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LCA FOR ENERGY SYSTEMS AND FOOD PRODUCTS

Environmental life cycle assessment of production of the non-nutritive sweetener sucralose (E955) derived from cane sugar produced in the United States of America: The SWEET project

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Abstract

Purpose There is increasing concern about the detrimental health effects of added sugar in food and drink products. Sweeteners are seen as a viable alternative. Much work has been done on health and safety of using sweeteners as a replacement for added sugar, but very little on their sustainability. This work aims to bridge that gap with a life cycle assessment (LCA) of sucralose derived from cane sugar grown in the United States of America (USA).

Methods An attributional, cradle-to-gate LCA was conducted on sucralose production in the USA. Primary data were derived from literature for the chlorination process, and all other data from background sources. Results are reported via the ReCiPe 2016 (H) method, with focus given to land use, global warming potential (GWP), marine eutrophication, mineral resource scarcity, and water consumption. Because sucralose has a much greater perceived sweetness than sugar, impacts are expressed both in absolute terms of 1 kg mass and in relative sweetness equivalence terms to 1 kg sugar. Scenario modelling explores the sensitivity of the LCA results to change in key parameters. This research was conducted as part of the EU Horizon 2020 project SWEET (Sweeteners and sweetness enhancers: Impact on health, obesity, safety and sustainability).

Results and discussion GWP for 1 kg sucralose was calculated to be 71.83 $kgCO_2$-eq/kg (sugar from sugarcane is 0.77 $kgCO_2$-eq/kg). However, on a sweetness equivalence basis, GWP of sucralose reduces to 0.12 $kgCO_2$-eq/kg_{SE}. Production of reagents was the main contributor to impact across most impact categories. Sugar (starting material for sucralose production) was not a majority contributor to any impact category, and changing the source of sugar has little effect upon net impact (average 2.0% variation). Instead, uncertainty in reference data is a greater source of variability: reagent use optimization reduces average impact of sucralose production by approximately 45.4%. In general, sucralose has reduced impact compared to sugar on an equivalent sweetness basis, however, due to data uncertainty, the reduction is not significant for all impact categories.

Conclusion This LCA is the first for sucralose produced from cane sugar produced in the USA. Results indicate that sucralose has the potential to reduce the environmental impact of replacing the sweet taste of sugar. However, data were derived from literature and future collaboration with industry would help in reducing identified uncertainties. Accounting for functional use of sucralose in food and drink formulations is also necessary to fully understand the entire life cycle impact.

Keywords Life cycle assessment · Non-nutritive sweetener · Sucralose · Sucrose · Sugar

1 Introduction

There is increasing interest in reducing added sugar in diets, because excess consumption is associated with adverse health effects such as obesity (Johnson et al. 2017) and tooth decay (Vaghela et al. 2020). One means of reducing added sugar is using non-nutritive sweeteners (NNS), or sweetness enhancers to replace the sweet taste of sugar. Therefore, there is also increasing interest in potential health benefits associated with consuming NNS instead of added sugar (O'Connor et al. 2021; McGlynn et al. 2022), and the World Health Organization (WHO) have released an extensive review on the subject (Rios-Leyvraz and Montez 2022).

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In parallel, there is great concern regarding the environmental impact of food production and consumption (e.g., Behrens et al. 2017; Ibarrola-Rivas and Nonhebel 2022). Yet, to date, there has been very little study of the sustainability of ingredients which may replace the sweet taste of sugar. For instance, there is only one relating to a sweetness enhancer, thaumatin (Suckling et al. 2023a). In terms of NNSs, studies are limited to six life cycle assessments (LCAs); five studies for steviol glycosides produced in various ways (PureCircle 2015; Cargill 2021; Gantelas et al. 2022; Milovanoff and Kicak 2022; Suckling et al. 2023b), and one for aspartame produced by fermentation, in the World Food LCA Database (Nemecek et al. 2019). There is no equivalent LCA for sucralose.

Sucralose is one of the most commonly consumed NNS along with aspartame and acesulfame-K (Le Donne et al. 2017; Buffini et al. 2018) and is increasing in popularity, recently surpasing that of aspartame in Slovenia (Hafner et al. 2021). It has been approved for use in the European Union as additive E955, as per requirements laid out in Regulation EC 1333/2008. Sucralose is produced by chlorination of sucrose molecules (Luo et al. 2008), a process which increases perceived sweetness by 600-times (Wang et al. 2011). This part plant derived production process sets it apart from other NNS which are either extracted from plant materials (e.g., steviol glycosides or thaumatin), or artificially produced (e.g., acesulfame-K or neotame).

If sucralose and other NNSs are to be considered replacements for added sugar in foods and drinks at a dietary level, it is necessary to investigate the sustainability ramifications of making such a change. However, in order to do that, the environmental impact of any NNS must first be understood. Due to the popularity of sucralose, any such dietary study should attempt to include it. Therefore, this study builds upon existing evidence for other NNS by being the first LCA conducted for sucralose.

The main objective of this study was to understand whether chlorination of sucrose reduces environmental impact of delivering a given level of perceived sweetness. In order to do that, the chlorination process must be scrutinized to understand inputs and outputs in terms of materials, energy, and emissions. However, due to the small nature of the NNS industry, issues of confidentiality can make it difficult for data to be divulged for such an LCA. Despite attempts to collaborate, it was not possible to engage a sucralose manufacturer in data collection for this LCA, with concerns over intellectual property and the small number of sucralose producers being raised when declining invitation to collaborate (private communication). Therefore, it was necessary to find an alternative approach to deriving the life cycle inventory. Examples of such approaches have been described previously by Hischier et al. (2005) and Mila i Canals et al. (2011). A more recent method developed for deriving process data for chemicals has been developed by Huber et al. (2022); the RREM. In that study, Huber et al. (2022) developed a four-step methodology for building up inventory for chemicals which are not present in databases, and proposed methods for dealing with assumptions arising from data gaps. This study took a similar approach wherein sucralose synthesis data were derived from patent US 7,884,203 (Wang et al. 2011) and uncertainties or gaps in data accounted for where possible. The results provide insight into the environmental impact of, and uncertainty relating to, producing sucralose, and the challenges associated with conducting an LCA of highly refined food additives in this manner. Outputs from the study can be used by other practitioners wishing to understand the environmental impact of NNS use within food and drink products. Due to the uncertainties in production processes uncovered in this study, the LCA programme files are made available in Supplementary Material as a file named Process Model (in. CSV format) so that findings presented here may be further explored, and other assumptions tested. This research is part of the large EU Horizon 2020 project SWEET (Sweeteners and sweetness enhancers: Impact on health, obesity, safety, and sustainability, http://www.sweetproject.eu).

In this manuscript, sucrose (a disaccharide of glucose and fructose) is the specific form of sugar used for sucralose synthesis. However, due to similarity between the written words *sucrose* and *sucralose*, "sugar" is used in place of "sucrose" for clarity and simplicity.

2 Overview of sucralose production process and LCA

The system diagram for sucralose production is shown in Fig. 1. Sucralose is produced by chlorination of sugar in a chemical process, as outlined in US 7,884,203. The process is described in terms of four steps: sucrose-6-acetate

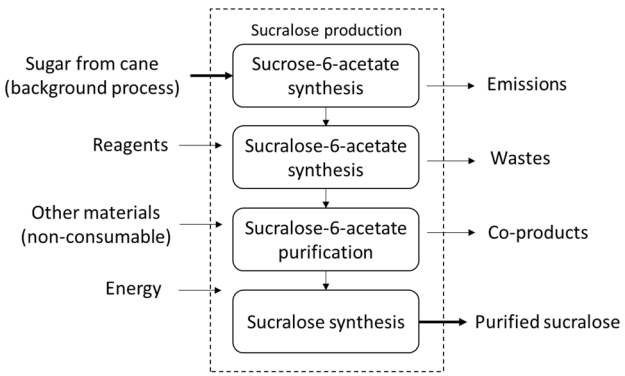

Fig. 1 Production process for sucralose showing main types of inputs and outputs

synthesis, sucralose-6-acetate synthesis, purification, and finally, sucralose synthesis. Each step is modelled separately in the LCA, to allow for parameterization of different data relating to each step. However, the whole process is assumed to occur within one factory. It is known that there is a sucralose plant in Alabama, USA (Tate and Lyle 2012) and, therefore, this is the assumed production location. The sugar is assumed to be produced from cane grown in Louisiana, USA (NASS 2018). It is likewise assumed that any supporting chemicals are produced in the USA. Alternative manufacturing locations for both sugar and chemicals are explored in scenario modelling.

The LCA environmental impact assessment was conducted using SimaPro 9.3 software and the ReCiPe 2016 Midpoint (Hierarchist) method (Huijbregts et al. 2016). Environmental impact within all impact categories of the ReCiPe 2016 method is reported, with focus given to global warming potential, land use, water consumption, marine eutrophication, and mineral resource scarcity.

2.1 Functional unit, goal, and scope

The goal of the LCA was to assess the environmental impact of producing 1 kg sucralose (E955) from sugar derived from sugarcane. As sucralose is a popular NNS used in many food and drink formulations, its use in each formulation is out of scope for this LCA, as is transport away from the factory. Therefore, the study is cradle-to-factory-gate. The functional unit is defined as "production of 1 kg purified sucralose". The LCA was undertaken in line with the ISO 14040:2006 (ISO 2010a) and ISO 14044:2006 (ISO 2010b) guidelines.

The study included all synthesis steps outlined in US 7,884,203 and background process data were taken from the Ecoinvent 3.8 and Agri-footprint 6.1 databases. Where an input material was not available in the databases, proxy processes were developed based upon literature sources. Related inventory data and references are given in Supplementary Material, Section 1, Tables S1 – S4. Where specific data relating to outputs, or co-products from reactions were not given in literature, stochiometric equations were used to derive quantities emitted. Formal disposal of wastes was not modelled, but instead, emissions of untreated wastes to the environment were assumed.

The functional unit is mass-based because 1 kg is an SI unit, but this does not reflect how sucralose is used within formulations. It is much sweeter than sugar, and smaller quantities are required to produce the same perceived sweetness. However, sweetness equivalence, or sucrose equivalence (both SE), is not exact, and varies depending upon application. Therefore, when comparison is offered to sugar, an SE of 600-times is used (Wang et al. 2011), and a mass of 1.67 g sucralose is used to provide equivalent sweetness to 1 kg sugar.

2.2 Allocation of impacts

All impacts are attributed to production of sucralose on an economic basis: all known by-products or reaction products were assumed to have no value. Cut-off criteria were applied to wastes exiting the system. Therefore, no burdens are associated with wastes (other than those relating to emission to the environment), likewise no benefits are carried (e.g., from recycling).

3 Life cycle inventory data

Sugar chlorination takes place over four steps as described in US 7,884,203 and shown in Fig. 1. A summary of material quantities and reaction conditions reported in the patent is given in the Supplementary Material, Section 2. Focus here is given to the quantity of materials and energy modelled for the baseline environmental impact results and are described as a function of production of 1 kg of each interim material and the final 1 kg sucralose product (and shown in Table 1). This reflects that each step in the process was modelled separately with 1 kg being the reference mass for each step (Supplemetary Material, Process Model). Masses of materials are those consumed by, or emitted from the reaction, and are inclusive of recovery rates as given in Table 2 and assumptions outlined in Section 3.1. All assumed quantities are parameterize and may be modified in the Process Model.

3.1 Assumptions

Information given in US 7,884,203 was not sufficient to model sucralose production directly. Therefore, the life cycle inventory needed to be filled in and the overarching process used here was in alignment with the RREM method developed by Huber et al. (2022). In summary, the steps were i) research on sucralose and its synthesis, ii) setting up of reaction equations and extending model if identified substances are lacking, iii) research on energy demand, and iv) modelling. The key assumptions are summarized as follows:

Yield In US 7,884,203, no reaction yields were stated. Instead, reagent masses and primary products are given. Implied molar yields derived from US 7,884,203 are 91.1% (sucrose-6-acetate synthesis), 65.4% (sucralose-6-acetate synthesis), and 68.0% (sucralose synthesis). No yield is given for sucralose-6-purification. However, it is not clear whether any discrepancies were due to unreacted reagents or from side-reactions occurring. Therefore, two approaches may be tested:

1. That imperfect yield is due to equilibrium in a reaction being reached, that only one reaction product is made, and that excess reagents are unreacted. In this

Table 1 Inventory data for production of 1 kg sucralose and preceding interim materials as used in baseline study

Sucrose-6-acetate synthesis			
Inputs	**Inputs per 1 kg**	**Outputs per 1 kg**	**Notes**
Sugar	899.1 g	8.36 g	Reagent (source material)
Acetic acid	156.5 g	95.00 mg	Reagent
DMF	12.41 g	12.41 g	Facilitator
DCC	285.7 mg	285.7 mg	Facilitator
Water	285.7 g	332.6 g	Facilitator & reaction product
Acetone	730.9 g	730.9 g	Facilitator
Transport	202.6 kg.km		Sugar transport
Transport	677.9 kg.km		Chemicals transport
Sucralose-6-acetate synthesis			
Inputs	**Inputs per 1 kg**	**Outputs per 1 kg**	**Notes**
Sucrose-6-acetate	918.7 g	44.66 g	Reagent
PCl_3	4.20 kg		Reagent
Water	11.07 kg	87.07 kg	Facilitator & reaction product
Sodium bicarbonate	14.84 kg		Reagent
DMF	21.62 g	21.62 g	Facilitator
TCA	480.9 g	480.9 g	Facilitator
DCM	1.13 kg	1.13 kg	Facilitator
CO_2		7.77 kg	Reaction product
Sodium chloride		4.96 kg	Reaction product
Transport	26.74 t.km		Chemicals transport
Sucralose-6-acetate purification			
Inputs	**Inputs per 1 kg**	**Outputs per 1 kg**	**Notes**
Sucralose-6-acetate	1.00 kg		Reagent
Methanol	5.94 g	5.94 g	Facilitator
Water	1.35 kg	1.35 kg	Facilitator
Transport	4.47 kg.km		Chemicals transport
Sucralose synthesis			
Inputs	**Inputs per 1 kg**	**Outputs per 1 kg**	**Notes**
Sucralose-6-acetate	1.16 kg	50.3 g	Reagent
Methanol	595.5 g	478.9 g	Reagent
Water	487.8 g	487.8 g	Facilitator
Potassium hydroxide	4.88 g	4.88 g	Facilitator
Activated carbon	128.0 g	128.0 g	Facilitator and reactivation process
Methyl acetate		1.86 g	Reaction product
Trisodium phosphite		8.71 kg	Reaction product
Transport	521.5 kg.km		Chemicals transport
Electricity	1.00 kWh		
Heat	2.00 kWh		
Sucralose factory	4.00×10^{-10}		Proxy process: organic chemicals factory (Facilitator)

instance, unreacted chemicals were assumed recovered and re-used in the system as much as possible, and unrecovered reagents were emitted, untreated to the environment (this assumption differs to that used in the RREM method (Huber et al. 2022)). This approach was used for the baseline environmental impact calculation in this study.

2. That complete reaction of reagents occurs, and that imperfect yield is due to side-reactions creating unwanted by-products. This assumption was tested in scenario modelling (Section 5.2). Masses of reagents consumed were estimated from stochiometric equations (Supplementary Materials, Section 3), with the stated product mass being used to define the input

Table 2 Recovery rates applied to reagents, catalysts, and products of sucralose synthesis

Main products		
Sucrose	90.33%	Assumed same as sucrose-6-acetate
Sucrose-6-acetate	90.33%	Chen et al. (2022)
Sucralose-6-acetate	90.33%	Assumed same as sucrose-6-acetate
Solvents/catalysts		
DMF	99.80%	Dou et al. (2019)
DCC	99.80%	Assumed same as DMF
Water	0.00%	Assumed
Acetone	67.37%	Nemeth et al. (2020)
TCA	82.00%	Assumed same a DCM
KOH	0.00%	Assumed
Methanol	95.00%	Dhar and Kirtania (2010)
DCM	82.00%	Ramalingam et al. (2011)
Reagents		
Acetic acid	99.90%	Fang et al. (2020)
By-products		
Trisodium phosphite	0.00%	Assumed
Carbon dioxide	0.00%	Assumed
Sodium chloride	0.00%	Assumed
Methyl acetate	99.00%	Zheng et al. (2015)

mass of reagents. Any stated excess of reagents was assumed converted into an equal mass of hazardous materials. Side-product disposal was modelled using a hazardous waste disposal process from Ecoinvent 3.8. It should be highlighted that this method required greater quantities of reagents and, therefore, net increase in consumed materials from each process step as described in Section 3.2.

Recovery rates Materials that are not consumed directly within the synthesis steps may be recovered. No recovery rates are stated in US 7,884,203. Therefore, where possible, recovery rates from literature were applied, as shown in Table 2. Recovery rates that could not be found were defined based upon assumptions relating to similar materials. Because material recovery is likely specific to the instance in which it is measured, and none of the rates found in literature pertained to sucralose synthesis, change in rate of recovery of key materials are tested in scenario modelling, Section 5.2. In addition, recovery rates are parameterized in the LCA model (Supplementary Material, Process Model) so practitioners may further explore them. It was assumed that recovered materials are recirculated until consumed in the production process. Any materials that are not recovered are emitted to the environment and quantities are defined in the process description.

Useful by-products Methyl acetate is thought to be produced from the reactions and has potential to be recovered and used elsewhere (NCBI 2023). However, in alignment with the cut-off principle, any benefits of use elsewhere are not counted as a reduction in impact of sucralose. Instead, it is assumed to leave the production system with no burden or benefits attached (aside from the fraction not recovered, which is emitted to water). The recovery rate applied is given in Table 2.

Material use Quantities of materials described in Examples in US 7,884,203 align with ranges stated in the Claims. However, there is one notable exception: phosphorus trichloride (PCl_3) in sucralose-6-acetate synthesis. The molar quantity given in Example 3 (approx. 8.8-times than that of sucrose-6-acetate) is greater than the range defined in Claim 3 (4- to 7-times). This was found to have an effect in the study presented here, because US 7,884,203 states that sodium bicarbonate is used to neutralize the reaction, but what it neutralizes is not clearly stated. From stochiometric equations (Supplementary Material, Section 3), a reaction product may be phosphorous acid. If it is phosphorous acid being neutralized, then an excess of PCl_3 leads to an excess of sodium bicarbonate consumption, a potentially unnecessary process efficiency reduction. Therefore, for this study, it was assumed that the quantity of PCl_3 consumed at baseline was that outlined in Example 3 (8.8-times), and scenario modelling explores taking the lower bound of that given in Claim 3 (4-times).

3.2 Production steps

In this section, total consumed resources are described, derived from US 7,884,203 and the assumptions outlined above. Each process step (Fig. 1) is described separately and quantities of materials, or resources such as energy and transport, are summarized in Table 1 as a function of process step.

1. *Sucrose-6-acetate synthesis*: 899.1 g of sugar from cane is reacted with 156.5 g acetic acid to produce 1 kg sucrose-6-acetate. Materials consumed in this step are as follows: 12.41 g N,N-dimethylformamide (DMF), 285.7 mg N,N-dicyclohexylcarbidiimide (DCC), 285.7 g decarbonized water, and 730.9 g acetone. The sugar is transported from Louisiana, USA, for 225.3 km by EURO 6 equivalent 32-ton capacity truck (202.6 kg.km). All chemicals are transported from Texas, USA, for 753.2 km (677.9 kg.km) by the same type of truck. Any materials not recovered are assumed emitted unchanged to water: 8.36 g sugar, 95.00 mg acetic acid, 332.6 g water, 730.9 g acetone, 12.41 g formamide (a proxy for DMF), and 285.7 mg DCC. DCC was not in available

LCI databases and, therefore, a proxy was created from data given in Vora et al. (2021), and reproduced in Supplementary Material, Section 1, Table S1.

2. *Sucralose-6-acetate synthesis*: 918.7 g sucrose-6-acetate is reacted with an excess of 4.20 kg PCl_3 to produce 1 kg sucralose-6-acetate. Materials consumed in this step are as follows: 11.07 kg water, 14.84 kg sodium bicarbonate, 21.62 g DMF, 480.9 g trichloroacetonitrile (TCA), 1.13 kg dichloromethane (DCM), and 106.7 g activated carbon. As before, all chemicals are transported from Texas for 753.2 km (26.74 t.km). Unrecovered materials are emitted to water: 11.07 kg water, 1.13 kg DCM, 21.62 g DMF (modelled as formamide). Excess PCl_3 reacts with water in the solution leading to products which are also neutralized with sodium bicarbonate (reaction equations given in Supplementary Material, Section 3). Therefore, all PCl_3 is assumed consumed. In addition, the following reaction products are emitted: 7.77 kg CO_2 to air, and 4.96 kg sodium chloride, 44.66 g sucrose-6-acetate (modelled as an "unspecified organic compound"), 8.71 kg trisodium phosphite (from neutralization reactions and modelled as "phosphorus containing compounds, unspecified"), and 76.0 kg water all emitted to water. In the patent, neither masses of DCM nor activated carbon are stated. Moreover, data relating to solubility of sucralose-6-acetate in DCM could not be found in literature. Therefore, the mass of DCM was estimated using a reference for sucralose solubility in methanol and the assumption that sucralose-6-acetate has the same solubility in DCM (Li et al. 2010). For activated carbon, the source used was commercial data (SAS 2022), with mass derived from an absorption efficiency of 33.3% activated carbon mass and 1% of reaction solution mass being absorbed. Effect on the LCA results of varying consumption of both DCM and activated carbon are explored in Section 5.2. TCA was not in available LCI databases; therefore, a proxy was created from data given in Kabisch (1956), and reproduced in Supplementary Material, Section 1, Table S3.
3. *Sucralose-6-acetate purification*: 1 kg sucralose-6-acetate is purified using 10% methanol in water (net consumption of 5.94 g methanol and 1.35 kg water after accounting for recovery rates). Transport of methanol is modeled as 4.47 kg.km as per chemicals in previous steps. Unrecovered solvents emitted to water are 1.35 kg water and 5.94 g methanol. No information on quantity or type of impurities removed is given in US 7,884,203 and, therefore, a 100% yield is assumed as the baseline case. A perfect yield is unlikely; therefore, the effect of a 90% yield is explored as a scenario (Section 5.2.), with impurities modelled as organic chlorine containing compounds emitted to water.
4. *Sucralose synthesis*: 1.16 kg sucralose-6-acetate is reacted with methanol (net consumed 595.5 g) to produce 1 kg sucralose. Solvents and catalysts consumed in the reaction are: 487.8 g water; 4.88 g potassium hydroxide; and 128.0 g activated carbon. Reactivation of 128.0 g activated carbon is also modelled using the process from the Ecoinvent 3.8 database. Transport of chemicals is modelled as per previous steps and is 521.5 kg.km. Unrecovered catalysts and solvents are emitted to water: 478.9 g methanol; 487.8 g water; potassium compounds 4.88 g (as a proxy for potassium hydroxide); and 50.3 g organic chlorine compounds (as a proxy for unreacted sucralose-6-acetate). From stochiometric equations in Supplementary Materials, Section 3, it is understood that methyl acetate is a by-product of the reaction and 1.86 g unrecovered methyl acetate is emitted to water. No masses of activated carbon or potassium hydroxide were stated in US 7,884,203; therefore, these were estimated, with mass of activated carbon derived as per step 2. For potassium hydroxide, a dissocaition constant for the mixture could not be found and, therefore, was assumed to be the same as in water ($k_b = 3.16 \times 10^{-1}$). Equations for dissociation are given in the Supplementary Material, Section 4. Change in the consumption of activated carbon and potassium hydroxide are explored in scenario modelling, Section 5.2.

No energy consumption was stated in US 7,884,203. Therefore, 2 $kWh/kg_{sucralose}$ heat and 1 $kWh/kg_{sucralose}$ electricity were assumed, which are similar to LCA data relating to a comparable food additive, aspartame (Nemecek et al. 2019) and in excess of the 0.5 $kWh/kg_{product}$ defined in Huber et al. (2022). Change in energy consumption is explored in scenario modelling, Section 5.2. Inventory data for the sucralose factory were not available and, therefore, a proxy organic chemical factory process from the Ecoinvent 3.8 database was used (4.0×10^{-10} units).

4 Results

In this section, results are presented for production of 1 kg sucralose for all ReCiPe 2016 (H) midpoint impact categories. For brevity, only impacts relating to global warming potential (GWP), marine eutrophication (MEu), land use (LU), water consumption (WC) and mineral resource scarcity (MRS) are discussed in detail.

Figure 2 shows the relative impact associated with different groups of inputs and emissions; sugar (black), energy (red), transport (blue), reagents (green), facilitators (e.g., solvents and catalysts; purple), and emissions (orange). Emissions here specifically refer to new materials which are either produced by synthesis steps described

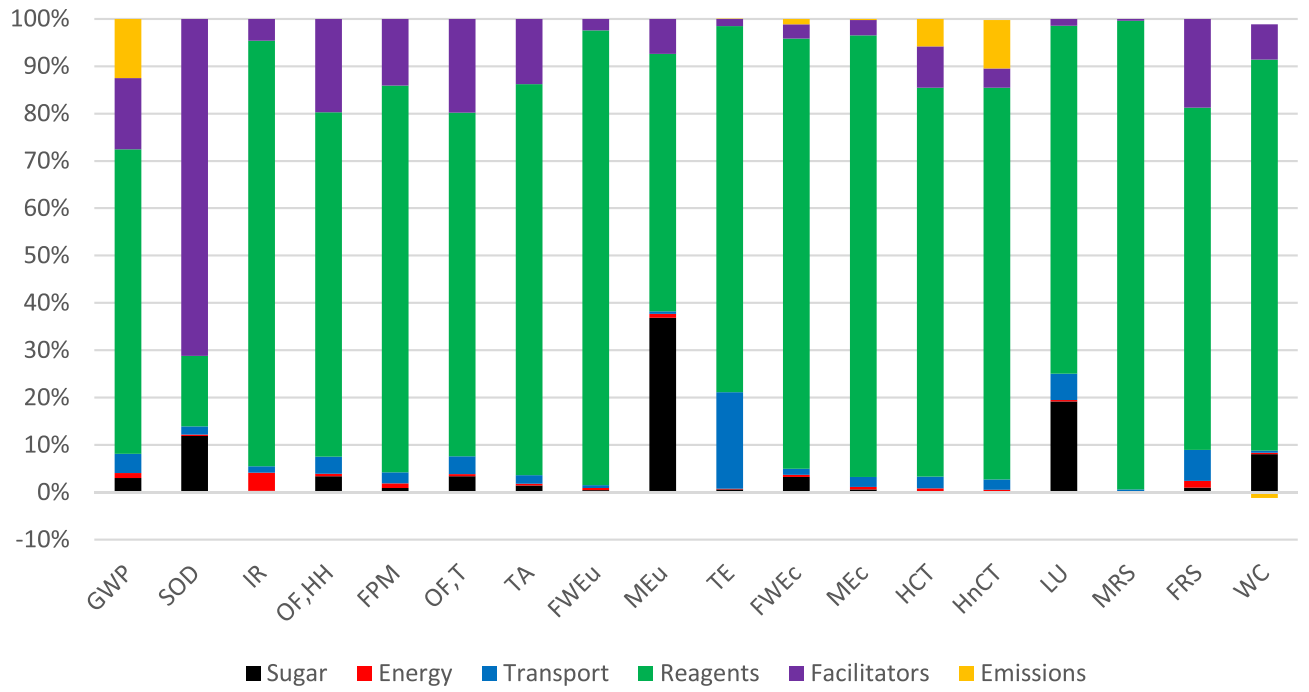

Fig. 2 Relative impacts of each input and output type in terms of all ReCiPe 2016 (H) midpoint impact categories. Inputs shown are sugar (black), energy (red), transport (blue), reagents (green), and facilitators (purple). Emissions shown as orange. GWP, global warming potential; SOD, stratospheric ozone depletion; IR, ionizing radiation; OF,HH, ozone formation, human health; FPM, fine particulate matter; OF,T, ozone formation, terrestrial; TA, terrestrial acidification; FWEu, freshwater eutrophication; MEu, marine eutrophication; TE, terrestrial ecotoxicity; FWEc, freshwater ecotoxicity; MEc, marine ecotoxicity; HCT, human carcinogenic toxicity; HnCT, human non-carcinogenic toxicity; LU, lane use; MRS, mineral resource scarcity; FRS, fossil resource scarcity; WC, water consumption

in this study, or input materials which are not recovered. Emissions arising from background processes are included in the impacts of those input materials, or resources (for example, energy). Absolute numerical data for all impacts are given in Table 3. In terms of GWP, the total impact is 71.83 $kgCO_2$-eq/$kg_{sucralose}$. The main contribution to impact comes from reagents at 46.19 $kgCO_2$-eq/$kg_{sucralose}$ (64.3% of total), facilitators at 10.81 $kgCO_2$-eq/$kg_{sucralose}$ (15.1%) and emissions at 8.99 $kgCO_2$-eq/$kg_{sucralose}$ (12.5%). Transport, energy, and sugar production are minor contributors, accounting for a total of 5.83 $kgCO_2$-eq/$kg_{sucralose}$ (8.1%). In terms of MEu, total impact is 3.38×10^{-3} kgN-eq/$kg_{sucralose}$. Main contributions are from reagents at 1.84×10^{-3} kgN-eq/$kg_{sucralose}$ (54.4%) and sugar at 1.24×10^{-3} kgN-eq/$kg_{sucralose}$ (36.9%). All other sources account for a total of 2.95×10^{-4} kgN-eq/$kg_{sucralose}$ (8.7%). In terms of LU, total impact is 4.50 m^2acrop-eq/$kg_{sucralose}$. Main contributions are from reagents 3.31 m^2acrop-eq/$kg_{sucralose}$ (73.4%) and sugar production 8.65×10^{-1} m^2acrop-eq/$kg_{sucralose}$ (19.2%). All other sources contribute a total of 3.31×10^{-1} m^2acrop-eq/$kg_{sucralose}$ (7.4%). In terms of WC, total impact is 1.29 $m^3/kg_{sucralose}$. Main contributions are from reagents at 1.09 $m^3/kg_{sucralose}$ (84.5%), sugar at 1.07×10^{-1} $m^3/kg_{sucralose}$ (8.3%), and facilitators at 9.82×10^{-2} $m^3/kg_{sucralose}$ (7.6%). All other sources contribute a total of -6.06×10^{-3} $m^3/kg_{sucralose}$ (-0.5%). The negative contribution is due to a net emission of water from the reactions (-1.53×10^{-2} $m^3/kg_{sucralose}$) which offsets consumption of the other inputs. Finally, in terms of MRS, total impact is 1.11 kgCu-eq/$kg_{sucralose}$. The main contributor is from reagents at 1.10 kgCu-eq/$kg_{sucralose}$ (99.0%). All the other groups contribute a total of 1.13×10^{-2} kgCu-eq/$kg_{sucralose}$ (1.0%). The main impact from sugar production is associated with growing the sugarcane crop (MEu, LU and WC). Across all impact categories, reagents are the greatest contributor, accounting for an average of 77.0%, followed by facilitators at 12.1%, and sugar at 5.3%.

For comparison, an equivalent cradle-to-gate environmental impact for sugar derived from sugar cane grown in the USA is 0.77 CO_2-eq/kg_{sugar} for GWP, 1.30×10^{-3} kgN-eq/kg_{sugar} for MEu, 9.06×10^{-1} m^2acrop-eq/kg_{sugar} for LU, 1.12×10^{-1} m^3/kg_{sugar} for WC, and 1.19×10^{-3} kgCu-eq/kg_{sugar} for MRS. Other impact categories are shown in Table 1. The impacts per kg for sugar are thus much lower than those for 1 kg of sucralose. This highlights the need for a 'functional' comparison of these ingredients based on their sweetness equivalence, rather than simplistically on mass alone.

The results for sucralose production demonstrate that reagents are the main source of impact, despite there being only four materials in that category (acetic acid, PCl_3, $NaHCO_3$, methanol). In contrast, the facilitators comprise nine

Table 3 Absolute numerical impact data supporting that shown in Fig. 2. Impact category abbreviations defined in caption of Fig. 2. Data shown as function of 1 kg sucralose. For comparison, Agri-footprint 6.1 cradle-to-gate data for sugar produced from sugarcane grown in the USA is given in right-hand column. Cells with zero impact denoted by a dash

	Sugar	Energy	Transport	Reagents	Facilitators	Emissions	Total	Sugar from sugarcane
GWP ($kgCO_2$-eq)	2.14	7.84×10^{-1}	2.91	46.19	10.81	8.99	71.83	7.67×10^{-1}
SOD (kgCFC11-eq)	1.42×10^{-5}	3.01×10^{-7}	2.07×10^{-6}	1.79×10^{-5}	8.1×10^{-5}	-	1.20×10^{-4}	8.76×10^{-6}
IR (kBqCo-60-eq)	1.28×10^{-2}	1.52×10^{-1}	5.34×10^{-2}	3.55	1.82×10^{-1}	-	3.95	1.34×10^{-2}
OF,HH ($kgNO_x$-eq)	5.52×10^{-3}	8.32×10^{-4}	5.85×10^{-3}	1.18×10^{-1}	3.21×10^{-2}	-	1.63×10^{-1}	5.78×10^{-3}
FPM (kgPM2.5-eq)	1.19×10^{-3}	1.36×10^{-3}	3.15×10^{-3}	1.10×10^{-1}	1.90×10^{-2}	-	1.35×10^{-1}	1.24×10^{-3}
OF,T ($kgNO_x$-eq)	5.55×10^{-3}	8.58×10^{-4}	6.20×10^{-3}	1.20×10^{-1}	3.27×10^{-2}	-	1.65×10^{-1}	5.82×10^{-3}
TA ($kgSO_2$-eq)	4.83×10^{-3}	1.38×10^{-3}	6.15×10^{-3}	2.84×10^{-1}	4.73×10^{-2}	-	3.43×10^{-1}	5.06×10^{-3}
FWEu(kgP-eq)	4.00×10^{-4}	3.96×10^{-4}	6.02×10^{-4}	8.67×10^{-2}	2.20×10^{-3}	-	9.03×10^{-2}	4.19×10^{-4}
MEu (kgN-eq)	1.24×10^{-3}	2.72×10^{-5}	1.87×10^{-5}	1.84×10^{-3}	2.49×10^{-4}	-	3.38×10^{-3}	1.30×10^{-3}
TE (kg1,4-DCB)	2.26	4.39×10^{-1}	71.69	272.49	5.34	1.71×10^{-1}	352.42	2.37
FWEc (kg1,4-DCB)	1.22×10^{-1}	1.73×10^{-2}	4.75×10^{-2}	3.37	1.14×10^{-1}	4.22×10^{-2}	3.74	1.27×10^{-1}
MEc (kg1,4-DCB)	3.04×10^{-2}	2.29×10^{-2}	1.01×10^{-1}	4.47	1.54×10^{-1}	1.13×10^{-2}	4.79	3.18×10^{-2}
HCT (kg1,4-DCB)	8.43×10^{-3}	2.72×10^{-2}	1.04×10^{-1}	3.47	3.68×10^{-1}	2.46×10^{-1}	4.23	8.83×10^{-3}
HnCT (kg1,4-DCB)	-2.22×10^{-1}	5.02×10^{-1}	1.94	74.41	3.61	9.22	89.46	-2.32×10^{-1}
LU (m^2a-crop-eq)	8.65×10^{-1}	1.31×10^{-2}	2.51×10^{-1}	3.31	6.67×10^{-2}	-	4.50	9.06×10^{-1}
MRS (kgCu-eq)	1.14×10^{-3}	5.30×10^{-4}	5.06×10^{-3}	1.10	4.60×10^{-3}	-	1.11	1.19×10^{-3}
FRS (kgoil-eq)	1.56×10^{-1}	2.42×10^{-1}	1.06	11.77	3.05	-	16.29	1.63×10^{-1}
WC (m^3)	1.07×10^{-1}	3.40×10^{-3}	5.82×10^{-3}	1.09	9.82×10^{-2}	-1.53×10^{-2}	1.29	1.12×10^{-1}

materials (Table 1). Therefore, contribution of individual reagents is explored in greater detail in Fig. 3. Shown are the relative impacts of acetic acid (black), PCl_3 (red), $NaHCO_3$ (blue), and methanol (green) to the total reagents' impact across all ReCiPe 2016 impact categories. The greatest contributors to impact are PCl_3 at an average of 47.6% across all

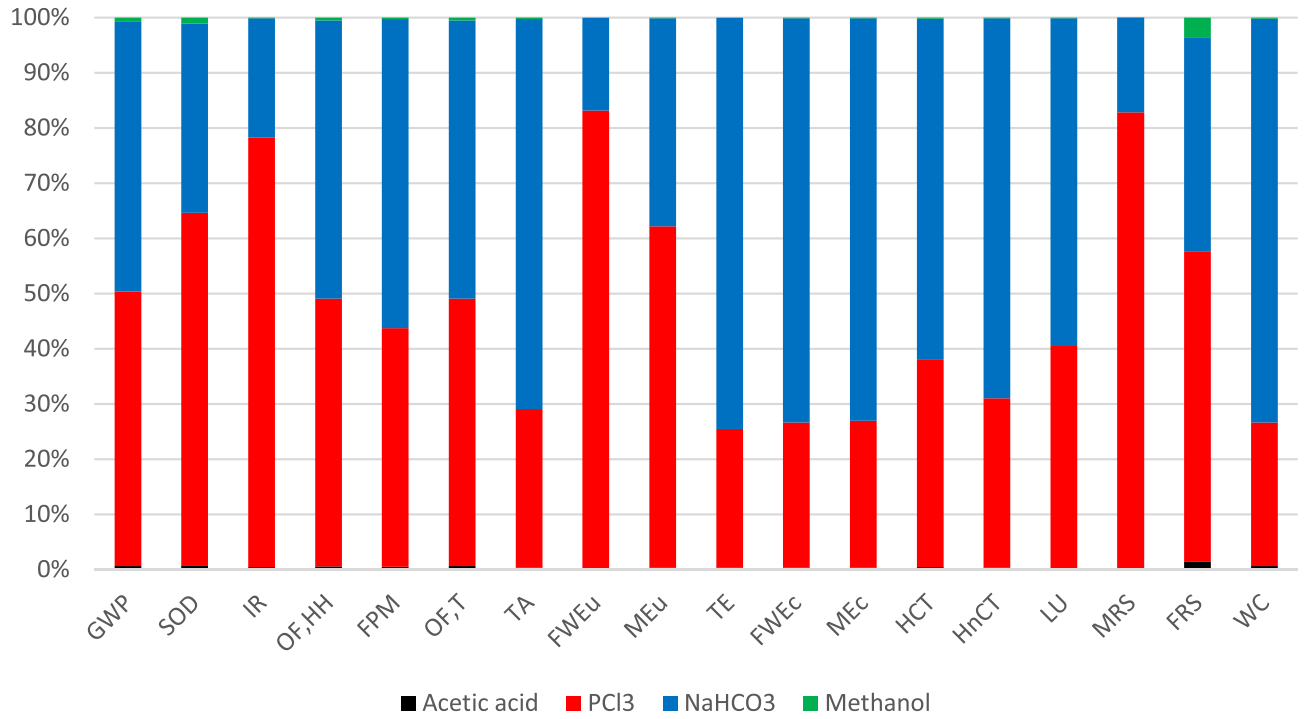

Fig. 3 Relative contribution of individual materials to net reagent impact: acetic acid (black), PCl_3 (red), $NaHCO_3$ (blue), and methanol (green). Key for impact category abbreviations given in Fig. 2

categories, and $NaHCO_3$ at 51.4%. Acetic acid and methanol together contribute 1.0%. PCl_3 is used in excess during chlorination of sucrose-6-acetate. A by-product of that reaction is phosphorous acid, which is neutralized using $NaHCO_3$ in water. However, a further reaction may occur between excess PCl_3 and the water, creating yet more phosphorous acid (Melhem and Reid 1998), which must be neutralized. Therefore, reducing excess PCl_3 may reduce impact due to both it and subsequent excess $NaHCO_3$. This was explored in scenario modelling.

4.1 Sweetness equivalence of sucralose

The results presented so far have been in terms of 1 kg sucralose. However, sucralose is approx. 600-times sweeter than sugar (Wang et al. 2011) and does not replace sugar on a like-for-like mass basis. Instead, only 1.67 g sucralose is needed to replace the sweetness of 1 kg sugar. Therefore, an alternative way of comparing environmental impact is sweetness equivalence (SE), whereby environmental impact of 1.67 g sucralose (called 1 kg_{SE}) is normalized to that of 1 kg sugar, as shown in Fig. 4. Two environmental impacts of sugar are shown: 1 kg US cane sugar (black) and 1 kg of a global sugar mix (red) of 80% sugar from cane, and 20% sugar from beet (ISO 2020; OECD et al. 2021). Full numerical data are given in Supplementary Material, Section 5, Table S5. The results show that although sucralose tends to reduce the environmental impact of providing 1 kg_{SE} by 80% or more across most impact categories, this is not true of all impact categories. The impact in GWP of sucralose on a sweetness basis is approx. 10% to 15% that of a global mix of sugar and US cane sugar respectively; MEu is between 0.3% and 0.4% respectively; LU between 0.5% and 0.8% respectively; and WC between 1 and 2% respectively. In contrast, the impact of sucralose is greater than sugar in MRS at 149% to 155%, respectively, because of demands placed by excess PCl_3 and sodium bicarbonate consumption. Finally, HnCT has a negative relative impact (not shown in Fig. 4, instead numerical data in Supplementary Material, Section 5, Table S5), which is due to background process data for sugar in the Agri-footprint database, showing a net absorption of certain toxic materials during sugarcane growth and reflects the cradle-to-gate nature of the study. Finally, the relative means for sucralose for both IR and HCT are less than for sugar but may exceed sugar when uncertainty is accounted for (Section 5.1).

In instances when sucralose can directly replace sugar (such as in drinks or tabletop sweeteners), the enhanced sweetness has potential to reduce land use. The impact category for land use in the ReCiPe 2016 (H) method is a measure of both land occupation and transformation, and as such also reflects biodiversity impact. However, land use may be used as an indication for potential land sparing and benefits that might arise from it. For instance, land use for producing 1 kg sugar from cane in the USA is 9.06×10^{-1} m^2acrop-eq/kg and from a global mix of sugar it is 1.39 m^2acrop-eq/kg. In contrast, 1 kg_{SE} sucralose requires $7.51 \times 10^{-3} \pm 1.44 \times 10^{-3}$ m^2acrop-eq/kg. This shows that chlorinating sugar into sucralose has potential for land sparing benefits.

5 Discussion

In Section 3, life cycle inventory data underpinning the baseline assessment were defined. At the same time uncertainties within the data and assumptions or estimates made to fill

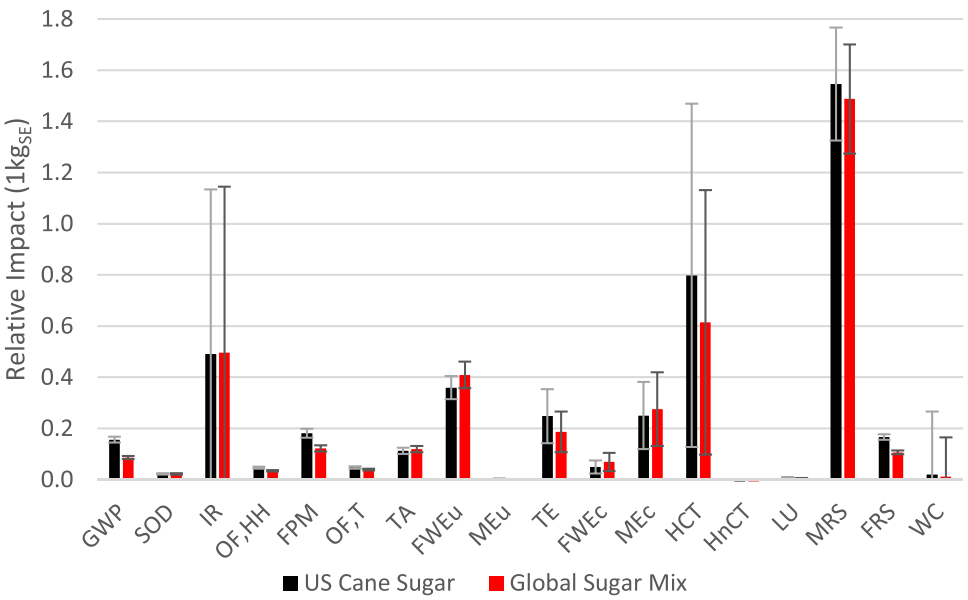

Fig. 4 Relative impact of 1kg_{SE} sucralose compared to 1 kg_{SE} sugar across all impact categories of the ReCiPe 2016 method. Sucralose compared to US cane sugar (black) and a global sugar mix (red). Error bars show standard deviation presented in Table 4. Results for 1 kg_{SE} sucralose are normalized to 1 kg sugar. Data for HnCT are negative (-0.64 ± 0.29 for US cane sugar, and -1.19 ± 0.53 for global sugar mix); numerical data given in Supplementary Material, Section 5, Table S5

data gaps were presented. Resulting variation in material or energy consumption are likely to impact upon the results. Therefore, in this section, the effect of uncertainty within the data are explored and their effect upon the environmental impact results quantified.

5.1 Uncertainty modelling

Table 4 shows sensitivity of the life cycle impact assessment to uncertainty within inventory data for 1 kg sucralose production. Uncertainty in both foreground and background data were modelled using the Monte Carlo simulation function available in SimaPro 9.3. Results are shown in terms of baseline impact, mean of sensitivity analysis, standard deviation from the mean, and standard deviation as a percent of mean value (relative standard deviation). All the means are shown to be close to the baseline results, with no significant deviation. Moreover, any changes are both up and down, indicating no skew resulting from uncertainty regarding a net reduction or increase in impact. However, within the results, three impact categories with greatest uncertainty are: WC, IR and HCT. In terms of WC, uncertainty (1263.21% relative standard deviation) relates to the greater quantity of water which flows through the product system, compared to that consumed: relatively small variation in net through-flow results in large apparent variation in consumption impact. For both IR and HCT (133.08% and 83.79% relative standard deviation respectively), uncertainty arises from background processes and does not appear to be greatly increased by foreground processes. Specifically, for IR, impact arises from electricity production, and majority electricity consumption is from PCl_3 production. Background uncertainty of IR from electricity processes used in PCl_3 production has a relative standard deviation 171.0%. For HCT, impacts arise from a greater variety of sources, but the majority appears to be from construction of organic chemical factories for sodium bicarbonate production. Uncertainty in those construction processes is 69.2% relative standard deviation.

5.2 Scenario modelling

In the life cycle inventory description (Section 3.2), several assumptions were made to enable environmental assessment. In this section, sensitivity of the results to changes in those assumptions are explored in detail.

The following scenarios and results are explored separately:

1. *Source of sugar*: It was assumed that all sugar was sourced from sugarcane grown in the USA. However, it could be sourced from a global commodities market. Therefore, change of sugar sourced from sugarcane grown in Louisiana, USA, to a global mix of 80% sugar from cane and 20% sugar from beet (ISO 2020; OECD et al. 2021) is explored. Results shown in Fig. 5.
2. *Chemicals source*: It was assumed that all chemicals were sourced from Texas, however, this might not be true in all instances. Therefore, change caused by sourcing chemicals from China instead is explored. This was modelled as a net increase in mass.distance from 27.94 t.km by road (as summed across Table 1) to 685.32 t.km by ship. All other data were kept the same as baseline. Results shown in Fig. 5.
3. *PCl_3 consumption*: It has been highlighted how the quantity of PCl_3 is stated as different in various parts of

Table 4 Sensitivity of the environmental impact assessment to uncertainty in foreground and background data

	Baseline	Mean	Standard Deviation	Relative Standard Deviation
GWP ($kgCO_2$-eq)	71.83	71.82	5.23	7.28
SOD (kgCFC11-eq)	1.20×10^{-4}	1.19×10^{-4}	1.28×10^{-5}	10.75
IR (kBqCo-60-eq)	3.95	3.88	5.17	133.08
OF,HH ($kgNO_x$-eq)	1.63×10^{-1}	1.63×10^{-1}	1.43×10^{-2}	8.75
FPM (kgPM2.5-eq)	1.35×10^{-1}	1.35×10^{-1}	1.31×10^{-2}	9.69
OF,T ($kgNO_x$-eq)	1.65×10^{-1}	1.66×10^{-1}	1.44×10^{-2}	8.71
TA ($kgSO_2$-eq)	3.43×10^{-1}	3.43×10^{-1}	3.63×10^{-2}	10.57
FWEu(kgP-eq)	9.03×10^{-2}	9.02×10^{-2}	1.14×10^{-2}	12.63
MEu (kgN-eq)	3.38×10^{-3}	3.38×10^{-3}	2.36×10^{-4}	6.69
TE (kg1,4-DCB)	352.42	352.05	149.51	42.47
FWEc (kg1,4-DCB)	3.74	3.74	1.95	52.09
MEc (kg1,4-DCB)	4.79	4.79	2.51	52.34
HCT (kg1,4-DCB)	4.23	4.24	3.55	83.79
HnCT (kg1,4-DCB)	89.46	89.80	39.78	44.35
LU (m^2a-crop-eq)	4.50	4.51	7.82×10^{-1}	17.35
MRS (kgCu-eq)	1.11	1.11	1.58×10^{-1}	14.33
FRS (kgoil-eq)	16.29	16.30	1.06	6.48
WC (m^3)	1.29	1.31	16.49	1263.21

US 7,884,203 (Section 3.1). Therefore, change in PCl_3 consumption from a molar quantity of 8.8-times that of sucrose-6-acetate (as given in Example 3 of US 7,884,203) to 4-times (as given in Claim 3 of the same) is explored. This was modelled as a reduction in PCl_3 consumption from 4.20 kg to 1.91 kg, and sodium bicarbonate from 14.84 kg to 5.86 kg. Similarly, CO_2 emission is reduced from 7.77 kg to 3.37 kg, trisodium phosphite emission from 8.71 kg to 3.44 kg, and reaction product water emission from 1.61 kg to 0.70 kg. Results shown in Fig. 5.

4. *Materials consumption*: Consumption rates of DCM, KOH, activated carbon and energy were not given in background literature and were derived from other literature, or assumed. Sensitivity of results to a five-times increase in consumption of all four during the production process is explored. Results shown in Fig. 6.
5. *Recovery rates*: Several material recovery rates had to be assumed. Therefore, change in recovery rate of DCC, TCA, sugar, and sucralose-6-acetate by ± 10% from that given in Table 2 is explored. Note: other recovery rates not explored here are parameterized in the Process Model (Supplementary Material) and can be further explored. Results shown in Fig. 7.

Yield was highlighted as a particular uncertainty from the process description in US 7,884,203. Therefore, two scenarios explore yield of different parts of the process:

6. *Sucralose-6-acetate purification yield*: Due to lack of information, yield of sucralose-6-acetate purification was assumed to be 100% for baseline results. This is unlikely. Therefore, a reduced yield of 90% sucralose-6-acetate (900 g product instead of 1000 g) is modelled alongside an emission of 10% (100 g) of chlorine containing organic compounds to water (a proxy as sucralose-6-acetate is not available in SimaPro). Results shown in Fig. 5.
7. *Other process yields*: In Section 3.1, yields for interim products and final sucralose inferred from US 7,884,203 were reported and two methods for approaching the issue of imperfect yields were suggested for this study. The baseline results assumed that reagents were not consumed in reactions and could be recovered for reuse. Instead, this scenario explores increased reagent consumption due to side-reactions producing unwanted by-products. For this scenario, sucrose consumption becomes 977.1 g (up from baseline of 899.1 g), acetic acid 251.4 g (up from 156.5 g), sucrose-6-acetate 1.34 kg (up from 918.7 g), sucralose-6-acetate 1.63 kg (up from 1.16 kg), and methanol consumption in the sucralose synthesis step 595.5 g (up from 559.5 g). As methanol is used in excess, the quantity emitted to water also changes from 478.9 g to 477.0 g. Side-products are modelled as hazardous waste treatment with a net mass of 1.20 kg. Quantity of PCl_3 consumed does not change because all of it is consumed, as described in Section 3.2. Results shown in Fig. 5.

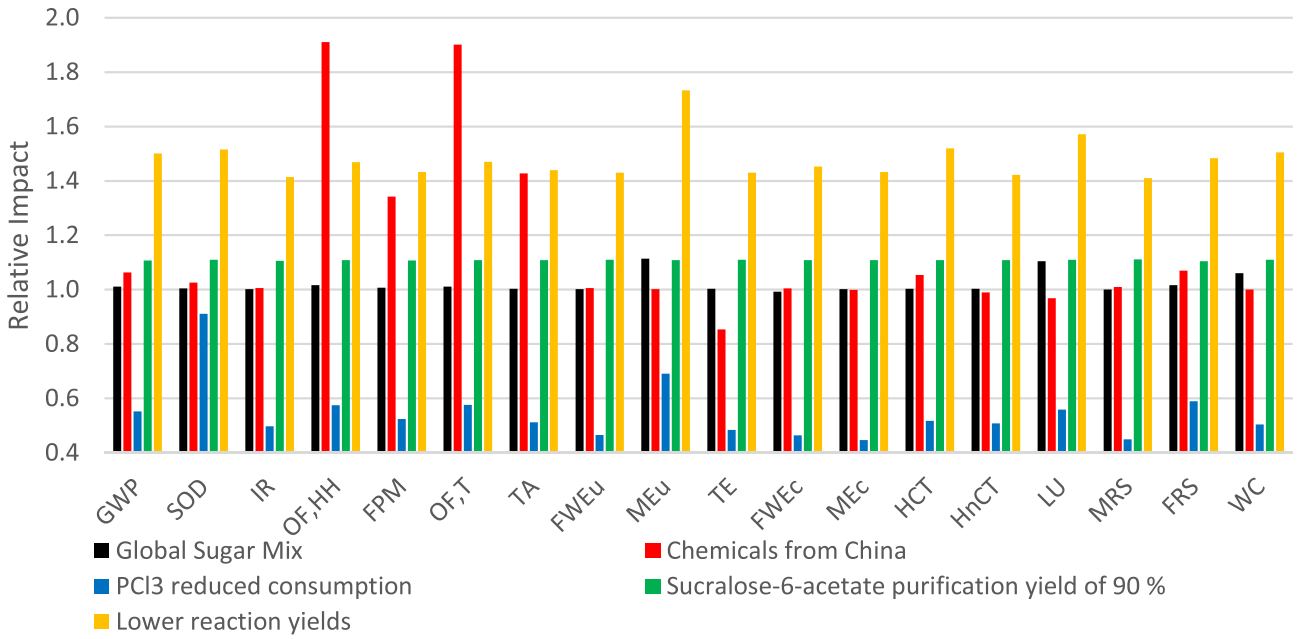

Fig. 5 Relative change in environmental impact of 1 kg sucralose production as a function of separate parameter change compared to baseline model. Effect of change in sugar source (black), chemicals source (red), PCl_3 consumption (blue), sucralose-6-acetate purification yield to 90% (green), and lower reaction yields (orange) shown. Baseline impact equates to 1. Key for impact category abbreviation given in Fig. 2

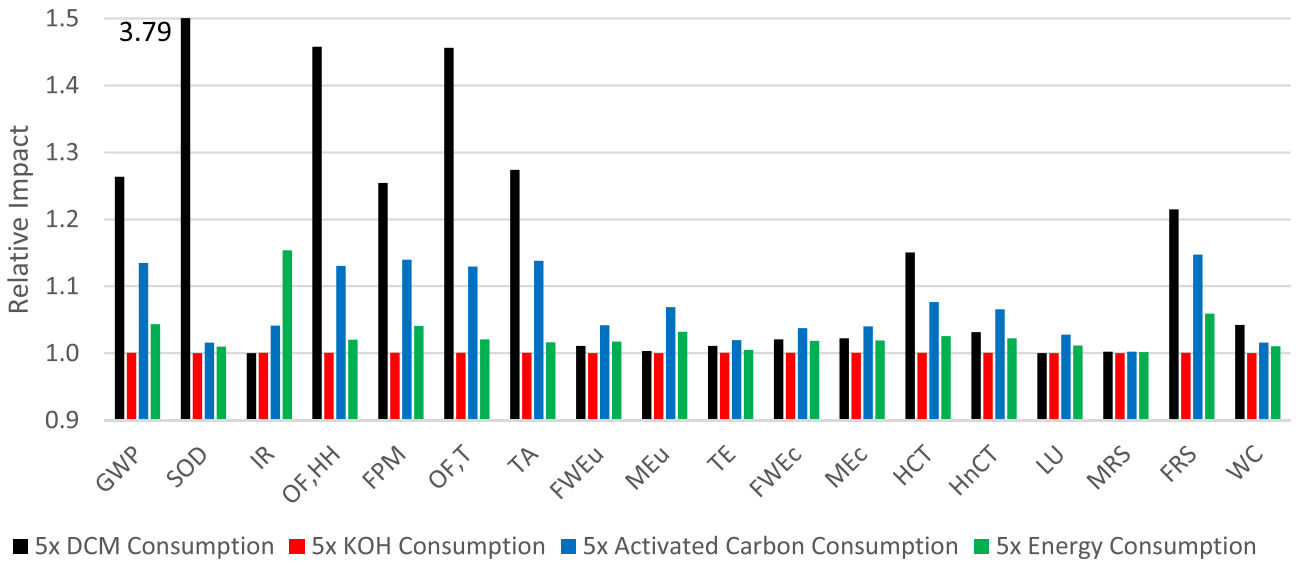

Fig. 6 Relative change in environmental impact of 1 kg sucralose production as a function of five-fold increase in consumption of each of DCM (black), KOH (red), activated carbon (blue), and energy (green) compared to the baseline model. Baseline impact equates to 1. Key for impact category abbreviation given in Fig. 2. Impact of SOD of DCM consumption data is greater than the 1.5 shown on scale at 3.79 (marked next to relevant column)

Figure 5 shows the relative change in environmental impact of producing 1 kg sucralose as a function of each scenario separately due to: change in source of sugar to a global mix (black), sourcing chemicals from China (red), and reducing PCl_3 consumption (blue), reduction in yield of sucralose-6-acetate purification to 90% (green), and lower reaction yields from all interim products (orange). Relative impact of the baseline assessment equates to 1 on the scale. Full numerical data for each separate scenario are given in Supplementary Material, Section 5, Table S6. It is shown that using sugar sourced from a global commodities market has relatively little impact upon net environmental impact. GWP increases by 1.1%, MEu by 11.4%, LU by 10.3%, WC by 6.0%, and MRS is unchanged. Average increase in impact

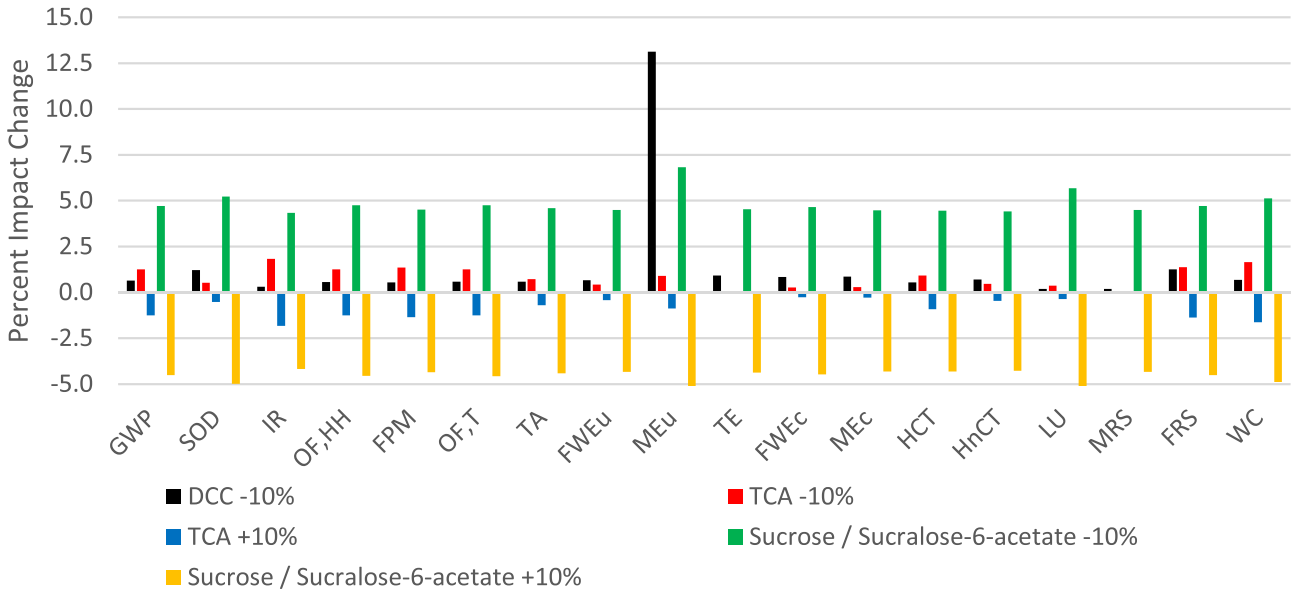

Fig. 7 Relative change in environmental impact of 1 kg sucralose production as a function of 10% change in recovery rate of each of DCC (black), TCA (red and blue), and sugar and sucralose-6-acetate (green and orange) compared to the baseline model. Key for impact category abbreviation given in Fig. 2

across all impact categories is 2.0%. Marginal increase in the given impact categories reflects efficiency of sugarcane production in US agricultural practice (85.4 t/ha), compared to global averages (70.6 t/ha) (FAOSTAT 2022). Change in sourcing chemicals from China causes an average increase of 14.6% across all impact categories, with an increase of 6.3% in GWP, 0.2% in MEu, 0.9% in MRS, and reduction of 3.2% LU, and no change in WC. Four impact categories (OF,HH; FPM; OF,T; and TA) show larger increases due to their connection with increased diesel combustion from longer shipping distances. Reduction in PCl_3 consumption causes an average reduction in impact of 45.4% across all categories, with reduction of 45.7% in GWP, 30.9% in MEu, 44.2% in LU, 55.1% MRS, and 49.6% in WC. This demonstrates that, out of scenarios 1 to 3, impact is most sensitive to reduction in PCl_3. In part, this is because reducing PCl_3 consumption also leads to a reduction in $NaHCO_3$ used for neutralizing PCl_3 by-products.

In terms of reducing yield of sucralose-6-acetate step from 100 to 90%, impacts are shown to increase almost linearly across all categories, with an average increase of 10.9%. The increase is similar for all impact categories and is due to an 11.1% increase in demand for materials and energy from the purification step and those preceding it. In contrast, reduced yields from side-reaction occurring, results in an average increase in impact of 47.9%: GWP increases by 50.1%, MEu by 73.3%, LU by 57.1%, WC by 50.5%, and MRS by 41.0%. Both sets of results from reduced yield further highlight the importance of process optimization in terms of mitigating environmental impact: cumulative inefficiencies between processes amplify environmental impacts arising from earlier process steps.

Figure 6 shows the relative change in environmental impact of producing 1 kg sucralose as a function of five-fold increase in consumption of DCM (black), KOH (red), activated carbon (blue), and energy (green). Each change is modelled and reported separately. Relative impact of the baseline assessment equates to 1 on the scale. Full numerical data are given in Supplementary Material, Section 5, Table S7. It is shown that a five-fold increase in both energy and KOH causes an average impact increase of 3.0% and 0.1%, respectively, across all impact categories. This demonstrates low sensitivity of results to large changes in these estimated inputs. In contrast, a five-fold increase in DCM and activated carbon consumption causes 27.8% and 7.1% increases in impact, respectively. For change in DCM consumption, GWP increases by 26.4%, MEu by 0.4%, MRS by 0.2%, and WC by 4.3%. Impact in LU is unchanged. For change in activated carbon consumption, GWP increases by 13.5%, MEu by 6.9%, LU by 2.8%, MRS by 0.3%, and WC by 1.6%. The uneven distribution of relative change across impact categories highlights the need for better information regarding consumption rates of both materials during sucralose production.

Figure 7 shows the relative change in environmental impact of producing 1 kg sucralose as a function of change in assumed recovery rate of DCC (black), TCA (red and blue), and sucrose and sucralose-6-acetate (green and orange). Each change is modelled in turn and reported separately. Full numerical data are given in Supplementary Material, Section 5, Table S8. Change in impact for TCA, and sugar and sucralose-6-acetate are ± 0.8% and + 4.8% / -4.6%, respectively. Change in impact from sucralose-6-acetate recovery is unequal because it is an interim product and change in impact from the upstream processes that create it is, therefore, also asymmetric for recovery rate. Impact change from reducing DCC recovery rate is 1.4%. However, change in MEu is 13.1%, which is notably larger than that of any other impact category and, excluding MEu, reduces the average increase to 0.7%. DCC was not available in the LCA databases and, therefore, it was recreated using proxy processes. The sensitivity of MEu to recovery rate change demonstrates that further research may be needed to better understand the manufacturing process of DCC. The results show that recovering sugar and intermediate products is important, but there is more to be gained by focusing on optimizing PCl_3 use and reaction yields.

5.3 Functional use of sucralose

Results presented in Section 4 are for sucralose in isolation of any food or drink formulation. It is not always possible to directly replace sugar with sucralose in a formulation. For instance, it is possible to directly replace sugar with sucralose in a drink but, in solid formulations, a bulking agent is required alongside sucralose to replace technical functions of sugar (e.g., mouth feel or hydroscopic control). Choice of bulking agents is formulation specific and, therefore, outside the scope of this study. However, the implications of using sucralose alongside a bulking agent can be explored here. It should be noted that exact quantities of sucralose and any bulking agent are also specific to the formulations in which they are used. Therefore, the discussion offered here is in terms of indicative quantities to highlight key aspects of using the two ingredients together.

One such bulking agent is sorbitol, for which the authors are aware of two LCA in the literature: Moreno et al. (2020) and Akmalina (2019). In terms of GWP, Moreno et al. (2020) reports an impact of between 2.20 $kgCO_2$-eq/$kg_{sorbitol}$ and 5.09 $kgCO_2$-eq/$kg_{sorbitol}$, depending on whether precursor glucose is hydrolyzed from starch by acid or enzymatic processes, respectively. Akmalina (2019) reports a GWP of 3.55 $kgCO_2$-eq/$kg_{sorbitol}$. To replace 1 kg sugar, approximately 998.33 g sorbitol might be used alongside 1.67 g sucralose. Therefore, net GWP according to Moreno et al. (2020) would range from 2.32 $kgCO_2$-eq/kg to 5.20 $kgCO_2$-eq/kg, sucralose accounting for between 5.2% and 2.3% net impact of the mixture. This

highlights the importance of having a clear understanding of how sucralose is used in each beverage or food formulation to best understand the net environmental impact of replacing sugar.

5.4 Limitations and further research

This LCA study is for sucralose production, and several instances of estimated or assumed data have been highlighted. Some materials had no existing background LCA processes and needed proxy processes. Further research into these materials would help in reducing uncertainty in the results.

The LCA study is only cradle-to-factory-gate and does not include use of sucralose in formulations. Therefore, further work to explore the impacts of sucralose in context of whole food or drink products, and within a dietary context, would allow better understanding of the whole life cycle impacts of producing and consuming sucralose.

Life cycle inventory data used in this study were derived from patent literature, and representativeness of the process chosen (US 7,884,203) was verified by industrial experts (private communication). However, due to intellectual property concerns, whether it is the actual process used for sucralose production is unknown. Future research would benefit from greater exploration of how the LCA data might be obtained from industrial sources without compromising confidentiality.

6 Conclusions

There is much interest in the potential to replace added sugar in foods and drinks with non-nutritive sweeteners or sweetness enhancers for consumer health benefits. However, at present, there is insufficient information about the environmental impact of NNSs to understand the ramifications of making such changes at food product or dietary levels. Most LCA studies are for steviol glycosides, with other NNSs under-represented. Therefore, this study aims to redress that imbalance with the first LCA of sucralose, one of the most popular NNSs.

The environmental LCA of producing 1 kg sucralose from chlorination of cane sugar grown in the USA has been presented in this study. It was not possible to engage an industrial producer in data provision. Therefore, life cycle inventory data for chlorination were derived from patent literature, and data for other input materials were taken from background LCA processes. Data from such an approach is prone to uncertainty and these uncertainties are explored throughout the study. Baseline results show that 1 kg sucralose has a greater impact than sugar, but this does not reflect how sucralose, which is 600-times sweetener that sugar, is used. Indeed, chlorination of sugar to enhance sweetness has potential to significantly reduce environmental impact across most categories when assessed on a sweetness equivalence basis. The extra impacts created from further processing are offset by increased sweetness of the product. However, this was not the case for all impact categories: mineral resource scarcity and human non-carcinogenic toxicity both showed an increased impact compared to sugar. Similarly, results for ionizing radiation and human carcinogenic toxicity did not show a significant reduction on a sweetness equivalence. Therefore, scenario modelling explored the uncertainties, and showed there is opportunity to reduce the environmental impact of sucralose by 50% or more via process optimization based on that modelled in this study's baseline. A reduced consumption of PCl_3 (and hence also $NaHCO_3$) was shown to offer a reduction in environmental impact. This highlights how collaboration with industry would both reduce uncertainty in, and improve the quality of, baseline impact results.

While this study presents the first cradle-to-factory-gate LCA of sucralose production, it does not include the use of sucralose in formulations or within a dietary context. However, we do illustrate how the need for extra bulking agents may affect environmental impact LCA calculations when replacing sugar in the context of a solid food. Finally, it will be valuable to extend LCA studies such as this to model the potential health benefit of consumption of sucralose and other NSSs, instead of added sugar, to gain 'whole system' or 'whole society' understanding of the ramifications.

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Data availability All data generated or analyzed during this study are included in this published article and its supplementary information files. The life cycle assessment process models used to calculate the results are provided in.CSV format in Supplementary Information. Uncertainties highlighted throughout the manuscript are parameterized to enable further exploration of the presented results.

Declarations

Conflict of interest The authors declare that they have no conflict of interest, except for: A. Raben, who has received honoraria from Unilever and the International Sweeteners Association; J.A. Harrold and J.C.G. Halford who have a grant from the American Beverage Association, and J.C.G. Halford who has in the past had consultancy (via the University of Leeds) with Mars Inc and DuPont.

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