Absolute Environmental Sustainability Assessment of Emerging Working Fluids in Organic Rankine Cycles

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Abstract

New working fluids (WFs) have been recently proposed to enhance the environmental performance of Organic Rankine Cycles (ORCs) in waste heat recovery systems. However, a critical gap remains in the comprehensive evaluation of their environmental impacts, particularly those associated with the production of these compounds and their use in ORC systems. This work addresses this gap by carrying out a comprehensive Life Cycle Assessment (LCA) to evaluate the environmental benefits of using emerging low-global-warming-potential WFs in comparison to traditional fluids like R245fa in ORC systems. An innovative methodology, combining process simulation with prospective analysis and the planetary boundaries (PBs) framework, is employed to quantify environmental benefits, including impacts associated with the WFs production processes. The results show that using low-GWP WFs reduces carbon footprint and most of the environmental categories analyzed, except for the ozone depletion (ODP) impact, although the PBs analysis indicates that the increase in ODP remains within sustainable limits. The prospective analysis highlights that the transition from current to low-GWP WFs for ORC systems could cut around 237 million tons of annual CO_2 emissions by 2050.

Keywords: ORC, Fluorinated Gases, LCA, Prospective LCA, Planetary Boundaries, Sustainability Assessment.

Synopsys: LCA highlights low-GWP working fluids’ potential to enhance Organic Rankine Cycle sustainability, reducing emissions while maintaining technical performance.

Introduction

Organic Rankine cycles (ORCs) are integrated thermodynamic cycles that efficiently generate electricity using thermal energy of low and medium temperature. ORCs play a key role in the development of sustainable energy systems, particularly through different applications such as waste heat recovery in industrial facilities and exploitation of renewable thermal energy (such as geothermal and solar)[1]. Their economic and environmental performance highly depend on the selected working fluid (WF). For that reason, significant efforts have been made in the last years to study and design novel and efficient WFs[2,3].

Traditional WFs used in ORCs are typically hydrofluorocarbons (HFCs), which have high global warming potentials (GWP)[4]. The Kigali Amendment to the Montreal Protocol[5], adopted in 2016, seeks to reduce the production and usage of HFCs by 80% by the late 2040s. This global agreement, aligned with the strict F-gas Regulation in Europe[6] and similar U.S. initiatives[7], highlights the urgency of reducing the use of HFCs, accelerating the search for alternative WFs[8]

The most common WFs used in ORC systems are R245fa (1,1,1,3,3-pentafluoropropane) and R134a (1,1,1,2-tetrafluoroethane), given their notable technical performance[9]. However, they have a high GWP (1030 and 1430 kg CO_2-eq for R245fa and R134a in a 100-year time horizon, respectively[10]). Consequently, low-GWP alternatives are continuously being explored. These include pure substances and mixtures designed to balance technical performance with environmental impact. For example, mixtures like R245fa/R600 (n-butane) and R1233ze(E) (trans-1,3,3,3-tetrafluoropropene)/toluene are being investigated for their potential to reduce GWP, while maintaining or even enhancing ORC efficiencies[11].

The transition from high-GWP fluids like R245fa to low-GWP fluids could substantially influence the environmental impact of ORC processes in terms of energy consumption, carbon footprint, and overall environmental sustainability. Comprehensive life cycle assessment (LCA) studies are hence essential to accurately evaluate the environmental benefits of these new WFs and to guide the development of sustainable ORC systems[12].

Several research studies about the environmental assessment of using different WFs in ORC systems have been recently published. Wang et al.[13] conducted a comparative techno-economic and environmental assessment of an ORC system with different mixtures recommending R245fa/R600 and R600/R600a as alternative WFs. Dawo et al.[14] investigated the hydrofluorolefins (HFOs) R1224yd(Z), R1233zd(E), and R1336mzz(Z) as potential replacements for R245fa in ORC systems. These novel HFOs, characterized by their low GWP, were first evaluated to analyze their thermophysical properties and compatibility with lubricants. Experimental testing in an ORC setup showed that R1224yd(Z) and R1233zd(E) were effective drop-in replacements with similar performance to R245fa, while R1336mzz(Z) exhibited a lower efficiency. Despite slight performance differences, an LCA established significant CO_2-equivalent reductions using the low-GWP fluids, particularly R1233zd(E) (67% reduction of CO_2-equivalent emissions) compared to R245fa in a theoretical geothermal power plant scenario. Heberle et al.[15] conducted an LCA for geothermal power production in Germany, evaluating subcritical and supercritical ORC systems. The study also found that R1233zd and R1234yf HFOs significantly reduced the environmental impacts compared to traditional WFs. In particular, the choice of R1233zd replacing R245fa decreased the ORC's global warming impact by 78% and reduced the carbon footprint of the process to 13 g CO_2/kWh_{el}.

However, while many studies focus on the technical performance and global warming impact of WFs, they often neglect the comprehensive LCA of WF production processes, ORC system operations, and broader environmental impacts beyond climate change, leaving critical sustainability aspects underexplored. Addressing this gap is essential for understanding the full environmental implications of emerging WFs compared to traditional compounds. By modeling WF production and the ORC process, we have conducted an LCA to estimate the environmental impacts of using different WFs involving R245fa, R1233zd(E) and mixtures combining them with R600 (n-butane) and toluene, respectively. Complementary prospective LCA and planetary boundaries (PBs) analyses are performed to assess the environmental sustainability of the proposed WF replacements. These evaluations will provide crucial insights into informed decision-making, promoting sustainable practices in ORC systems.

Methodology

Working Fluid Production Modeling

Four different WFs are examined in the ORC model: R245fa as a benchmark WF and three suggested alternative low-GWP WFs (R1233zd(E)[14], R245fa/R600 (composition 56/44 % w/w)[13] and R1233zd(E)/toluene (composition 83/17 % w/w)[16]. The properties of the examined WFs are provided in Section S.1 in the Supporting Information (SI). Notably, the compounds R245fa and R1233zd(E), considered in this work as WFs, are not modeled in the Ecoinvent 3.9.1 database. To perform the environmental sustainability assessment, the production of these WFs was modeled using different patents found in the literature, while the methodology from Piccino et al.[17] is employed to estimate the life cycle inventories (LCI) of the production phase (mass and energy foreground flows) through a scale-up of the synthesis methods found in several production patents. The production of R245fa encompasses two steps: the first one is the manufacture of 1,1,1,3,3 pentachloropropane (R240) from carbon tetrachloride and vinyl chloride, whose information is based on a patent of Honeywell International[18]. The second step consists of producing R245fa reacting R240 with hydrogen fluoride and antimony pentachloride, based as well on a subsequent patent of Honeywell International[19]. The production of R1233zd(E) is studied through a three-steps process: firstly, R240 is produced with the above-mentioned process. The second step is producing 1,1,3,3-tetrachloro-1-propene (TCP) by dehydrochlorination of R240 using iron chloride according to a patent of Arkema France[20]. Finally, R1233zd(E) is produced from the fluorination with hydrogen fluoride of TCP according to a patent of the company Spolchemie Zebra[20]. Additionally, the Ecoinvent 3.9.1 database is used to complete the information for toluene and R600 (n-butane), which are involved in the mixtures studied in this work.

ORC Process Modeling

The ORC process is simulated in Aspen Plus V12 with the REFPROP method, which is suitable and accurate for the description of the thermophysical properties of fluorinated refrigerants and their mixtures. A basic flowsheet that generates 1 kW of electrical power from a simulated waste heat stream of 200 ºC was created using the modeling approach of Shalaby et al.[21] (see Section S.2 in SI, Figure S1). The ORC modeled is a basic cycle composed of 4 steps: (1–2) pumping the WF to increase the pressure, (2–3) evaporating the pressurized WF in the evaporator, (3–4) expanding the evaporated WF in a turbine to generate electrical power, and (4–1) condensing the WF in the condenser. The efficiency of the driver in the pump and the isentropic efficiency in the turbine are considered 75% and 84%, respectively. In the proposed ORC, water is used at 27 ºC and 1 bar for cooling the WF in the condenser[21]. The power required for pumping cooling water was also considered for the LCA. The WF flow rate, pressures and temperatures are established following the methodology of Shalaby et al.[21] The temperature and pressure of the evaporator, the flow rate of WF and the pump pressure are adjusted for each WF until achieving the optimal cycle efficiency (η_{ORC}) obtained with the benchmark WF (R245fa; η_{ORC} = 9% ±0.5%). η_{ORC} is calculated with Equation 1, where E_{el} is the electricity produced in the turbine, E_{pump} is the energy of the ORC cycle pump and Q_{in} is the heat exchanged in the evaporator.

$$\eta_{ORC} = \frac{E_{el} - E_{pump}}{Q_{in}} \qquad \text{Eq:1}$$

Life Cycle Impact Assessment

In this contribution, an integrated attributional LCA framework has been developed to quantify the environmental sustainability level of replacing high-GWP WFs (such as R245fa) by low-GWP WFs, aimed to produce electricity with ORC from waste heat. First, following the ISO 14040[22] and ISO 14044[23] guidelines, we adopt a cradle-to-grave approach, meaning boundaries of the system (Figure 1) encompass all life-cycle phases: (1) raw material extraction, (2) WF production, (3) use of WF to generate electricity in the ORC, (4) the construction of the ORC plant and (5) the end-of-life of the plant.

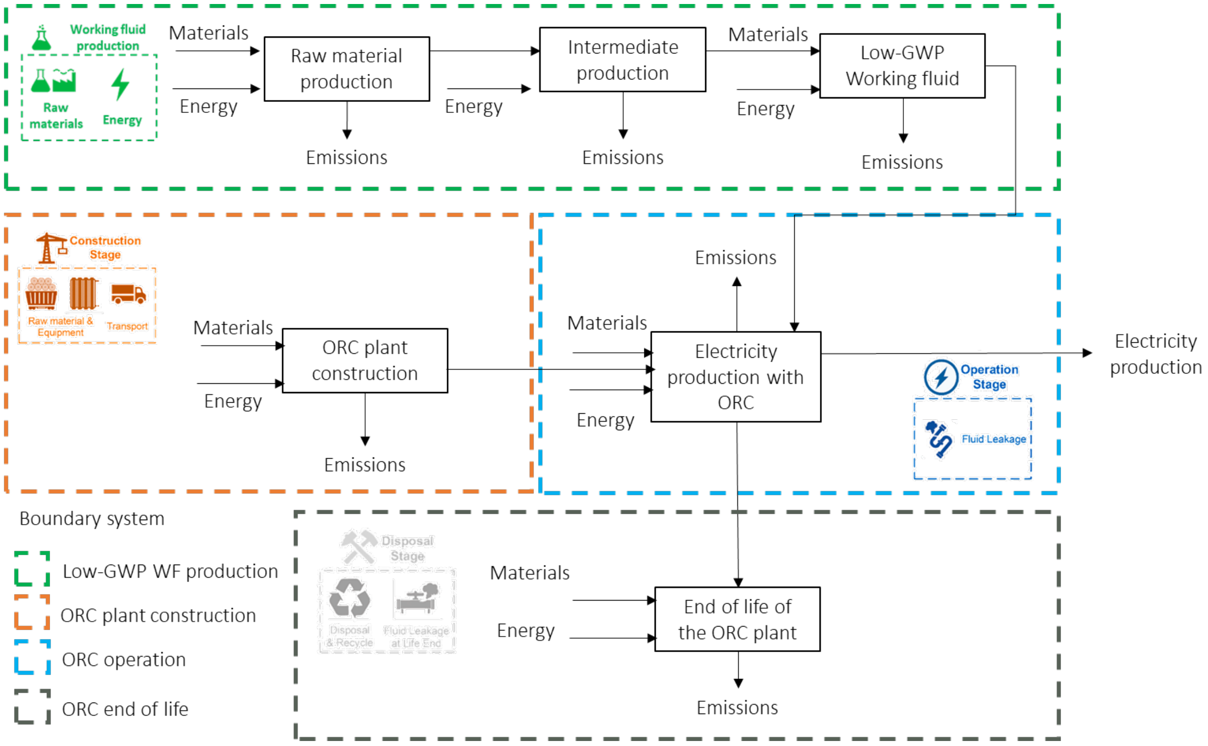


Figure 1: Cradle-to-grave LCA system boundary of the ORC system.

Second, the life cycle inventories (LCIs) are generated. Although the LCA community has made considerable progresses in generating wide LCI databases for various applications, there are still challenges that need to be tackled[24]. For example, there are no activities in the Ecoinvent database about the production of the WFs considered in this work. The LCIs herein combine data of patents and process simulation (foreground system) with data from the Ecoinvent 3.9.1 database (background system), using the allocation method "cut-off by classification"[25]. The LCIs to produce the WFs and electricity with ORC are obtained from the process models' energy and mass balances. The LCA is modeled using Brightway2[26], through the Activity Browser graphical interface. LCI data of the foreground system is retrieved from the Ecoinvent 3.9.1 database[25].

Assumptions and considerations adopted for the LCIs are provided in Section S.3 and Table S2 of the SI.

In the third phase of the LCA, the impacts are first evaluated using the Environmental Footprint (EF) as the life cycle impact assessment (LCIA) methodology. This approach is later completed with two additional studies, including a prospective analysis and a planetary boundaries (PB) evaluation.

The impact of generating 1 kWh of electrical energy with the ORC (functional unit (FU)) is evaluated by analyzing the 16 midpoint impact categories outlined in the EF method (EF 3.1), suggested by the European Commission for LCA studies[27]. In this stage, the LCI elementary flows $f \in F$ (such as emissions and natural resource use) are converted into potential impacts using characterization factors (CF). The impact assessment follows the EF methodology with two exceptions: the IPCC 2021 GWP for a 100-year time frame[28] to measure the carbon footprint, and the updated LANCA model[29] for evaluating the land use impacts.

For a general case, the environmental impact on the 16 EF impact categories $b \in B$ for each scenario $s \in S$ ($EI_{b,s}$) is calculated with Equation 2:

$$EI_{b,s} = \sum_{f \in F} I_{s,f} \cdot CF_{b,f} \cdot FU \qquad \forall\, b \in B, s \in S \qquad \text{Eq: 2}$$

where $I_{s,f}$ denotes the elementary flow quantity related with producing 1 FU, $CF_{b,f}$ is the characterization factor of the elementary flow f regarding impact category b, and FU is the amount of functional unit studied. The environmental impact is analyzed for 4 ORC scenarios (S≔{R245fa, R1233zd(E), R245fa/R600, R1233zd(E)/toluene}).

A prospective analysis is then carried out employing the open-source tool Premise v2.1.0[30] to modify the Ecoinvent database. These adjustments are made according to the scenario outcomes generated by the Integrated Assessment Model (IAM) IMAGE[31]. Premise updates the LCIs for sectors such as steel, cement, transport and electricity production to represent how production and consumption patterns will evolve over time based on three climate scenarios: 1.5 °C, 2 °C, and baseline (3.5 °C) average global warming. All the scenarios follow a "Middle of the Road" socioeconomic pathway (SSP2), indicating that economic and societal development trends are consistent with historical patterns.

For the prospective analysis, a compound annual growth rate of 17.3% in ORC installed power is considered to achieve in 2050 a scenario where all the global heat waste (GHW) could be used to produce electricity via ORC. According to Forman et al.[32] estimation, GHW from exhaust and effluent sources, with medium-grade (100-299 ºC) and low-grade (<100 ºC) temperatures, suitable for ORC recovery, could produce up to 652 GW, based on 7474 hours of annual operating time (AOT) and an ORC thermal efficiency (η_{ORC}) of 9%. To calculate the net global electricity that could be generated with ORC (GE^{ORC}), the value of net electrical efficiency (η_{el}) obtained for the benchmark R245fa (77.8%) is used in this work according to Equation 3. This efficiency means that 0.222 kWh of electricity are needed to power pumps of the ORC system to obtain 1 kWh in the generator of the turbine. The installed global initial ORC power in 2022 is 4.15 GW according to Wieland et al[33].

$$GE^{ORC,2050} = GHW \cdot \eta_{el} \cdot AOT = 652\,GW \cdot 0.778 \cdot 7474h = 3.79 \cdot 10^{6} GWh \quad \text{Eq: 3}$$

Finally, the methodology developed by Sala et al.[34] is applied to contextualize the environmental impacts of the EF method considering the PBs concept. For this analysis the FU (Equation 4) corresponds to the satisfaction of the world annual generation of electricity considering the global installed electrical power in 2023 (EP_{Glo}=3746 GW)[35] and 7474 hours of AOT.

$$FU = EP_{Glo} \cdot AOT = \ 3746\ GW \cdot 7474h = 2.80 \cdot 10^{7} GWh \qquad \text{Eq: 4}$$

A comparison of the impacts of electricity generation with ORC, assuming that all the estimated GHW could be recovered with ORC systems, is done with the safe operating space (SOS) of the Earth for each impact category. Since the SOS is based on global sustainability thresholds, they must be allocated when analyzing specific industrial systems.

In this part of the study, a total of four scenarios have been evaluated. First, two different business-as-usual (BAU) scenarios, where electricity is only obtained from the grid, are considered: current (BAU) and projected in 2050 (BAU 2050). Second, two additional scenarios where all the expected GHW is used in ORC systems operated with a high-GWP (R245fa) or low-GWP (R1233zd(E)/toluene) WF to cover part of the electricity demand. Therefore, for the four scenarios studied now, $S' \coloneqq \{BAU, BAU2050, R245fa, R1233zd(E)/toluene\}$, the parameter GE_s^{ORC} in the PB analysis is defined as:

$$GE_s^{ORC} = \begin{cases} 0\ kWh & s \in \{BAU, BAU2050\} \\ GE^{ORC,2050} = 3.79 \cdot 10^{6}\ GWh & s \in \{R245fa, R1233zd(E)/toluene\} \end{cases}$$

The environmental impact of grid electricity production in scenario s on the 16 EF impact categories b ($\mathrm{EI}_{b,s}^{Grid}$) is calculated with Equation 5:

$$\mathrm{EI}_{b,s}^{Grid} = \sum\nolimits_{f \in F} \mathrm{I}_{s,f}^{Grid} \cdot CF_{b,f} \cdot (FU - GE_{s}^{ORC}) \qquad \forall\, b \in B, s \in S' \qquad \text{Eq: 5}$$

where $I_{s,f}^{Grid}$represents the elementary flow quantity connected with the generation of 1 kWh of electricity from the grid (modelled as the activity from Ecoinvent: market group for electricity mix, medium voltage, GLO), with the current impact and the projected impact for 2050 obtained from Premise.

The environmental impact of the fraction of electricity that could be produced with ORC on the 16 EF impact categories ($\mathrm{EI}_{b,s}^{ORC}$) is calculated with Equation 6:

$$\mathrm{EI}_{b,s}^{ORC} = \sum\nolimits_{f \in F} \mathrm{I}_{s,f}^{ORC} \cdot CF_{b,f} \cdot GE_{s}^{ORC} \qquad \forall\, b \in B, s \in S' \qquad \text{Eq: 6}$$

where $\mathrm{I}_{s,f}^{ORC}$represents the elementary flow quantity connected with the generation of 1 kWh of electricity produced with ORC. Similar foreground inventories to those detailed previously are used, although the analysis is conducted for the year 2050 under a climate scenario of 2 ºC using Premise.

To perform the absolute environmental sustainability assessment, the transgression level (TL) of scenario *s* with respect to the downscaled SOS ($\mathrm{SOS}_{\mathrm{EL,b}}$) is calculated for each EF impact category *b*, according to Equation 7.

$$TL_{b,s} = \frac{(EI_{b,s}^{Grid} + EI_{b,s}^{ORC})}{SOS_{EL,b}} \qquad \forall\, b \in B, s \in S' \qquad \text{Eq: 7}$$

Ryberg et al.[36] explored different downscaling methods for allocating shares of the global SOS (SOS_{GLO}) to specific products. These downscaling principles are grounded in distributive justice theory, which allocates a fair share of the total SOS_{GLO} to an activity based on different factors (i.e., currency, geographical scope, target, pattern, constraints, clauses and temporal scope). The selection of a downscaling method may strongly influence the results and conclusions of the analysis. Therefore, two downscaling methods were used in this work to assess the status of the ORC market within the LCIA-based PBs for the EF impact categories framework: the grandfathering method[37] (explained in the coming paragraph) and the utilitarian principle[38] (detailed in Section S.4 of the SI).

$SOS_{EL,b}$ is computed employing a grandfathering downscaling methodology. This approach determines for each EF impact category *b*, the share of the global SOS ($SOS_{GLO,b}$) corresponding to the BAU technology (the electricity obtained from the grid). The $SOS_{EL,b}$ is given by the ratio between the environmental impact of the BAU technology in one year ($EI_{BAU,b}$), assuming it is used to fulfill the full demand of electricity, and the total environmental impact of all anthropogenic activities in the same year ($EI_{GLO,b}$), according to Equation 8. $EI_{GLO,b}$ is obtained from the global normalization factors reported by Sala et al[34] (see Table S3 in Section S.4 of the SI).

$$SOS_{El,b} = SOS_{GLO,b}\frac{EI_{BAU,b}}{EI_{GLO,b}} \qquad \forall\, b \in B \qquad \text{Eq: 8}$$

In the final stage of the LCA, the implications of using different WFs to power the ORC in 2050 are assessed. A $TL_{b,s}$ value below 1 means that scenario *s* remains within the allocated SOS for EF impact category *b*, indicating that the system is considered environmentally sustainable in that category. Conversely, with a $TL_{b,s}$ value higher than 1, scenario *s* exceeds the allocated SOS for the EF impact category *b*, so the system is considered environmentally unsustainable. For a sustainable system, $TL_{b,s}$ values must be below 1 across all PBs. However, it is important to carefully interpret claims of environmental sustainability taking into account the uncertainties involved in the results obtained and the assumptions made. Additionally, due to the use of downscaling, exceeding the SOS share does not indicate that all anthropogenic activities will collectively surpass the total SOS[39], as high impacts in one activity could be offset by low impacts in others.

Results and Discussion

Material and Energy Flow Analysis of the Production of Working Fluids

The production of 1 kg of R245fa and R1233zd(E), both compounds missing in Ecoinvent, has been studied through a material flow analysis (MFA) and energy flow analysis (EFA). The work of Piccino et al.[17] is used to scale up the experiments (mass and energy) found in the patents. Figure 2 shows the MFA and EFA obtained for the production of each WF. The MFA reveals that the production of 1 kg of R245fa and 1 kg of R1233zd(E) requires 6.72 kg and 4.72 kg of raw materials, respectively, while the total amount of mass recycled or emitted during the production is 5.72 kg and 3.73 kg, representing 85 wt % and 79 wt % of these raw materials. Concerning the EFA, the production of 1 kg of R245fa requires 3.07 kWh of energy (split in 90% thermal energy and 10% electricity), while the production of 1 kg of R1233zd(E) only needs 1.18 kWh (89% thermal energy and 11% electricity). These results clearly show that the production of R245fa requires a higher amount of mass and energy than that of R1233zd(E). The MFA and EFA are used to prepare the LCIs for the production of the WF (see Section 5 in the SI, Tables S4 and S5).

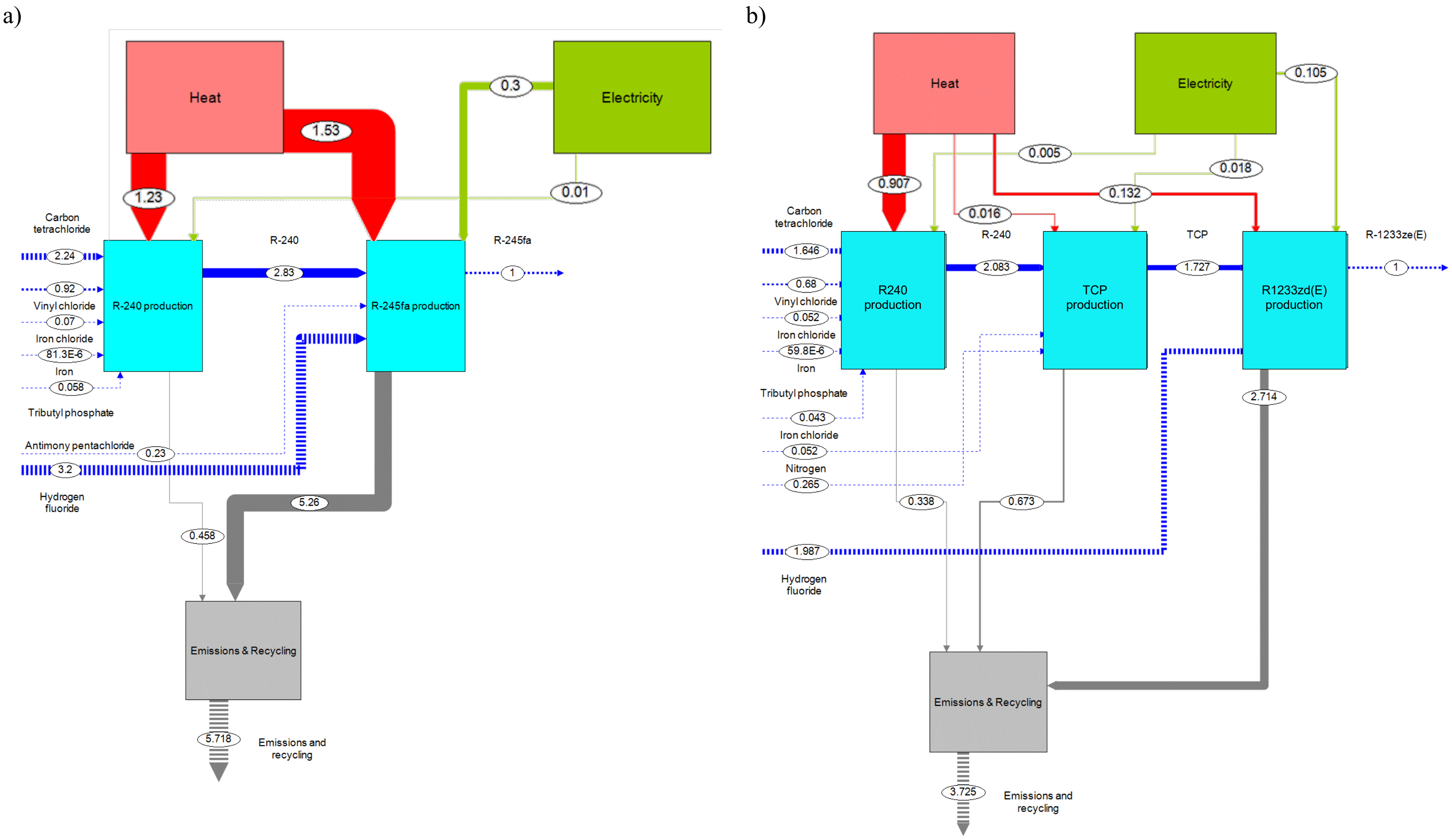


Figure 2: MFA (kg) and EFA (kWh) to produce 1 kg of a) R245fa and b) R1233zd(E). Blue arrows represent mass flow, grey arrows are emissions or recycled flow, red arrows represent heat (kWh$_{th}$), and green arrows represent electricity (kWh$_{el}$). The thickness of the line shows the relative mass or energy flow.

Environmental Impact Analysis of the Production of Working Fluids

The impact associated with the production of different WFs has been carried out through a cradle-to-gate LCA (details are shown in Section 5 of the SI, Table S6 and Figures S2 and S3). The LCIA results (Table S6 of the SI) show that the production of R1233zd(E)/toluene mixture exhibits the lowest impact across all categories, except for ozone depletion potential (ODP) and human toxicity, carcinogenic categories. Notably, the climate change impact is significantly reduced with the production of low-GWP alternatives. However, the impact on ozone depletion increases notably with the WFs containing R1233zd(E), due to the presence of a chlorine atom. The production of R245fa exhibits the highest carbon footprint among all WFs, with 18.5 kg CO_2-eq/kg, followed by the R245fa/R600 mixture, with 12 kg CO_2-eq/kg. R1233zd(E) and R1233zd(E)/toluene exhibit lower carbon footprints with 7.49 and 6.49 kg CO_2-eq/kg, respectively.

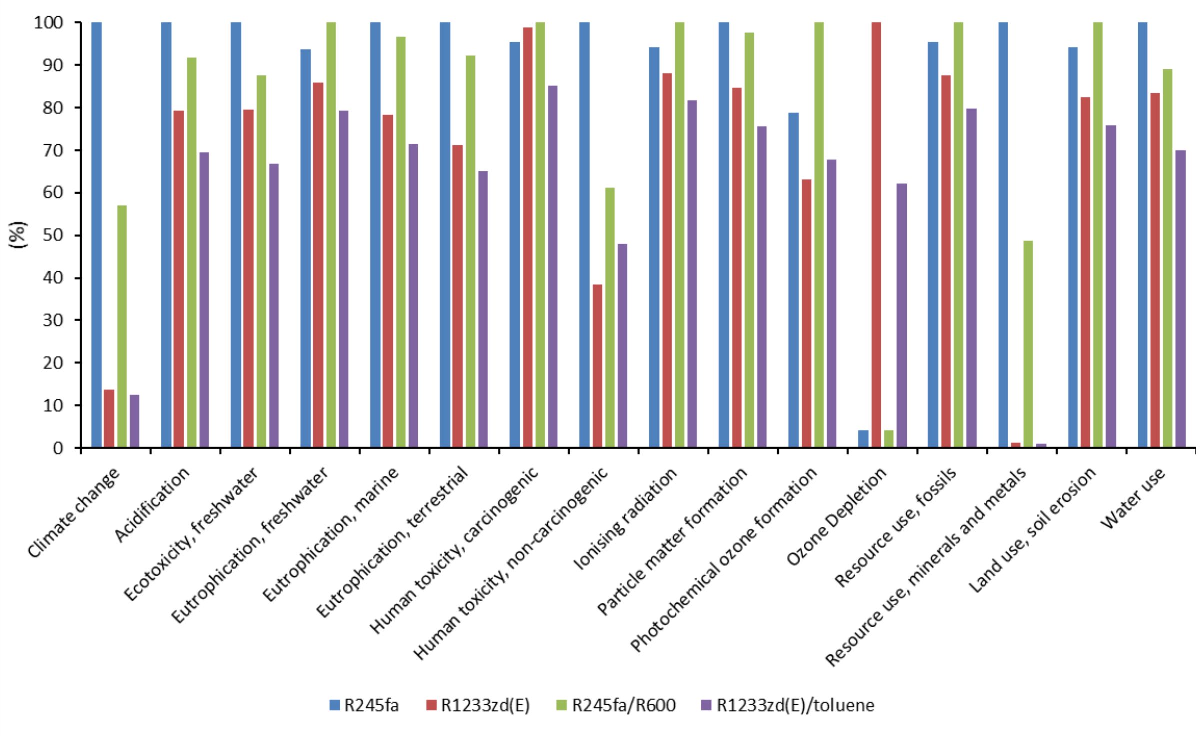
Figures S2 a) and b) in the SI show the main process contributions to the carbon footprint and ozone depletion, respectively, for the production of 1 kg of WF. Electricity, the use of carbon tetrachloride as raw material, and fugitive emissions in the WFs containing R245fa represent the highest contributions to the cradle-to-gate carbon footprint. Regarding ozone depletion, the highest contributors are the use of vinyl chloride and chlorine as raw material, and the fugitive emissions in the case of the WFs containing R1233zd(E) (contributing more than 37%).

Environmental Impact Analysis of the Production of Electricity with ORC

Next step concerns the environmental impact of an ORC using the previous WFs. ORC simulations are evaluated using the Aspen Plus v12 software and the main results are summarized in Table S7 (Section S.6 of SI). With the simulation results and the data compiled in Table S8 the LCI for producing 1 kWh is generated (Table S9). The LCIA results presented in Figure 3 a) (additional details in Table S10 and Figure S4 of SI) show that the R1233zd(E)/toluene mixture exhibits the lowest impact across all categories except for ODP, photochemical ozone formation, and human toxicity, non-carcinogenic categories. Figure S5 of SI shows the breakdown of the environmental impacts for all the WFs. Focusing on the carbon footprint, an uncertainty analysis using Montecarlo simulation has been carried out (see Figure S6 of SI), considering the implicit uncertainty of the background life cycle inventories in the Ecoinvent database. According to the results, the carbon footprint for R245fa is 74±4 g CO_2-eq/kWh, decreasing till 44±5 g CO_2-eq/kWh for the R245fa/R600 mixture. R1233zd(E) and R1233zd(E)/toluene exhibit similar lower values (12±4 and 11±3 g CO_2-eq/kWh, respectively). The carbon footprints for the pure components (R245fa and R1233zd(E)) are in agreement with those reported by Heberle et al.[15] who estimated carbon footprints of 69.9 g CO_2-eq/kWh and 21.5 g CO_2-eq/kWh for R245 and R1233zd(E) respectively.

Figure 3 b) shows that fugitive emissions and end-of life activities are the largest contributions to the carbon footprint of the production of 1 kWh with an ORC in the scenarios with WFs containing R245fa. Concerning ozone depletion, the results of Figure 3 c) indicate that these two items highly contribute in the scenarios with WFs containing R1233zd(E).

a)


100
90
80
70
60
50
40
30
20
10
0
(%)
Climate change
Acidification
Ecotoxicity, freshwater
Eutrophication, freshwater
Eutrophication, marine
Eutrophication, terrestrial
Human toxicity, carcinogenic
Human toxicity, non-carcinogenic
Ionising radiation
Particle matter formation
Photochemical ozone formation
Ozone Depletion
Resource use, fossils
Resource use, minerals and metals
Land use, soil erosion
Water use
R245fa
R1233zd(E)
R245fa/R600
R1233zd(E)/toluene

b)

c)

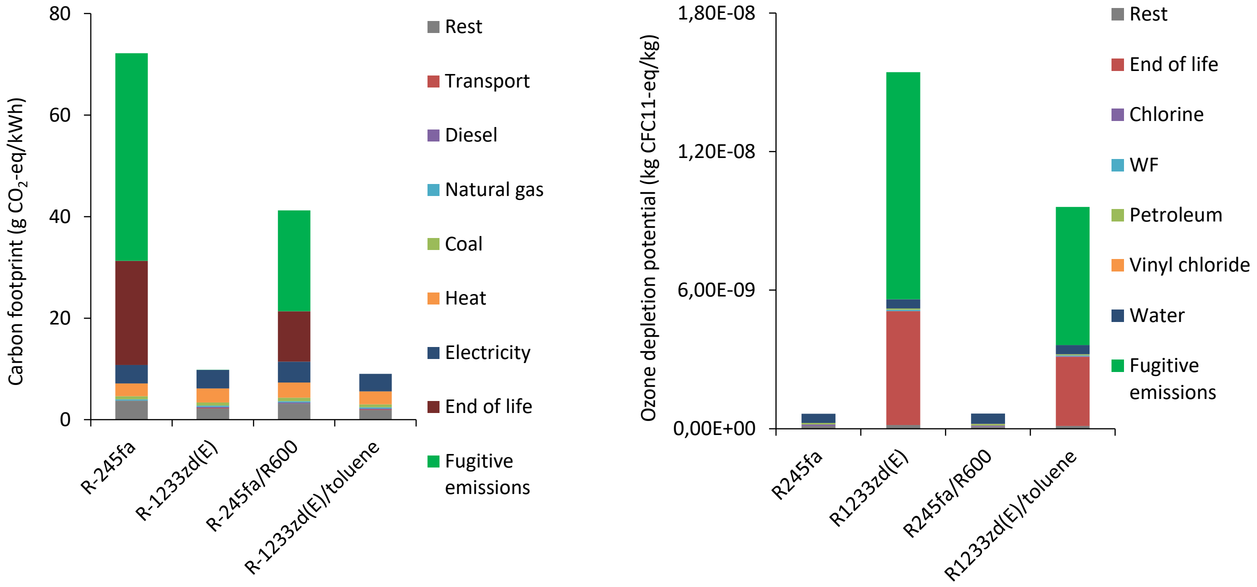


Figure 3: a) LCIA of the production of 1 kWh in ORC using different WFs. b) Carbon footprint and c) Ozone depletion with the main process contributions.

Prospective Analysis

Figures 4 a) and b) compare the global 100-year average cradle-to-grave climate change and ozone depletion impacts for global electricity mix from the grid and from electricity produced with ORC, using R245fa and the mixture R1233zd(E)/toluene as WFs, from current to 2100 in three climate policy scenarios. The emissions are obtained using the average impacts as determined by prospective LCA. In the case of electricity from grid, lower CO_2-eq emissions are observed because of more ambitious policies (1.5 °C and 2 °C scenarios), due to the decarbonized generation of electricity.

From Figure 4 a), the carbon footprint of the electricity grid in 2100 is projected to be comparable to that of the ORC using R1233zd(E)/toluene assuming the most favorable climate scenario (1.5 ºC). In all other scenarios, the electricity produced with ORC using R1233zd(E)/toluene exhibits a lower carbon footprint. However, the ozone depletion results in Figure 4 b) reveal that the production of electricity with ORC using R1233zd(E)/toluene is approximately 1.8 times worse than the scenario of electricity from the grid, based on the 2°C increase scenario projected for 2050. In contrast, the ozone depletion in the ORC scenario using R245fa is almost 8 times better than that of the electricity grid.

Figure 4 c) shows the installed power capacity of ORC systems in 2020 and projects future growth with a compound annual growth rate of 17.3%, reaching a net electrical power of 507 GW by 2050. This projection assumes the utilization of all the waste heat estimated by Forman et al.[32], with an ORC efficiency (η_{ORC}) of 9 % and an electrical efficiency (η_{el}) of 77.8%. Finally, Figure 4 d) depicts global CO_2-eq and CFC11-eq emissions associated to the power shown in Figure 4 c) using electricity from grid, as well as ORC using the WFs R245fa and R1233zd(E)/toluene in a 2 ºC scenario. According to the results, changing a high-GWP WF by low-GWP fluids could save around 237 million tons of CO_2/year in 2050. On the other hand, the emissions of CFC11-eq will increase in the case of the scenario with R1233zd(E)/toluene compared to the scenario of electricity from the grid due to the fugitive emissions considered in the LCA. The emissions of CFC11-eq in the ORC scenario using R245fa are practically always lower than in the other scenarios.

a) b)

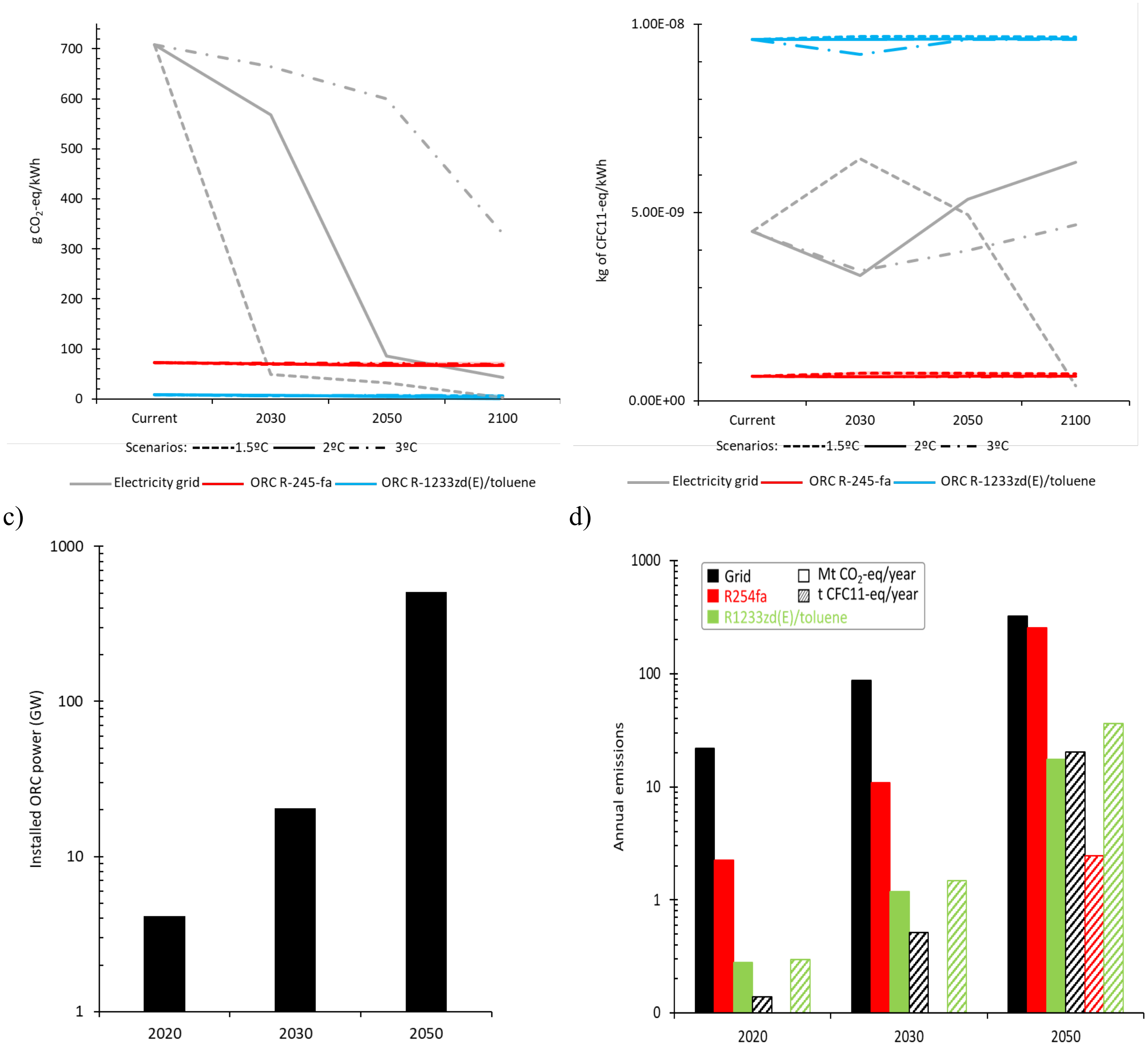


Figure 4: a) Global 100-year average cradle-to-grave climate change impacts and b) ozone depletion for global electricity obtained from grid (grey) and electricity produced with ORC using R245fa (red) and the mixture R1233zd(E)/toluene (blue) as working fluid from current to 2100 in three climate policy scenarios. c) Installed power with ORC systems in 2020 and future projections with a compound annual growth rate of 17.3% to reach in 2050 an ORC installed power of 507 GW. d) Emissions of CO$_2$-eq (full bars; Mt CO$_2$-eq/year) and of CFC11-eq (dashed bars; t CFC-11-eq/year) of electricity mix (grid) (black), and electricity obtained with ORC systems using R245fa (red) and R1233zd(E)/toluene (green) in a 2 ºC scenario. These emissions are associated to the installed power of Figure 4 c).

Planetary boundaries analysis

Figure 5 shows the results of life cycle indicators, showing the TL in each PB using the grandfathering downscaling method. The background color coding highlights the status of the PB for each impact category, with green indicating within the SOS (TL lower than 1), yellow within the zone of uncertainty, and red signifying high-risk areas. The scenarios evaluated include business-as-usual (BAU) for electricity production using the current electricity mix, business-as-usual in 2050 (BAU 2050) for electricity production using the predicted electricity mix in 2050 (climate scenario of 2ºC) and two additional scenarios for 2050 where part of the electricity will be supplied using all the potential global waste heat with ORC with two different WFs (R245fa and R1233zd(E)/toluene).

The implementation of the two ORCs scenarios improve almost all of the TLs compared to the BAU scenarios. In particular, there are only two impact categories using ORC that are worse than in the BAU current benchmark case: the resource use, mineral and metals, and the ozone depletion. From one side, the TL of the resource use, mineral and metals is higher than that of the BAU in all the 2050 scenarios (BAU 2050, R245fa and R1233zd(E)/toluene) due to the increased resource use in 2050 electricity (higher percentage of renewable energy). From the other side, the R1233zd(E)/toluene scenario has a higher TL for ozone depletion compared to the other scenarios, due to the fugitive emissions of WF. However, it remains below 1, indicating that it is still within the SOS. It is important to note that, when using the utilitarian downscaling method (Section S.7, Figure S7 in the SI) the ozone depletion in the ORC scenarios still remains within the SOS, ensuring the validity of this outcome.

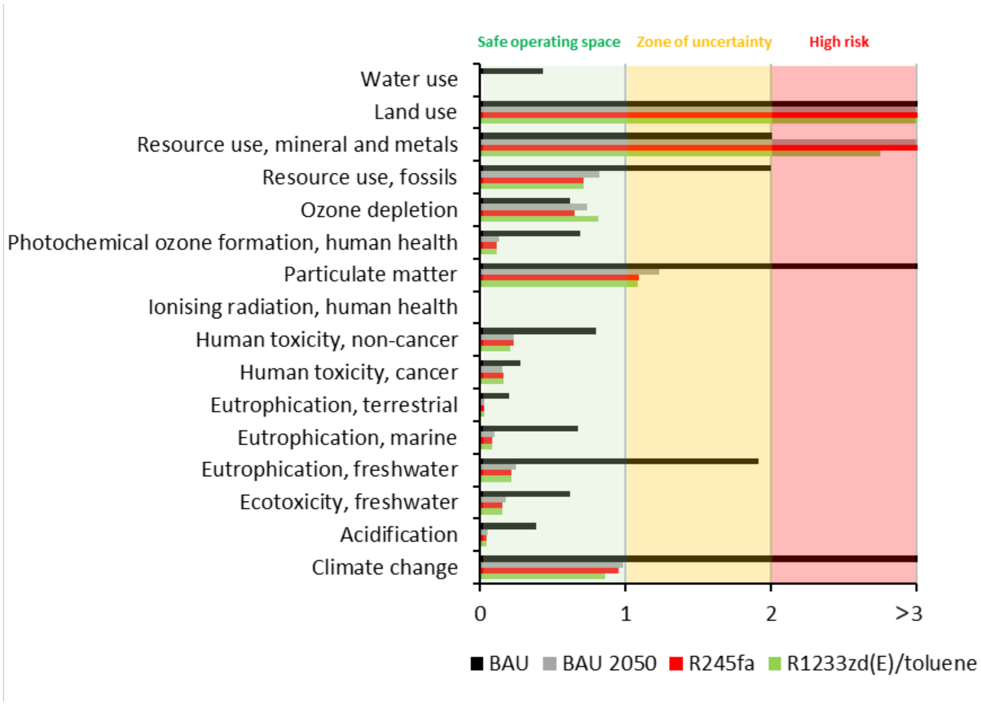


Figure 5: Life cycle indicators' results, as total impacts, compared to global impacts and PBs with grandfathering downscaling. The color code of the background reflects the status of the PB for each impact category: green = below the PB; yellow = within the zone of uncertainty of the PB; red = in a high-risk area. The scenarios analyzed are: BAU, business as usual producing electricity with current electricity mix obtained from Ecoinvent; BAU 2050, business as usual producing electricity with electricity mix in 2050 in a climate scenario of 2ºC obtained from Premise; R245fa producing in 2050 part of the electricity with ORC using R245fa (high GWP) and R1233zd(E)/toluene producing in 2050 part of the electricity with ORC using R1233zd(E)/toluene (low GWP).

Conclusion

This study provides a comprehensive LCA of ORC systems, focusing on their environmental impacts and sustainability level across multiple scenarios using different WFs, these being R245fa (high GWP), R245fa/R600 (medium GWP), R1233zd(E) (low GWP) and R1233zd(E)/toluene (low GWP). The results demonstrate that the replacement in ORC systems of high-GWP fluids by low-GWP alternatives can significantly improve the carbon footprint and most of the environmental categories, with the exception of the ozone depletion. The prospective analysis under different climate policy scenarios indicates that ORC systems can play an important role in reducing greenhouse gas emissions when integrated into the global electricity mix. These findings also suggest that transitioning from high-GWP to low-GWP WFs in ORC systems could cut global CO_2 emissions by approximately 237 million tons annually by 2050, demonstrating the role that ORC systems can play in mitigating climate change. Furthermore, the comparison with PBs shows that, while there is burden-shifting from the climate change PB toward the ozone depletion PB when using low-GWP WFs, the system remains within its SOS. This work highlights the necessity for continuous evaluation and improvement of ORC technologies to maximize their environmental benefits, paving the way for more sustainable energy solutions.

▪ ACKNOWLEDGMENTS

This research is supported by projects NEW-F-Tech (TED2021-130959B-I00) and RE(F)CICLA (PID2023-149713OB-I00) funded by MICIU/AEI/10.13039/501100011033/ and by the European Union NextGeneration EU/PRTR (NEW-F-Tech) and ERDF/EU (RE(F)CICLA). Recognition from AGAUR as Consolidated Research Groups for GESPA (2021 SGR 00321) and AGACAPE (SGR 2021-00738) is gratefully appreciated. The authors would like to thank Professor Gonzalo Guillén-Gosalbez from ETH Zürich for his recommendations and constructive discussions, as well as to Lucas Francisco dos Santos, Juan Diego Medrano and Jorge Cuesta, from the same institution, for their help with Brigthway2.

ABBREVIATIONS

AOT, Annual Operating Time; BAU, Business As Usual; EF, Environmental Footprint; EFA, Energy Flow Analysis; FU, Functional Unit; GHW, Global Heat Waste; GWP, Global Warming Potential; HFC, hydrofluorocarbon; HFO, hydrofluorolefin; IPCC, Intergovernmental Panel on Climate Change; LCA, Life Cycle Assessment; LCI, Life Cycle Inventory; LCIA, Life Cycle Impact Assessment; MFA, Mass Flow Analysis; ODP, Ozone Depletion Potential; ORC, Organic Rankine Cycle; PB, Planetary Boundaries; SOS, Safe Operating Space; TCP, tetrachloro-1-propene; TL, Transgression Level; WF, Working Fluid; WHR, Waste Heat Recovery.

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