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Full length article



Environmental assessments of scales: The effect of ex-ante and ex-post data on life cycle assessment of wood torrefaction

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ABSTRACT

Life Cycle Assessment (LCA) is a powerful tool for achieving sustainability. Traditional LCAs analyze well defined and developed industrial systems, but recent developments of LCA focus on analyzing emerging technologies which are not yet optimized with respect to energy and materials. Therefore, LCA results of ex-ante applications can be very different from ex-post applications for the same system. The purpose of this study is to show the different effects of data scales on LCA results regarding global warming, fine particulate matter formation, terrestrial acidification and freshwater eutrophication potentials. For this purpose torrefaction technology was selected as the case study and assessed based on bench scale data, lab scale data, data derived from process simulations, pilot scale data and commercial scale data. Considered environmental impacts were global warming, fine particulate matter formation, terrestrial acidification and freshwater eutrophication. Results showed that process efficiencies improved significantly between the bench scale system and systems with higher technology readiness levels (TRLs), such as pilot, process simulations and commercial scale systems. Furthermore, process simulations result in scores closer to commercial scale regarding all considered environmental impacts. However, if LCA practitioners focus only on global warming impact, then pilot scale is also a good alternative. Finally, due to torrefaction technology being relatively simple in terms of raw materials input, we suggest more complex chemical systems to be assessed with LCA in various TRLs.

1. Introduction

Data produced from lab or bench scale apparatuses are used to perform ex-ante life cycle assessment (LCA) studies of emerging technologies. On one hand, ex-ante assessments are preliminary because they concern scales significantly smaller than commercial and this difference in scales results in large differences in process efficiencies and operating conditions. On the other hand, commercial data for emerging technologies may not exist and regarding the process industry the use of preliminary data may result in LCA studies with applicable results. In this work we investigated what is the effect of different data scales in assessing the environmental performance of wood torrefaction with LCA.

LCA was standardized by ISO (International Standard Organization, 2006) in 2006 and is already considered a powerful tool for achieving sustainability. ISO classifies LCA in two types, the attributional LCA and the consequential LCA. The former concerns the environmental

footprint of a process, product or system and is typically used in carbon accounting. The latter concerns the environmental consequences due to a change in a system and is typically used in policy making, when a decision is to be made. This way, LCA practitioners can assess the environmental performance of the system now and after implementing the change. However, regarding energy transition and circular economy, many emerging technologies are developing and their environmental performance is investigated with data derived from modeling and/or laboratory experiments.

A recent review Santos et al. (2019) about the application of LCA on the chemical industry concluded that LCA is typically used for identifying hotspots of studied systems and the omission of uncertainty analysis is crucial for research results. Among 46 reviewed LCA studies, Santos et al. (2019) presented that typical system boundaries are cradle-to-gate, the functional unit is in mass units and the most considered commodity chemicals are petrochemicals. Databases are the most common source of data because they are used for background data.

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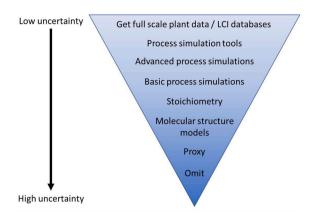


Fig. 1. Uncertainty in LCA studies, adapted from Parvatker and Eckelman, (2019).

On the other hand, foreground data are collected from simulations, literature, industrial data, experimental tests and site investigation. Therefore, foreground data sources may concern different scales and typical life cycle inventory data are expected to change when scaling up technologies, such as conversion efficiency of processes, energy efficiency of processes and equipment used.

Traditional LCA studies analyze well defined and developed industrial systems in an ex-post manner. In this case, a classical uncertainty analysis which focuses on "known unknowns" can happen (van der Giesen et al., 2020). Fig. 1 illustrates how the sources of LCA data result in high or low uncertainty. However, recent developments in LCA literature focus on assessing emerging technologies based on lab or bench scale data. The LCA application in this so-called ex-ante manner supports early design improvements and puts claims of environmental sustainability (Cucurachi et al., 2018). In LCA of emerging technologies a classical uncertainty analysis is not enough due to unknown future situations. Therefore, quantifying uncertainty in ex-ante LCA adds another dimension of quantifying "unknown unknowns". For simplicity purposes data in ex-ante LCA will be also called ex-ante data, and data in ex-post LCA will be called ex-post data in our study. Ex-ante data derives from small scale rigs or process modeling, and ex-post data derives from industrial systems. Small scale test rigs exist at universities or research institutes in order to perform research. Their main disadvantage is that many steps in an operational protocol of a thermochemical process are done manually and this adds uncertainty to the results because researchers may perform the same functions in different ways. For instance, start-up operation and problem solving can vary among research labs. Furthermore, the smaller the scale of a system, the lower its efficiency is. For instance, energy losses of a process can be much higher in a bench scale unit than in an industrial scale unit due to energy optimization because an industrial unit needs to be cost effective. In addition, process modeling is performed with specialized software, such as Aspen Plus (Aspen Technology, Inc., 2013), CHEMCAD, COMSOL Multi-physics, etc.

Using ex-ante in relation to ex-post data is not thoroughly researched in the LCA community. There are limited studies (Cucurachi et al., 2018; Fernandez-Dacosta et al., 2019; Piccinno et al., 2016; Tan et al., 2018; Tecchio et al., 2016; van der Giesen et al., 2020; van der Hulst et al., 2020; Villares et al., 2017) which focus on the effect of using ex-ante data instead of ex-post on LCA applications because It is challenging to find comparable data for a specific technology in different technology development levels. Therefore, some of these studies focus on suggesting guidelines on how up-scaling ex-ante data can happen in LCA (Cucurachi et al., 2018; Piccinno et al., 2016; Tecchio et al., 2016; van der Giesen et al., 2020; van der Hulst et al., 2020; Villares et al., 2017), while other studies aim to compare LCA results with different data scales or data sources (Fernandez-Dacosta et al., 2019; Tan et al., 2018). For

instance, Tecchio et al. (2016) suggested that investigated biotechnological processes must be described in literature and considered feasible, and the analysed products are likely to be produced in large quantities in a reasonable future scenario. Cucurachi et al. (2018) concluded that using ex-ante LCA is a mean of increasing LCA application on emerging technologies. Villares et al. (2017) concluded that LCA results based on an ex-ante context cannot be considered accurate but a good foundation to build upon. Piccinno et al. (2016) developed a framework regarding scaling up chemical process data based on lab-scale data. However, these researchers did not validate their framework with a case study, nor provided values for the reliability of their framework because their proposed scale-up framework is "a complementary approach, which adds another dimension in the scale-up of chemicals processes for LCA studies" (Piccinno et al., 2016). Van der Hulst et al. (2020) developed an organized procedure to conduct ex-ante LCA and applied it in a case study about copper indium gallium (di)selenide (CIGS) photovoltaic laminate. Tan et al. (2018) used ex-ante data based on lab-scale production and an up-scaled process design. These researchers concluded that when the R&D advances into the engineering phase, improving process efficiency becomes the key focus of technology development. As a result, substantial impact reduction can be expected by the first process design. So far, only Fernandez-Dacosta et al. (2019) investigated the environmental performance of an industrial system in relation to performing an ex-ante LCA of the same system. Their case study was the production of innovative bio-based chemicals.

Torrefaction is a mild thermochemical process occurring from 200 to 300 °C in an inert atmosphere to convert biomass to a more coal-alike fuel because its energy density is increased. Partial biomass devolatilization during torrefaction results in biomass becoming more brittle, hydrophobic and less prone to microbial and fungal degradation (van der Stelt et al., 2011). Torrefaction lowers the biomass oxygen content and increases the aromatic fraction of bio-oil when it is used as feedstock for fast pyrolysis (Meng et al., 2012). In addition, biomass co-firing can already be a near-term and low-risk option regarding biomass integration to European energy infrastructure depending (primarily) on carbon price (Cutz et al., 2019). Therefore, torrefied biomass can be a promising coal replacement fuel for boilers and gasifiers from a technical (Tsalidis et al., 2017a) and environmental perspective (Tsalidis et al., 2017b, 2014), and a promising feedstock for bio-oil production via pyrolysis (Kumar et al., 2020).

The aim of this study is to use ex-ante experimental data, data derived from simulations, and ex-post empirical data in a case study of the Dutch torrefaction industry and investigate the effect of various data scales on LCA results. We investigate if ex-ante data, under certain conditions, can decrease the type of ex-ante uncertainty which exists due to unknown future situations, and be used instead of ex-post to yield comparable results. For this purpose, we modelled a bench scale, lab scale, pilot scale, commercial scale and simulations of torrefaction technology. As far as the authors are aware, this is the first LCA study that compares LCA results from different data scales of torrefaction technology.

2. Methodology

2.1. Case study

The selected case study regards the torrefaction technology combined with pelletization because applying LCA requires a specific scope. Torrefaction combined with pelletization as a case study has specific characteristics because it is a rather simple thermochemical technology due to consisting of two stages and having two critical parameters, mainly temperature and, to a lesser extent, residence time (Van der Stelt et al., 2011). Furthermore, several commercial torrefaction plants operate worldwide (Thrän et al., 2016) and among the potential various types of feedstock, wood is quite common, abundant and well employed.

Table 1Details of every considered torrefaction plant.

<u> </u>					
Input	Bench	Lab	Simulation	Pilot	Commercial
LCA study type	Ex-	Ex-	Ex-ante	Ex-post	Ex-post
	ante	ante			
System	S1	S2	S3	S4	S5
Year of data	2005	2016	2010	2016	2017
TRLa	3	4	_	7–8	9
Size of plant (kg wood chips input)	<0.01 ^b	0.1 ^b	17,260	50–100	23,464 ^c
Type of feed wood	Willow	Pine	Pine	Pine	Round wood
Torrefaction temperature (°C)	300	270	300	270	300
Residence time (min)	10	30	_d	10	_d
Calorific value of torrefied pellet (MJ/kg)	21	19.4	21	20.9	20.6

a stands for technology readiness level.

2.2. Goal and scope

The goal of this study is assess how much ex-ante uncertainty exists in LCA bioenergy studies when researchers model their systems with exante data instead of ex-post data. Therefore, process data exist on two levels:

- Ex-ante: experimental data collected from bench scale and lab scale
 tests at early development of torrefaction technology or generated
 data from specialized software for process flowsheet simulation, i.e.
 Aspen Plus (Aspen Technology, Inc., 2013). Aspen Plus (Aspen
 Technology, Inc., 2013) is used from bulk, specialty chemical and
 pharmaceutical industries to optimize throughput, quality and energy use. Modeling in Aspen Plus concerns steady state of chemical
 systems and, thus, it yields results relevant to feasibility studies.
- Ex-post: empirical data collected from a large pilot plant and a commercial torrefaction plant located in the Netherlands.

Based on different data types and sources the following systems are presented below and in Table 1:

- 1 Ex-ante system S1: bench scale torrefaction derived from the very early days of torrefaction and used in a proof-of-concept scheme.
- 2 Ex-ante system S2: lab scale torrefaction, with torrefaction feedstock as auxiliary fuel.
- 3 Ex-ante system S3: simulation of a torrefaction facility with Aspen Plus software and FORTRAN programming.

- 4 Ex-post system S4: (large) pilot scale torrefaction which was used to conclude the market readiness of torrefied solid biofuels, with torrefaction feedstock as auxiliary fuel.
- 5 Ex-post system S5: commercial scale torrefaction based on an existing Blackwood B.V. torrefaction plant in the southern part of the Netherlands.

2.2.1. Functional unit

The main functionality of the torrefaction systems is the production of torrefied wood pellets which are typically co-fired with coal for electricity generation (Kumar et al., 2017). Furthermore, lab scale and pilot scale tests were performed at lower temperature than the rest. A higher temperature will result in higher devolatilization rate, a lower mass yield and a higher calorific value. Therefore, the effect of temperature on torrefied pellets can be overcome (to a large extent) if the functional unit is energy related. The functional unit was selected to be 1 GJ of torrefied wood pellets.

2.2.2. System boundaries

Fig. 2 presents the system boundaries of initial system and scenario A. System boundaries of the initial system were gate-to-gate because they focused on the operation of the torrefaction plant. Thus, system boundaries started with the delivery of wood chips at the torrefaction plant entrance gate and finished with the production of torrefied wood pellets. However, due to the fact that wood chips may come with a certain environmental footprint, even if they were produced from forest management residues, we developed a scenario where the entire supply chain of torrefied pellets is assessed. This is done to show the contribution of torrefaction process of different scales in the entire supply chain.

Data on infrastructure construction and demolition is needed. However, LCA studies have mentioned that for cradle-to-grave or cradle-to-gate systems, the contribution of a 30 year-lifetime plant to the environmental performance is negligible (Damen and Faaij, 2003; Tsalidis et al., 2017b). Furthermore, it was not possible to collect reliable data for construction and demolition stages of torrefaction units in considered systems. Therefore, we have excluded construction and demolition from the system boundaries.

2.2.3. Assumptions

The study (Prins et al., 2006), based on which the bench scale data (S1) was collected, does not include a pelletization stage downstream torrefaction. Thus, it was assumed that the same pelletization process with S2 (McNamee et al., 2016) is employed. Furthermore, S1 and S5 systems employ willow and round wood, respectively, instead of pine wood as systems S2, S3 and S4 do. It was assumed that employing willow and round wood instead of pine wood will result in effects to an extent due to the similar feedstock' characteristics (as presented in Table A1). Derks, (2018) mentioned that roundwood regards lower quality trees

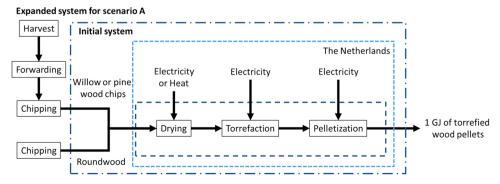


Fig. 2. System boundaries of S1-5.

^b batch experiments.

 $^{^{\}rm c}$ continuous operation in kg. h^{-1} .

^d not mentioned by Derks (2018).

Table 2
Consumables per 1,000 kg torrefied wood pellets.

Input	Bench	Lab	Simulation	Pilot	Commercial
Wood chips (kg)	1497	1777	1726	2122	2460
Electricity (kWh)	51,753	303	146	121	155
Heat (kWh)		355 ^a	87.5	322^{b}	

^a some derived from feedstock combustion.

which are not acceptable for saw wood and chip-n-saw wood purposes but have sufficient quality to be employed by the pulp and paper industry. Thus, pulpwood was selected as a good proxy for roundwood. Last, the electricity system was the same for all systems, even though some systems were based on 2005 and 2010 data which concerned an electricity system with lower renewable energy share and larger

environmental footprint. A larger environmental footprint results in larger environmental burdens due to the electricity consumption during torrefaction and pelletization. Due to the fact that we aimed to show the effect of technology scales on LCA results we assumed the same electricity system to all considered systems

2.2.4. Impact categories

The systems under study belong to the energy sector. Thus, the considered impact category indicators were: global warming potential, fine particulate matter formation potential, terrestrial acidification potential and freshwater eutrophication potential.

2.3. Life cycle inventory

The life cycle inventory quantifies all relevant energy and material

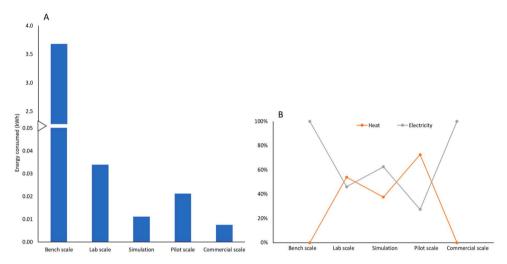


Fig. 3. Absolute (A) and relative (B) energy consumption per functional unit.

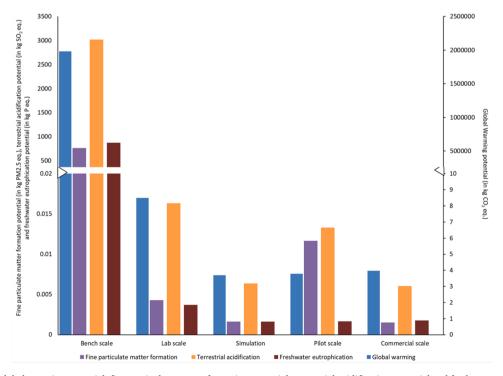


Fig. 4. LCA results of global warming potential, fine particulate matter formation potential, terrestrial acidification potential and freshwater eutrophication potential per system.

b all derived from feedstock combustion.

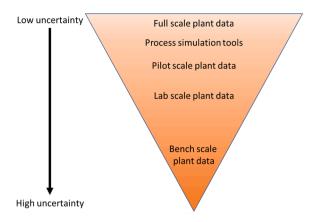


Fig. 5. Hierarchy of data scales based on results.

Table 3Environmental results per functional unit of the entire supply chain, in brackets the initial systems' contribution.

Environmental impact	S1A (S1)	S2A (S2)	S3A (S3)	S4A (S4)	S5A (S5)
Global Warming (kg CO_2 eq.1 GJ^{-1})	1985,073 (99.8%)	11.83 (71.7%)	6.63 (55.6%)	7.61 (49.7%)	7.33 (54.2%)
Fine particulate matter formation (kg PM2.5 eq.1 GJ ⁻¹)	770.1 (98.9%)	0.0088 (48.2%)	0.0056 (28.9%)	0.0169 (68.3%)	0.0063 (23.9%)
Terrestrial acidification (kg SO_2 eq.1 GJ^{-1})	3043.7 (99.2%)	0.0272 (59.9%)	0.0159 (39.9%)	0.0258 (51.5%)	0.0178 (33.9%)
Freshwater eutrophication (kg P eq.1 GJ ⁻¹)	881.9 (99.4%)	0.0039 (94.4%)	0.0018 (89.3%)	0.0019 (86.7%)	0.0029 (60.3%)

Table A1Wood feedstock composition of torrefaction.

	Willow wood	Pine wood	Roundwood (mixed wood)
Moisture (as received weight %)	3.35	7.1	30–55
Fixed carbon (dry weight %)	17	15.9	15–25
Volatile matter (dry weight %)	78	83.8	70–84
HHV (MJ/kg)	18.7	19.1	18.2

requirements as well as air, water and land emissions for the entire life cycle of a product. Inventory data was classified as foreground and background data. Foreground data consisted of data collected from literature regarding torrefaction on different scales (Derks, 2018; McNamee et al., 2016; Prins et al., 2006; Thrän et al., 2016; Yun et al., 2020). Background data, such as electricity generation in the Netherlands was collected from Ecoinvent database v.3.4 (Wernet et al., 2016).

2.3.1. Processes

This section provides a brief description of processes in the system boundaries. Systems S1 - S5 concerned the same unit processes. However, feedstock and process efficiencies were different among scales, as presented in Tables 1 and 2.

2.3.2. Torrefaction process

Typical torrefaction energy efficiency and mass efficiency of woody

biomass is approximately 90% (Nanou et al., 2016) and 70%, respectively (Van der Stelt et al., 2011). This means that 90% and 70% of wood's energy and mass are transferred to the main product, respectively. It is possible in torrefaction process to produce part of the heat needed for drying via the combustion of torrefaction gas. This way moisture can decrease from 40 to 50% to approximately 15% on a wet fuel basis (Tsalidis et al., 2014). Furthermore, another source of heat can be torrefaction's feedstock itself. In both cases, CO2 generated from torrefaction gas or wood chips combustion is biogenic and not contributing to climate change (IEA Bioenergy, 2000). The rest of needed heat is generated via natural gas combustion in a boiler with an efficiency of 90%, as shown in Fig. 1. Data on the process level has been collected from literature (Derks, 2018; McNamee et al., 2016; Prins et al., 2006; Thrän et al., 2016; Yun et al., 2020). Torrefaction can be followed by pelletization because of the energy efficiency benefits. Power needed for size reduction and densification of torrefied wood chips is 70-90% (Bergman et al., 2005) and 70% (Uslu et al., 2008) less than consumed power for pelletization of wood chips, respectively.

2.3.3. Pelletization process

In torrefaction plants, pelletization is typically integrated down-stream torrefaction. The reason for this integration is not only the energy consumption decrease, but also safety. It is less probable that torrefied pellets self-ignite, which is crucial during storage and transportation stages (Nunes, 2020). In our study, this integration happens in systems: S3, S4 and S5. However, S1 and S2 regard small experimental torrefaction units, where pelletization was not integrated with torrefaction. Energy consumption data during pelletization were published in S2 (McNamee et al., 2016), but not in S1 (Prins et al., 2006). Table 2 presents a combined version of consumables for the production of 1 ton of torrefied pellets for each considered system. A detailed version of Table 2 exists in the Appendix, see Table A3.

2.3.4. Electricity and heat

Background data concerning electricity generation and heat generation for chemical plants in the Netherlands was acquired from Ecoinvent database v.3.4 (Wernet et al., 2016). Furthermore. In systems S2 and S4, part of the received wood chips is burned to generate heat.

2.3.5. Scenario A - Harvest, forwarding and chipping

The first stage of each supply chain system in Scenario A regards the harvest of wood by the forest owner. Then wood is forwarded and chipped on site to produce wood chips. Fuel consumption and emissions produced during tree harvesting, forwarding and chipping pine and willow woods were collected from Ecoinvent database v.3.4 (Wernet et al., 2016).

3. Results and discussion

3.1. Effect of data scale on technical parameters

Energy consumption is usually a good predictor of environmental footprint because electricity and heat generation typically employ fossil resources in Europe (European Environment Agency, 2018). Therefore, it is important to show first effects of data scale on operational parameters, such as energy consumption. Fig. 3A shows the total energy (in kWh) consumed per functional unit and how much of this energy derives from heat or electricity in percentage (Fig. 3B). First, it is clear that torrefaction's process efficiency has vastly improved between the first bench scale experiment and other systems. This improvement is up to 99.8% (for S5). This happened not only due to the scale, but also because S1 data were produced in 2005, much earlier that other systems considered in our study. Smaller scales result in larger heat losses, therefore, for a thermochemical process, heat losses will greatly affect the overall efficiency. Furthermore, torrefaction practitioners tested the employment of heat generation via torrefaction gas combustion.

Table A2 LCA results based on Recipe 2016 midpoint (E) impact model.

Impact category	Unit	Bench scale	Lab scale	Pilot scale	Commercial scale	Simulation
Global warming	kg CO ₂ eq	1,982,033	8.489392	3.780877	3.974591	3.687739
Stratospheric ozone depletion	kg CFC11 eq	1.730413	9.38E-06	6.94E-06	3.47E-06	3.66E-06
Ionizing radiation	kBq Co-60 eq	349,058.7	1.485592	0.843439	0.699971	0.647335
Ozone formation, Human health	$kg NO_x eq$	1768.718	0.012028	0.019526	0.003547	0.004285
Fine particulate matter formation	kg PM2.5 eq	761.8632	0.004279	0.011647	0.001528	0.001644
Ozone formation, Terrestrial ecosystems	kg NOx eq	1785.574	0.012171	0.019815	0.003581	0.004332
Terrestrial acidification	kg SO2 eq	3019.413	0.016332	0.013305	0.006055	0.006377
Freshwater eutrophication	kg P eq	876.3006	0.003724	0.001674	0.001757	0.001624
Marine eutrophication	kg N eq	60.55765	0.00026	0.000123	0.000121	0.000113
Terrestrial ecotoxicity	kg 1,4-DCB	336,009.7	5.632296	8.852229	0.673804	1.561222
Freshwater ecotoxicity	kg 1,4-DCB	24,666.36	0.112053	0.058091	0.049464	0.047323
Marine ecotoxicity	kg 1,4-DCB	2.71E + 08	1263.158	694.3804	542.6855	526.7418
Human carcinogenic toxicity	kg 1,4-DCB	3,447,826	14.66381	6.542193	6.913961	6.391793
Human non-carcinogenic toxicity	kg 1,4-DCB	2.24E + 08	1049.768	582.8128	448.4828	436.6185
Land use	m²a crop eq	56,163.47	2.453938	1.646353	0.112625	0.5986
Mineral resource scarcity	kg Cu eq	244.7361	0.001174	0.000728	0.000491	0.000483
Fossil resource scarcity	kg oil eq	646,826.3	2.769018	1.275029	1.297088	1.203151
Water consumption	m ³	24,605.2	0.104514	0.057687	0.049341	0.045585

Table A3Detailed version of Table 2 of the manuscript with references

Detailed version of Table	2 of the m	anuscri	pt with references.		
Bench scale (Prins et al., 2	006)				
Torrefaction					
Input			Output		
Willow wood	1497	kg	Torrefied willow wood	1000	kg
Electricity	51,659	kWh	CO ₂ CO (from CO ₂)	59.9 28.2	kg kg
Lab scale (McNamee et al.	, 2016)				-
Torrefaction					
Input	Value	Unit	Output	Value	Unit
Pine wood chips	1777	kg	Torrefied pine wood chips	1000	kg
Dryer duty	102.83	kWh			
Torrefier duty	105.81	kWh			
Additional energy from auxiliarry fuel Pelletization	355	kWh			
Torrefied pine wood	1020	lr.c.	TOD pollete	1000	lr.c.
chips	1020	kg	TOP pellets	1000	kg
Electricity	95	kWh	Waste wood chips	20	kg
Simulations (Yun et al., 20	20)				
Torrefaction integrated with pelletization					
Input	Value	Unit	Output	Value	Unit
Pine wood chips	1726	kg	Torrefied pine wood pellets	1000	kg
Heat (from burning woodchips)	87.5	kWh			
Primary energy (electricity)	145.8	kWh			
Pilot scale (Thrän et al., 20)16)				
Torrefaction with integrated pelletization					
Input	Value	Unit	Output	Value	Unit
Pine wood chips	2122	kg	Torrefied pine pellets	1000	kg
Heat (from burning pine chips)	321.71	kWh			
Electricity	121.47	kWh			
Commercial scale (Derks, 2	2018)				
Torrefaction with integrated pelletization					
Input	Value	Unit	Output	Value	Unit
Roundwood chips	2460	kg	Torrefied wood 1000 pellets		kg
Energy	155.14	kWh	÷		

Therefore, the need for heat can be significantly decreased with scale. For instance, S3 of (Yun et al., 2020) assumed that the energy in torrefaction gas is enough to achieve auto-thermal operation of torrefaction; i.e. all the energy needed for torrefaction can be supplied from the heat in the torrefaction gas. Second, S1 and S5 consume only electricity, while S2, S3 and S4 consume a mixture of electricity and heat with most energy being heat for S2 and S4. Due to S1 being bench scale, it was expected that researchers (Prins et al., 2006) would employ electricity as the energy source for torrefaction. However, employing only electricity was not expected for S5 (commercial scale). It is not clear if the authors (Derks, 2018) mentioned that due to confidentiality reasons because this data derives from a commercial torrefaction plant.

Another important effect of scale on technology development was the replacement of natural gas as the fuel for heat with wood chips which is torrefaction's feedstock. This way, the carbon footprint of torrefaction product can be lowered, but there may be a trade-off in other environmental impacts which wood chips production and wood chips combustion contribute to. Such trade-offs are presented in the following section.

3.2. Effect of data scale on LCA results

The results of ex-ante and ex-post LCA systems are presented in Fig. 4, all LCA results can also be found in Table A2 of Supplementary Materials. First of all, Fig. 4 shows at first glance that LCA results of S1 are several orders of magnitude larger than S2, S3, S4 and S5, and LCA results of S3 and S5 are quite similar regarding the considered environmental impact indicators. Furthermore, Fig. 5 presents a modified data hierarchy based on our results, with S5 being the system with no exante uncertainty due to being full scale.

Results show that for global warming potential simulations, pilot scale and commercial scale data result in similar values, 3.7, 3.8 and 3.9 kg of CO2-eq., respectively. On the other hand, bench scale data show by far the highest global warming potential. The efficiency improvement of 99.1-99.8% between S1 and S2-5 resulted in a 99.9% improvement of the global warming potential score. A major difference between S1 and S2–5 systems is the employment of a dryer unit upstream torrefaction. The drying process is energy intensive and the initial moisture content of wood is typically 50% (Menon et al., 2020). Furthermore, as stated earlier minimization of heat losses during torrefaction and re-circulation of torrefaction gas to burn it and re-use the heat contribute to decreasing the global warming score. S3 and S4 result in better global warming score than S5 due to the better torrefaction efficiency in terms of mass. S5 employs roundwood which according to (Derks, 2018) concerns lower quality trees. In addition, the assumption of Yun et al. (2020) for S3 that torrefaction operation is auto-thermal resulted in even lower

global warming score than S4. However, the difference of global warming scores of S3, S4 and S5 is so small that they can be considered the same.

The effect of scale to fine particulate matter formation potential is similar to global warming potential. There is a significant decrease from bench scale (S1) to simulations, lab and pilot commercial scales. However, S4 results in a higher fine particulate matter formation potential score than S2. This happens because S4 employs wood chips combustion for the entire employed heat and the wood chips production stage contributes to fine particulate matter formation. The same reason exists for terrestrial acidification potentials of S2 and S4 in comparison with S3 and S5. The former two systems include in the system boundaries wood chips production for heating, while the other two do not, thus emissions contributing to acidification are higher. Lastly, freshwater eutrophication potential is also several orders of magnitude higher in S1 than S2–5. Furthermore, freshwater eutrophication potential of S2 is almost double the potential of S3-5, and the freshwater eutrophication potential scores of S3-5 are almost the same, the same way as in the case of global warming impact.

Excluding S1 which resulted in very large environmental burdens, we find that with higher data scale alternative heat sources were employed instead of natural gas, such as wood chips. On one hand, wood chips production and combustion resulted in lowering the global warming and freshwater eutrophication potentials. On the other hand, wood chips production contributed to fine particulate matter and terrestrial acidification potentials due to fossil fuels use in that stage. Especially, due to S4 employing only wood chips to generate heat resulted in higher terrestrial acidification potentials than S5, even though S5 showed a similar global warming potential. Last, S2 would have resulted in larger environmental burdens if data for electricity at 2010 would have been used instead of data for the current electricity production system.

Our results are in agreement with Fernandez-Dacosta et al. (2019) and Tan et al. (2018): i) Fernandez-Dacosta showed that ex-ante LCA resulted in worse environmental performance than ex-post LCA of lactic acid production regarding global warming and eutrophication potentials. Furthermore, the contribution of process energy was higher for the ex-ante system, similar to our results between S1 and S2, and S4 and S5. ii) Tan presented that with increasing development stage, energy consumption and GHG emissions decrease. Both studies show a significant improvement of GHG reduction 91.5% and 78%, and Tan et al. report an improvement of fossil energy use by 96% and conclude that substantial impact reduction can be expected by the first process design. The latter is obvious in our study with S1.

3.3. Effect of scale on the entire supply chain of Dutch torrefied wood pellets

Table 3 shows the effect of data scale on the entire supply chain of torrefied wood pellets due to the expansion of the initial system boundaries (of Fig. 2). First of all, it is evident that the supply of wood chips contributes mainly to fine particulate matter formation and terrestrial acidification potentials. This happens due to diesel oil burned in mobile harvesting equipment and other machines. This contribution is the highest in S3A and S5A due to the initial low scores of S3 and S5 systems in relation to S4. The same effect is not seen in S4A because the initial score of fine particulate matter formation for S4 is higher. Similarly, the environmental footprint of S1 was so large that any effect of the supply chain is insignificant, and the environmental footprint (for all considered environmental impacts) of S2 contributes highly to the S2A footprint due to its low mass and energy efficiencies.

The comparison among S3A, S4A and S5A changes when compared to Fig. 4. This happens due to the larger needs of S5 for woodchips input than S3 and S4. In addition, the supply chain of these three systems can contribute as high as approximately 76% (Fine particulate matter formation of S5A) or as low as approximately 13% (freshwater

eutrophication potential of S4A). Furthermore, Table 3 shows that S3A and S4A resulted in better and worse global warming score by 9.6% and 3.8% than S5A, respectively. The supply chain of roundwood for S5A results in a better environmental performance with respect to global warming than supply chains of pine wood and willow wood chips even though roundwood needs to be chipped at the commercial torrefaction plant with an industrial chipper. However, concerning S3A, Aspen Plus simulations overestimate the torrefaction mass efficiency (when compared to S5) in terms of how many tons of woodchips input are required to produce torrefied pellets of 1 GJ. Therefore, S3A requires less woodchips to be harvested, forwarded and chipped than S5A. On the other hand, S4A results in slightly worse global warming potential due to its supply chain.

3.4. Limitations

A major limitation of our study is torrefaction technology itself and the number of studies per TRL. Torrefaction is rather simple in terms of raw materials. However, at the same time this fact offered the opportunity to find comparable torrefaction systems of different TRLs. Furthermore, in order to assess comparable systems, one study was selected per TRL. It was not completely clear if the commercial plant (S5) employs only electricity. This was stated in the data source (Derks, 2018), but replacing fossil dominated Dutch electricity with wood chips to generate heat (similar to S4) would improve even more the environmental performance of Blackwood torrefied pellets system. Thus, this may happen in Blackwood's facility and it could affect its environmental results. Additionally, not the same wood species is employed by all systems. However, the fact that all wood species have similar proximate analysis and in combination with the selected functional unit, the effect of wood species has to torrefaction's products is limited to a certain extent. Last, S1, S2 and S5 regard torrefaction systems operating at 300 °C, and S2 and S4 regarded systems at 270 °C. Therefore, S2 and S4 will result in lower consumption of electricity and/or heat due to a lower torrefaction temperature than the same systems operating at 300 °C. Literature (Chih et al., 2019; Keivani et al., 2018; Simonic et al., 2020; Urbancl et al., 2019) shows that such a temperature difference will affect the torrefaction product (primarily) in terms of solid yield and heating value, and (secondarily) composition because a lower temperature results in a lower degree of devolatilization. For instance, regarding pine wood such a torrefaction temperature difference can result in varying solid yield and heating value between 65% and 53% and 25 MJ/kg and 28.7 MJ/kg, respectively (Keivani et al., 2018). Thus, we aimed to reduce such a torrefaction temperature effect on torrefaction product in an LCA context by choosing an energy functional unit (see Section 2.2.1). In contrast, additional effects of torrefaction temperature on the torrefaction product, such as density, hardness, and durability (Manouchehrinejad and Mani, 2018; Simonic et al., 2020), were not considered and may affect the following stage of pelletization because grindability is improved.

4. Conclusions

The purpose of this study was to show the different effects of data scales in LCA studies for the process industry and torrefaction technology was selected as the case study. We found that (based on the source for) simulations result in better scores regarding all considered impacts than bench, lab and pilot scales when scores of industrial scale is considered as reference or the system with no ex-ante uncertainty. However, if LCA practitioners focus only on global warming impact, then data derived from pilot plants is also a good alternative. In addition, the expansion of system boundaries to the entire supply chain shows that simulations can underestimate the global warming potential due to the fact that differences in process efficiencies of foreground systems based on simulations can increase unevenly footprints of upstream processes. However, for the rest considered impact indicators, simulations are

sufficiently accurate.

We recommend researchers to duplicate the method that we applied, collecting data from processes of various scales, but to select a more complicated technology than torrefaction. A chemical process with more consumables will result in accounting for the manufacturing of more chemical products which will consequently result in larger differences among systems of different scales.

5. Disclosure statement

No potential conflicts of interests were reported by the authors.

CRediT authorship contribution statement

Georgios Archimidis Tsalidis: Conceptualization, Data curation, Formal analysis, Methodology, Writing – original draft, Writing – review & editing. **Gijsbert Korevaar:** Writing – original draft, Writing – review & editing.

Declaration of Competing Interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

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Appendix

The appendix contains the composition of considered wood types in each LCA system and a detailed version of all the generated LCA results.

Table A1 presents considered wood types' composition with respect to percentages of moisture, fixed carbon, volatile matter and higher heating value (HHV).

Table A2 is a detailed version of Fig. 4 in the main text. Table S2 all the LCA results as generated from SimaPro software.

Table A3 regards a detailed table of Table 2 from the main text.

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