego, 2022). In addition, transparent and science-based information—especially in the case of novel forest products—is often lacking. For stakeholders such as companies, suppliers, customers, civil society, NGOs, and politicians, such information is not only essential to informed discussion and decision-making but also serves to facilitate constructive societal discourse and the generation of shared objectives (i.e., "joint purposes") in the value creation process (Breuer & Lüdeke-Freund, 2017; Freudenreich et al., 2020). Conflicts and uncertainties often result from inadequate information, leading to the creation of a challenging operational environment both for the businesses and their stakeholders. Näyhä (2019, 2020) concluded that creating a shared understanding among the different actors was one of the key issues in promoting transition in the Finnish forest-based sector.

1.2 | Biorefining of wood-based lignin

A major material under consideration in biorefining is forest-based kraft lignin (e.g., for lightweight materials and phenol-based aromatic chemicals; European Commission, 2019b). An estimated 40–50 million tonnes of such lignin are produced globally per year (e.g., Cline & Smith, 2017). Currently, it is largely burnt on-site in pulp mills for the recovery of process chemicals and in order to gain energy (e.g., Cline & Smith, 2017). However, a surplus amount is also said to be available, and it is this which could be used to generate value-added products, while maintaining the energy supply needed on-site in the pulp mill (Dessbesell et al., 2018b; Holladay et al., 2007). The kraft lignin is, due to its availability and chemical structure, considered to be a promising bio-based compound and is expected to play a major role in biorefinery development (e.g., Ragauskas et al., 2014). Its potential for replacing fossil-based substances and its use in the development of a wide variety of non-energy products are currently under investigation (e.g., Isikgor & Becer, 2015; Ragauskas et al., 2014). Hence, among the top 20 bio-based product innovations (European Commission, 2019b), six are based on lignin as their main feedstock (i.e., plant-fiber reinforced lignin bio-composites, high-purity lignin, lignin-based carbon nanofibers, lignin bio-oil, lignin-based phenolic resins, and bio-BTX aromatics).

The industries affected by such developments, such as the forest or chemical industry, are usually science driven and path dependent (i.e., the new technologies build upon the previous ones), and innovations are usually based on technology-focused research and development (R&D) projects, rather than on consumer markets or consumer trends (e.g., Bröring et al., 2006; Hansen, 2010). Accordingly, in the biorefinery area, research at various levels, in particular in the natural sciences and engineering fields, is often driven by the idea of replacing fossil with bio-based resources in order to generate more sustainable products on the markets (e.g., Hurmekoski et al., 2019). In order to guide investment and research activities, this often entails assessment of economic feasibility and of related (mostly environmental) impacts. Such assessment may also be required by funding agencies (e.g., Mahmud et al., 2021; Scown et al., 2021; Thomassen et al., 2019). Common examples here entail optimization/design approaches (Elaradi et al., 2021; Mansoornejad et al., 2010; Murillo-Alvarado et al., 2013; Santibañez-Aguilar et al., 2014), as well as prospective techno-economic approaches (e.g., as reviewed by: Scown et al., 2021; Lo et al., 2021) and life cycle analyses (e.g., as reviewed by Parajuli et al., 2015; Vance et al., 2022). These are usually intended to narrow the scope for potential action (e.g., by means of comparisons with alternatives or by the stipulation of benchmarks) and are applied to rather specific cases. In a similar vein, technical investigations relating to lignin applications (e.g., on chemical, process engineering, and analytical issues) have been the focus of research for many years (e.g., Wenger et al., 2020). The potential macro-scale impacts that may arise during the establishment of biorefineries within the forest-based bioeconomy were investigated by Asada et al. (2020) and Jonsson et al. (2021). In contrast, the level of knowledge concerning the market environment and innovation diffusion of lignin remains rather low, and only relatively few research papers are currently available (Lettner et al., 2020; Wenger et al., 2020). Earlier research papers on the (techno-)economic aspects of kraft lignin innovations (Wenger et al., 2020) tended to focus mainly on the internal (direct) factors influencing the success of commercialization (e.g., improving technology, performance, reducing costs, and optimizing processes), while the external (indirect) factors (e.g., substitute markets, demands, and regulatory issues) were barely taken into account. In general, approaches allowing for (techno-economic) technology evaluation and technology foresight, while simultaneously including a value creation perspective for biorefinery innovations, are largely absent.

1.3 | Research aims and questions

In view of the above, the consideration of intra-organizational techno-economic aspects alone seems insufficient when developing novel forest-based products and thus a wider systemic perspective is called for, one which also takes into account the external innovation environment—including diverse needs, values and goals of the various stakeholders—as well as the potential (sustainability-related) consequences of the innovations once spread. Bennich et al. (2018) stated that as socio-ecological systems are complex and that there is a clear risk of unintended consequences and trade-offs arising in any transition towards a bioeconomy. Several authors have addressed the potential related to the modeling of innovation pathways in improving knowledge creation and communication among various bioeconomy stakeholders, and in enhancing understanding of multi-actor systemic level change processes towards sustainability (e.g., Bennich et al., 2018; Yang et al., 2022). In our study, we take such a systemic approach to knowledge and value creation in novel biorefinery production. Our aim is to model and simulate potential innovation diffusion pathways for lignin-based products using an agent-based approach. By engaging diverse actors and variables from different socio-technical levels, this approach generates information for various stakeholders in lignin biorefining. Thus, the use of a systems approach to integrate both internal and external variables helps creating a more holistic understanding of how the transition to a bioeconomy may be achieved (cf. Bennich et al., 2018; Bauer et al., 2017; Wenger et al., 2020).

The objective of the present paper is therefore to model and simulate potential innovation diffusion pathways for lignin-based products by means of an agent-based approach.

The simulation allows us to address the following research question and sub-questions:

- **What are the conditions needed to encourage the innovation diffusion of kraft lignin as a (partial) replacement for fossil-based feedstock in selected material applications?**

- How is the simulated lignin innovation diffusion process affected by the case-specific conditions (e.g., cost conditions) for high-value (carbon fibers, CFs) and low-value (lignin phenol formaldehyde—LPF—resins) products, and by scenarios involving the supply and pricing of commodities (separated kraft lignin and crude oil-based counterparts)?
- How can policy measures, such as carbon pricing, affect the innovation diffusion patterns?
- What are the potential annual emission savings resulting from the input substitutions by 2030/2050, as derived from selected scenario results?
- How sensitive are the selected parameters and, where there are different diffusion patterns, how do the observed sensitivities vary with respect to parameters (i.e., related to techno-economic versus socio-economic contexts) and to the different cases (i.e., phenol for LPF resins versus CFs)?
- How can the information provided by the simulation promote collaboration and shared value creation among the stakeholders/actors involved?

Overall, the outcomes of the study serve to indicate the potential areas of conflict among the diverse stakeholders involved in the biorefining value network. The study produces knowledge that can facilitate the formulation of a shared understanding among stakeholders and thus help establish the achievement of a commonly shared set of goals with respect to sustainability transition.

2 | THEORETICAL AND CONCEPTUAL BACKGROUND

2.1 | Collaborative efforts for shared value creation

Despite its various historical roots (Wagner Mainardes et al., 2011), the modern development of stakeholder theory and conceptualization was initiated by the work of Freeman (1984). A central tenet of stakeholder theory is that business organizations need to focus on the interests of all stakeholders and not merely on those of shareholders (Freeman, 1984, 2010). A vast stakeholder literature now exists, incorporating quite diverse theoretical developments, views, interpretations, and applications.

Stakeholder theory perspectives have also been applied in the context of sustainability management as well as in sustainable value creation and business model studies (e.g., Freudenreich et al., 2020; Hörisch et al., 2014; Lüdeke-Freund et al., 2020). Sustainable alternatives for traditional value creation and business models aim to solve current sustainability challenges by adapting more holistic perspectives, by considering the needs of various stakeholders, and by developing new collaborative solutions when meeting demands (Hörisch et al., 2014; Pedersen et al., 2021). According to Freudenreich et al. (2020, with reference to Bocken et al., 2013; Lüdeke-Freund & Dembek, 2017; Schaltegger et al., 2015; Stubbs & Cocklin, 2008; Upward & Jones, 2016), sustainable business model literature, in particular, highlights value creation as a process entailing various outcomes for different stakeholders. For Lüdeke-Freund et al. (2020, p.81), the cornerstones of theorizing about sustainable value creation center on the issues of (a) what is value; (b) for whom is it created; (c) how is value created; and (d) who captures the value. The framework thus emphasizes (a) a need for a stakeholder-responsive definition, which in turn necessitates identifying the fundamental needs of stakeholders. It is also essential (b) to consider the respective boundaries of the systems and stakeholder networks as well as to take account diverse levels as well as spatial and temporal aspects. Further, the framework highlights that (c) new value is created in various stakeholder relationships and collaborative value creation processes, whereby the various roles of the stakeholders are taken into account. This means it is important (d) to evaluate value capture from every stakeholder's perspective and to take relevant power relations into account (Lüdeke-Freund et al., 2020). Accordingly, Pedersen et al. (2021) emphasize the importance of cross-sector collaborations as a means of "*providing voice to new stakeholder groups*" (p. 1042) whose views are often neglected in more traditional sustainability approaches. This thus highlights such form of collaboration as a key enabler of transition (see also Rey-García et al., 2021).

In alignment with the key principles of sustainable, cross-sectoral value creation and collaborative business models, network management scholars emphasize a need for supportive ecosystems around new innovations supplementing single company's resources and capabilities. Thus, customers and users, distributors, suppliers, and investors are all needed in performing practical commercialization tasks, facilitating innovation diffusion and in creating new markets (Möller & Svahn, 2009; Sandberg & Aarikka-Stenroos, 2014). Oskam et al. (2020) explored the tensions existing between various actors in innovation ecosystems with sustainability goals. They suggest that when developing a sustainable business model innovation, ecosystems need to engage in a process which they call "valuing value," that is, a process in which the aim is to search for a result that satisfies all participants and thus one which facilitates collaborative processes among cross-sectoral actors. In a similar manner, Breuer and Lüdeke-Freund (2017) emphasize the crucial role of the networks and shared values of the stakeholders involved in the innovation processes and the related management. Further, they argue that values-based innovation networks and business models can help significantly when addressing complex sustainability challenges.

All in all, solving difficult sustainability problems requires collaborative, cross-sectoral effort and resources among stakeholders, and this needs to be guided by shared values and objectives. In practice, however, establishing and managing such networks and finding solutions fulfilling the demands of multiple actors is highly challenging. The present paper attempts to provide an approach aimed at facilitating knowledge exchange and at increasing understanding among the various actors, and thus at mitigating related tensions.

2.2 | Agent-based simulation of bio-based (eco-) innovation diffusion pathways

Traditional models of innovation diffusion are in general often based on the Bass model (Bass, 1969), and tend to focus on aggregate trends and behavior rather than on the decisions and interactions of individuals (e.g., Kiesling et al., 2012; Zhang & Vorobeychik, 2017). However, several relevant aspects, such as actor communications, networks, heterogeneity (as described by Rogers, 1983), and the inclusion of variables helpful for decision-makers (i.e., providing predictive and/or explanatory power in such models), are difficult to capture with such aggregate models (Kiesling et al., 2012; Zhang & Vorobeychik, 2017). Agent-based models (ABMs) represent one possible approach to dealing with such challenges by modeling complex emergent phenomena bottom-up (agents' micro-level interactions) and have therefore gained popularity in innovation diffusion research (e.g., Garcia, 2005; Kiesling et al., 2012; Zhang & Vorobeychik, 2017). In the realm of *eco-innovations*, which can be defined as innovations that (intentionally or unintentionally) "*improve the environmental performance*" (e.g., Carrillo-Hermosilla et al., 2010, p. 1075), technological innovations (including both preventive and curative environmental measures) are a common focus of research. The organizational, social, and institutional innovations, however, have so far received comparably little attention in this context (Rennings, 2000). While these types of innovations are said to be more challenging to coordinate in practice, targeting them in addition to the more commonly considered technological innovations may lead to higher environmental benefits overall (Machiba, 2010). In exploring innovation diffusion phenomena and underlying actor behavior, ABMs can improve explanatory power by incorporating elements from (neo-)institutional economics (e.g., bounded rationality) (e.g., Kiesling et al., 2012; Moncada et al., 2017). Also, ABMs are capable of including both the technical considerations and the social structures relevant in technology innovation diffusion (e.g., Moncada et al., 2017). This contrasts with the comparatively limited explanatory power of innovation diffusion models based on classical economics which depend on relatively restrictive assumptions, for example, on homogeneous actors with complete information (Kiesling et al., 2012; Moncada et al., 2017). In addition, agent-based simulation is considered especially appropriate where communication within a social network is important (Macy & Willer, 2002), and where the diffusion of innovations may be regarded as a communication process for increasing awareness of the innovation (Rogers, 1983). Previous studies have shown that the topology of an underlying network has a significant impact on innovation diffusion (e.g., Bohlmann et al., 2010; Kiesling et al., 2012; Garcia, 2005; commonly used network types in ABMs: Barabási & Albert, 1999; Watts & Strogatz, 1998; Erdös & Rényi, 1961). Conceptual ABMs are seen "*as ideal* learning tools *for scientists to understand a system under a variety of conditions by simulating the interactions among agents*" (Zhang & Vorobeychik, 2017, p. 3), and thus do not always aim at being descriptively accurate and/or predictive (Garcia, 2005). However, owing to problems related to the relative simplicity of agent rules ("toy models") (Garcia & Jager, 2011; Zhang & Vorobeychik, 2017) and to predictive validity (Kiesling et al., 2012; Zhang & Vorobeychik, 2017), empirically grounded ABMs—that is, where empirical data are used for initialization, parametrization, and/or validity evaluation—are increasingly being applied to tackle real-world problems (Kiesling et al., 2012; Zhang & Vorobeychik, 2017). In particular, such empirically grounded ABMs (e.g., Garcia & Jager, 2011) may be used for the purposes of foresight, policy analysis, and decision support (e.g., by enabling a better understanding of how and why innovation diffusion pathways shape up) (e.g., Kiesling et al., 2012). The reviews by Kiesling et al. (2012) and by Zhang and Vorobeychik (2017) summarized several approaches in these areas and elaborated on the challenges and progress regarding model validation, since "*all of them are, at least to some extent, speculative thought experiments until data for validation becomes available*" (Kiesling et al., 2012, p. 219). Nevertheless, it is believed that empirically grounded ABMs are becoming more and more acceptable, both as a research tool (e.g., in the facilitation of theory construction) and as a decision-support tool (e.g., for managerial diagnostics and policy recommendation) (Kiesling et al., 2012).

With respect to innovation diffusion ABMs, to date, the main areas of application for ABMs have been agriculture, transportation, energy, and environmental innovation (Kiesling et al., 2012). There are, for example, agent-based approaches on specific wood markets which, while not explicitly relating to biorefinery operations, do include industrial/pulp wood consumers in some way (e.g., Holm et al., 2018a, 2018b; Kostadinov et al., 2014; Scholz et al., 2020). In the area of biorefineries and related innovation diffusion processes, most research papers deal with the topic of biofuels (e.g., Günther et al., 2011; Moncada et al., 2017; Stummer et al., 2015; van Tol et al., 2021; Yang et al., 2022). As one example, Moncada et al. (2017) placed a particular conceptual focus on institutions, and related this to the conceptual underpinnings of complex adaptive systems theory, (neo-)institutional economics (e.g., bounded rationality), and socio-technical systems, and also investigated import tariffs and international trade flows (Moncada et al., 2017; van Tol et al., 2021). These authors also noted that ABMs, in comparison to optimization approaches, were suitable for addressing socio-economic aspects, such as the relevant behavior of supply chain actors, particularly since the biofuel supply chains' economic performance "*depends on the interaction of technical characteristics (technological path-ways and logistics) and social structures (institutions and actors behavior)*" (Moncada et al., 2017, p. 895). In another paper, Yang et al. (2022) developed a community communication tool for miscanthus-based biofuels, which was based on multiple sources and included a range of actor groups (farmers, industry, community, government, and biofuel consumers). Based on these previous works on (agent-based) innovation diffusion modeling and innovation-related studies in the bio-based area, the present paper has aimed at developing a similar approach using a case study on kraft lignin and derived products (LPF resins and CFs).

3 | MATERIAL AND METHOD

To gain insight into the diffusion process of kraft lignin innovations as a replacement for fossil-based feedstock, we developed an agent-based model. Its main goal is to quantify the success rate of the diffusion (i.e., the amount of kraft lignin traded in the market relative to the theoretical maximum). The model uses various input parameters that can be changed to investigate different scenarios or possible future developments, including the price development of crude oil, the number of kraft lignin producers, and details about the produced good and its substitute.

The main feature of the model is a virtual market on which the agents (i.e., producer and consumer actors) can interact by exchanging goods. Furthermore, goods producers (GPs) need to decide whether they should switch to using kraft lignin instead of the incumbent crude oil-based counterparts. This decision is made using probabilistic decision rules based on potential profit (i.e., economic feasibility is required), willingness to accept risk, and network effects. The model is empirically grounded (see, e.g., Zhang & Vorobeychik, 2017; Kiesling et al., 2012) and is based on previous studies on biorefineries and lignin research and implementation (techno-economics, preceding systematic literature reviews), trade and market data and expert knowledge, as well as on innovation and diffusion theory.

3.1 | Model overview

The main agent groups and decision mechanisms of the Biorefinery Products Innovation Diffusion (BioPID) ABM, are described in the following, taking the example of the innovation diffusion of kraft lignin-containing products, and are illustrated in Figure 1. In brief, the main actor groups (agents) in the BioPID ABM are the commodity producers (kraft lignin or crude oil-based counterpart—i.e., phenol or acrylonitrile), the (potential) processors of the bio-based commodity that can either continue to use the crude oil-based input or adopt the lignin-based input to produce (resins or CFs), and the consumers. The main change factors in the model are (1) the techno-economic potential regarding the bio-based commodity (extracted kraft lignin) producers, (2) the scenarios covering the GPs (based on oil-based commodity price projections, with and without carbon pricing, as well as lignin producer variants with regard to their number, capacity, and pricing strategies), and (3) the demand for bio-based-products (including the willingness-to-pay more/less for these) on the consumer side. The main result of a simulation run is then the amount of kraft lignin traded on the market each year as an indicator of the speed and success of the innovation diffusion process under the circumstances investigated.

Details regarding the behavior and data foundation of the respective agent groups are given in Section 3.2. The simulation mechanism is described thereafter, in Section 3.3. The two case studies included are described in Section 3.4. In Section 3.5., the scenario development is described (including variations in future oil prices and variations in lignin prices, lignin pricing strategies, and the number/capacities of potential lignin producers).

3.2 | Agents

The fundamental characteristics of the four agent groups—the crude oil commodity producer, lignin producers, lignin processors (GPs), and consumers—are described in the following. Further related information and specifications (concerning the model mechanisms, scenarios, and parameter specifications) can be found in the respective sections below.

3.2.1 | Crude oil commodity producer

The main role of the crude oil commodity producer is to satisfy the respective demand on the market, using realistic prices. It was developed on the basis of international trade data (United Nations, 2021), and the corresponding price developments were derived from the

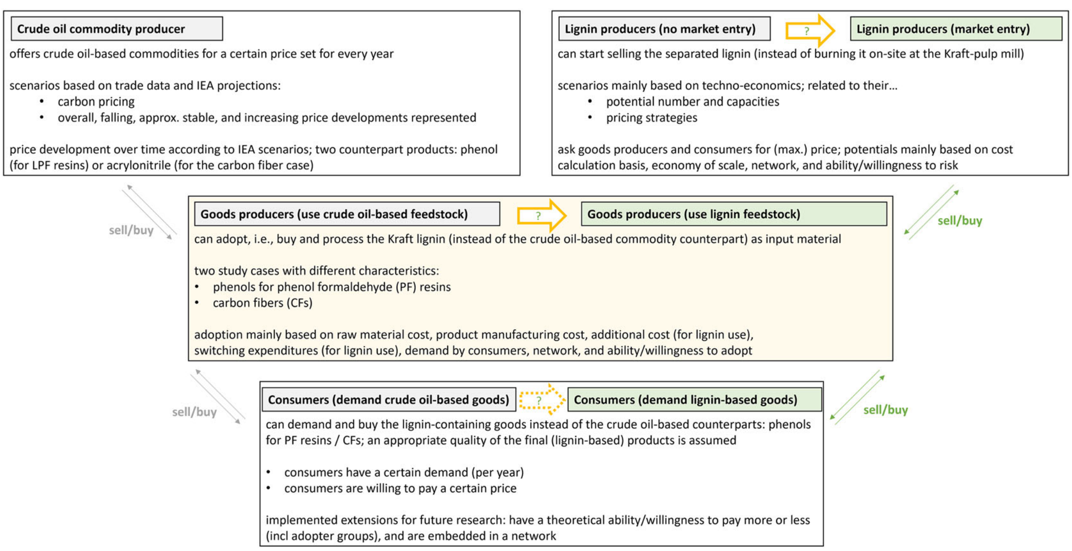

FIGURE 1 Actor groups and main decision-making principles in the BioPID ABM.

crude oil price projections made by the International Energy Agency (International Energy Agency, 2021). These prices serve as a reference for the GPs, who can then choose between the fossil-based and lignin-based raw material. The fossil-based commodity producer agent is used to represent the global prices and price developments of commodities that are potentially replaced by the lignin-based commodities under investigation. Historic prices of the crude oil-based commodities were extracted from the UN Comtrade Database (United Nations, 2021), and the dollar prices were converted to euro prices using the respective annual exchange rates (Deutsche Bundesbank, 2022). The selected commodities are "phenol (hydroxybenzene), salts agent" (code 290711) for the LPF resin case and "nitrile-function compounds: acrylonitrile" (code: 292610) for the CF case, using import data of the EU-28 (reporter) from the world (WLD, partner ISO). The ratios of crude oil price (average closing prices, converted to €/t; MacroTrends.net, 2022; Deutsche Bundesbank, 2022; BP p.l.c., 2021) to commodity prices were calculated for each year, and the average conversion factors (2010–2019) were used for determining the starting commodities' prices in 2021; these factors were 2.31 (standard deviation: 0.18) and 3.36 (standard deviation: 0.52) for phenols and acrylonitrile, respectively.

3.2.2 | Bio-based commodity producers (lignin producers)

The bio-based commodity producers can produce kraft lignin and sell it once they have entered the market. Contrary to the single crude oil commodity producer, embodying the dominant role of global prices and price developments in this market, a larger number of agents were employed in the bio-producer group in order to account for the lignin producers' heterogeneity. In the model, the potential producers of kraft lignin are equipped with respective cost and production capacity structures, are part of a network (pulping industries), and are assigned specific innovation-adoption probabilities. These structures—depending on the respective variants—are based on the relevant scientific literature (techno-economic studies and innovation diffusion) and on International Energy Agency (IEA) crude oil price projections (for opportunity costs). Kraft lignin producers decide on whether to enter the market or not. The main criterion for the decision-making of the raw lignin producers is profitability, and is additionally influenced by their respective *network*, *ability/willingness to bear risk*, and *economies of scale* (*EoS*) (relation of production capacity and costs per unit). Techno-economic assessments (TEAs) have frequently identified the cost of the lignin feedstock as a major, sensitive, input factor (e.g., as reviewed by Wenger et al., 2020). However, its determination is tricky since it is dependent on various considerations, for example, cost allocation procedures in multi-product systems (cf., e.g., Hermansson et al., 2020; Cherubini et al., 2011; Wenger et al., 2022), the basis used for its determination (e.g., the opportunity costs of the energy source replaced, recovery boiler debottlenecking considerations, the market expectations for fossil-based substitute products, investment considerations, capital and operating cost etc.).

3.2.3 | Goods producers (commodity processors)

The GPs buy either kraft lignin or crude oil on the market, and they produce goods for sale. The GPs are the core element of the model: as soon as they change their production process, the innovation is regarded as adopted (whereby we assume that once they have changed, they stay in the bio-based market). The lignin processors can either source the raw lignin or the fossil-derived counterpart. Their decision to (not) adopt the lignin is strongly based on economic feasibility—including *raw material purchasing cost* (of lignin or of the oil-based counterpart), the *switching cost*, in the case of switching to bio-based production (this includes depreciation of capital expenditure—takes account of economy of EoS considerations—and, in a broader sense, also switching costs), the *additional cost*, in the case of switching to bio-based production (e.g., for lignin modification or other regular additional costs), and *production cost of resin/CF* (including *EoS* considerations).

The GPs (processing the lignin) exhibit a specific cost structure regarding their production (depending on EoS), including feedstock and lignin modification costs. As is the case for the kraft lignin producers, they are part of a network (phenol formaldehyde resin or CF production) and are assigned appropriate adoption probabilities. These actors can either follow the status quo and use fossil-based inputs (i.e., phenol or acrylonitrile) or use kraft lignin to produce their products—(lignin) phenol formaldehyde resins or CFs.

The structure of the respective expenditures is now described below. The detailed assumptions employed in the respective cases can be retrieved from Tables 1 and 2. The first cost component is the purchasing cost of the main raw material—either the respective oil-based commodity (phenol, acrylonitrile) or the "raw" separated kraft lignin (solid). The cost for either feedstock is determined by the respective scenarios under investigation. In general, forecasting the costs of technologies is a challenging task, though several approaches exist that improve understanding of the underlying mechanisms and/or improve relevant models and predictions (e.g., Alberth, 2007; Daugaard et al., 2014; Lieberman, 1984). In line with this, the estimation of capital and operating costs for the LPF and CF cases is also associated with major uncertainties, in particular, owing to variations in (plant or cumulated) production capacities, and to the difficulties entailed in taking account of realistic capacity ranges for future biorefineries.

Generally speaking, the cost per unit of production tends to decrease as the (cumulated) production capacity increases. Potential reasons for this include EoS effects and learning/experience effects (Lieberman, 1984; Thomassen et al., 2020). The standard literature commonly takes account of such impacts on cost (both on the plant level and on the cumulated capacity level) by using a power law function $C = C_o(M/M_o)^{\alpha}$, where C and C_o refer to the (base) costs, M and M_o refer to the (base) plant capacity, and α refers to the power law exponent (e.g., Couper et al., 2008). As major uncertainties exist regarding quantification of the exponent for technologies under development, a variety of recommendations can be found in the literature (as applied to biorefinery cases: e.g., Dessbesell et al., 2018b;

TABLE 1 Description of model case parameters (lignin phenol formaldehyde resins).

Lignin-based phenol for formaldehyde resins (TRL 8)		
Parameter	**Initial parameter setting**	**Reference**
Initial fossil product price ("phenol (hydroxybenzene) and its salts") [€/t]	976	United Nations (2021)
Number of goods producer agents	26	Based on Risi Inc. (2016), Mordor Intelligence (2021b), and own assumptions
Formula for capacity-cost-ratio [result in €/t]; capacity range [t/year]	768*(capacity/25,000)^−0.4388 [capacities: 2,700–135,300 t/year phenolic resins]	Based on Khanal et al. (2021) and Risi Inc. (2016)
Amount of lignin used for 100 t of the product (i.e., for the phenol substitute) [t]	111	Dessbesell et al. (2018a), phenol scenario; approx. 50% of the phenol for the resin can be replaced without compromising product quality (European Commission, 2021b; Gong et al., 2022)
Total market (phenols from lignin for resins) [t/year]	1,000,000	Based on Risi Inc. (2016) (note: phenolic share in resin end product estimated at ~15–20%)
Base costs (for lowest capacity) [€/t]	1,000	United Nations (2021) ("amino-resins, phenolic resins, polyurethanes, primary", and "acrylonitrile"), and own assumption (resin production cost minus precursor cost)
Switching expenditures (lowest cap., min.) [€]	3,700,000	Dessbesell et al. (2018a)
Depreciation time [years]	10	Assumption (same as in Otromke, 2018)
Additional costs (basic assumption) [€/t]	540	Based on Dessbesell et al. (2018a) (excluding lignin feedstock and resin preparation); assumption made for low capacity (EoS)

Abbreviation: TRL, technology readiness level.

TABLE 2 Description of model case parameters (carbon fibers).

Lignin-based carbon fibers (TRL 4–6)		
Parameter	**Initial parameter setting**	**Reference**
Initial fossil product price ("acrylonitrile" + preparation costs to PAN precursor) [€/t]	(1,422 * 2) + 3,000	Based on United Nations (2021) ("acrylonitrile"), Baker and Rials (2013), European Commission (2021b), and own assumptions (preparation of PAN from AN)
Number of goods producer agents	12	Based on Risi Inc. (2016), Mordor Intelligence (2021a), and own assumptions
Formula for capacity-cost-ratio [result in €/t]; capacity range [t/year]	13,840*(capacity/120)^-0.166 [capacities: 100–10,000 t/year CF]	Based on Ellringmann et al. (2016), Groetsch et al. (2021), and Risi Inc. (2016)
Amount of lignin used for 100 t of the product (i.e., for CF) [t]	250	Baker and Rials (2013); Souto et al. (2018) (yield ~40–45%)
Total market (CF from lignin) [t/year]	20,000	Based on Risi Inc. (2016) (CF from lignin)
Base costs (for lowest capacity) [€/t]	6,000	Based on Ellringmann et al. (2016) (adjusted to lower-cost CF; CF production cost minus base PAN precursor cost is ~50% of CF cost)
Switching expenditures (lowest cap., min.) [€]	1,169,795	Based on Otromke et al. (2019) and calculated to resp. capacities
Depreciation time [years]	10	Otromke (2018)
Additional costs (basic assumption) [€/t]	1,458	Lignin precursor preparation costs based on Otromke (2018) (excluding lignin feedstock and by-product credits); assumption made for low capacity (EoS); further processing costs to final CF assumed to be alike

Abbreviations: CF, carbon fiber; TRL, technology readiness level.

Farag & Chaouki, 2015). For the operational costs of phenol-formaldehyde resins and CFs, our cost-estimation approach was simplified such that cases (with different capacities) were taken from the relevant literature (PF: Khanal et al., 2021; CF: Ellringmann et al., 2016, and Groetsch et al., 2021) and the respective exponents (α) were calculated on the basis of these cases (excluding the feedstock cost) in order to estimate current EoS for the production processes. The resulting values were in reasonable agreement with publicly available market data and were therefore found to be realistic approximations for current cost-to-capacity ratios. Assumptions regarding the potential capacity ranges for lignin-derived products (LPF, CF) were derived from related TEAs and from the lignin report by Risi Inc. (2016) (see detailed descriptions and tables in Section 3.4). Only in the case of lignin purchase was an additional cost included in order to account for the additional costs required, in particular, for raw lignin modification, and for other regular costs that may be indicated on a per tonne basis. Additional costs were derived from TEAs. However, owing to the major uncertainties still present, several variations were tested and sensitivity analyses were carried out. The capital investment necessary to switch to lignin-based goods production was calculated on the basis of TEAs. For the capital investment, exponents of 0.8–0.6 are commonly assumed in the TEA literature (Couper et al., 2008); the so-called "six-tenth-rule" is applied in the present study, and the formula applied is given by *(investment based on TEA* [capacity*capacity based on TEA]$^{0.6}$/switching time/capacity).*

3.2.4 | Goods consumers

The goods consumers are the buyers of the products (resins and/or CFs). They exhibit a certain demand for a final product per year and they are—in the base simulation runs carried out in this paper—willing to pay an equal or lower price for the alternative bio-based goods. Theoretically, for further extension of the model, they can also be willing to pay more (or less, e.g., because of inferior product quality) for the bio-based alternative (cf., e.g., Ruf et al., 2022; Zwicker et al., 2023), they can be assigned a certain adoption probability, and they are embedded in a network (consumers network). As current empirical findings on the *willingness to pay* for bio-based products (usually expressed as a percentage of the alternative fossil-based product price) are quite contradictory (Ruf et al., 2022), the *willingness-to-pay* parameter implemented in the present model is set to zero in the scenarios described.

3.3 | Simulation mechanism

The basic mechanism of the model may now be described as follows. The bio-based commodity producers (kraft lignin producers) check with the GPs and with the goods consumers, what they would be willing to pay for the lignin. Regarding the GPs, this entails ascertaining whether their cost of goods production (i.e., of CF or resins) would be equal or lower when switching to lignin; for the consumers, the kraft lignin producers must ascertain their willingness to pay more for the bio-based variant. If this is not zero, then this price level is taken as the upper cost limit. Assuming these conditions are acceptable for the kraft lignin producer and depending on individual switching probabilities (which result from both the network and the risk affinity of the assigned adopter group), this agent may then produce the lignin at the end of the time step. In the subsequent time step, the kraft lignin producer offers this lignin on the market. The consumers can then decide whether or not they want to order the lignin-containing product from the GP. This decision depends on things such as the good's price and willingness to pay. Following this, and in a similar fashion, GPs have to decide whether or not to switch to using the bio-based lignin. Assuming the latter is found to be acceptable (this depends on lignin availability, ascertained profitability of bio-based goods production, and individual switching probabilities which result from both the network and the risk affinity of the assigned adopter group), the GPs start producing the product—that is, CF or phenol formaldehyde resin—at the end of this time step. This product is then bought in the subsequent time step by the consumer. Once a GP has switched production to bio-based feedstock use, we assume that this process will not be reversed (e.g., owing to contractual obligations, investments made etc.).

Computationally, a simulation run is implemented as follows: To initialize the model, the following agents are generated: a single crude oil producer, the kraft lignin producers, the GPs, and the goods consumers. Agents within the same agent group are connected in a network. In the present study, we use a small-world network (Watts & Strogatz, 1998). This is commonly applied in innovation diffusion research owing to its similarities with real-world social networks (e.g., Bohlmann et al., 2010; Kiesling et al., 2012), and to the fact that it shows "*properties of both random graphs (small diameters) and regular lattices (high degree of clustering)*" (Bohlmann et al., 2010, p. 747). Note, that the proximity of two agents need not be spatial in nature. For example, proximity may exist in terms of joint research projects, existing collaborations, or even competition.

Once the agents are set up, the simulation begins in discrete time steps. Here, the resolution chosen is 1 year. During each time step, the different agent types perform different actions. The crude oil producer produces and sells oil to all GPs who demand it. Since this producer represents the global oil market, it is modeled as a single agent with infinite capacity and the price is given by the respective oil price projections (International Energy Agency, 2021). Lignin producers exhibit similar behavior. Based on their ability/willingness to bear risk, they may enter the lignin market and sell lignin to GPs. In contrast to the oil producer, the capacity of lignin producers is finite and their prices are not uniform. Of all agents modeled, the GPs (i.e., the lignin processors) exhibit the most complex behavior. They first undertake a feasibility analysis in order to compare their cost of production using the crude oil-based commodity to the cost of production using lignin. Since base costs are the same in both variants, the relevant comparison is $P_{oil} > (P_{lig} + C_{add}) * A_{lig} + C_{swi}$.

This shows the price of oil P_{oil}, the price of kraft lignin P_{lig}, the additional cost C_{add}, the relative amount of lignin needed when compared to oil A_{lig}, and the cost of switching the production to bio-based materials C_{swi}. If the feasibility check reveals that switching to lignin is profitable, the GPs check the market in order to verify that enough lignin is available to satisfy their demand. Two factors influence the probability of adoption in the BioPID ABM. The first is related to the ability/willingness of an individual potential adopter and represents a proxy for various internally based pre-conditions (i.e., an umbrella term for individual and internal factors, such as the presence of existing patents), which given the context of the present paper, we have based on Rogers (1983, 2002). Hence, the agents were divided into five categories: *innovators* (2.5%), *early adopters* (13.5%), *early majority* (34%), *late majority* (34%), and, finally, *laggards* (16%) (Rogers, 1983). These adopter groups can be regarded as "ideal types", that is, a conceptual formulation of five categories from a continuous innovativeness variable (Rogers, 1983). To define a base chance of adoption per year, we used these five categories and their respective distribution. The initial base chances of adoption (i.e., the respective probabilities) for the various categories were set as follows: innovators: 25%, early adopters: 16%, early majority: 9%, late majority: 4%, and laggards: 1%. These figures are used to represent the likelihood that producers begin with lignin production, the likelihood that GPs buy and use the lignin in their production, and the likelihood that consumers are willing to pay more for the lignin-containing product (in cases where the respective parameter is set to >0).

In addition to this rather internal, adopter-related parameter, the second factor influencing the possibility of adoption is network effects, that is, those items representing the organization's external innovation environment (e.g., engaging in research collaboration). Where network neighbors have already adopted the new technology, the base chance is multiplied by ($1 + [n/10]$), with n being the number of neighbors that have already adopted. This means, for example, that for an early adopter with five network neighbors already using the innovation, its own probability of adoption rises from 16% to 24%.

Once a GP switches to lignin-based production, it buys lignin from lignin producers instead of buying the crude oil-based commodity from the oil producer. In every time step, the amount of lignin traded provides a quantitative measure of how well the innovation is diffusing throughout the system. The specific cases investigated are described in detail in the following sections.

3.4 | Biorefinery study cases

The respective product cases (lignin phenol formaldehyde resins, lignin-based CFs) are now described below. In both cases, there is one supplier for the respective fossil-based counterpart, and 100 consumers among which the total demand (phenol for LFP resins or CFs, depending on the case) is evenly allocated. The number of repetitions was 200 for the main results and 50 for the sensitivity analysis results. At the end of the section, the approach taken to estimate the potential emissions savings resulting from the corresponding substitutions is then briefly presented.

3.4.1 | Phenolic resins from lignin

The use of kraft lignin for phenol-formaldehyde resins (LPF resins) has been dealt with extensively in several research papers (e.g., Donmez Cavdar et al., 2008; El Mansouri et al., 2011; Kouisni et al., 2011; Tejado et al., 2007) and policy documents (European Commission, 2019b, 2021b). The issues covered have included the barriers and drivers commonly faced with respect to commercialization (European Commission, 2019b; Lettner et al., 2020; Stern et al., 2012) and issues relating to process-specific techno-economics (e.g., Bangalore Ashok et al., 2018; Dessbesell et al., 2018a; Khanal et al., 2021). The technology readiness level (TRL) of phenolic resins from lignin is estimated to be 8 (European Commission, 2021b). Compared to the TRLs for other innovative material applications of kraft lignin, this is relatively high. The LPF resins are intended, for example, for application in engineered wood products such as particle boards (European actors in that field are UPM-Biofore, Prefere Resins, StoraEnso, VTT, and Avalon Industries) (European Commission, 2021b). The relevant model assumptions are given in Table 1.

3.4.2 | Carbon fibers from lignin

In the production of current CFs, the cost of the precursor is considered to be the decisive factor (as it accounts for an estimated 51% of the total costs) (Baker & Rials, 2013). The most widely used precursor is crude oil-based acrylonitrile (polymerized to polyacrylonitrile, PAN). Other common precursors are cellulosic (e.g., Rayon) or pitch based (Souto et al., 2018). This leads to variations in CF properties, depending on the feedstock and processes employed (Souto et al., 2018). Extensive research has also been carried out on the preparation and properties of lignin-based CF in different applications and on the related barriers and drivers (e.g., Baker & Rials, 2013; Choi et al., 2019; Qu et al., 2021; Souto et al., 2018). Lignin-based CF applications are commonly discussed in the context of the automotive industry. The aim here is to reduce product cost and weight with a view to lowering fuel consumption and emissions (Baker & Rials, 2013; Mainka et al., 2015; Souto et al., 2018). The estimated technology readiness level for such lignin-based applications is 4–6 (European Commission, 2021b). In choosing from the rather wide price ranges for PAN precursors, as indicated in various sources (e.g., Choi et al., 2019; European Commission, 2021b; Souto et al., 2018), we assumed relatively low reference prices due to the estimated lower quality of lignin precursors compared to PAN precursors. Since no techno-economic estimations were available on the further processing steps of the lignin precursor to the CF (i.e., melt spinning, thermal stabilization, and carbonization), it was assumed that such steps were comparable to PAN-based CF. The relevant model assumptions are given in Table 2.

3.4.3 | Estimation of potential emission savings

To monitor the potential emission savings arising from the material substitutions investigated in the case studies, an estimate was made of the environmental impact resulting from replacing fossil-based feedstocks by lignin-based feedstocks. For this purpose, we conducted an environmental impact analysis (carbon footprint) and used an attributional approach (Hauschild et al., 2018). We simplified the analysis by assuming that the extraction of lignin and/or reduced production of phenols and acrylonitrile has no consequences on other parts of the economy. Furthermore, the effects on the internal material and energy balances of kraft pulp mills arising from lignin extraction are ignored. The total emission savings for each scenario are calculated by subtracting the avoided burden of the production of phenols or acrylonitrile from the impact of lignin extraction in kraft pulp mills.

The environmental impacts are based on the Ecoinvent database (Wernet et al., 2016) and were calculated for the production of phenol (RER, market for phenol) and for the production of acrylonitrile (GLO, market for acrylonitrile). Data for the extraction of kraft lignin was derived from Culbertson et al. (2016). The resource extraction and production phase are taken account of in the analysis. The global warming potential indicator (GWP; IPCC, 2013) was used for the life cycle impact analysis in the present study. As a functional unit, 1 kg of kraft lignin has been chosen.

3.5 | Scenario development

The model is used to investigate and compare the diffusion processes arising in different scenarios. Several authors have recommended that, concerning innovation in the forestry sector, greater emphasis be placed in the pulp and paper industry on developing an innovation-friendly culture, on cooperation and collaboration, and on targeting market and customer needs (e.g., Hansen, 2010; Leavengood & Bull, 2013; Näyhä & Pesonen, 2014). To date, however, innovation in this industry—which is considered to be relatively capital intensive and risk averse—tends to be rather incremental and production-oriented, with cost-reduction and/or quality improvement playing major roles (e.g., Hansen, 2010; Leavengood & Bull, 2013; Näyhä & Pesonen, 2014). The model scenarios were therefore designed in such a way that price developments (fossil-based and bio-based), pricing strategies, techno-economic considerations (bio-based), and production capacities (bio-based) play major roles. The scenarios developed are designed to reflect different possible combinations of (1) future oil prices and (2) lignin pricing strategies, including variations in number/capacities of potential lignin producers.

3.5.1 | Fossil-based commodity prices

With respect to the oil price, we investigated variants based on projected oil price developments as well as variants that additionally include carbon pricing.

Different potential commodity price developments based on oil price projections are considered. For this, prices in the model develop annually until 2050 in accordance with the four crude oil price development projections published by the IEA, each with or without carbon pricing (International Energy Agency, 2021). As oil commodity prices correlate with oil prices (illustrated in Figure 2), the IEA oil price projections (International Energy Agency, 2021: price scenarios, page 101, Table 2.2) were taken as reference in order to model commodity prices. The IEA projections are related to four "scenarios," that is, *Net Zero Emissions by 2050 (NZ)*, *Sustainable Development (SD)*, *Announced Pledges (AP)*, and *Stated Policies (SP)*, for all of which crude oil price levels were indicated for 2030 and 2050, respectively. The stated prices were converted to €/t (exchange rate of 2021; Deutsche Bundesbank, 2022; BP p.l.c., 2021) and, for the sake of simplicity, it was assumed that the annual model prices always developed linearly across the given projections, starting from 2021. The resulting changes in prices (€/t) were then transferred to the commodity cases.

The *NZ* and *AP* scenarios were then subject to further investigation. The former represents the scenario with the strongest price decrease, and the latter the scenario with approximately stable prices (AP).

To take account of carbon pricing, we used the IEA CO_2 price projections for the years 2030, 2040, and 2050 (International Energy Agency, 2021: projections for European Union (SP), Advanced economies with net zero pledges (AP, SD), and Advanced economies (NZ), page 329, Table B2), starting from 0 €/t in 2021 and then with prices always developing linearly across the given projections. For the fossil carbon pricing, the CO_2 emissions per commodity tonne were calculated in a simplified fashion using the chemical formulas of the commodities (phenol C_6H_6O, [poly-]acrylonitrile C_3H_3N) and then calculating the carbon content per tonne of commodity (phenol 76.6% m/m, [poly-]acrylonitrile 67.9245% m/m). Here, it was assumed that one molecule of CO_2 would be formed from one molecule of carbon (resulting in 2.81 t CO_2 from 1 t phenol and 2.49 t CO_2 from 1 t [poly-]acrylonitrile).

The price developments of the commodities for the model runs (eight projections—i.e., four with, and four without, carbon pricing) are illustrated in Figure 2. For further investigation, the AP scenario with carbon pricing (*AP* + *CT*) was chosen, representing the scenario with the strongest price increase.

3.5.2 | Structure of kraft lignin producers (pricing strategy and potential capacity)

The variations developed for the kraft lignin producers (with variations in number of producers, capacities, and pricing strategies for separated lignin) are based on (1) kraft lignin production costs derived from TEAs, (2) a kraft lignin price as commonly assumed in the literature (see, e.g., Gosselink, 2011; Hodásová et al., 2015; Gabriel et al., 2017), whereby we assume the latter to be based primarily on basic separation expenditures and opportunity costs, and (3) minor-change assumptions, with only few producers present in the market taken as a reference.

For analyzing the lignin producer configurations, which are based on TEAs (variant), EoS were derived from 42 published TEAs (see also Krassnitzer et al., 2023), dealing either with obtaining lignin from black liquor by acid precipitation or by membrane filtration (Arkell et al., 2014; Axelsson et al., 2006; Benali et al., 2014; Culbertson

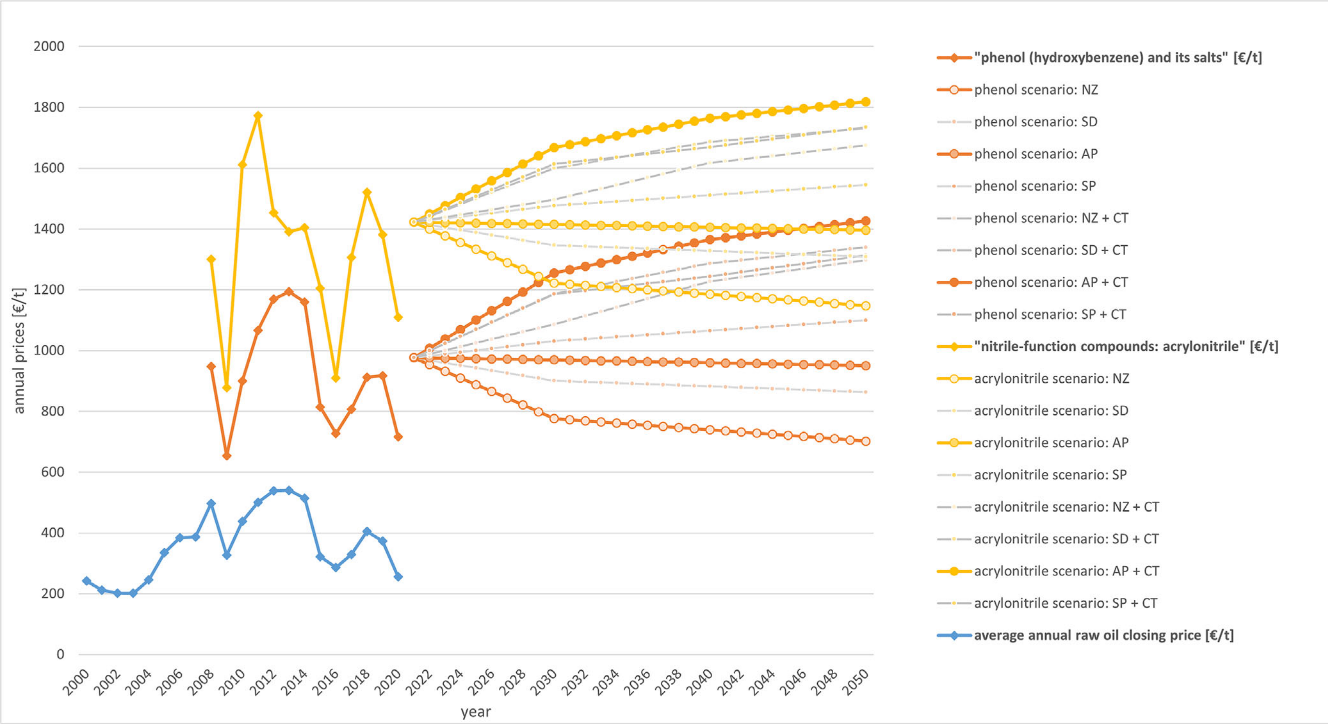

FIGURE 2 Historic prices of crude oil, phenol, and acrylonitrile [€/t] (United Nations, 2021); price assumptions [€/t] from 2021 to 2050 derived from IEA scenarios (NZ, SD, AP, SP) with and without carbon pricing (CT) scenarios included (International Energy Agency, 2021). AP, announced pledges; IEA, International Energy Agency; NZ, net zero emissions by 2050; SD, sustainable development; SP, stated policies.

et al., 2016; Davy et al., 1994; Dieste et al., 2016; Holmqvist et al., 2005; Jönsson et al., 2008; Jönsson & Wallberg, 2009; Kannangara et al., 2012; Laaksometsä et al., 2009; Lindorfer et al., 2019; Loutfi et al., 1991; McKeough et al., 2014; Olsson et al., 2006; Tomani, 2010; Uloth & Wearing, 1989). For detailed numbers, see Table A1. These 42 cases are modeled as respective agents in the model. The structure of the lignin producers as illustrated in Figure 3 represents the scenario *TEA*. The kraft lignin price (which equals the cost of production in this scenario) is on average 252 €/t in this lignin producer variant, and the average capacity is 44,853 t/year (in total, approximately 1.9 million tonnes per year).

In the variations where the lignin producer configuration is based on lignin market price expectations (***PEX and PEXx*** variants), there are also 42 potential kraft lignin producers and the lignin production capacities as in the TEA variant, but the cost of lignin production (in our model this is also the selling price) is (initially) set to 300 €/t, which represents a price per tonne of kraft lignin commonly assumed in the literature (e.g., Gosselink, 2011; Hodásová et al., 2015; Gabriel et al., 2017). Price estimations of lignin in the literature are often based on lignin type and grade, and usually start at approximately 50 €/t (estimated fuel value, where the basis for comparison is often the price per energy unit of natural gas) and may reach 750 €/t and more, also depending on purification costs etc. (Gosselink, 2011). We assume in the *PEX* variant, that a market exists at a stable price of 300 €/t for basic quality kraft lignin, and that this can be sold to processors for further modification. In *PEXx*, we start with 300 €/t for kraft lignin, with the price changing in accordance with changes in crude oil prices (described in the following section). It is assumed that besides being based on basic preparation costs (separation, drying etc.), this price is also based on opportunity costs related to alternative oil-based products. The lignin producer variants capture 42 potential lignin producers and are thus believed to be reasonably representative of a potential European-level kraft lignin market.

Given the currently rather low innovation diffusion level of kraft lignin (with only four major suppliers in Europe and America) (e.g., Dessbesell et al., 2020), the variants with 42 potential lignin producers are quite optimistic. Therefore, in order to establish a fairly realistic point of reference, we analyzed lignin producer configurations based on only minor changes of the status quo (***MC*** and ***MCx*** variants). Here, a total of four potential kraft lignin produces is considered with a total capacity of 107, 000 t of kraft lignin per year. Similar to *PEX* and *PEXx*, there is an *MC* variant with a stable price of 300 €/t lignin, and an additional *MCx* variant with kraft lignin prices following crude oil prices. These minor change variants, in terms of producer capacities and pricing characteristics, more closely resemble the potential for kraft lignin production in Austria. In order for innovation diffusion to occur in the simulation, the willingness/ability to bear risk was set as described in Section 3.3. This setting is likely to be more optimistic than that found in the status quo.

For each of the two study cases, 40 combinations were initially simulated. These resulted from the eight fossil-based commodity price variants and from the five variants for lignin pricing/capacity. After an

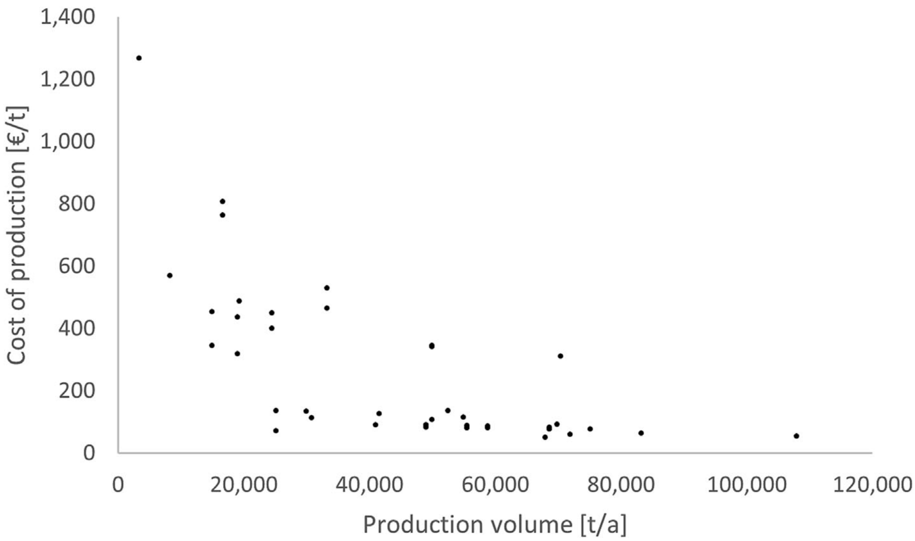

FIGURE 3 Production costs and volumes (economies of scale) of black liquor-derived kraft lignin production (calculated from techno-economic assessments on lignin separation; Krassnitzer et al., 2023; see also Table A1).

TABLE 3 Screened and selected commodity producer scenarios (green check marks: considered in detail; yellow check marks: considered for discussion).

Fos. / Lig.	NZ 1	SD 2	AP 3	SP 4	NZ+CT 5	SD+CT 6	AP+CT 7	SP+CT 8
MC	☑ (yellow)	☐	☑ (green)	☐	☐	☐	☑ (yellow)	☐
MCx	☑ (yellow)	☐	☑ (yellow)	☐	☐	☐	☑ (yellow)	☐
PEX	☑ (yellow)	☐	☑ (green)	☐	☐	☐	☑ (green)	☐
PEXx	☑ (yellow)	☐	☑ (yellow)	☐	☐	☐	☑ (yellow)	☐
TEA	☑ (yellow)	☐	☑ (yellow)	☐	☐	☐	☑ (green)	☐

Abbreviations: AP, announced pledges (oil price projection variant); CT, carbon pricing; Fos., oil price projections; Lig., lignin producer variants; MC, stable lignin producer variant "minor change"; MCx, lignin producer variant "minor change" with lignin price development following the oil price development; NZ, net zero emissions by 2050 (oil price projection variant); PEX, stable lignin producer variant "price expectation"; PEXx, lignin producer variant "price expectation" with lignin price development following the oil price development; SD, sustainable development (oil price projection variant); SP, stated policies (oil price projection variant); TEA, stable lignin producer variant based on techno-economic assessments.

initial screening of the results, the most significant scenarios were picked out for purposes of comparison and for ascertaining the major findings of the whole study (see Table 3).

4 | RESULTS

In this section, the major results of the simulations are illustrated and described, starting with the selection of scenarios, minor-change scenario (MC3), lignin upscaling scenarios (PEX3 and PEX7), and individual lignin pricing scenario (TEA7), then moving on to the potential emission savings that result from substituting the respective bio-feedstocks for oil-based inputs.

4.1 | Scenario selection

In order to highlight the key results and findings of the model runs, the four scenarios with a green check mark, shown in Table 3, are dealt with in detail in the following sections. Scenario MC3, being closest to the current status quo, was selected as a reference scenario, and TEA7 was chosen because it showed the most stable patterns of innovation diffusion; PEX3 (representing a larger number of potential producers) was selected as a counterpart mainly to MC3, and PEX7 (representing a different pricing scheme of the potential lignin producers) was chosen as a counterpart mainly to TEA7. The other selected scenarios (see yellow check marks in Table 3) were chosen to cover as wide a range as possible of the fossil-based commodity price developments and all respective lignin producer scenarios (i.e., covering number of potential adopters, their capacities, and pricing strategies). While the four main scenarios are considered in detail in the following sections, the other 11 scenarios are mainly used to illustrate the possible consequences of further variations in fossil-based and commodity-based price developments (the associated plots for those can be found in Appendix A).

Figure 4 provides an example of basic monitoring of a single model run, including the adopted kraft lignin and the crude oil commodity replaced over time, the respective adoption feasibilities, and behavior of (lignin and goods) producers, as well as the average cost comparison procedure of actors during the decision process.

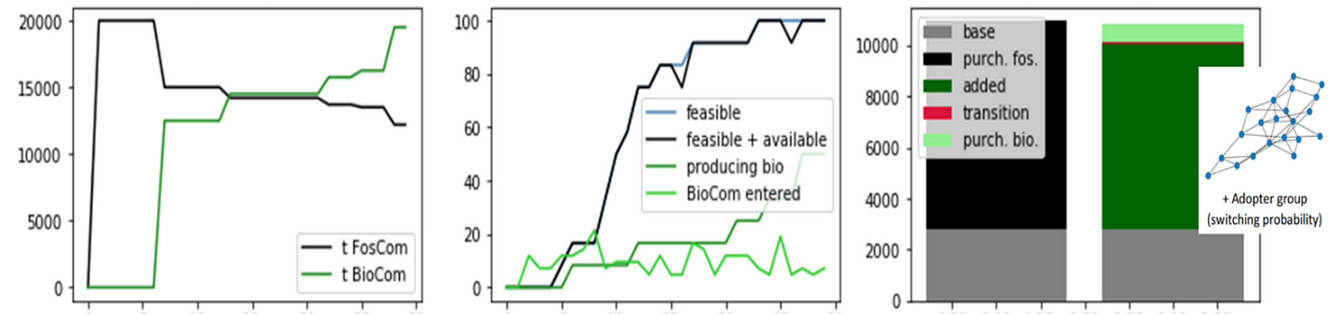

FIGURE 4 Example of monitoring a single model run (carbon fiber case with 1,458 €/t additional costs); (left) adopted kraft lignin (t) over time; (middle) lignin commodity producers entered the market, and goods producers switch to bio-based production (with the number of potential innovation adopters expressed as a percentage of the respective agent group); and (right) average cost comparison procedure of actors during the decision process.

TABLE 4 Adopted tonnes of kraft lignin and crude oil-based commodities replaced in 2030/2040/2050 for the phenol-for-LPF resins and carbon fiber cases in selected scenarios (MC3, PEX3, PEX7, and TEA7).

Product	Scenario	Add. cost (€/t)	Lignin used 2030 (t)	Lignin used 2040 (t)	Lignin used 2050 (t)	FosCom repl. 2030 (t)	FosCom repl. 2040 (t)	FosCom repl. 2050 (t)
Phenols for LPF-resins	**rMC3**	540	19,730	41,625	53,141	2%	4%	5%
	rPEX3	540	338,692	606,678	746,313	31%	55%	67%
	rPEX7	540	330,139	600,436	740,740	30%	54%	67%
	rTEA7	540	330,203	595,321	733,730	30%	54%	66%
CF	**cMC3**	1,458	8,110	17,399	23,425	16%	35%	47%
	cPEX3	1,458	19,573	30,493	36,628	39%	61%	73%
	cPEX7	1,458	19,141	30,756	37,078	38%	62%	74%
	cTEA7	1458	17,424	29,054	36,073	35%	58%	72%

Abbreviations: CF, carbon fiber; LPF, lignin phenol formaldehyde.

4.2 | Minor-change scenario (MC3)

The assumptions of the MC3 reflect a situation close to the current one whereby technical lignin is used as a feedstock. This means, the scenario assumes a small number of potential providers (four) who would offer lignin after taking account of (mainly) the opportunity costs, that is, accounting for the basic lignin separation costs and not using it as a fuel. Furthermore, in order to allow innovation diffusion to be observed, it is assumed that certain structures also exist within the innovation environment (e.g., in terms of innovativeness and investment opportunity) that would favor the adoption of the innovation. Simulation runs indicate that, under these conditions, diffusion occurs slowly and only reaches a relatively limited market share in both application fields. In total, the use of lignin in this scenario remains clearly below the technical potential. Here, diffusion in CF applications is more dynamic, while phenols for LPF resin application require the use of a larger total amount of lignin. As shown in Table 4 and in Figure 5, lignin would replace up to 47% (by mass) of the fossil-based counterpart (acrylonitrile) in the assumed lignin CF market by 2050, but only up to 5% of the phenol in the potential, lignin-containing, phenolic resin market. In total numbers, given the respective assumptions, about 9,000 t/year of CFs would be produced in this scenario, and assuming a total share of 15–20% (by mass) phenols in the final LPF resins, this would mean that approximately 200,000–300,000 t/year of resins would contain a share of lignin-derived phenolics. The higher relative market penetration in the case of CFs reflects the different market structure prevailing, for example, with smaller total capacity, a different GP structure, and higher estimated value added. As a consequence, innovation diffusion in this field of application is also less influenced by increasing additional processing costs (see Table A2). In contrast, the amount of lignin needed to cover 5% of the phenolics in the resin market is likely to be almost twice that needed to reach 47% of the CF market. Regarding the lignin producers, on average, two lignin producers are sufficient to satisfy respective lignin demands, while due to the different market structure in the phenol and CF cases, about three and eight GPs, respectively, would enter the market. The simulation indicates that the rate of innovation diffusion in both application fields is lower in the period 2040 to 2050 than in 2030 to 2040.

These results of the MC3 are used as a reference for interpreting other scenario results.

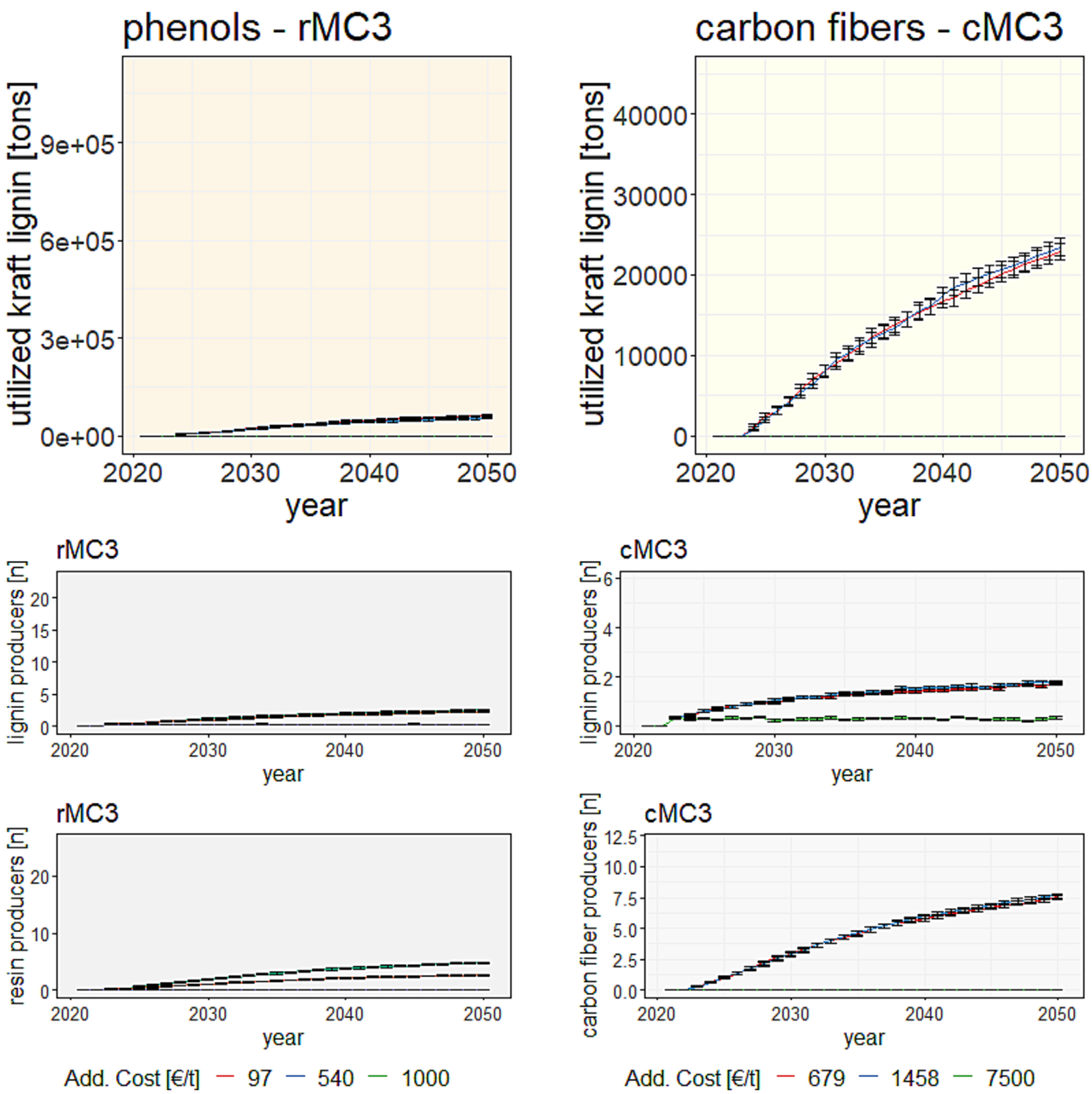

FIGURE 5 Minor-change scenario of the LPF resin (left column; rMC3) and carbon-fiber (right column; cMC3) cases (average values from 200 repetitions, including standard error bars); upper row: tonnes of utilized kraft lignin per year; middle row: number of lignin producers on the market per year; lower row: producers of phenols for LPF resins and carbon fibers from lignin per year. LPF, lignin phenol formaldehyde.

4.3 | Scale-up scenarios (PEX3 and PEX7)

The simulations of these scenarios reveal that assuming a larger number (42) of potential suppliers, as compared to the MC3, results in a much larger market share being reached (illustrated in Figure 6). Simulations indicate that 67% (in the LPF resin case) to 74% (in the CF case) of the target application market share is acquired by 2050 (Table 4). In terms of adopted lignin, and when assuming low to medium additional cost levels, the variation in oil prices, for example, due to the introduction of carbon pricing (PEX3 versus PEX7), exerts only a minor influence on the innovation diffusion process. There is, however, a marked difference between the PEX3 and the PEX7 scenarios in the case of high additional cost levels. Low crude oil prices together with high additional costs make lignin use economically unfeasible and result in no innovation diffusion. In contrast, high oil prices seem to offset the impact of high additional costs over time and, thus, allow more actors to switch to bio-based production. Up to an average of 22 (in the phenol case) and 6 (in the CF case) lignin producers sell their lignin in these scenarios, resulting in up to 19 phenol or 9 CF producers that switch production. In the simulation variants where lignin prices move in accordance with the oil prices over time (see Appendix A, scenario rPEXx3/cPEXx3), the results in the roughly constant oil price scenario (AP3) are similar to their constant lignin price counterpart variants. However, in the falling and rising oil price variants, the respective results of the lignin price-adjusted scenarios become more similar to each other since the oil price fluctuations are offset to a large extent (e.g., in the case of higher additional cost variants

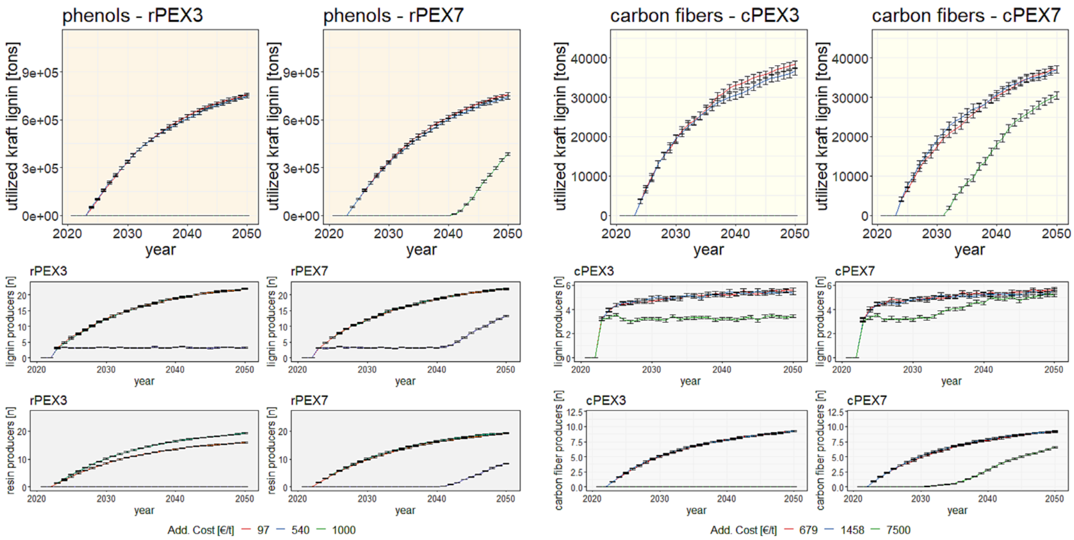

FIGURE 6 Scale-up scenarios of the LPF resin (two columns on the left: rPEX3 and rPEX7) and carbon fiber (two columns on the right: cPEX3 and cPEX7) cases, with and without carbon pricing assumption (average values from 200 repetitions, including standard error bars); upper row: tonnes of utilized kraft lignin per year; middle row: number of lignin producers on the market per year; lower row: producers of phenols for LPF resins and carbon fibers from lignin per year. LPF, lignin phenol formaldehyde.

and rising oil prices, innovation diffusion of lignin no longer occurs when its price also increases over time).

4.4 | Individual pricing scenario (TEA7)

Assuming that the pricing strategy of potential lignin suppliers is not driven solely by opportunity cost considerations but also by individual firm strategy and site-specific production costs, when compared to the PEX7-scenario, similar results to PEX7 are observed, in particular, for low and medium additional costs (illustrated in Figure 7 and Table 4). This indicates a relatively saturated diffusion path. This pattern, however, changes under high additional costs. A small number of lignin producers providing lignin at relatively low prices enables early diffusion, even under high additional costs, or at least under high uncertainty regarding such costs. In particular, regarding the application in CFs, the production cost-oriented pricing favors early diffusion of lignin even under high additional cost assumptions. This can be explained by the much smaller overall market size. In such a market, only a small number of lignin producers, supplying at the lowest prices, are sufficient for effective diffusion. In the case of phenol resin applications, this pattern changes. In the larger overall market, the early diffusion under high additional costs is slower compared to that in the low and medium additional cost scenarios. However, the effect levels out by 2050 as a result of the rising oil prices. Thus, from an aggregate perspective, the combination of individual lignin prices that do not increase over time, with rising crude oil prices, can be regarded as the least risky scenarios in terms of overall lignin innovation diffusion. In this diverse structure of heterogeneous lignin suppliers and processors, there is more scope for finding respective "matches" that are economically feasible and thus, theoretically, also better for coping with any additional costs potentially incurred in the lignin processing. Regarding the lignin producers, however, the average number of lignin producers that provide lignin is lower with individual pricing (15 and 4 producers for phenols and CFs, respectively) than in the PEX scenarios, because the larger producers profit more from EoS. Furthermore, like in the PEX scenarios, up to 19 (phenol) and 9 (CF) lignin processors switch production in the individual pricing scenario.

In several of the scenarios involving falling crude oil prices (see Figures A5 and A6; NZ1 scenarios), no matter which lignin pricing strategy is followed, switching is initially feasible, but then the lignin use gradually becomes unprofitable as a result of increased cost pressure, and thus, from the perspective of GPs, this would be a misinvestment.

4.5 | Potential emission savings

The potential emission savings were estimated for two selected scenarios: MC3, which is closest to the status quo, and TEA7, which showed the most stable innovation diffusion patterns. Figure 8 depicts the potential emission savings gained by replacing fossil raw materials (phenols and acrylonitrile) with extracted lignin. The dashed line in each graph represents the potential upper limit of emission savings, based on the theoretical maximum amount of fossil raw materials replaced when the predicted respective markets are fully saturated (1,000,000 t and 20,000 t in the phenol and CF cases, respectively). The potential emission savings differ in the two cases. On the one hand, potential emission savings are influenced by the respective innovation diffusion rates prevailing in the scenarios investigated. On the other hand, emission savings also vary as a result of differences in lignin to commodity substitution proportions, in market potential, and

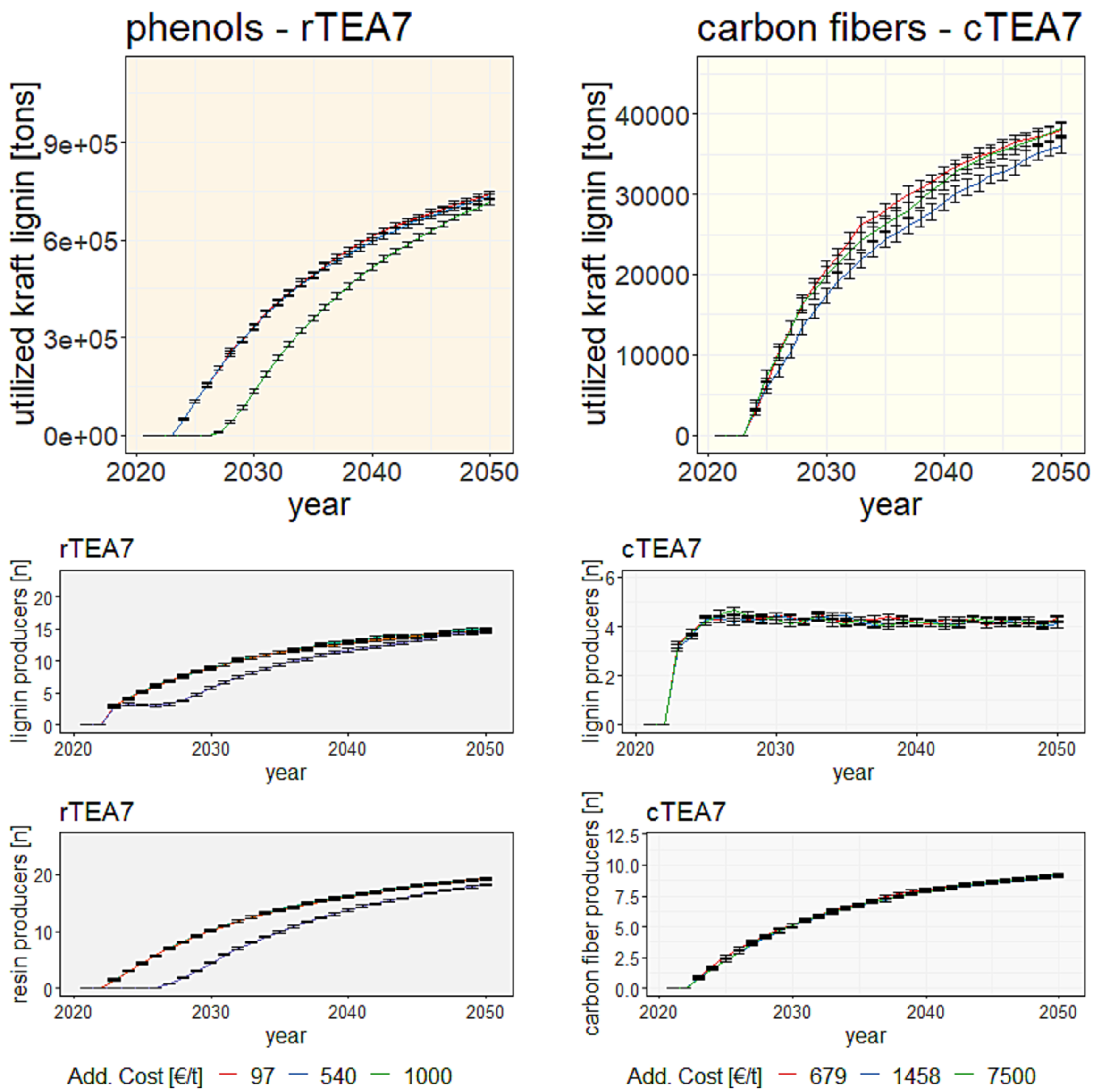

FIGURE 7 Individual pricing scenario of the LPF resin (left column: rTEA7) and carbon fiber (right column: cTEA7) cases, including carbon pricing assumption (average values from 200 repetitions, including standard error bars); (upper row) tonnes of utilized kraft lignin per year; (middle row) number of lignin producers on the market per year; and (lower row) producers of phenols for LPF resins and carbon fibers from lignin per year. LPF, lignin phenol formaldehyde.

in the respective impacts of the commodities replaced (phenols [RER, market for phenol] and acrylonitriles [GLO, market for acrylonitrile]). Here, the impacts resulting from the processes required for the respective raw lignin modifications have not been considered due to the lack of relevant data concerning mass and energy balances. Life-cycle phases such as the use and end-of-life were also not considered.

Nevertheless, due to the overall forecasted market size, the potential for emission savings appears vastly higher in the phenolic resin case. Although the production of acrylonitrile from fossil feedstocks has a larger carbon footprint than that of phenol production (3.62 kg CO_2-Eq/kg compared to 2.94 kg CO_2-Eq/kg), the replacement of fossil-based feedstocks in the phenolic resin market may lead to higher overall emission savings. By contrast, due to the small market size and relatively rapid saturation in the CF case, a relatively large part of the emission savings potential is already exploited in the scenario with minimal changes (cMC3), compared to the savings in the stable, high diffusion scenario (cTEA7).

4.6 | Sensitivity analyses

In order to validate the model and gain insight into how sensitive the results are with respect to specific input parameters, a one-factor-at-a-time sensitivity analysis was performed. As a starting point for this, we chose the TEA7 scenario, as this showed the most promising and stable results. For each parameter sweep, we only modified one parameter, keeping all others constant, and observed the outcome of the innovation diffusion process. The latter is quantified in terms

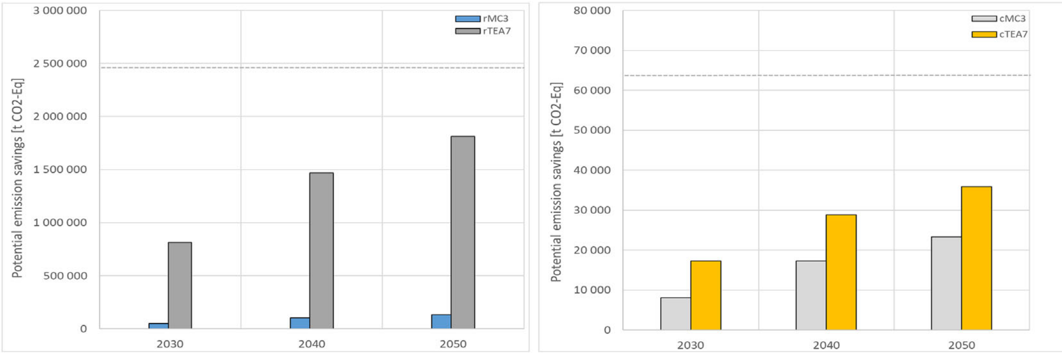

FIGURE 8 Potential emission savings in the scenarios rMC3 and rTEA7 as well as in cMC3 and cTEA7; the dashed lines represent the maximum potential emission savings when the respective lignin product markets are saturated.

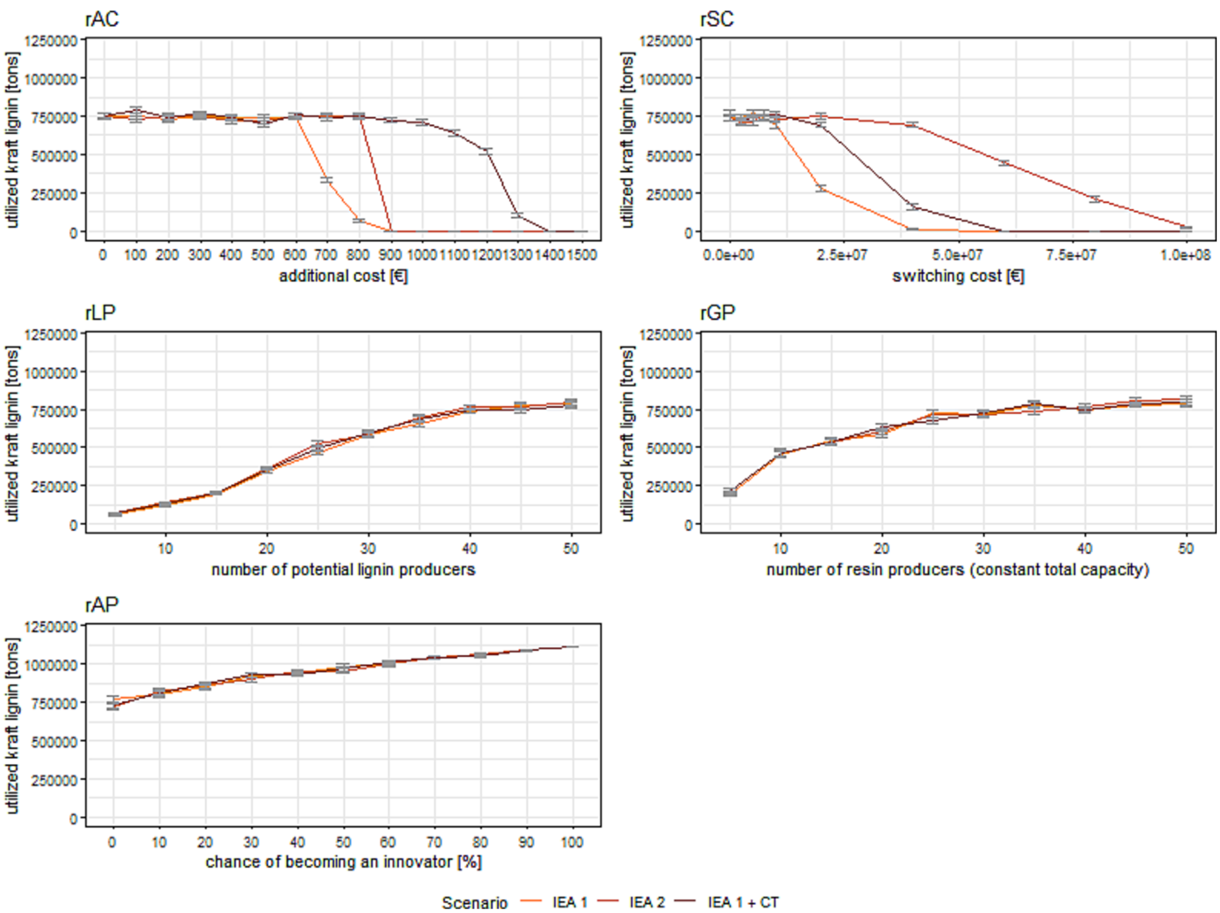

FIGURE 9 Sensitivity analysis results for the LPF resin case (year 2050); **rAC**: variation of additional costs (lignin scenario: TEA); **rTC:** variation of switching/transition cost (lignin scenario: TEA; additional cost: 540 €/t); **rLP**: variation of potential lignin producers on the market (additional cost: 540 €/t; lignin price: as in TEA); **rGP**: variation of potentially adopting resin producers on the market (total capacity constant at 1,000,000 t/year phenol for resins needed; lignin scenario: TEA; additional cost: 540 €/t); **rAP**: probability of producers becoming assigned to the innovator adopter group (lignin scenario: TEA; additional cost: 540 €/t). LPF, lignin phenol formaldehyde; TEA, techno-economic assessment.

of the amount of lignin traded in the year 2050. The results of this analysis are presented in Figure 9 (LPF resin) and Figure 10 (CF).

Concerning the additional cost, most of the time the actual value of the additional cost has no significant effect on the diffusion process. However, the diffusion process is hindered once the additional cost is large enough to make the overall production cost, when using lignin, comparable to that when using crude oil. Depending on the investigated scenario and product, this break-even point or "deterministic feasibility" is found at different values. Since the transformation expenditures (depreciation) represent only a tiny fraction in the

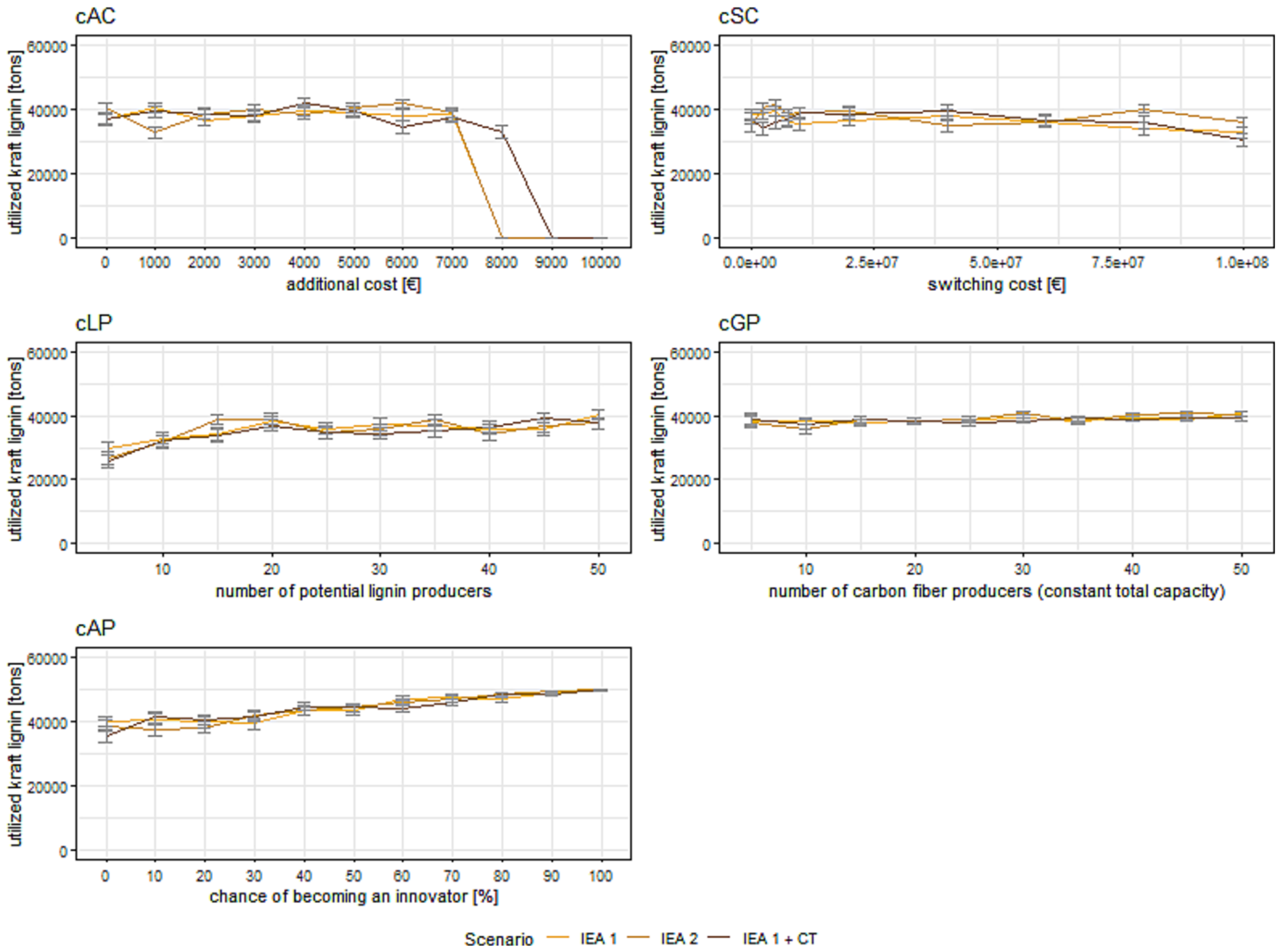

FIGURE 10 Sensitivity analysis results for the carbon fiber case (year 2050); **cAC**: variation of additional costs (lignin scenario: TEA); **cTC:** variation of switching/transition cost (lignin scenario: TEA; additional cost: 1,458 €/t); **cLP**: variation of potential lignin producers on the market (additional cost: 1,458 €/t; lignin price: as in TEA); **cGP**: variation of potentially adopting carbon fiber producers on the market (total capacity constant at 20,000 t/year carbon fibers potentially from lignin; lignin scenario: TEA; additional cost: 1,458 €/t); **cAP**: probability of producers becoming assigned to the innovator adopter group (lignin scenario: TEA; additional cost: 1,458 €/t). TEA, techno-economic assessment.

overall production cost structure (see red bar in Figure 4)—when calculated per tonne of lignin and depreciated over 10 years—they have no significant influence on diffusion in our model, unless values are increased to (probably) unrealistic levels. However, in practice, this parameter would not only include expenditures related to the investment but also switching costs of various kinds, and thus, the maximum value used for such costs was € 100,000,000.

To analyze the influence of the number of potential lignin producers, we initialized the model in the TEA scenario, yet we generated more or fewer lignin producer agents by randomly removing or duplicating those from the baseline scenario. This also changed the overall amount of lignin available on the market. This analysis provides different results for the two products investigated. While the CF case is not much influenced by a reduced amount of available lignin (because the projected market for this product is saturated relatively fast), the LPF resin case is nearly linearly dependent on the number of lignin producers, until saturation is reached at a point of roughly 40 producers. We performed a similar analysis for the number of GPs. Here, we kept the overall production capacity constant but varied conditions to reflect whether capacity is generated by a few large or by many smaller companies. Again, the LPF resin case shows much more sensitivity, especially for a low number of GPs.

Finally, the influence of the innovativeness of the firms was investigated. When initializing the simulation, each firm was assigned a probability of moving into the most innovative adopter group (see Section 3.3 for details). This resulted in an increase in the amount of traded lignin for both the products investigated. Note that the amount of traded lignin surpasses that reached when compared to the situation where there are no additional costs.

5 | DISCUSSION

5.1 | Discussion of key results

The major results and their interpretation are given in Table 5, and the related implications are discussed in the subsequent subsection.

TABLE 5 Summary of key results and interpretations thereof.

	Result	Interpretation
1	**Number of potential lignin suppliers (MC3 and other scenarios)**: In the “minor-change scenario” (MC3) with four lignin suppliers, innovation diffusion occurs slowly and only reaches a relatively limited market share below the technical potential expected for lignin in both application fields. On assuming a larger number (42) of potential suppliers, this pattern changes.	Particularly with respect to the anticipated technological potential, the relatively limited number of lignin suppliers on the market represents a major challenge in innovation diffusion (low supply, low network effects).
2	**Phenols and carbon case comparison (MC3)**: There is a higher relative market penetration (corresponding to the much lower absolute amounts of lignin adopted) and a higher number of goods producers entering the market in the case of carbon fibers. The innovation diffusion in this field of application is also less influenced by increasing additional processing costs.	Innovation diffusion patterns (e.g., absolute/relative market penetration; impact of additional processing costs) differ across product categories, which not only reflects different product-related characteristics but also the different respective market structures prevailing.
3	**Price and cost levels (PEX3 and PEX7)**: In terms of adopted lignin, and when assuming low to medium additional cost levels, the variation in oil prices (including the carbon pricing in PEX7) exerts only a minor influence on the innovation diffusion process. In the case of high additional cost levels, these, along with low crude oil prices, make lignin use economically unfeasible and result in no innovation diffusion. In contrast, increasing oil prices seems to offset the impact of high additional costs over time and, thus, allows more actors to switch to bio-based production.	Because the overall cost competitiveness results from different variables (e.g., feedstock costs, switching costs, lignin processing costs, carbon pricing for fossil feedstocks; respective developments over time), this can lead to low costs in one area compensating for higher costs in another area. However, given the large associated uncertainties (including over time), the investment risk increases in the cases of relatively high costs incurred in bio-based production or relatively low costs incurred in fossil-based production (i.e., the narrower the cost gap becomes).
4	**Lignin price dependent on crude oil price (PEXx3)**: In the simulations where lignin prices move in accordance with the oil prices over time, and in particular in the falling and rising oil price variants, the respective results of the lignin price-adjusted scenarios become more similar to each other since the oil price fluctuations are offset to a large extent.	In the case of a larger established kraft lignin market, the exact relationship of lignin price developments along with crude oil price developments still remains unclear. The stronger their correlation, the more likely the effect of carbon pricing on the lignin innovation diffusion may be cushioned.
5	**Pricing strategies (TEA7 and PEX7):** Assuming that the pricing strategy of potential lignin suppliers is not driven solely by basic preparation and opportunity cost considerations but also by individual firm strategy and site-specific production costs, and under high additional costs, a small number of lignin producers providing lignin at relatively low prices enables early diffusion.	In the diverse structure of heterogeneous lignin suppliers (TEA7) and processors, there would be more scope for finding respective “matches” that are economically feasible and thus, theoretically, also better for coping with any additional costs potentially incurred in the lignin processing. The combination of individual lignin prices that do not increase over time, with rising crude oil prices (including carbon pricing), can be regarded as the least risky scenario in terms of overall lignin innovation diffusion.
6	**Phenols and carbon case comparison (TEA7):** In the carbon fiber case, early diffusion of lignin happens even under high additional cost assumptions, which can be explained by the much smaller overall market size (only a small number of lignin producers, supplying at the lowest prices, are sufficient for effective diffusion). In the case of phenol resin applications, this pattern changes: In the larger overall market, the early diffusion under high additional costs is slower compared to that in the low and medium additional cost scenarios.	Major barriers to overall innovation diffusion differ in the cases studied. In the phenol case (higher TRL, higher volumes, lower prices), the low lignin availability and issues regarding economic feasibility (low phenol price, high lignin price, high additional costs, EoS considerations) are the main barriers. In the carbon case (lower TRL, lower volumes, higher prices), barriers seem to center on the low TRL and associated uncertainties, on competition from other bio-based feedstocks, as well as on the potentially low level for emission savings given that the total market here is expected to be rather small.
7	**Lignin producers on the market (PEX3/7 and TEA7):** Regarding the lignin producers, the average number of lignin producers that provide lignin is lower with individual pricing than in the PEX scenarios, while earlier diffusion occurs in the TEA scenarios.	The larger lignin producers profit more from EoS; therefore, fewer producers are required in the TEA scenarios. This highlights potential conflicting goals and points to game-theoretic implications: e.g., in terms of how individual actors or groups of actors might maximize benefits (e.g., via corresponding pricing mechanisms; high-value products) versus how the overall innovation diffusion process might be most effective and, thus, could benefit the environment as well as more actors (e.g., total tonnes of lignin adopted; overall environmental impacts; number of adopter firms).
8	**Falling crude oil price scenarios (with constant lignin prices)**: In several of the scenarios involving falling crude oil prices, no matter which lignin pricing strategy is followed, switching is initially feasible, but then the lignin use gradually becomes unprofitable as a result of increased cost pressure.	Falling crude oil prices—even where bio-based production may initially appear profitable—raise the risk of investments in bio-based production becoming unprofitable, and thus, from the perspective of goods producers, this would be a misinvestment.

TABLE 5 (Continued)

	Result	Interpretation
9	**Emissions (phenols and carbon case comparison):** Although the production of acrylonitrile from fossil feedstocks is associated with a larger carbon footprint than that of phenol production, the replacement of fossil-based feedstocks in the phenolic resin market may lead to higher overall emission savings (due to the overall forecasted market size). By contrast, due to the small market size and relatively rapid saturation in the carbon fiber case, a relatively large part of the emission savings potential is already exploited in the scenario with minimal changes (MC3), even when compared to the savings in the stable, high diffusion scenario (TEA7).	The potential emission savings (simplified approach – see limitations) differ in the two cases studied. On the one hand, potential (overall) emission savings are influenced by the respective innovation diffusion rates prevailing in the scenarios investigated. On the other hand, emission savings (per unit) vary as a result of differences in lignin to commodity substitution proportions, in market potential, and in the respective impacts of the commodities replaced.
10	**Sensitivity (TEA7, additional costs):** The actual value of the additional cost only hinders the innovation diffusion process once the additional cost is large enough to make the overall production price (when using lignin) comparable to that when using crude oil. Depending on the investigated scenario and product, this break-even point or "deterministic feasibility" is found at different values.	Profitability is not only influenced by the (internal, techno-economic) costs incurred in the lignin processing but also by external factors (e.g., crude oil price developments) which influence where the break-even point will be. This is associated with uncertainties and will, e.g., depend on future price development scenarios.
11	**Sensitivity (TEA7, number of producers):** While the carbon fiber case is not influenced by a reduced amount of available lignin, the LPF resin case is nearly linearly dependent on the number of lignin producers, until saturation is reached (at a point of ∼40 producers). When the number of goods producers is varied (production capacity kept constant), the LPF resin case shows more sensitivity, especially for a low number of goods producers.	The sensitivities of producer-related variables are different in the respective cases, with higher sensitivities (number of lignin producers, number of goods producers) in the phenols case.
12	**Sensitivity (TEA7, innovativeness):** Varying the ability/willingness parameter, there is a steep increase in the amount of traded lignin for both the products investigated. With a high chance of becoming an innovator, the amount of traded lignin surpasses that reached in the situation where there are no additional costs.	Financial incentives alone do not seem to be enough to lead to (nearly) complete innovation diffusion. The socio-economic context, as well as the level of firm innovativeness (here expressed using the ability/willingness parameter) seem paramount in the innovation diffusion process.

Abbreviations: EoS, economies of scale; LPF, lignin phenol formaldehyde; TEA, techno-economic assessment; TRL, technology readiness level.

5.2 | Theoretical and practical implications

Novel forest-based businesses are important in the transition towards a more sustainable circular bioeconomy. The successful diffusion of innovations—such as the substitution of kraft lignin-based products for their fossil-based counterparts—is not possible unless the stakeholders involved engage in some form of collective effort and pursuit of shared goals. This includes actors directly connected to the lignin-based supply chains as well as wider societal groups. There is a potential of goal conflict (**Table 5, items 5, 7, and 9**), for example, in terms of how individual actors or groups of actors might maximize benefits (e.g., with respect to various pricing mechanisms) versus how the overall innovation diffusion process might be most effective (which in turn could benefit the environment as well as actors). Agent-based simulation of innovation diffusion pathways for kraft lignin products using BioPID not only introduces multi-faceted situations and mechanisms behind potential diffusion pathways but also acts as a tool enabling diverse societal stakeholders to engage in informed knowledge exchange and communication (cf., e.g., Macy & Willer, 2002; Yang et al., 2022). In other words, information provided by BioPID can promote dialogue between different actors, thus helping them to set common goals (or joint purposes, see Breuer & Lüdeke-Freund, 2017; Freudenreich et al., 2020).

Despite wide-scale agreement on the need to abandon fossil-based production, barriers to change still exist in the form of social and political resistance, inflexible planning policies, general reluctance, etc. (e.g., Béfort, 2020). The creation of a suitable political environment and power structure is imperative in supporting any transition towards a non-fossil society (e.g., Köhler et al., 2019; Meadowcroft, 2011). In the context of bioeconomy businesses, coherent, long-term policies play a crucial role (Kelleher et al., 2019). Political factors are also important drivers in the case of lignin production and processing, where the limited number of lignin suppliers on the market, as well as the high level of uncertainty related to the additional costs of lignin processing, represent major challenges for innovation diffusion. The results described above show that the interplay of several different variables is decisive for the successful, "lower-risk" diffusion of bio-based innovation (**Table 5, items 3, 4, 8, and 10**). Once again, this stresses the need for coherent, long-term policies. Often, dominating incumbent actors in the regime level aim to prevent the (market) entry of new business entrants into regime (Geels, 2010). In such a case, the bio-based materials would have to compete with their fossil-based counterparts in the petro-chemical industry. Despite the relatively blurred boundaries between niche and regime players in the case of several bioeconomy applications (see, e.g., Hermans, 2018), the pulp and paper companies may be regarded as mature regime-level actors, and the processing of lignin to (partly) replace crude oil-based products would require niche-level innovations and their scaling up to more large-scale production. However, this is likely to entail overcoming a range of challenges related to lock-ins and path dependencies of the mature forest-based companies (e.g., Markard et al., 2012). Overall, public policies should thus provide a stronger normative directionality (see Köhler et al., 2019) and create a more compelling environment in order to enable easier entrance and participation of various actors in the markets and greater market functionality (e.g., avoidance of monopolies and improved security of lignin supply). BioPID can provide policy makers in all societal levels involved in bioeconomy development with better understanding of the lignin-based innovation system, and thus promote better informed and coherent decision-making in the transition towards non-fossil societies.

Further, promoting the diffusion of lignin-based products requires a collaborative effort among niche companies: they need to collaborate horizontally with other niche actors as well as vertically with the regime actors providing raw material. The results of the BioPID approach indicate that both a limited number of lignin suppliers and GPs (phenols) on the market (**Table 5, items 1 and 11**) as well as a lower level of innovativeness among respective actors (**Table 5, item 12**) pose challenges to innovation adoption and subsequent diffusion. While the setting of shared goals with suppliers and producers would promote collaboration, the establishment of relationships with traditional and dominant regime actors (i.e., lignin producers) with rigid organizational cultures still remains a challenge (e.g., Kuhmonen et al., in press). Collaborative efforts and potential joint strategies among niche actors can provide a way forward in these relationships. The crucial importance of collaboration has also been highlighted by many management studies on cross-sectoral value creation, networks, business ecosystems, and open innovations. Melander and Wallström (2022), for example, highlighted the importance of horizontal collaboration in finding innovative, more environmentally friendly solutions. At the same time, they highlighted that environmental and economic incentives as well as trust between the companies are a prerequisite for establishing collaborative relationships. However, niche companies are often very reluctant to share proprietary knowledge on their business models and technologies, since their competitiveness is based on these unique solutions and this may weaken their competitive position and increase the risk of them being exploited by other firms (e.g., Kuhmonen et al., in press; Melander & Paziraandeh, 2019). Nevertheless, areas of potential collaboration still exist, for example, in lobbying campaigns, and in learning processes relating to their (shared) suppliers, customers, investors, or infrastructure. They can also jointly promote suitable legislation and regulative networks. In the case of lignin-based value creation, this could mean, for example, establishing common infrastructure for material characterization, or that knowledge gained throughout research projects—which often receive funding from the public budget—is made available to potential adopters in order to reduce information asymmetries and increase innovativeness. In addition to relationships between the companies, supportive ecosystems around new innovations include actors such as customers and end users as well as investors (see, e.g., Möller & Svahn, 2009; Sandberg & Aarikka-Stenroos, 2014). All these actors can utilize the information created by BioPID when making their (more conscious) purchasing or investing decisions. Altogether, in the realm of innovation in the bio-based field, major challenges exist in relation to organizational culture, cooperation, and collaboration (e.g., Bröring et al., 2020; Golembiewski et al., 2015; Hansen, 2010; Leavengood & Bull, 2013; Näyhä & Pesonen, 2014). Companies in the forest-based sector are often reluctant to participate in open networks and open innovating (D'Amato et al., 2020; Näyhä, 2021). The knowledge provided by BioPID may serve to reduce mistrust among different companies and stakeholders and thus help to create a more secure basis for collaboration.

Given both the different innovation diffusion patterns arising from the two product categories studied (**Table 5, items 2, 6, 9, and 11**), as well as the high number of potential lignin applications currently being researched (e.g., Wenger et al., 2020), it is important not to neglect the need for generating balanced product portfolios while considering issues at different levels of analysis (e.g., firm-level, market structures in socio-technical system, and macro-level consequences). This is a challenge, particularly from the perspective of the companies involved and their strategic management and decision-making. Given such a context, we believe that BioPID can provide managers with more relevant information for decision-making on their product portfolios.

By enhancing the availability and flow of information among actors in diverse interactions, and thus serving to increase transparency and decrease mistrust among various actors, the BioPID has value for diverse actors in the operating environment of companies. In sum, therefore, by reducing levels of uncertainty, we believe that BioPID can make the fundamental needs of diverse stakeholders more visible in value creation processes (see Lüdeke-Freund et al., 2020, p. 81).

5.3 | Limitations and outlook

As acknowledged by several authors (e.g., Kiesling et al., 2012; Zhang & Vorobeychik, 2017), the (predictive) validation of prospective agent-based innovation diffusion simulation remains challenging for several reasons (e.g., lack of appropriate data). This is also the case for the BioPID approach (an exploratory tool rather than a predictive tool). Particular strong variations exist in the literature regarding the expected additional costs and, in particular, with respect to CF (cf., e.g., referenced sources in Section 3.4.2). This is at least partly related to the lower TRL as compared to that of phenolic resins (e.g., European Commission, 2019b), resulting in higher associated levels of design uncertainty, and, possibly, of higher design freedom (eco-design paradox; e.g., Genus & Stirling, 2018; Poudelet et al., 2012). In general, it is assumed that the quality of the bio-feedstock is such that it can be used in the respective products and markets, which implies that current technological challenges—for example, concerning lignin characterization, constant homogeneity, etc. (e.g., Holladay et al., 2007; Ragauskas et al., 2014)—can be adequately addressed in the future, which may appear rather optimistic at this point. Several scientific sources point to the relevance of "learning effects" in technology development (e.g., Daugaard et al., 2014; Lieberman, 1984; Thomassen et al., 2020). These are expected to occur as cumulative capacity rises, and in addition to the benefits of EoS, contribute to a lowering of unit production costs. Currently, due to the lack of relevant data available, the quantification of "learning effects" remains a difficult task. Overall, to address (some of the) prevailing uncertainties—both with regard to the data and potential future preconditions—several scenarios were introduced (e.g., with regard to raw material prices and pricing strategies), broad ranges and combinations of prices and costs were tested in a range of simulation runs (including indication of standard errors), and sensitivity analyses were conducted on a range of parameters.

In the BioPID model, once basic criteria had been fulfilled, the lignin was adopted as soon as a lignin producer and a GP entered a contractual agreement, which probably is a shortcoming in our current assumptions (e.g., no minimum number of lignin suppliers required on the market and no possibility to switch back). Related expenses only became a significant decision criterion when they were relatively high. Thus, further adaptations of the model could be made in regard to the actual switching to lignin (e.g., introducing entry barriers or by refining estimations concerning the extent or nature of expenditures). The perspectives of various affected actor groups (e.g., company representatives, societal actors, and land owners)—including their different perceptions, needs, and (partly conflicting) goals—need to be better understood and ecological aspects need to be considered more strongly for the biorefinery innovation diffusion pathways to actually contribute to sustainable development (e.g., Dieken et al., 2021; Mustalahti, 2018; Näyhä, 2019; Tan et al., 2019). Closer examination of such issues could include analyzing the various preconditions faced by individual actors (ability/willingness) and network structures representing the embedding of actors in (external) social structures (e.g., Bohlmann et al., 2010; Kiesling et al., 2012). The gathering of survey data (e.g., from respective actor groups) could help generate more empirical information on social structures, to refine the BioPID parameters accordingly, and thus introduce a stronger empirical reliability and validity into the model. In the current BioPID model, a major focus was placed on supply chain actors (who are equipped with a certain heterogeneity). Other actors have so far only been included implicitly: for example, in the current BioPID model, high costs of crude oil-based inputs could be interpreted as government measures (including carbon pricing), low "additional costs" for bio-based innovations as incentive measures, or an increased innovativeness (see sensitivity analysis) as the promotion of network activities and R&D projects. Other (horizontal) actor groups such as regulatory organizations thus could receive more emphasis in the future. With regard to the actor groups explicitly included, some issues that could be further explored are related to lignin market requirements from the perspectives of the potential lignin buyers (market structure such as minimum number of lignin suppliers on the market, required lignin qualities, etc.), refinement of the preconditions and behaviors of the consumer agents (e.g., willingness to pay for a bio-based counterpart product, attitudes towards partly bio-based materials; Günther et al., 2011; Stummer et al., 2015; Zwicker et al., 2023; Ruf et al., 2022), and analysis of actor networks (e.g., empirically derived, actual networks; loose/highly connected networks) and corresponding refinement of the model networks.

Regarding the sustainability-related impacts, in the present paper, calculation of possible emission savings merely served to establish a link between the BioPID model and approaches to analyzing potential sustainability consequences arising from corresponding innovation diffusion pathways. However, considerations of possible changes to previous mass and energy balances arising during production, of subsequent life-cycle stages (e.g., lightweight carbon fiber materials in vehicles could lead to reduced fuel consumption and emissions), of geographical issues (e.g., regional energy mixes), or modeling efforts to address the uncertainties of parameters, just to name a few examples, were beyond the scope of this paper and remain the subject of future research. The highlighted potential goal conflicts and trade-offs (see Table 5), including analysis of which individual actors or actor groups win or lose in different scenarios, may also be an issue worth exploring further. With regard to some issues, the BioPID ABM already allows for more extensive analyses than those conducted in the present paper. For example, at the level of the GPs, it would be possible to put the focus of analysis on individual actors, for example, the respective successful production capacities of GPs adopting lignin, as well as on the resulting price (ranges) of the final products (phenol for LPF resins and CFs) in different scenarios. Focusing on individual actors' characteristics could provide valuable insight into the potential roles and outcomes relating to individual actors in the different scenarios and could also be a starting point for better incorporating management perspectives. This could be supported by participative and collaborative approaches using BioPID as a facilitator (e.g., Yang et al., 2022). On the system level, new and radical biorefinery innovation pathways require active forms of collaboration (ideally based on shared values), multidisciplinary, multi-objective and participatory approaches, more efficient (environmental) management practices, and improved and more transparent decision-making processes (Dieken et al., 2021; Mustalahti, 2018; Näyhä, 2019; Tan et al., 2019).

6 | CONCLUSIONS

The significance of forest-based businesses is often stressed when discussing transition towards a more sustainable circular bioeconomy. In particular, innovations in kraft lignin, a by-product from the pulping industry, and in related biorefineries are believed to offer considerable potential in this area. For such transition pathways to be successful, however, the appropriate interplay of a range of variables on different levels (e.g., technology development on the niche-level, barriers and drivers prevailing in the socio-technical environment, and policies supporting more sustainable practices) is decisive. The facilitation of shared goals and collective effort among various societal actors with different needs and understandings will be required to overcome current sustainability challenges. So far, lignin researchers have focused mainly on internal (direct) factors, have not yet adequately considered external (indirect) factors in the operational environment, and to the current authors' knowledge, have not yet analyzed the interplay between these two areas. The present paper thus aimed at addressing this research gap by applying an empirically grounded agent-based simulation approach, BioPID, in order to explore the interaction of diverse intra- and extra-organizational factors in the innovation diffusion of two different, novel biorefinery products. This entailed examining the intersection of techno-economic issues, innovation research (diffusion and socio-technical perspectives), and the related potential impact in terms of sustainability (greenhouse gas emission savings) in the model.

The simulation results outlined in Table 5 indicate that the current relatively low level of innovation diffusion for technical lignin in material applications may be explained (apart from technological issues) by (1) the rather small number of lignin providers applying relatively homogeneous pricing strategies based on opportunity and basic preparation costs; and, (2) major unknowns regarding the associated additional costs arising in the required lignin processing, which represent a major investment risk (aggravated by the uncertain price developments of fossil and bio-based raw materials in the future). Innovation diffusion processes may thus be improved by reducing (uncertainties regarding) the additional costs arising in lignin processing and by increasing the diversity of lignin providers. With respect to overcoming the cost barriers to diffusion, one essential, but as yet unrecognized, finding is the impact of site-specific and production cost-specific pricing strategies. These could enable innovation diffusion even in the face of very high costs or cost uncertainty, and/or allow for greater room for maneuver when dealing with the additional costs. In the case of the analyzed higher-value product, successful innovation–diffusion appears to happen more unwaveringly as the additional costs play a relatively smaller role. However, as this is associated with limited market volumes, expected overall emission savings are relatively low when compared to the higher-volume (but lower-value) product analyzed, and in practice, other barriers such as lower technology readiness level and stronger competition with other feedstock may hinder innovation diffusion in this case.

The BioPID approach also highlighted that the development and adoption of biorefinery innovations depend on the interaction of a variety of actors (e.g., public institutions, firms, and consumers) and points out potential areas of conflict. It thus highlights the importance of shared value creation among stakeholders. In this regard, the BioPID can be used as an explorative knowledge-exchange and communication tool in multi-actor biorefinery development. The model can facilitate the setting of common goals ("joint purposes") for the actors' shared value creation processes. It can be used to uncover basic mechanisms underlying biorefinery innovation diffusion pathways, to develop a more systemic understanding thereof, including potential consequences, and to help identify knowledge gaps. Political factors are considered important drivers in the case of lignin, and the BioPID can provide politicians involved in bioeconomy development with a multi-faceted and more holistic understanding of the lignin-based innovation system, thus promoting better informed and coherent decision-making in any transition towards non-fossil societies. The BioPID approach can also be used to increase knowledge and decrease mistrust among the niche level companies, both when constructing horizontal collaborations and when establishing niche-regime vertical interactions. Furthermore, the approach can also facilitate dialog between different companies and wider groups of stakeholders, helping to create the basis for collaboration, and create greater awareness among company managers engaged in developing new product portfolios. Overall, a novelty of the BioPID simulation approach is that it allows for iterative technology evaluation and technology foresight analysis of biorefinery projects in a structured manner (e.g., by combining techno-economic, socio-technical, innovation theory, and sustainability aspects). Thus, on the one hand, actors in management and policy areas (who focus more strongly on the external innovation environment) can monitor the potential consequences of targeting specific innovation diffusion pathways, and on the other hand, technology-focused actors (who deal more strongly with internal aspects of innovations) can develop a broader understanding of the innovation system which can be helpful in their decision-making on the micro-level.

While the model attempts to generate new perspectives on this complicated issue, critical reflection concerning the approach is still needed. A range of limitations were identified and discussed above, relating, for example, to data issues (e.g., quality, availability, and uncertainty), the relative emphases placed on various items (e.g., regarding the assumptions related to adopters' behaviors), complexity versus comprehensiveness, and empirical reliability and validity of the model (which may be regarded as an explorative but not a predictive tool). Accordingly, several suggestions were made for future research, for example, on how to address particular limitations, how to refine or augment the model (e.g., regarding actors' preconditions and behaviors; focus on individual actors), and how to deal with trade-offs and potential areas of conflict arising in biorefinery innovation diffusion pathways. Applying the model to other biorefinery case studies, and establishing a more sophisticated linkage between the BioPID and sustainability impact analysis would be helpful in future research.

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CONFLICT OF INTEREST STATEMENT

The authors declare no conflict of interest.

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APPENDIX A

More information on specific model assumptions are given in Table A1 and in Table A2 in the Appendix. More detailed results including the results related to other investigated scenarios can be found in the Appendix as well (Table A3 and Figures A1–A7)

TABLE A1 Assumed costs and capacities of lignin producers in the TEA scenarios (based on techno-economic assessments of lignin separation pathways; Krassnitzer et al., 2023).

Separation approach	First author	Publication year	Cost of production (own calc.) [€/t]	CapEx[€]	CapEx/ t[€/t]	OpEx [€/year]	OpEx/ t[€/t]	Cost of capital (3–5 years) [€/year]	Total cost [€/year]	CapEx [€/a]	CapEx allocated to x years [a]	Production volume[t/a]
Acid precipitation	Benali	2012	**806**	33,737,685	2,024	6,081,967	365	5,672,586	13,441,437	7,359,470	5	**16,667**
Acid precipitation	Benali	2012	**762**	37,128,407	2228	4,605,064	276	6,242,695	12,704,180	8,099,116	5	**16,667**
Acid precipitation	Tomani	2009	**107**	11,462,840	229	2,829,151	57	1,927,339	5,329,632	2,500,481	5	**50,000**
Acid precipitation	Uloth	1989	**70**	4,637,489	184	751,488	30	779,738	1,763,100	1,011,612	5	**25,200**
Acid precipitation	Laasksometsä	2009	**111**	10,303,051	335	1,176,542	38	1,732,334	3,424,029	2,247,487	5	**30,800**
Acid precipitation	Dieste	2016	**1,266**	6,710,489	1,974	2,839,801	835	1,128,288	4,303,613	1,463,812	5	**3,400**
Acid precipitation	Loutfi	1991	**487**	19,523,678	1,007	5,178,808	267	3,282,672	9,437,663	4,258,855	5	**19,380**
Acid precipitation	Culbertson	2016	**136**	14,511,581	276	3,964,400	76	2,439,948	7,129,927	3,165,527	5	**52,500**
Acid precipitation	Kannangara	2015	**448**	11,843,396	483	8,403,435	343	1,991,325	10,986,930	2,583,495	5	**24,500**
Acid precipitation	Kannangara	2015	**399**	15,171,292	619	6,641,608	271	2,550,870	9,784,648	3,143,040	5	**24,500**
Acid precipitation	Davy	1993	**344**	7,657,653	512	2,856,574	191	1,914,091	5,153,547	2,296,973	3	**14,960**
Acid precipitation	Davy	1993	**317**	8,847,626	465	3,382,491	178	2,211,534	6,036,407	2,653,916	3	**19,040**
Acid precipitation	Davy	1993	**453**	7,901,056	528	4,408,370	295	1,974,932	6,778,354	2,369,984	3	**14,960**
Acid precipitation	Davy	1993	**436**	9,594,988	504	5,417,215	285	2,398,343	8,295,308	2,878,093	3	**19,040**
Acid precipitation	Lindorfer	2019	**310**	11,000,000	156	19,419,124	276	1,849,518	21,818,642	2,399,518	5	**70,428**

(Continues)

TABLE A1 (Continued)

Separation approach	First author	Publication year	Cost of production (own calc.) [€/t]	CapEx[€]	CapEx/ t[€/t]	OpEx [€/year]	OpEx/ t[€/t]	Cost of capital (3–5 years) [€/year]	Total cost [€/year]	CapEx [€/a]	CapEx allocated to x years [a]	Production volume[t/a]
Acid precipitation	McKeough	2014	**343**	29,810,120	596	10,665,335	213	5,012,214	17,168,055	6,502,720	5	**50,000**
Acid precipitation	McKeough	2014	**341**	40,456,592	809	8,237,423	165	6,802,290	17,062,543	8,825,120	5	**50,000**
Acid precipitation	Olsson	2006	**82**	9,756,445	199	1,908,656	39	1,640,429	4,036,907	2,128,251	5	**49,050**
Acid precipitation	Olsson	2006	**79**	10,884,296	185	2,290,387	39	1,830,064	4,664,665	2,374,278	5	**58,860**
Acid precipitation	Olsson	2006	**77**	11,939,013	174	2,672,118	39	2,007,402	5,276,470	2,604,352	5	**68,670**
Acid precipitation	Olsson	2006	**80**	10,517,347	189	2,163,143	39	1,768,366	4,457,376	2,294,233	5	**55,590**
Acid precipitation	Olsson	2006	**77**	11,939,013	174	2,672,118	39	2,007,402	5,276,470	2,604,352	5	**68,670**
Acid precipitation	Olsson	2006	**75**	12,608,794	168	2,926,605	39	2,120,017	5,677,062	2,750,457	5	**75,210**
Acid precipitation	Olsson	2006	**80**	10,517,347	189	2,163,143	39	1,768,366	4,457,376	2,294,233	5	**55,590**
Acid precipitation	Benali	2015	**464**	27,586,303	828	9,447,310	283	4,638,305	15,464,930	6,017,620	5	**33,333**
Acid precipitation	Benali	2015	**529**	37,200,987	1,116	9,503,326	285	6,254,899	17,618,275	8,114,949	5	**33,333**
Acid precipitation	Axelsson	2006	**86**	12,108,206	218	2,163,143	39	2,035,849	4,804,403	2,641,260	5	**55,590**
Acid precipitation	Axelsson	2006	**89**	11,232,210	229	1,908,656	39	1,888,561	4,358,827	2,450,171	5	**49,050**
Acid precipitation	Axelsson	2006	**89**	11,232,210	229	1,908,656	39	1,888,561	4,358,827	2,450,171	5	**49,050**
Acid precipitation	Axelsson	2006	**85**	12,530,661	213	2,290,387	39	2,106,880	5,023,800	2,733,413	5	**58,860**
Acid precipitation	Axelsson	2006	**83**	13,744,914	200	2,672,118	39	2,311,042	5,670,406	2,998,288	5	**68,670**
Membrane filtration	Jönsson	2009	**54**	15,351,169	142	2,463,693	23	2,581,115	5,785,366	3,321,673	5	**108,000**

TABLE A1 (Continued)

Separation approach	First author	Publication year	Cost of production (own calc.) [€/t]	CapEx[€]	CapEx/ t[€/t]	OpEx [€/year]	OpEx/ t[€/t]	Cost of capital (3–5 years) [€/year]	Total cost [€/year]	CapEx [€/a]	CapEx allocated to x years [a]	Production volume[t/a]
Membrane filtration	Jönsson	2008	**59**	11,408,165	158	1,745,293	24	1,918,146	4,233,847	2,488,554	5	**72,000**
Membrane filtration	Holmqvist	2005	**126**	14,151,101	340	1,461,949	35	2,379,338	5,256,397	3,794,448	4	**41,625**
Membrane filtration	Holmqvist	2005	**63**	13,323,552	160	1,690,318	20	2,240,195	5,262,868	3,572,550	4	**83,250**
Membrane filtration	Holmqvist	2005	**115**	17,981,475	327	1,483,474	27	3,023,369	6,304,990	4,821,516	4	**54,945**
Membrane filtration	Holmqvist	2005	**91**	17,307,613	247	1,709,269	24	2,910,067	6,350,097	4,640,828	4	**69,930**
Membrane filtration	Uloth	1989	**135**	7,857,481	312	1,686,000	67	1,321,141	3,400,015	1,714,015	5	**25,200**
Membrane filtration	Arkell	2014	**88**	2,500,898	61	3,077,074	75	420,496	3,622,615	545,541	5	**41,000**
Membrane filtration	Arkell	2014	**50**	1,098,614	16	3,134,928	46	184,719	3,374,578	239,650	5	**68,000**
Membrane filtration	Arkell	2014	**569**	2,835,836	342	4,108,150	495	476,812	4,726,753	618,603	5	**8,300**
Membrane filtration	Arkell	2014	**134**	1,628,700	54	3,652,233	122	273,846	4,007,514	355,281	5	**30,000**

TABLE A2 Number and respective capacities [t/year] of goods producers.

Goods producers			
Phenols for LPF resins		**Carbon fibers**	
1	2,700	1	100
1	3,000	1	200
1	4,000	1	300
1	5,000	2	400
2	10,000	1	500
2	15,000	1	600
2	20,000	1	700
2	25,000	1	800
2	30,000	1	1,000
2	35,000	1	5,000
2	40,000	1	10,000
2	50,000		**20,000**
1	60,000		
1	70,000		
1	80,000		
1	90,000		
1	100,000		
1	135,300		
	1,000,000		

Abbreviation: LPF, lignin phenol formaldehyde.

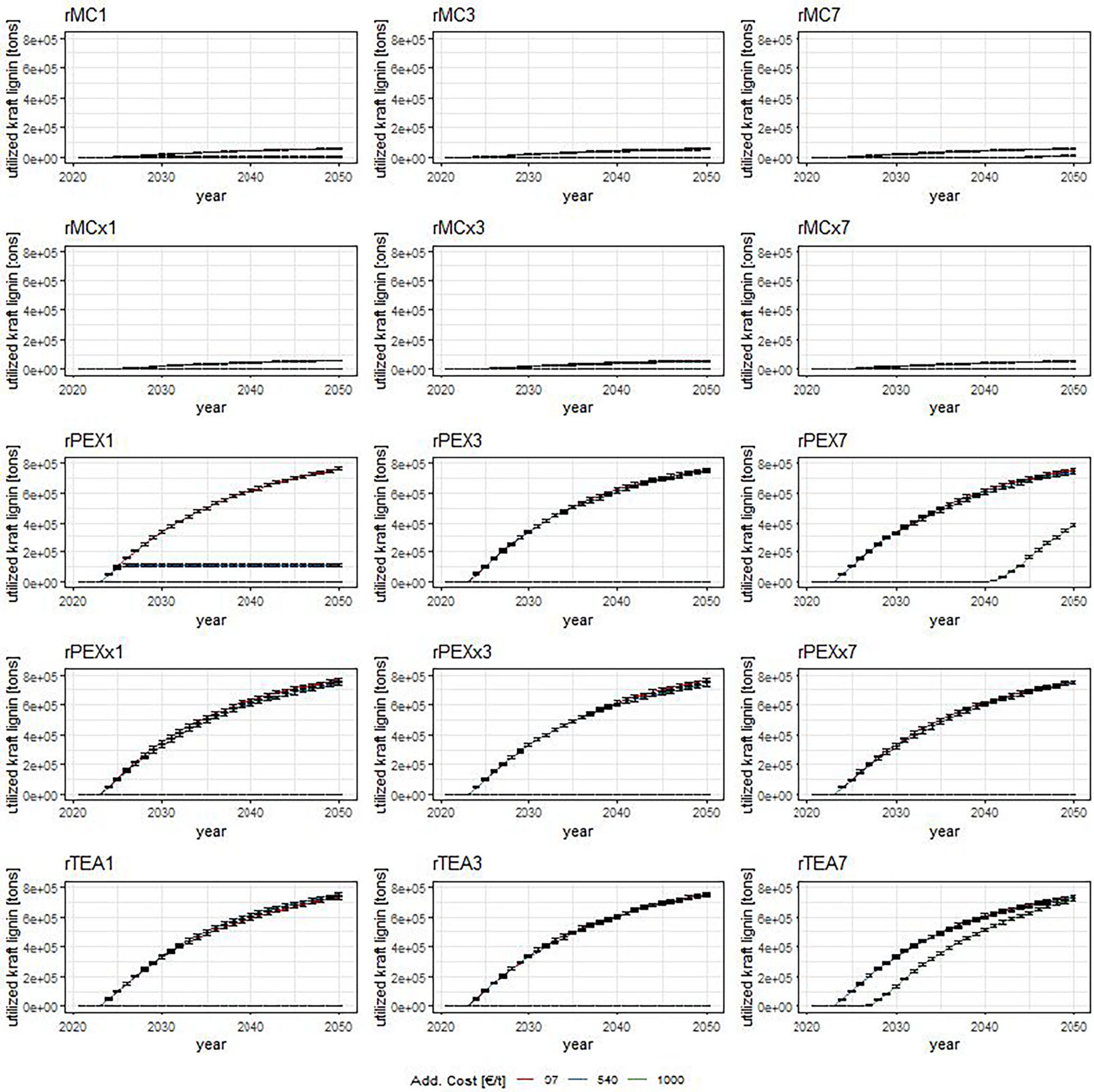

FIGURE A1 Phenol-for-LPF-resins case; kraft lignin utilization development over time (in metric t; $n = 200$; including standard error bars); rows represent five lignin production scenarios, columns represent three crude oil commodity (phenol) price scenarios (column 1: NZ; column 2: AP; column 3: AP including carbon pricing scenario), and respective colored curves represent three different additional cost assumptions. AP, announced pledges (oil price projection variant); LPF, lignin phenol formaldehyde; NZ, net zero emissions by 2050 (oil price projection variant).

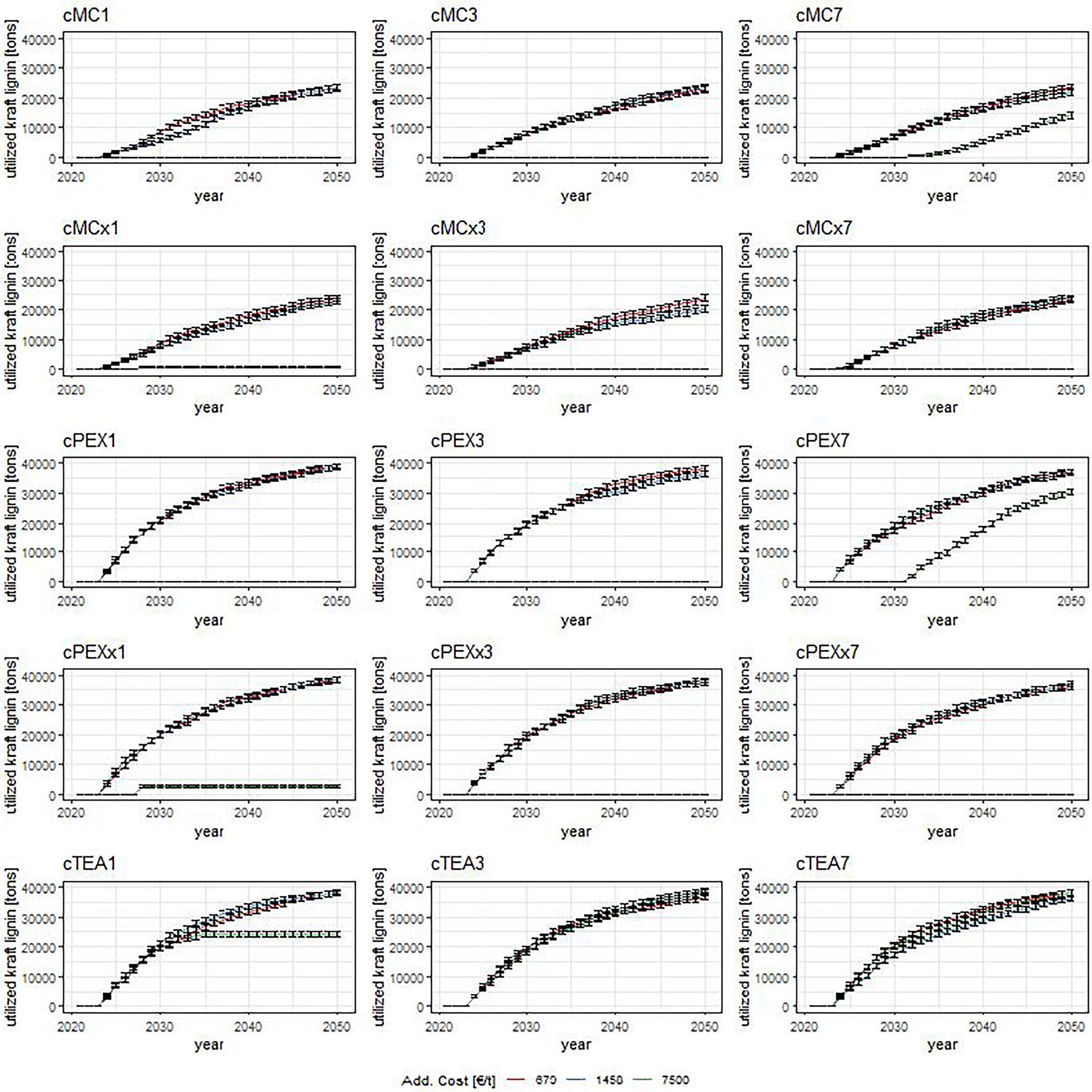

FIGURE A2 Carbon fiber case; kraft lignin utilization development over time (in metric t; $n = 200$; including standard error bars); rows represent five lignin production scenarios, columns represent three crude oil commodity (poly-acrylonitrile) price scenarios (column 1: NZ; column 2: AP; column 3: AP including carbon pricing scenario), and respective colored curves represent three different additional cost assumptions. AP, announced pledges (oil price projection variant); NZ, net zero emissions by 2050 (oil price projection variant).

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TABLE A3 Phenol-for-LPF-resins resp. carbon fiber case; adopted tonnes of kraft lignin and substituted fossil-based commodity in 2030/2040/2050 for respective scenarios (including additional costs).

Product	Scenario	Add. cost (€/t)	Lignin used 2030 (t)	Lignin used 2040 (t)	Lignin used 2050 (t)	Foss. com. subst.2030 (t)	Foss. com. subst.2040 (t)	Foss. com. subst.2050 (t)
Phenols for LPF-resins	rSQ3	97	21,525	47,828	61,606	19,392	43,089	55,501
		540	19,730	41,625	53,141	17,775	37,500	47,875
		1,000	-	-	-	-	-	-
	rPEX3	97	335,369	623,443	756,598	302,135	561,660	681,620
		540	338,692	606,678	746,313	305,128	546,557	672,355
		1,000	-	-	-	-	-	-
	rPEX7	97	335,968	616,916	759,327	302,674	555,780	684,079
		540	330,139	600,436	740,740	297,423	540,934	667,333
		1,000	-	-	383,673	-	-	345,652
	rTEA7	97	334,631	610,008	738,992	301,470	549,557	665,759
		540	330,203	595,321	733,730	297,481	536,326	661,018
		1,000	133,971	515,793	714,684	120,695	464,678	643,860
Carbon fibers	cSQ3	679	8,034	16,805	22,923	3,214	6,722	9,169
		1,458	8,110	17,399	23,425	3,244	6,960	9,370
		7,500	-	-	-	-	-	-
	cPEX3	679	19,324	33,033	38,311	7,730	13,213	15,325
		1,458	19,573	30,493	36,628	7,829	12,197	14,651
		7,500	-	-	-	-	-	-
	cPEX7	679	17,514	30,211	37,096	7,006	12,085	14,839
		1,458	19,141	30,756	37,078	7,657	12,303	14,831
		7,500	-	17,893	30,478	-	7,157	12,191
	cTEA7	679	20,745	32,561	38,103	8,298	13,025	15,241
		1,458	17,424	29,054	36,073	6,970	11,622	14,429
		7,500	20,005	31,534	38,274	8,002	12,614	15,310

Abbreviation: LPF, lignin phenol formaldehyde.

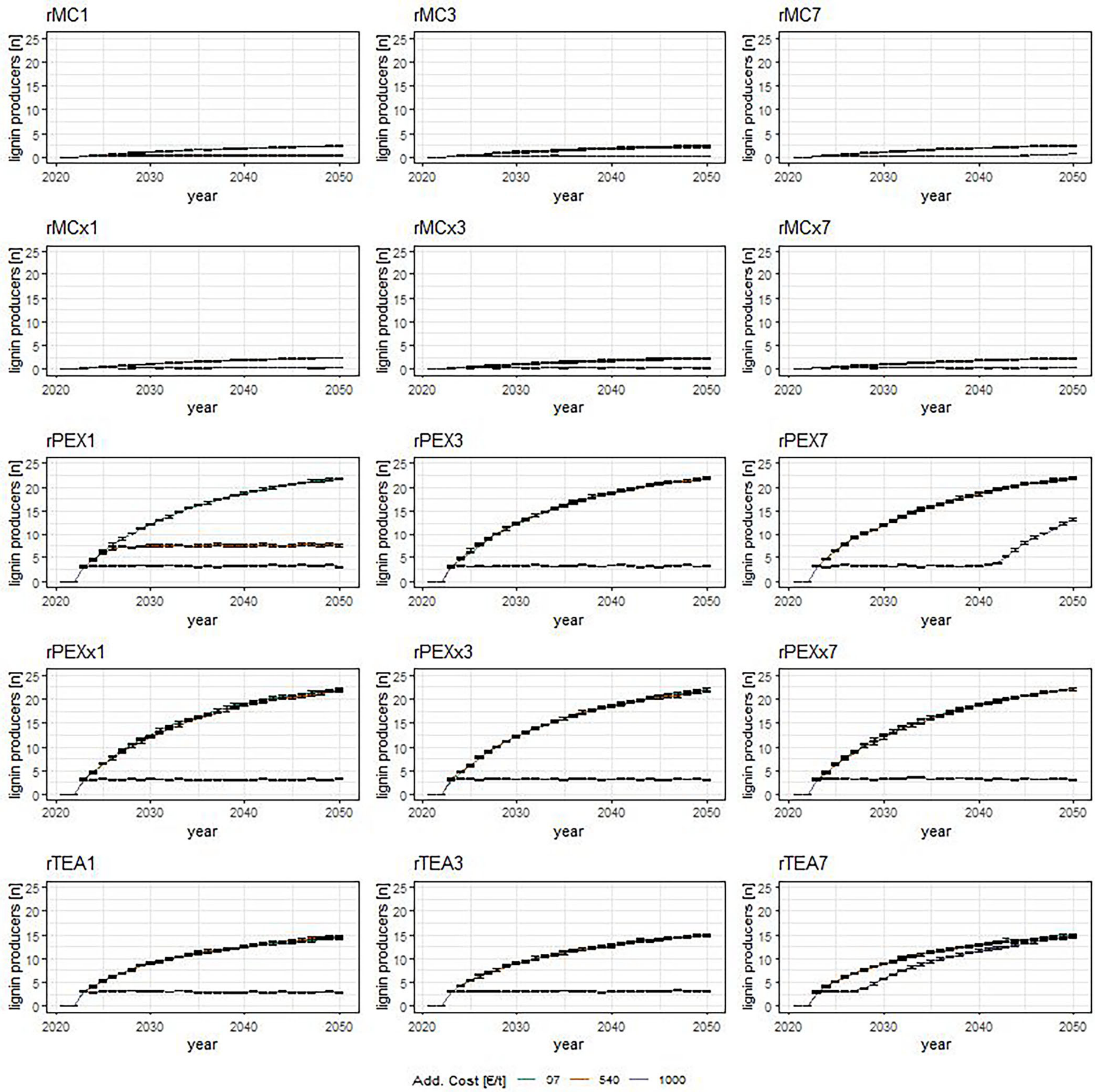

FIGURE A3 Phenol-for-LPF-resins case; number of lignin producers over time ($n = 200$; including standard error bars); rows represent five lignin production scenarios, columns represent three crude oil commodity (phenol) price scenarios (column 1: NZ; column 2: AP; column 3: AP including carbon pricing scenario), and respective colored curves represent three different additional cost assumptions. AP, announced pledges (oil price projection variant); LPF, lignin phenol formaldehyde; NZ, net zero emissions by 2050 (oil price projection variant).

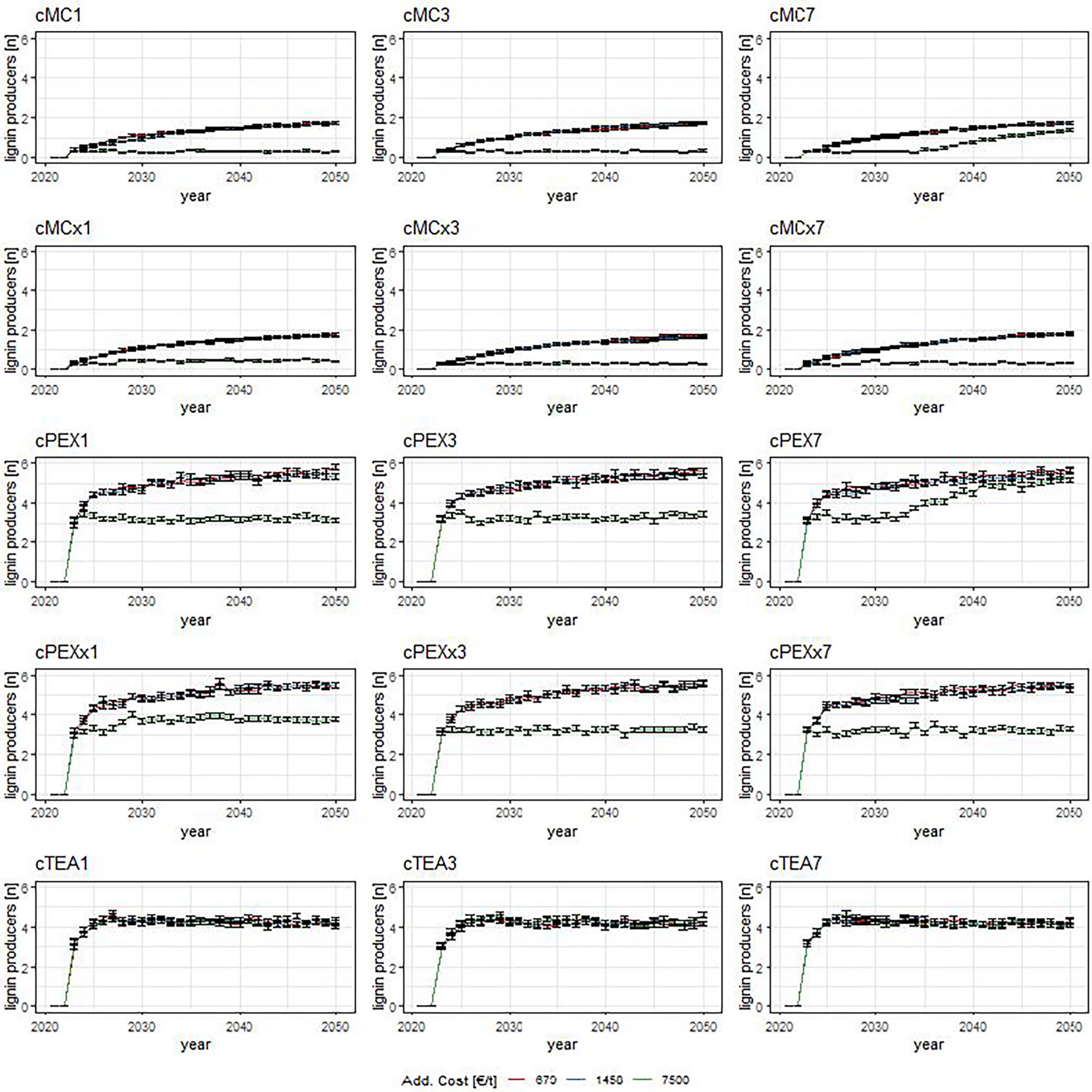

FIGURE A4 Carbon fiber case; number of lignin producers over time ($n = 200$; including standard error bars); rows represent five lignin production scenarios, columns represent three crude oil commodity (phenol) price scenarios (column 1: NZ; column 2: AP; column 3: AP including carbon pricing scenario), and respective colored curves represent three different additional cost assumptions. AP, announced pledges (oil price projection variant); NZ, net zero emissions by 2050 (oil price projection variant).

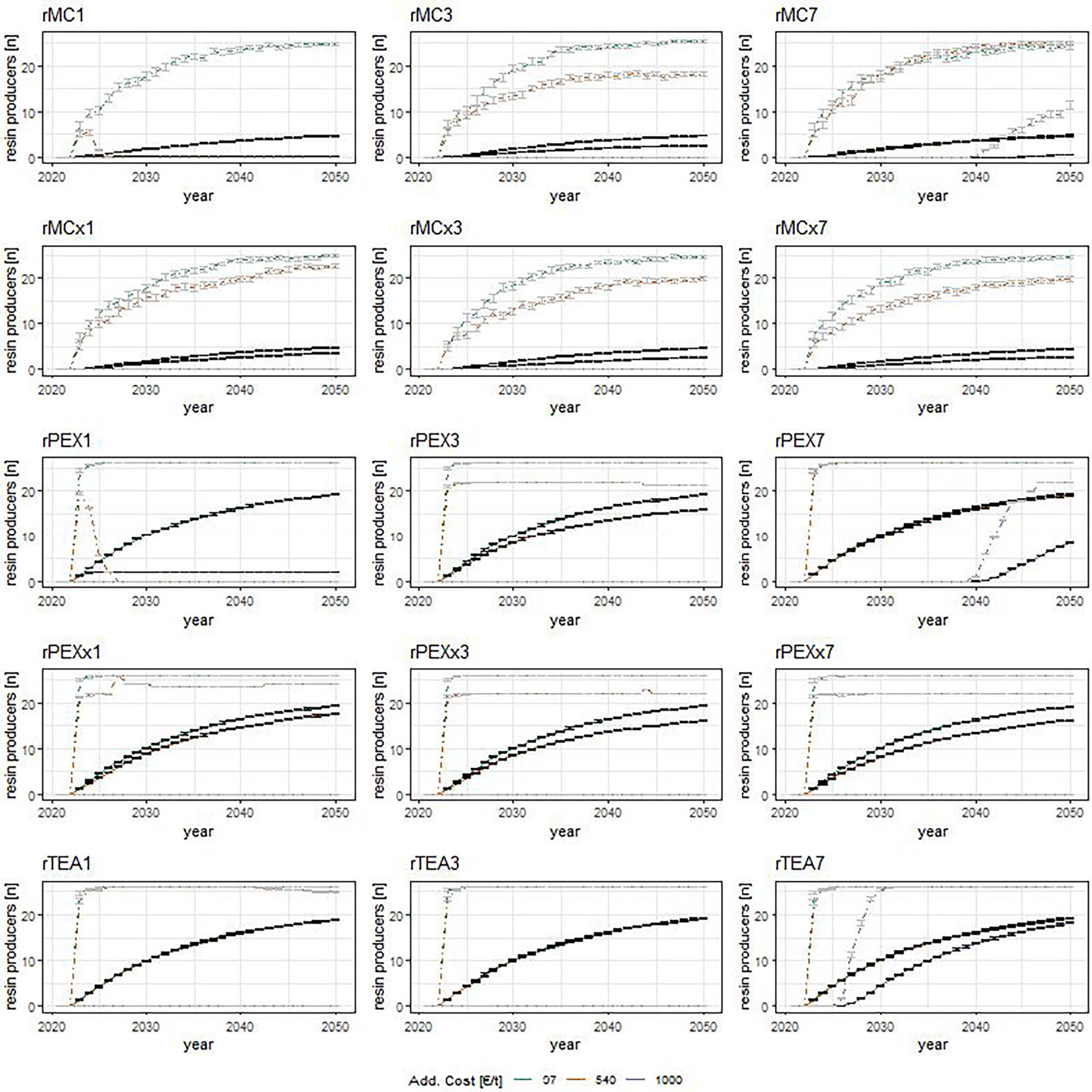

FIGURE A5 Phenol-for-LPF-resins case; number of phenols (resin) producers over time ($n = 200$; including standard error bars); rows represent five lignin production scenarios, columns represent three crude oil commodity (phenol) price scenarios (column 1: NZ; column 2: AP; column 3: AP including carbon pricing scenario), and respective colored curves represent three different additional cost assumptions; light dotted curves represent goods producers for whom adoption seems feasible in a certain time step. AP, announced pledges (oil price projection variant); LPF, lignin phenol formaldehyde; NZ, net zero emissions by 2050 (oil price projection variant).

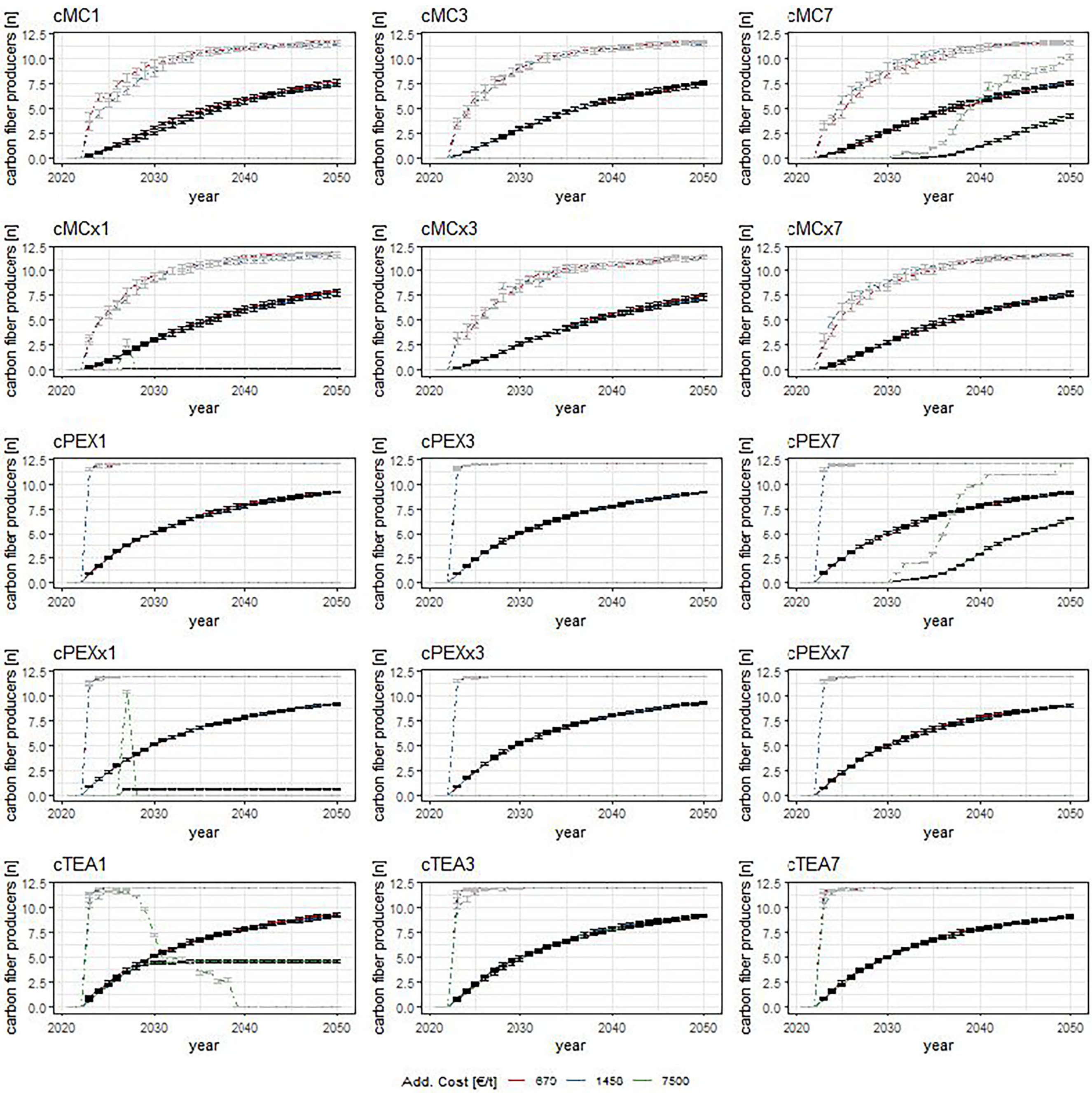

FIGURE A6 Carbon fiber case; number of carbon fiber producers over time ($n = 200$; including standard error bars); rows represent five lignin production scenarios, columns represent three crude oil commodity (phenol) price scenarios (column 1: NZ; column 2: AP; column 3: AP including carbon pricing scenario), and respective colored curves represent three different additional cost assumptions; light dotted curves represent goods producers for whom adoption seems feasible in a certain time step. AP, announced pledges (oil price projection variant); NZ, net zero emissions by 2050 (oil price projection variant).

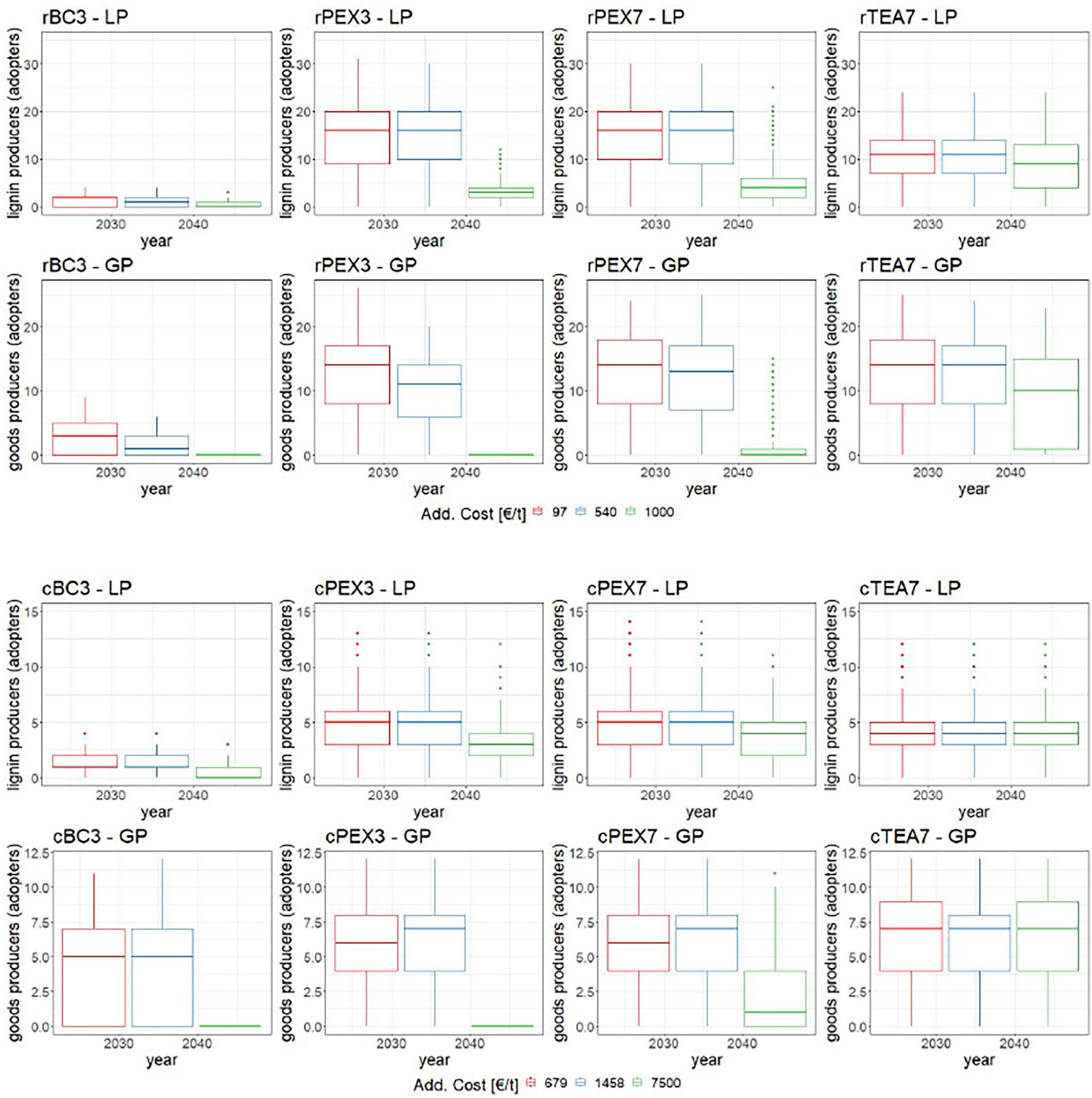

FIGURE A7 Distribution of the adopting lignin and goods producers in the phenols and carbon fiber case; number of adopting producers in 2030, 2040, and 2050.