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RESEARCH ARTICLE

A consequential approach to life cycle sustainability assessment with an agent-based model to determine the potential contribution of chemical recycling to UN Sustainable Development Goals

Raoul Voss[1,2,3] | Roh Pin Lee[1] | Magnus Fröhling[3]

[1]Institute of Energy Process Engineering and Chemical Engineering, Technische Universität Bergakademie Freiberg (TUBAF), Freiberg, Germany

[2]Fraunhofer Institute for Microstructure of Materials and Systems IMWS, Branch Lab Freiberg – Circular Carbon Technologies, Freiberg, Germany

[3]Chair of Circular Economy, Technical University of Munich (TUM), Munich, Germany

Correspondence
Raoul Voss, Institute of Energy Process Engineering and Chemical Engineering, Technische Universität Bergakademie Freiberg (TUBAF), Fuchsmühlenweg 9D, 09599 Freiberg, Germany.
Email: raoul-lukas.voss@iec.tu-freiberg.de

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Abstract

Chemical recycling (CR) could support a circular approach for municipal solid waste (MSW) treatment. In promoting the recirculation of recyclable carbon-containing waste as secondary feedstock for chemical production, it could contribute to resource conservation, emissions reduction, and supply security. To evaluate CR's contribution to the transition from a linear to a circular carbon economy—and correspondingly to the achievement of environmental, economic, and social sustainability as indicated in the UN Sustainable Development Goals (UN-SDGs)—this study builds on extant literature of life cycle sustainability assessment (LCSA) to investigate consequential environmental, economic, and social CR impacts. Specifically, an integrated approach whereby process-based life cycle assessment, techno-economic analysis, and social indicators are linked in the framework of an agent-based model is developed to investigate sustainability consequences of CR via gasification of residual MSW in Germany. Results suggest that CR contributes to reducing climate change and to addressing terrestrial acidification and fossil resource scarcity. However, its deployment will be associated with significant system costs. Hence, to promote CR implementation, measures such as obliging direct waste incineration to trade CO_2 certificates—provided that certificate prices increase sharply in the future—as well as implementing a recycling rate are found to be necessary to gap economic disadvantages. This study not only contributes to extending life cycle approaches for LCSA methodologically, it furthermore provides valuable insights into temporal and spatial interactions in waste management systems to inform science, industry, and politics about the sustainability impacts of CR on the achievement of the UN-SDGs. This article met the requirements for a gold-gold *JIE* data openness badge described at http://jie.click/badges.

KEYWORDS
circular economy, gasification, industrial ecology, municipal solid waste, techno-economic analysis, waste incineration

1 | INTRODUCTION

Today, municipal solid waste (MSW) remains predominantly landfilled or incinerated in numerous countries (Kaza et al., 2018). These linear “cradle-to-grave” disposal pathways are associated with significant environmental and social impacts. With global annual MSW quantities anticipated to reach around 3.5 billion tonnes in 2050 (Chen et al., 2020; Riahi et al., 2017), the sustainable management of MSW is becoming an increasingly urgent priority for many nations (Lee et al., 2020). At the same time, precarious developments ranging from climate change, depleting natural resources, to disruptions in industrial production resulting from bottlenecks along international supply chains are additional drivers for the transformation towards a circular approach for MSW treatment. The goal is to recover recyclable materials and to contribute to resource conservation, emission reduction, supply security, and competitiveness (United Nations Industrial Development Organization, 2019, 2021).

With its Circular Economy Action Plan—one of the main pillars of the European Green Deal—the EU has taken a pioneering role in the transition toward a circular economy (European Commission (EC), 2020). In this context, increasing interest in chemical recycling (CR) is observable from science, industry, politics, and the civil society in recent years (Lee et al., 2021; Nessi et al., 2021; Rollinson & Oladejo, 2020; Voss et al., 2021; Zero Waste Europe, 2019). Other than conventional (mechanical) recycling technologies, CR technologies alter the chemical structure of carbon-containing waste per thermochemical processes or the application of chemical agents to produce basic chemicals as feedstocks for the chemical industry, while the recirculation of inorganic waste materials as secondary feedstocks for chemical production is typically not referred to as CR in current discussions. CR technologies are classified generally into solvent-based purification, depolymerization, pyrolysis, and gasification (Keller et al., 2022; Smet & Linder, 2019). In particular, gasification has been identified as a potential alternative to waste incineration for the treatment of heterogenous and “dirty” carbon-containing waste (Lee et al., 2021; Voss et al., 2021). As highlighted by Voss et al. (2021), by focusing on heterogenous waste such as residual MSW (rMSW)—the remaining fraction of MSW following source separation of hazardous and recyclable waste fractions mainly in households or offices which is currently incinerated and/or landfilled (Beylot & Villeneuve, 2013; Sahimaa et al., 2015; Umweltbundesamt (UBA), 2018c)—CR in the form of gasification will not compete with mechanical recycling for pure waste streams. Rather, it will enable the recirculation of a wider spectrum of carbon-containing waste as secondary carbon feedstock back into the production loop—instead of as an energy feedstock for waste incineration—for higher value-added production.

In supporting the transition toward a circular carbon economy, CR in the form of gasification (cf. Section 2.3) could contribute to environmental, economic, and social sustainability as indicated in the 17 UN Sustainable Development Goals (UN-SDGs). Specifically, 12 of the 17 UN-SDGs within the UN Post-2015 Development Agenda explicitly or implicitly call for sustainable waste treatment and the global transformation from (linear) value chains to value cycles to facilitate a sustainability transition in our society (Wilson et al., 2015). To determine the contribution of gasification to the achievement of the UN-SDGs, it is necessary to quantify the systemic and multidimensional consequences which will be associated with its deployment in comparison to the linear status quo.

However, to date, CR literature—with its predominant focus on evaluating the technical applicability of CR technologies (Ragaert et al., 2017; Solis & Silveira, 2020; Thiounn & Smith, 2020)—provides limited insights to support a systemic evaluation of its potential impacts and contribution to environmental, economic, and social sustainability. To address this gap, current life cycle assessments (LCA) for CR (de Andrade et al., 2016; Keller et al., 2020; Voss et al., 2022; Zamani et al., 2015) can provide a methodological basis, but need to be further developed regarding four central shortcomings:

- The top-down, aggregate, and point-in-time nature of archetypal LCA, which neglects relevant economic or social impacts,
- the predominance of isolated process evaluations that ignore systemic issues such as intersectoral linkages and industrial dynamics (Davidson et al., 2021; Shen et al., 2010),
- the lack of consequential assessments which limits knowledge about the systemic impacts of regulatory decisions on CR (Fröhling & Hiete, 2020; Voss et al., 2021),
- and the focus on the pyrolysis of pure (plastic) waste streams which represents a potential competition to mechanical recycling (Ragaert et al., 2017; Rollinson & Oladejo, 2020), and which neglects/ignores the potential applicability of CR for heterogenous and “dirty” waste (BASF, 2020; Davidson et al., 2021; Shen et al., 2010; Wollny et al., 2001; Volk et al., 2021; Zhang et al., 2020).

To address the identified shortcomings, this study develops a comprehensive life cycle sustainability assessment (LCSA) approach which links (1) process-based LCA methods, (2) techno-economic analysis (TEA), and (3) social indicators within the framework of an agent-based model (ABM) to investigate consequential environmental, economic, and social impacts that will be associated with gasification's deployment for CR so as to determine its potential contribution to achieving a circular carbon economy and consequently, the UN-SDGs. Compared to traditional equilibrium or optimization models, ABM refers to a bottom-up modeling paradigm for complex systems of heterogeneous agents that communicate, perceive system states, evolve, and make decisions to represent multiple solutions and path dependencies in technological transformation processes (Breun et al., 2017; Mercure et al., 2016). Previous research has shown that the combination of ABM with LCSA can support a realistic mapping of agent interactions and resulting sustainability dynamics in adaptive waste management systems (Hatik et al., 2020; Wu et al., 2017; Zupko, 2021).

The investigation focuses on Germany—a pioneer in waste separation and recycling with numerous chemical sites for direct integration of CR products into existing production chains (Lee et al., 2020)—to investigate environmental, economic, and social impacts which will be associated with CR of heterogenous and "dirty" waste in the form of rMSW via gasification on a country level (i.e. entire German territory). The methodological objective is to elaborate that an integrated LCSA approach linking LCA, TEA, and social indicators to an ABM can contribute quantitative insights into systemic impacts (i.e., temporal and spatial interactions) on waste management systems as well as impacts of emergent regulatory and market dynamics on CR and demonstrate its applicability through the described case of Germany.

The study is structured as follows: Section 2 introduces the study context, while Section 3 presents the integrated LCSA approach. Then, Section 4 reports and discusses central modeling results, before Section 5 concludes with a summary of key findings, limitations, and suggestions for future research.

2 | STUDY CONTEXT

2.1 | Residual municipal solid waste

In Germany, rMSW includes waste assigned to waste code numbers EAV-20030100-U for "not differentiable mixed municipal waste" and EAV-20030101-U for "household waste, household-type commercial waste" in the national waste classification system (Statistisches Bundesamt (DESTATIS), 2020a). As of 2018, 15 million tonnes rMSW is produced in the country with fractional composition and chemical characteristics as discussed in Section 3.1.3 (DESTATIS, 2021). Note that Figure S1 in Supporting Information S1 illustrates the spatial distribution of waste production based on data for the 401 administrative areas (NUTS 3) in Germany (DESTATIS, 2020b).

2.2 | Current treatment of rMSW in Germany

After its production in administrative areas, rMSW is transported to primary treatment plants. Today, primary treatment plants include 66 municipal solid waste incinerators (MSWIs) where unsorted rMSW is incinerated to produce electricity/heat, and 44 mechanical–biological treatment (MBT) plants where rMSW is processed via mechanical sorting to separate—inter alia—metals, in addition to biological treatment to stabilize organic contents for deposition (DESTATIS, 2021; UBA, 2018b, 2018c). Besides metals, mechanical sorting also separates high calorific value fractions such as plastics to produce a refuse-derived fuel (RDF) for energetic utilization in secondary treatment plants. Secondary treatment plants include 32 RDF power plants where RDF is incinerated to produce electricity/heat, 8 coal power plants with the permission to substitute coal per RDF for electricity/heat generation, and 36 cement works where RDF is utilized to provide thermal energy for clinker burning (UBA, 2018b, 2018c). Note that Figure S1 in Supporting Information S1 illustrates the location of all primary/secondary treatment plants in Germany according to UBA (2018c).

2.3 | Alternative treatment of residual municipal solid waste via waste gasification

Due to its heterogeneous composition, rMSW is challenging to recycle not only per conventional mechanical recycling techniques, but also per CR processes such as depolymerization and pyrolysis (Ragaert et al., 2017; Seidl et al., 2021). As a significant source of secondary carbon, rMSW is thus used mainly as an energy feedstock for electricity/heat production in Germany today (cf. Section 2.2). Via incineration, 100% of the carbon contained in rMSW will be emitted into the environment mainly as CO_2 (Lee et al., 2018). Thus, incineration is associated with diverse climate and social challenges ranging from air pollution through particulate matter, safe disposal of toxic fly ash, to public resistance (Lee et al., 2020, 2021). In order to achieve the goals stated in the European Green Deal and in the UN-SDGs, there is thus revived interest in a circular utilization of rMSW as a chemical feedstock via gasification (Enerkem, 2019; Lee et al., 2020; Voss et al., 2021).

Gasification refers to the thermochemical conversion of carbon resources under high temperatures and mostly high-pressure conditions (Lee et al., 2020; Voss et al., 2021). It produces a synthetic gas (syngas) consisting of carbon monoxide and hydrogen which can be processed to produce fuels or chemical intermediates such as methanol/olefins via synthesis processes (Keller et al., 2020; Scheithauer et al., 2021). Due to high process temperatures (1000–1400°C), gasification is robust against feedstock impurities (Seidl et al., 2021). This represents a significant advantage for the application to heterogeneous rMSW compared to alternative CR technologies such as solvent-based purification, depolymerization, and pyrolysis (Janajreh & Raza, 2015; Lee et al., 2021). Pioneering developments in the co-utilization of rMSW with coal for chemical production via gasification were carried out in Berrenrath and Schwarze Pumpe in Germany in the 1990s to 2000s (Lee et al., 2017a, 2017b; Schmalfeld & Arendt, 2008). Today, rMSW gasification is also carried out, for example, by Enerkem in Edmonton in Canada, with diverse other international projects in the pipeline (cf. Lee et al., 2021 for an overview of previous and current waste gasification activities).

As key chemical intermediates, olefins—the basic materials for the production of polyolefins (i.e., plastics)—are produced today mainly via steam cracking from crude oil in Germany (Keller et al., 2020). rMSW—in the form of RDF following treatment in MBT plants—can also be used as an alternative carbon feedstock for olefins production via waste gasification. Fleiter et al. (2013) report nine chemical production sites in Germany that are equipped with a steam cracking plant (cf. Supporting Information S1, Figure S1). These sites present attractive locations for CR implementation as they not only have the essential infrastructure to enable immediate feed-in of gasification products, they furthermore possess the appropriate know-how and trained personnel in chemical conversion processes (Keller et al., 2020; Ren et al., 2006). The present study thus investigates the systemic and multidimensional impacts which will be associated with olefins production via rMSW gasification—with site integration in existing chemical production sites—compared to the linear status quo.

3 | METHODS

This research applies integrated LCSA, facilitating consequential assessments of sustainability impacts associated with rMSW treatment via linking process-based LCA, TEA, and social indicators in an ABM framework. Specifically, it develops an LCSA environment including all relevant treatment pathways for rMSW in Germany (Section 3.1). Then, following consequential principles, an ABM captures temporal system dynamics resulting from interactions between waste producers and processors under dynamic framework conditions (Section 3.2).

3.1 | Life cycle sustainability assessment

3.1.1 | Goal and scope definition

Goal is to assess environmental, economic, and social impacts of CR for rMSW treatment in Germany to understand CR's contribution to achieving UN-SDGs. The functional unit is defined as treating the total amount of wet rMSW produced annually in Germany. The geographic scope is set to the national borders without consideration of waste imports/exports, representing an exception for German rMSW (DESTATIS, 2020b, 2021).

3.1.2 | System boundary definition

Figure 1 presents the system environment extending from rMSW production in administrative areas to product distribution after one/two stages of waste treatment. Upstream rMSW generation impacts are excluded due to a zero-burden approach (Montejo et al., 2013). Supply and product impacts are accounted for by system expansion per background system, assuming that treatment products substitute conventional market products. Applied background system data (cf. Supporting Information S1, Table S1) refer to specific or market average values and are drawn from GaBi (2019) and United Nations (2021). Based on Montejo et al. (2013), recovered ferrous and non-ferrous scraps substitute primary steel and aluminum at 87% and 79% ratios, respectively. In contrast, substitution coefficients for electricity/heat and chemical products are set to 100% as conventional product quality is assumed (Keller et al., 2020; Voss et al., 2021).

3.1.3 | Waste characterization

Fractional rMSW composition (cf. Supporting Information S1, Table S2) and chemical characteristics (cf. Supporting Information S1, Table S3) are assumed based on Voss et al. (2021) as national averages.

3.1.4 | Inventory analysis

Waste and RDF are transported per fully loaded semitrailer truck consuming 0.021 L diesel tonnes^{-1} km^{-1} (Olesen, 2013). Additionally, the inventory includes information about six relevant rMSW/RDF treatment processes (cf. Table 1). Process inventories are generated from LCA studies, technical reports, scientific publications, and LCA databases. Specifically, applied inventory data for MSWIs, MBT plants, RDF power plants, and CR plants are based on Voss et al. (2021) (cf. Supporting Information S1, Tables S4 to S14). Inventories for RDF utilization in cement works and coal power plants are generated from Reza et al. (2013) where RDF replaces conventional fuel at equivalent thermal energy production (cf. Supporting Information S1, Tables S15 to S21).

TABLE 1 Process inventories

	MSWI	MBT plant	RDF-PP	Cement work	Coal-PP	CR plant
Ref. capacity [kt a^{-1}]	310	110	190	73	240	480
FCI [MEUR]	160	43	110	2.6	32	580
Process steps						
Delivery	●	●	●	●	●	●
Grate firing	●		●			
Metal separation	●		●			
Mechanical treatment		●				
Anaerobic digestion		●				
Biogas combustion		●				
Tunnel rotting		●				
Lignite substitution				●		
Hard coal substitution					●	
Gasification						●
(Flue) gas treatment	●	●	●		●	●
Syntheses to olefins						●
Labor						
Skilled labor [TEH a^{-1}]	14	13	12	0.45	0.68	12
Unskilled labor [TEH a^{-1}]	79	73	69	2.5	3.8	66
Supplies						
Activated carbon [kg t^{-1}]	0.8	–	0.8	–	0.8	–
Ammonia [kg t^{-1}]	5.9	–	5.9	–	–	–
Calcium carbonate [kg t^{-1}]	12	–	12	–	–7	–
Diesel [L t^{-1}]	0.71	1.6	0.63	–	–	-
Electricity [kWh t^{-1}]	–	–	–	10	29	420
Fuel oil [L t^{-1}]	2	–	2	–	–	–
Nitric acid [kg t^{-1}]	–	3.5	–	–	–	–
Sodium hydroxide [kg t^{-1}]	3	–	3	–	12	9
Products						
Chemical by-products [kg t^{-1}]	–	–	–	–	–	45
Electricity [kWh t^{-1}]	320	120	910	–	–	–
Ethylene [kg t^{-1}]	–	–	–	–	–	120
Fe scrap [kg t^{-1}]	6.8	6.5	4.7	–	–	–
Heat [kWh t^{-1}]	930	86	2200	–	–	710
N-Fe scrap [kg t^{-1}]	1	5.8	0.86	–	–	–
Propylene [kg t^{-1}]	–	–	–	–	–	130
Emissions						
Bottom ash/slag [kg t^{-1}]	170	–	95	–	–	99
CO_2-eq [kg t^{-1}]	270	6.5	820	810	810	410
Composting residues [kg t^{-1}]	–	260	–	–	–	–
Fly ash [kg t^{-1}]	26	–	14	–	–	–
RDF [kg t^{-1}]	–	250	–	–	–	–
SO_2-eq [kg t^{-1}]	0.23	0.023	0.31	0.3	0.3	0.17

Abbreviations: CR, chemical recycling; FCI, fixed capital investment; Fe, ferrous; LPG, liquified petroleum gas; MBT, mechanical–biological treatment; MSWI, municipal solid waste incinerator; N-Fe, non-ferrous; PP, power plant; RDF, refuse-derived fuel; rMSW, residual municipal solid waste; TEH, thousand employee hours.

Underlying values are rounded to two significant digits. Dataset available at: https://doi.org/10.5281/zenodo.6323442

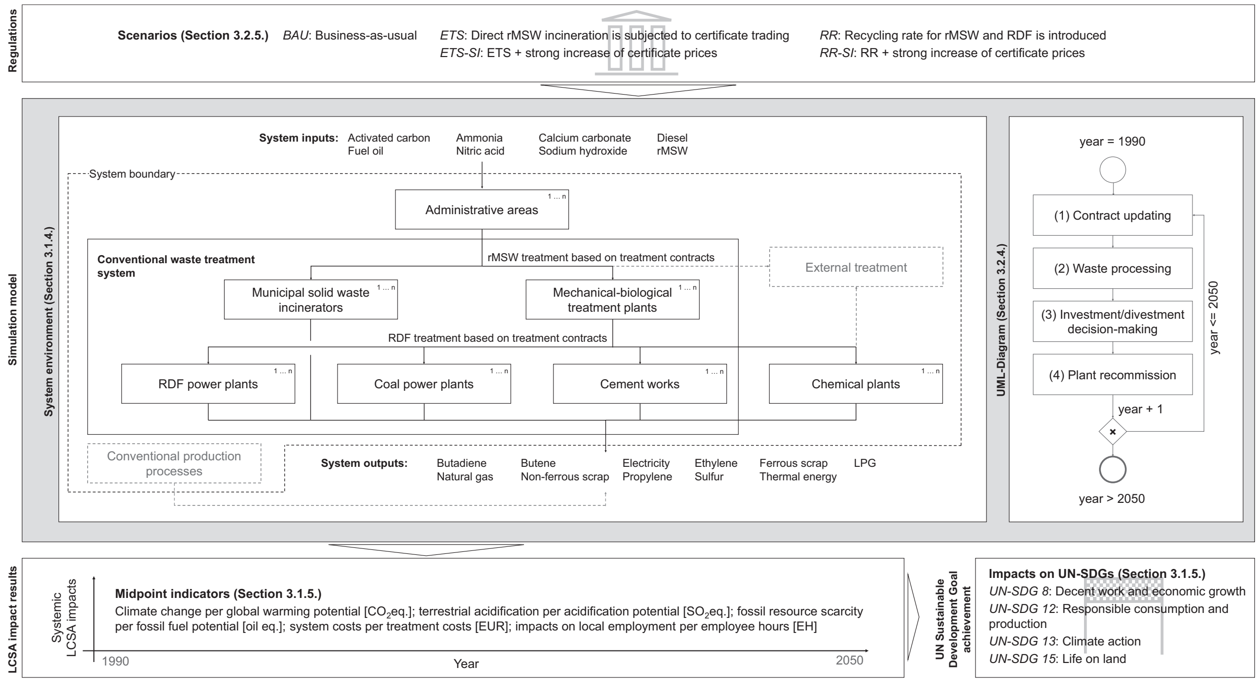


FIGURE 1 Consequential life cycle sustainability assessment (LCSA) system. BAU, business-as-usual; EH, employee hours; ETS, emission trading system; LPG, liquified petroleum gas; MEUR, million euros; RDF, refuse derived fuel; rMSW, residual municipal solid waste; RR, recycling rate; SI, strong increase; UN-SDG, UN Sustainable Development Goal

TABLE 2 LCSA midpoint indicators and associated SDGs

Sustainability dimension	Midpoint indicator	Mechanism	Associated SDG
Environmental	Climate change	Global warming potential (GWP100) based on Intergovernmental Panel on Climate Change (IPCC) (Pachauri & Mayer, 2015)	UN-SDG 13 *Climate action* based on Wilson et al. (2015)
	Terrestrial acidification	Acidification potential (AP) based on ReCiPe (Huijbregts et al., 2017)	UN-SDG 15 *Life on land* based on Kan and Meijer (2020)
	Fossil resource scarcity	Fossil fuel potential (FFP) based on ReCiPe (Huijbregts et al. 2017)	UN-SDG 12 *Responsible consumption and production* based on Harmes and Meijer (2020)
Economic	System costs	Treatment costs (TC) based on Voss et al. (2021)	UN-SDG 8 *Decent work and economic growth* based on Wilson et al. (2015)
Social	Impact on local employment	Employee hours (EH) based on Wu et al. (2017)	UN-SDG 8 *Decent work and economic growth* based on Wilson et al. (2015)

3.1.5 | Impact assessment

Table 2 presents applied LCSA midpoint indicators (MI) along environmental, economic, and social dimensions including their connections with UN-SDGs. Environmental sustainability is assessed based on Voss et al. (2022), Keller et al. (2020), and Meys et al. (2020) with a global warming emissions factor for biogenic carbon emissions equal to zero (Pachauri & Mayer, 2015). Economic sustainability is assessed based on Voss et al. (2021) per MI *System costs* reflecting the decision-relevant component of environmental life cycle costs (eLCC). Social sustainability is assessed based on Wu et al. (2017). Note that, as per Wu et al. (2017), the integration and temporal dynamization of impacts from individual LCSA dimensions per systemic modeling is focused in this research rather than exploring an extensive number of impact categories.

3.2 | Agent-based model

3.2.1 | Agent-based model characteristics

The ABM regulating systemic waste flows is implemented per MATLAB R2019a (MathWorks, 2019). The simulation period extends from 1990 to 2050 to also cover previous system developments for model validation. The temporal resolution is set to 1 year of waste production/treatment.

3.2.2 | Agent characteristics

The agent system (cf. Supporting Information S1, Figure S1) includes 401 administrative areas and 195 primary/secondary treatment plants (cf. Section 2). Administrative areas are characterized by geographic location and annual rMSW production volumes. Geographic location data are generated with QGis V3.12 based on digital map data provided by German authorities (Bundesamt für Kartographie und Geodäsie, 2019; QGis Development Team, 2009). Annual rMSW production volumes (cf. Supporting Information S1, Table S22) refer to data by the German Federal Statistical Office as further described in Supporting Information S1, Section 5 (DESTATIS, 2020b, 2021).

Treatment plants are characterized by geographic location, treatment capacity, year of commission, and fixed capital investment (FCI). Geographic location, treatment capacity, and year of commission are drawn from UBA (2018c). FCI for each plant is calculated as per Equation (1) (Peters et al., 2004; Sinnott & Towler, 2020). Specifically, FCI data as displayed in Table 1 drawn mainly from Voss et al. (2021) and UBA (2018b) are adjusted per power factor applied to a capacity ratio approach for individual treatment plants to reflect economies of scale (Brennan, 2020). Additionally, the Chemical Engineering Plant Cost Index (CEPCI) is applied for temporal price adjustments (Chemical Engineering, 2020). A detailed overview of treatment plant data is provided in Supporting Information S1, Tables S23 to S32.

$$FCI = FCI_{rp} \left(\frac{cap}{cap_{rp}} \right)^{\varkappa^{inv}} \left(\frac{pindex}{pindex_{ry}} \right) \tag{1}$$

where

cap … Capacity [t]

cap_{rp}… Capacity of reference plant [t]

FCI … Fixed capital investment [€]

FCI_{rp} …Fixed capital investment of reference plant [€]

$pindex_{ry}$ … Price index in reference year [-]

$pindex$ … Price index in year of commission/recommission [-]

$\varkappa^{inv}$ … Scaling power factor [-]

3.2.3 | Transportation distances

A dataset for transportation distances to primary/secondary treatment plants is generated per self-programmed Microsoft Excel macro for aggregated Microsoft Bing queries (Microsoft Corporation, 2019, n.d.).

3.2.4 | Model iteration steps

As illustrated in Figure 1, each model iteration reflects 1 year of rMSW production/treatment including four consecutive steps: (1) contract updating, (2) waste processing, (3) investment/divestment decision-making, and (4) plant recommission:

In step (1) contract updating, treatment contracts between administrative areas and primary treatment plants as well as between MBT plants and secondary treatment plants are updated. Specifically, treatment contracts are limited by time (1–5 years) and closed via competitive tendering (Jänicke, 2020; UBA, 2018b). A tendering competition is initiated by an administrative area or MBT plant if the rMSW or RDF production volume exceeds the volume that is covered by pending treatment contracts. In a tendering competition, primary or secondary treatment plants provide a treatment offer on the condition they have capacity available. Available capacity is defined as 90% of total plant capacity reduced by pending treatment contract volumes and capacities blocked by system external waste fractions such as bulky waste (SWB, 2020; UBA, 2018c; Voss et al., 2021; Wolfersdorf et al., 2017). Blocked capacity (cf. Supporting Information S1, Table S33) is estimated by applying data on fraction-specific treatment quantities for all plant types provided by DESTATIS (2021) as further described in Supporting Information S1, Section 7. If the available plant capacity is sufficient, a treatment offer is calculated.

Treatment offers are calculated with a plant internal view to reflect the restricted flow of information in German tendering competitions causing imperfect agent knowledge (Bundesamt für Justiz (BfJ), 2022; Vergabe24, 2022): First, based on Voss et al. (2021), total plant costs are calculated including capital expenses, maintenance and repair costs, labor costs, and so on (cf. Equations 2–11). Second, processed waste for the year is estimated at minimum 80% of plant capacity corresponding to a 20% plant idle time that includes (1) reduced availability due to maintenance and repairs and (2) decreasing ability to accept new treatment contracts as plant capacity utilization increases (cf. Equation 12). Third, applying Equation (13), total plant costs are divided by processed rMSW/RDF in the year and augmented by transportation costs and plant internal profits—modeled as the cost gap to the best competitor in the tendering competition—to determine the treatment cost offer (cf. Supporting Information S1, Table S34 for economic parameters). Note that for lignite or hard coal substitution in cement works or coal power plants, Equation (14) is applied that additionally considers cost savings due to reduced conventional fuel consumptions (Gendebien et al., 2003; Reza et al., 2013).

$$CF_1 = \frac{FCI}{olt} \tag{2}$$

where

CF_1 … Capital expenses [€]

FCI … Fixed capital investment [€]

olt … Operational lifetime [a]

$$CF_2 = FCI\,(insur + lTax) \tag{3}$$

where

CF_2 … Local taxes and insurances [€]

FCI … Fixed capital investment [€]

$insur$ … Insurances percentage [%]

$lTax$ … Local taxes percentage [%]

$$CF_3 = FCImaint\,(1 + consum) \tag{4}$$

where

CF_3 … Maintenance and repair [€]

$consum$ … Consumables percentage [%]

FCI … Fixed capital investment [€]

$maint$ … Maintenance and repair percentage [%]

$$CF_4 = (sEmploysRate + usEmployusRate)\,(1 + supervis) \tag{5}$$

where

CF_4 … Labor [€]

$sEmploy$ … Skilled employee hours [h]

$sRate$ … Hourly rate for skilled labor [€ h^{-1}]

$supervis$ … Supervision percentage [%]

$usEmploy$ … Unskilled employee hours [h]

$usRate$ … Hourly rate for unskilled labor [€ h^{-1}]

$$CF_5 = CF_4 overhd \tag{6}$$

where

CF_4 … Labor [€]

CF_5 … Overhead [€]

$overhd$ … Overhead percentage [%]

$$CF_6 = \frac{CF_4 admin}{1 + supervis} \tag{7}$$

where

admin … Administration percentage [%]

CF_4 … Labor [€]

CF_6 … Administration [€]

supervis … Supervision percentage [%]

$$CF_7 = \sum_s requi_s price_s \tag{8}$$

where

CF_7 … Supplies [€]

$price_s$ … Price for *s* [€ t^{-1}]

$requi_s$ … Total requirements *s* [t]

s … Supply [-]

$$CF_8 = \sum_{str} outp_{str} dist_{str} tRate \tag{9}$$

where

CF_8 … Transportation [€]

$dist_{str}$ … Transportation distance for *str* [km]

$outp_{str}$ … Output of *str* [t]

str … Solid treatment residue [-]

tRate … Transportation cost rate [€ t^{-1} km^{-1}]

$$CF_9 = \sum_{em} outp_{em} costs_{em} \tag{10}$$

where

CF_9 … Environmental expenses [€]

$costs_{em}$ … Price for handling/treatment of *em* [€ t^{-1}]

em … Emission/contaminant [-]

$outp_{em}$ … Output of *em* [t]

$$CF_{10} = -\sum_{prod} outp_{prod} price_{prod} \tag{11}$$

where

CF_{10} … Revenues [€]

$outp_{prod}$ … Output of *prod* [t]

$price_{prod}$ … Selling price for *prod* [€ t^{-1}]

prod … Product [-]

$$appcap = \begin{cases} curcap & curcap > 0.8 \\ 0.8 & curcap \leq 0.8 \end{cases} \tag{12}$$

where

appcap … Applied capacity utilization rate [%]

curcap … Current capacity utilization rate [%]

$$TO = \frac{\sum_{k=1}^{10} CF_k}{appcap * cap} + disttRate2 + profits \tag{13}$$

$$TO_{substitution} = \frac{\sum_{k=1}^{7} CF_k}{appcap * cap} + disttRate2 + profits - fcosts \frac{fcal}{wcal} \tag{14}$$

where

appcap … Applied capacity utilization rate [%]

cap … Plant capacity [t]

dist … Transportation distance [km]

fcal … Fossil resource calorific value [GJ t^{-1}]

fcosts … Fossil resource costs [€ t^{-1}]

profits … Plant internal profits [€ t^{-1}]

TO … Treatment offer [€ t^{-1}]

$TO_{substitution}$ … Treatment offer for substitution [€ t^{-1}]

tRate … Transportation cost rate [€ t^{-1} km^{-1}]

wcal … Waste calorific value [GJ t^{-1}]

Administrative areas or MBT plants decide for the best offer they receive according to the "Principle of Economical Budget Management" (Jänicke, 2020). Note that based on Skeldon et al. (2018), administrative areas or MBT plants close contracts with system external plants if they receive no offer (cf. Figure 1). System external plants include plants not reflected in the system as they belong to plant types that are underrepresented in Germany or designed primarily for the treatment of other waste fractions such as bulky waste sorting plants (UBA, 2018b). External treatment costs are set to €50/150 $tonne^{-1}$ rMSW/RDF in 1990 with a 5% annual increase. Environmental and social impacts for external treatment are modeled per annual average values for system internal treatment.

In step (2) waste processing, sustainability impacts (cf. Section 3.1.5) are calculated for each plant—based on processed rMSW/RDF as fixed in pending treatment contracts—before they are aggregated for the entire system. Specifically, to determine environmental sustainability, process impacts are considered in addition to upstream and downstream impacts (cf. Section 3.1.2). To determine economic sustainability, total rMSW treatment costs including transportation are determined for all administrative areas. Eventually, to determine social sustainability impacts, required employee hours for rMSW/RDF treatment is determined via subtracting required labor to process system external waste fractions from total required labor in all treatment plants.

Step (3) investment/divestment decision-making involves decisions about treatment plant constructions/deconstructions. For MSWIs, MBT plants, and RDF power plants, investment/divestment decision-making involves multiple steps: First, a waste processing estimate (WPE) is generated for the next year per first-order linear regression applying previous waste processing volumes. Then, the WPE is increased by 20% reflecting plant downtimes or non-utilized capacity, and subsequently reduced by already realized capacity (RC) to calculate the investment/divestment capacity (IDC) (cf. Equation 15).

$$IDC = 1.2WPE - RC \tag{15}$$

where

IDC … Investment/divestment capacity [t]

RC … Realized capacity [t]

WPE … Waste processing estimate [t]

For negative IDC, treatment plants with equivalent capacity are decommissioned, with plants operating most inefficiently based on current capacity utilization being decommissioned first. For positive IDC, treatment plants with equivalent capacity are commissioned at one of 16 potential sites located in the centers of the 16 German states (NUTS 2) as illustrated in Supporting Information S1, Figure S2. For location identification, the net present value (NPV) criterion—the difference between the total present value of all cash flows and the present value of all capital investments (Peters et al, 2004)—is applied (cf. Equation 16). For NPV calculation, market research is conducted at each potential location to determine regional rMSW/RDF treatment prices. Then, the location with the highest NPV is selected for plant construction.

$$NPV = \sum_{n=1}^{t} \frac{\sum_{k=1}^{10} CF_{n,k}}{(1+i)^n} - FCI \tag{16}$$

where

$CF_{n,k}$ … Annual cashflow [€]

FCI … Fixed capital investment [€]

i … Discount rate [%]

k … Cashflow index [-]

n … year [a]

TABLE 3 Examined scenarios

No	Scenario	Abbr.	Details
1	Business-as-usual	BAU	Current regulation is maintained
2	Emission trading adjustment	ETS	Direct incineration of rMSW in MSWIs is assumed to be subjected to emissions trading which is not the case in Germany so far (UBA, 2019)
3	Recycling rate	RR	An obligatory rate for MBT treatment of rMSW and CR of RDF is introduced that annually increases by 3.5% to reach 100% by 2050, i.e., ban on direct/indirect incineration to support the European goal of climate neutrality (EC, 2019)
4	Emission trading adjustment at strong increase in certificate prices	ETS-SI	Scenario ETS + certificate prices increase linearly to €880 in 2050 based on IPCC (2018) instead of to €180 based on Wagner et al. (2019) in Scenarios BAU, ETS, and RR
5	Recycling rate at strong increase in certificate prices	RR-SI	Scenario RR + certificate prices increase as in ETS-SI

Abbreviations: CR, chemical recycling; MBT, mechanical-biological; MSWI, municipal solid waste incinerator; RDF, refuse-derived fuel; rMSW, residual municipal solid waste.

NPV … Net present value [€]

t … Investment period [a]

CR plants—unlike MSWIs, MBT plants, and RDF power plants—are currently not represented in the German system. Thus, IDC that is derived from previous treatment volumes (cf. Equation 15) is inapplicable. To simulate market entry of waste gasification, NPV calculation including market research to determine regional rMSW/RDF treatment prices is conducted annually after 2021 for a plant that is assumed to be average in size (cf. Table 1) based on Voss et al. (2021) and Poganietz et al. (2019) at all chemical sites equipped with steam cracking (cf. Section 2.3). Specifically, CR will be introduced to the market when one potential construction location yields a positive NPV value. Subsequently, waste gasification capacity development is modeled analogous to MSWIs, MBT plants, and RDF power plants (see above).

The plant portfolio of coal power plants and cement plants is assumed independent of the modeled system: For coal power plants, Ørsted (2020) reports decommission years for all plants in Germany under the "Energy Transition" (BfJ, 2020; Bundesamt für Wirtschaft und Klimaschutz (BMWI), 2020). For cement works, a stable plant portfolio is assumed up to 2050 based on Verein Deutscher Zementwerke e.V. (2020).

In step 4) recommission, FCI data for plants are updated in case their operational lifetime—assumed unified at 30 years for all plants (Voss et al., 2021)—has expired but they are not decommissioned according to step (3) investment/divestment decision-making. Specifically, FCI is updated per Equation (1) to reflect rising capital expenditures.

3.2.5 | Scenarios

Environmental regulation could significantly impact the diffusion of CR in the future (cf. Section 1). Scenario analysis is utilized to identify regulatory barriers and accelerators for gasification-based CR deployment in five individual scenarios presented in Table 3.

3.2.6 | Consideration of uncertainties

Central uncertainties exist in (1) model-inherent logics including applied mechanisms for treatment plant investments/divestments (cf. Section 3.2.4) and (2) parameter assumptions including assumed prices for supplies/products (cf. Supporting Information S1, Table S1). Dysfunctional model logics could result in unreliable and unrealistic model execution behaviors, while incorrect parameter assumptions could lead to systematic errors in the magnitude and temporal appearance of sustainability impacts. Model execution behavior including the plausibility of system dynamics is addressed as per white box validation—referring to the correctness of internal model mechanics—throughout model application as discussed in Sections 4.1 and 4.2 (Utomo et al., 2018). Systemic errors due to parameter uncertainties are addressed as per black box validation—referring to direct model input and output relationships—via comparing model results to empirical rMSW treatment observations in terms of pathway utilization and treatment prices in Section 4.3 (Montanola-Sales et al., 2011).

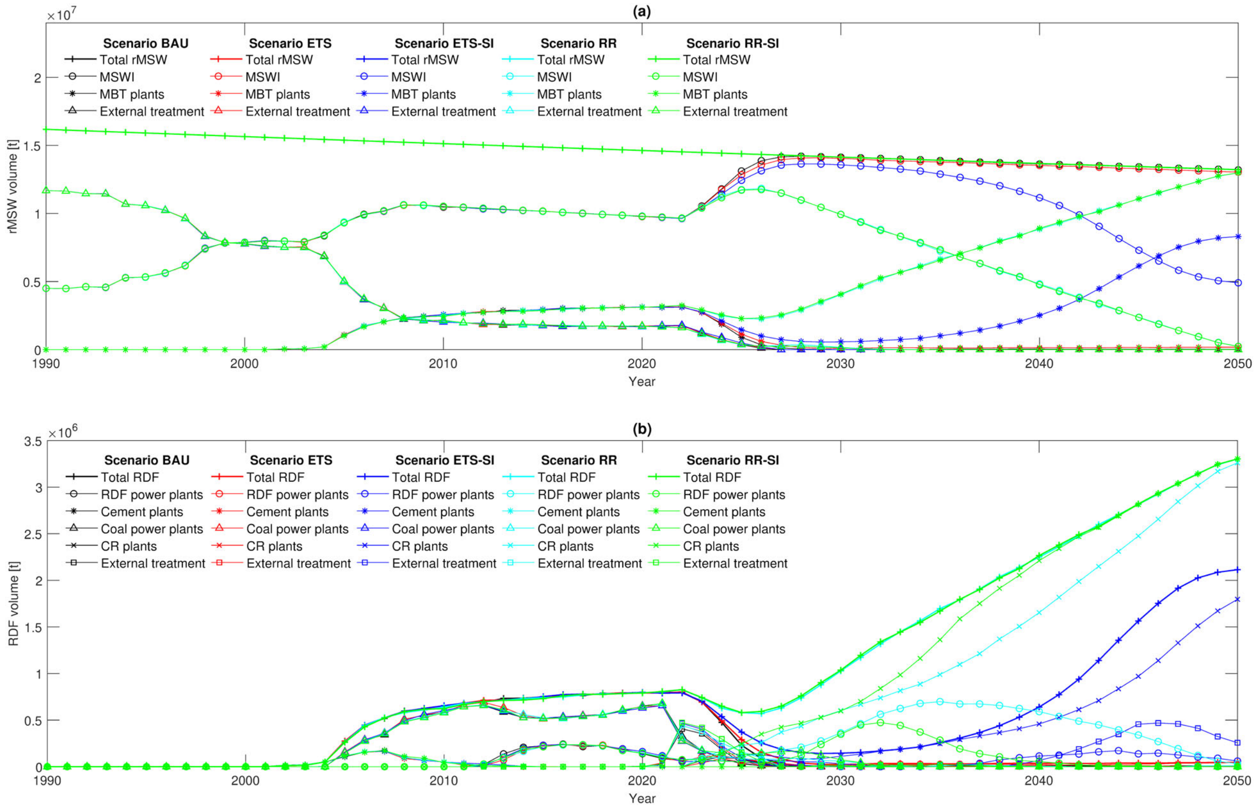


FIGURE 2 (a) rMSW and (b) RDF treatment pathways in all scenarios. BAU, scenario business-as-usual; CR, chemical recycling; ETS, scenario emission trading system adjustment; MBT, mechanical–biological treatment; MSWI, municipal solid waste incinerator; rMSW, residual municipal solid waste; RR, scenario recycling rate; SI, strong increase of ETS prices. Dataset available at: https://doi.org/10.5281/zenodo.6323442

4 | RESULTS AND DISCUSSION

4.1 | Treatment pathway utilization

Figure 2 summarizes results on rMSW and RDF treatment pathway development in all scenarios from 1990 to 2050. As scenarios cause similar model behavior until 2021 (i.e., lines overlap), results for this period are reported jointly. Due to dissimilar model behavior between 2021 and 2050, results are examined individually.

According to model results, rMSW treatment starts in 1990 with a dominance of system external treatment including landfilling, while direct incineration in MSWIs is underrepresented and indirect treatment via MBT is not practiced at all. For 2021, model results show a strong direct incineration dominance, while indirect incineration via MBT has entered the market and system external treatment pathways are significantly reduced. This diffusion of direct/indirect incineration until 2021 corresponds to actual system developments described by the Arbeitsgemeinschaft stoffspezifischer Abfallbehandlung e. V., explained via stricter landfill regulations manifested in the European Landfill Directive and corresponding German directives (EC, 1999). From 2021, discrepancies between results for the five model scenarios (cf. Section 3.2.5) highlight potential environmental regulation impacts on rMSW treatment in the future. As illustrated in Figure 2 scenarios BAU and ETS lead to a future increase in direct incineration dominance, while scenarios ETS-SI, RR, and RR-SI promote gasification-based CR deployment. Specifically, direct incineration expansion observed in scenario BAU suggests that without regulatory adjustments, CR will not be deployed in the future. That scenario ETS generates similar results indicates that obligating MSWIs to trade CO_2 certificates at moderately increasing certificate prices neither creates a stimulating environment for CR. On the other hand, a sharp certificate price increase for scenario ETS-SI is observed to significantly reduce direct incineration, with 64% rMSW being processed in MBT plants and nearly 86% RDF in CR plants by 2050. This suggests that obligating MSWIs in Germany to trade CO_2 certificates at higher certificate prices can be effective in promoting CR. Eventually, modeling results show that the introduction of a recycling rate in both scenarios RR and RR-SI is highly effective in promoting CR, leading to nearly 100% rMSW being processed per CR pathway. Note that additional information on scenario results including capacity developments is provided in Supporting Information S2.

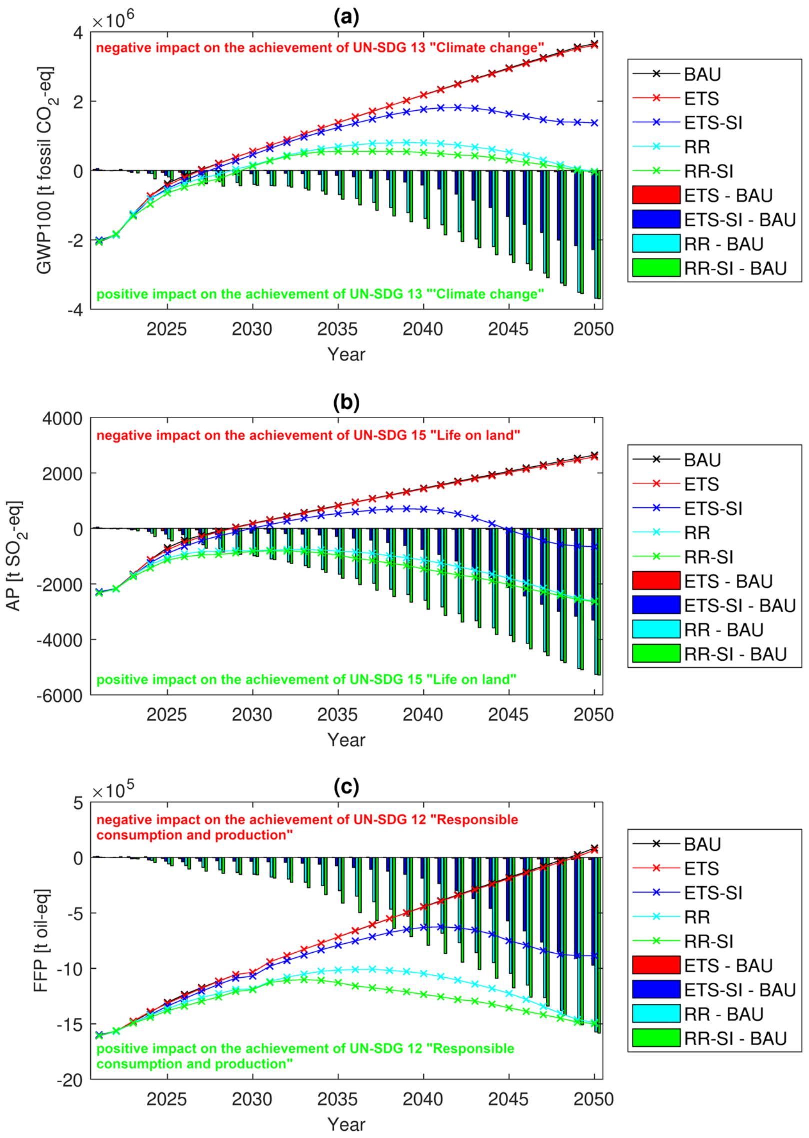


FIGURE 3 Environmental midpoint indicators for categories (a) Climate change, (b) Terrestrial acidification, and (c) Fossil resource scarcity. AP, acidification potential; BAU, scenario business-as-usual; CO_2-eq, carbon dioxide equivalent; ETS, scenario emission trading system adjustment; FFP, fossil fuel potential; FRS, fossil resource scarcity; GWP, global warming potential; oil-eq, crude oil equivalents; RR, scenario recycling rate; SI, strong increase of certificate prices; SO_2-eq, sulfur dioxide equivalent; TA, terrestrial acidification; UN-SDG, UN Sustainable Development Goal. Dataset available at: https://doi.org/10.5281/zenodo.6323442

4.2 | LCSA impacts

4.2.1 | Environmental impacts

In Figure 3a, total annual impacts are indicated with line charts while impact reductions/increases in reference to scenario BAU are presented via bar charts for MI *Climate change* between 2021 and 2050. For total impacts, scenarios BAU and ETS show a linear increase from negative to positive GWP100 values, attributable to massive energy system transformations in upcoming years due to the German "Energy Transition" (BMWI, 2020). Specifically, emission credits for conventional electricity/heat substitution via direct incineration will be reduced as the energy system shifts to renewable energies (cf. Supporting Information S1, Table S1). While emission credits today overcompensate for process emissions of direct incineration, decreased credits will lead to net CO_2-eq in the future. For scenarios ETS-SI, RR, and RR-SI, this development is moderated by CR deployment, leading to lower total emissions mainly due to lower process emissions (cf. Table 1). Total impact reductions compared to scenario BAU are 17, 36, and 40 Mt CO_2-eq in scenarios ETS-SI, RR, and RR-SI, respectively. Results thus suggest a significant positive CR deployment impact—especially via recycling rate implementation—on MI *Climate change* contributing to UN-SDG 13 *Climate action*.

Figure 3b,c presents results for MIs *Terrestrial acidification* and *Fossil resource scarcity*. Similar to MI *Climate change*, scenarios BAU and ETS lead to adverse total environmental impacts for the system by 2050. In comparison, for scenarios ETS-SI, RR, and RR-SI, CR is associated with significant savings in terms of SO_2-eq emissions and oil-eq depletion. Specifically, compared to scenario BAU, 27, 62, and 67 kt SO_2-eq emissions are saved in the scenarios ETS-SI, RR, and RR-SI, respectively. Additionally, 7.2, 15, and 18 Mt oil-eq are saved in scenario ETS-SI, RR, and RR-SI, respectively. Results thus suggest a positive CR deployment impact on MIs *Terrestrial acidification* and *Fossil resource scarcity*, and correspondingly on UN-SDGs 15

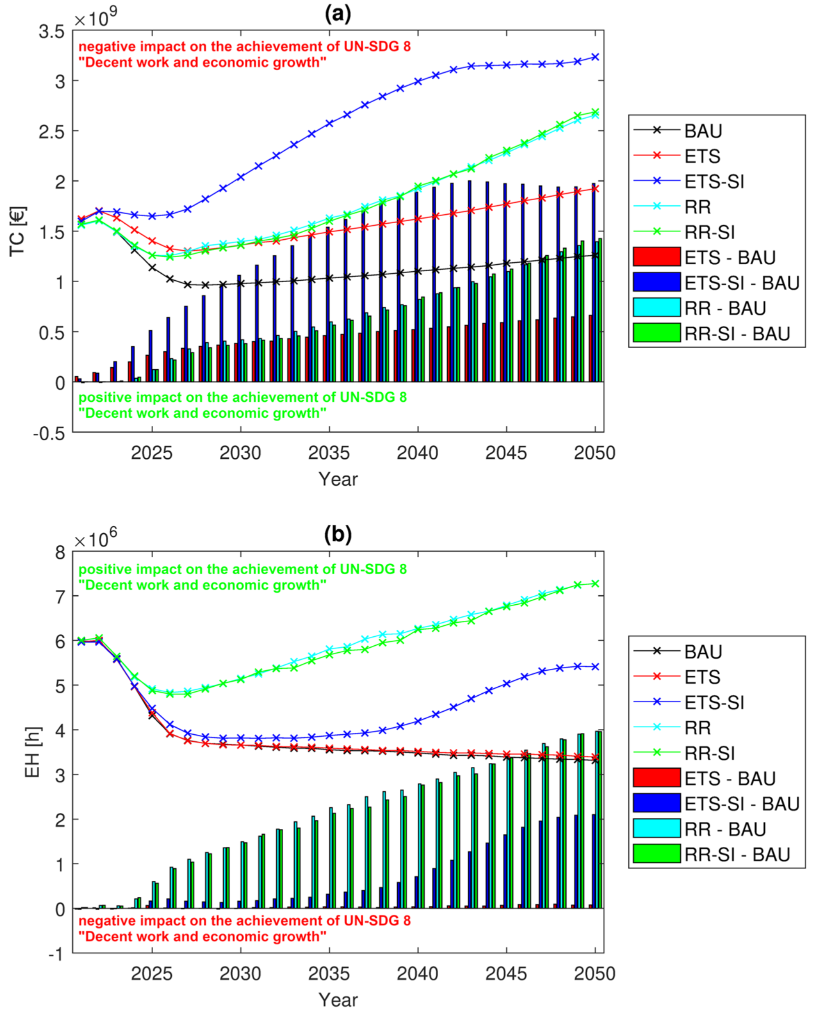


FIGURE 4 Economic and social midpoint indicators for categories (a) System costs and (b) Local employment. BAU, scenario business-as-usual; EH, employee hours; ETS, scenario emission trading system adjustment; RR, scenario recycling rate; SI, strong increase of certificate prices; TC, treatment costs; UN-SDG, UN Sustainable Development Goal. Dataset available at: https://doi.org/10.5281/zenodo.6323442

Life on land and 12 *Responsible consumption and production*. As for MI *Climate change*, a recycling rate introduction appears to trigger more positive effects compared to ETS adjustment.

In the model, German coal power plants are phased out by 2038 based on current political plans (BfJ, 2020). However, due to an ongoing sustainability shift in the German socio-political realm, calls for an accelerated phase-out are increasingly voiced (Löffesend & Becker, 2018; Westdeutscher Rundfunk, 2021). With coal power plants playing no significant role after 2021 for all scenarios, an accelerated process would have minor effects on RDF treatment pathways (cf. Figure 2). However, significant indirect effects might occur due to an accelerated change in the German energy system. Specifically, emission credits for conventional electricity/heat substitution via incineration-based treatment (cf. Section 3.1.2) would be reduced more rapidly leading to increased negative environmental impacts, especially in scenarios BAU and ETS where waste incineration dominates until 2050.

4.2.2 | Economic impacts

Figure 4a displays results for MI *System costs*. In scenario BAU, total costs first decrease before they gradually increase until 2050. The initial decrease is attributable to the systemic shift toward 100% direct incineration in this scenario, which is highly cost efficient (cf. Figure 2). The subsequent increase is explained by—inter alia—inflation, rising labor costs, and increased capital expenditures. For scenario ETS, emission certificates for direct incineration in MSWIs contribute €13B additional cost for the period from 2021 to 2050 compared to scenario BAU. In scenario ETS-SI, an even stronger increase in systemic costs is observed at €41B. In scenarios RR and RR-SI, corresponding costs are lower at €19BB. The higher absolute system costs observed for scenarios ETS, ETS-SI, RR, and RR-SI indicate a negative impact on UN-SDG 8 *Decent work and economic growth*.

These results possess high relevance for political decision-making processes, as they oppose the positive environmental impacts especially for CO_2-eq emissions observed in Section 4.2.1. A possible solution to this conflict is the integration of both sustainability dimensions: Carbon abatement costs reflect the costs per tonne of CO_2-eq emissions reduced (Friedman et al., 2020; Voss et al., 2021). Drawing on total CO2-eq emission results from Section 4.2.1, lowest carbon abatement costs are attained for Scenarios RR and RR-SI at €540 and €480 tonne^{-1} CO_2-eq, respectively (€35K and €2.4K for scenarios ETS and ETS-SI, respectively). These costs can serve as a benchmark for evaluations of other sustainable rMSW treatment pathways in Germany or comparable cases.

4.2.3 | Social impacts

Figure 4b presents results for MI *Impact on local employment*: In scenarios BAU and ETS, a continuous decrease of rMSW production in the future underpins the continuous decline in employee hours observed (cf. Figure 2). For scenarios ETS-SI, RR, and RR-SI, significant increases in employee hours are observed due to the deployment of labor-intensive CR including two treatment steps, MBT treatment and gasification. Specifically, in scenario ETS-SI, 21M additional employee hours are generated compared to scenario BAU. For scenarios RR and RR-SI, this effect—at 64M and 63M employee hours, respectively—is even greater due to earlier systemic transformations. The German "Structural Transformation," as part of the decarbonization of the domestic energy system, is associated with significant societal challenges, including the loss of 20,800 jobs in lignite mining and lignite power plants due coal phase-out (UBA, 2018a). Based on modeling results combined with data from VGB Powertech e.V. (2009), the positive labor effect of an efficient CR implementation for rMSW until 2050 in scenarios RR and RR-SI, is estimated at roughly 1500 additional jobs. Thus, CR could contribute to mitigating social challenges—especially in the coal regions—brought about by sustainability transformations in Germany in upcoming years. In conclusion, results suggest that CR of rMSW can lead to significant positive effects for MI *Impact on local employment* and thus UN-SDG 8 *Decent work and economic growth*. Furthermore, a recycling rate introduction triples the effect compared to subjecting direct rMSW incineration to emissions trading.

4.3 | Black box validation

Figure 5a compares modeled rMSW treatment quantities and percentage treatment pathway utilization rates in Germany to validation data provided by DESTATIS (2021). For all treatment pathways, simulation and reference data show good agreement. Additionally, Figure 5b compares modeled rMSW treatment prices to lower and upper treatment price bounds reported by Hugo (2020). As for treatment pathway utilization, simulation and reference data exhibit a satisfactory agreement.

5 | CONCLUSION

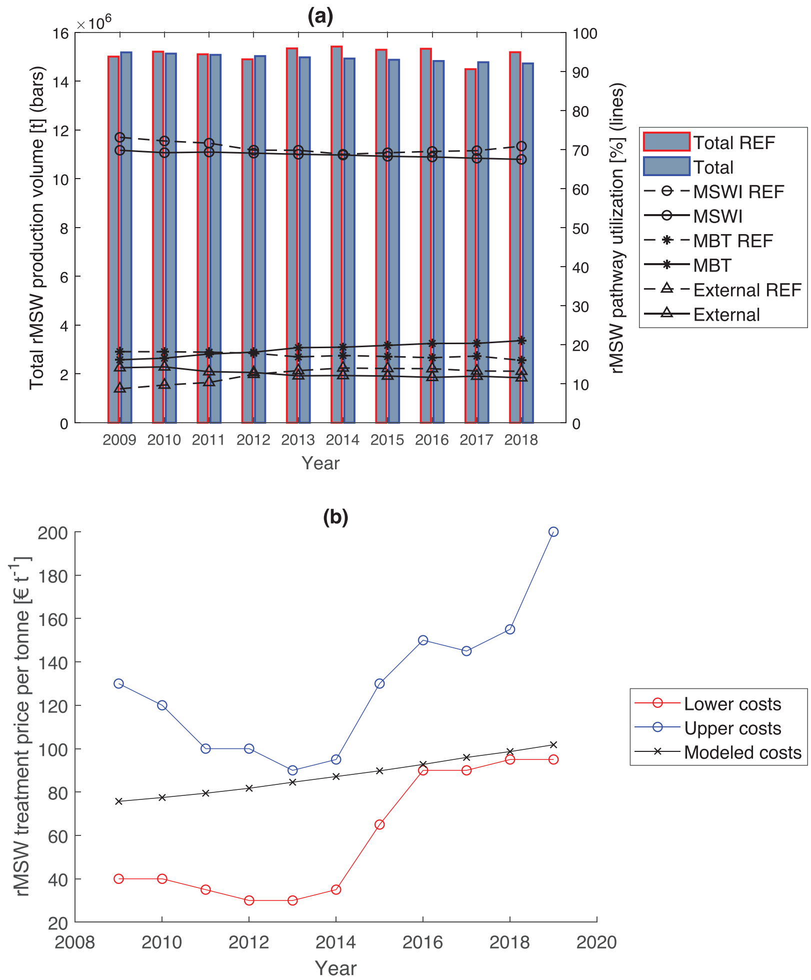
Extending LCSA literature, this study develops and implements a multidimensional and interdisciplinary approach linking process-based LCA, TEA, and social indicators in the framework of an ABM to investigate environmental, economic, and social impacts of chemical recycling for German rMSW. Eventually, this innovative method enables a consequential LCSA that facilitates quantitative insights into how chemical recycling implementation in modern and adaptive waste management systems could potentially contribute to the achievement of individual UN-SDGs.

Results indicate that the German rMSW treatment system could become an environmental burden prospectively. Today, positive impacts of fossil energy substitution are observed to overcompensate for negative environmental impacts due to process emissions. However, as the energy system shifts toward renewables leading to reduced environmental credits for energy substitution, rMSW treatment will produce significant negative environmental impacts beyond the loss of valuable resources. Results show that gasification could counter this development via reducing 40 Mt CO_2-eq and saving 18 Mt oil-eq, for instance. Additionally, gasification could contribute positive social effects of 1500 additional jobs. However, the applied model approach reveals that unfavorable framework conditions for chemical recycling implementation will require regulatory adjustments to bridge the existing cost gap to conventional treatment and trigger corresponding technology deployments. Whether the integration of waste incineration into emission trading is effective will depend on certificate price developments. In contrast, a recycling rate introduction is observed to be associated with more positive environmental, economic, and social impacts compared to emission trading system adjustments. Taken together, study findings provide a deeper understanding of potential contributions of chemical recycling to the achievement of the UN-SDGs, as well as the effectiveness of alternative measures to directly or indirectly promote its deployment.

While the present study provides valuable first insights, a central limitation is represented by the significant number of assumptions and simplifications made regarding model mechanics, modeling scope, and model results that could be further addressed in following research:

- In regard to model mechanics, system external restrictions to the construction and dismantling of treatment plants including political or social resistance are not included, potentially leading to overfast system adaption behaviors (cf. Section 3.2.4). Additionally, the partly generalized economic logic of agents with regard to the assumption of fixed tax rates is simplifying (cf. Section 3.2.4). Eventually, waste composition and

FIGURE 5 Validation of (a) rMSW treatment pathway utilization and (b) rMSW treatment costs based on data provided by DESTATIS (2021) and Hugo (2020). Dataset available at: https://doi.org/10.5281/zenodo.6323442



chemical characteristics refer to national instead of regional data (cf. Section 3.1.3). Corresponding factors could be added in follow-on versions of the model to further align it with the real system and increase result validity.

- In regard to the modeling scope, the focus of this research on the current context may limit its transferability to other waste fractions or nations. Future research could thus benefit from extending the implemented approach to other countries/systems to investigate sustainability impacts under different baseline conditions in terms of treatment plant infrastructure or regulatory framework. Alternatively, the developed system could be equipped with additional technologies to support comparative sustainability assessments or with additional waste fractions to reflect the modeled system in greater detail.
- In regard to model results, the spectrum of applied LCSA impact categories in this study is limited to a number of five (cf. Section 3.1.5) and could be extended in future model applications to attain additional insights into environmental, economic, and social impacts of chemical recycling.

Despite these potentials for research, this study promotes a deeper understanding about the opportunities and challenges associated with chemical recycling for mixed waste under different regulatory conditions that can support political or industrial representatives in objectifying their decision-making. Additionally, it advances the research field of LCSA by applying a consequential approach linked to the achievement of UN-SDG.

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CONFLICT OF INTEREST

The authors declare no conflict of interest.

DATA AVAILABILITY STATEMENT

The data that support the findings of this study are either openly available in repository Zenodo at https://doi.org/10.5281/zenodo.6451976 or in the supporting information of this article. Data on municipal solid waste treatment volumes for Germany used in this study are provided by the German Federal Statistical Office (DESTATIS) and are openly available in (1) the GENESIS-ONLINE database, reference number 32111-0004, at https://www.destatis.de/DE/Home/_inhalt.html, and (2) the REGIONAL database, reference number 32121-01-02-4, at https://www.regionalstatistik.de. Data on German waste treatment plant infrastructure used in this study are provided by the German Environment Agency (UBA) and are openly available in the study "Energieerzeugung aus Abfällen Stand und Potenziale in Deutschland bis 2030," reference number 51/2018, at https://www.umweltbundesamt.de/publikationen. The data on sustainability footprints are available from GaBi Databases 2019 Edition, provided by Sphera Solutions. Restrictions apply to the availability of secondary data used for this study. Corresponding data are available from the authors with the permission of Sphera Solutions or directly from Sphera Solutions. Data on prices for market products and supplies are provided—inter alia—by the UN and are openly available in the UN Comtrade Database at https://www.comtrade.un.org/. Additional data are derived from sources as referenced in the main text and in the supporting information.

ORCID

Raoul Voss https://orcid.org/0000-0001-7097-7958
Roh Pin Lee https://orcid.org/0000-0001-9536-7750
Magnus Fröhling https://orcid.org/0000-0001-5429-1163

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SUPPORTING INFORMATION

Additional supporting information can be found online in the Supporting Information section at the end of this article.

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