Supplementary Information

Nitrous oxide as a green oxidant: a holistic evaluation based on economic, environmental, and safety metrics

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1. Process modelling methodology

The process flow diagrams for nitrous oxide (N_2O, **Figs. S1,S2**), hydrogen peroxide (H_2O_2, **Fig. S3**), and phenol (**Figs. S4,S5**) production were simulated using standard process models in Aspen Plus v12.1, employing the NRTL fluid package. The latter was selected to describe phase equilibria, given the polar, non-electrolytic nature of the compounds studied at pressures below 10 bar. Simulation results, including input-output data for mass and energy flows and process unit sizes, were used for the economic, environmental, and safety assessments. **Table S1** provides the mass and energy balances for N_2O production via the one-step direct ammonia (NH_3) oxidation and the five-step ammonium nitrate (NH_4NO_3) decomposition pathways. For the one-step route, we assume 100% conversion and selectivity towards N_2O. For the five-step route, the simulation was performed using literature data on temperature, pressure, conversion, and selectivity.[1–4]

Similarly, for H_2O_2, we consider the anthraquinone autoxidation (AO) process, which produces H_2O_2 from hydrogen (H_2) and oxygen (O_2) using 2-ethylanthraquinone as the working solution. This simulation was also based on literature data on temperature, pressure, conversion, and selectivity.[5] **Table S2** presents the mass and energy balances for the H_2O_2 production route via the AO process.

For phenol production, we analysed the traditional cumene oxidation route and compared it to emerging methods involving the direct oxidation of benzene using either N_2O or H_2O_2. Conversion, selectivity, and operating conditions for the reactions were based on literature values for the direct oxidation of benzene to phenol with N_2O[6] and H_2O_2,[7] respectively. **Table S3** provides the mass and energy balances for the phenol production routes. The mass and energy balances for the traditional cumene oxidation-based phenol production route were sourced from Ecoinvent v3.10 database.[8] For further details, please refer to the techno-economic assessment (**Section 2** of the SI) and life cycle assessment (**Section 3** of the SI).

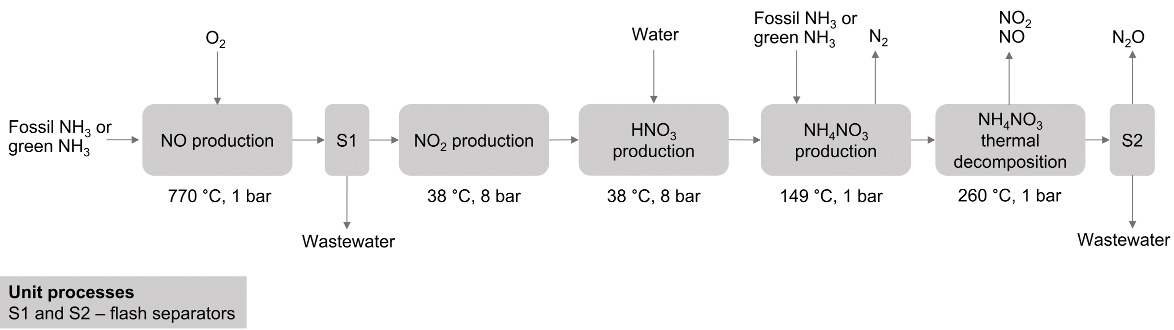

Fig. S1 | Process block diagram for the production of N_2O via the multi-step NH_4NO_3 thermal decomposition. An annual production of 130 kt N_2O was considered. All process models were simulated using Aspen Plus v12.1, employing the NRTL fluid package. For simplicity, compressors, pumps, valves, heaters, and coolers are omitted from the process block diagram. Heat integration was performed using the Aspen Energy Analyzer v12.1. The simulation was performed using literature data on temperature, pressure, conversion, and selectivity.[1–4]

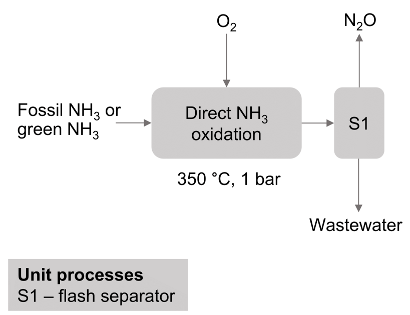

Fig. S2 | Process block diagram for the production of N_2O via the one-step direct NH_3 oxidation. An annual production of 130 kt N_2O was considered. All process models were simulated using Aspen Plus v12.1, employing the NRTL fluid package. For simplicity, compressors, pumps, valves, heaters, and coolers are omitted from the process block diagram. Heat integration was performed using the Aspen Energy Analyzer v12.1.

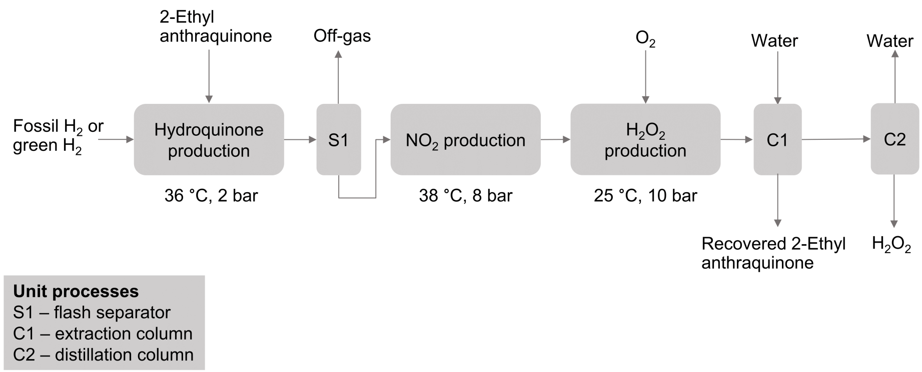

Fig. S3 | Process block diagram for the production of H_2O_2 via the AO process. An annual production of 130 kt H_2O_2 was considered. All process models were simulated using Aspen Plus v12.1, employing the NRTL fluid package. For simplicity, compressors, pumps, valves, heaters, and coolers are omitted from the process block diagram. Heat integration was performed using the Aspen Energy Analyzer v12.1. Conversion, selectivity, and operating conditions for the reactions were based on literature.[5]

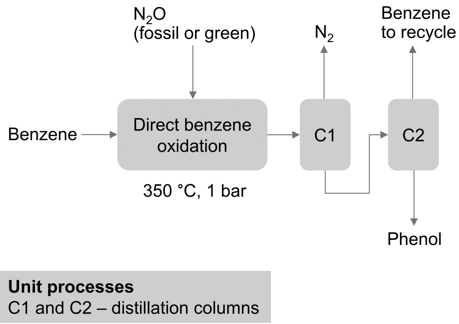

Fig. S4 | Process block diagram for the production of phenol via the one-step oxidation of benzene using N_2O. An annual production of 130 kt phenol was considered. All process models were simulated using Aspen Plus v12.1, employing the NRTL fluid package. For simplicity, compressors, pumps, valves, heaters, and coolers are omitted from the process block diagram. Heat integration was performed using the Aspen Energy Analyzer v12.1. Conversion, selectivity, and operating conditions for the reactions were based on literature.[6]

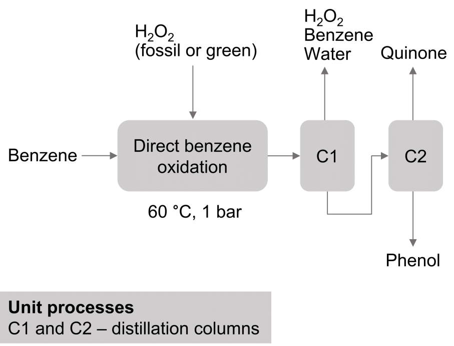

Fig. S5 | Process block diagram for the production of phenol via the one-step oxidation of benzene using H_2O_2. An annual production of 130 kt phenol was considered. All process models were simulated using Aspen Plus v12.1, employing the NRTL fluid package. For simplicity, compressors, pumps, valves, heaters, and coolers are omitted from the process block diagram. Heat integration was performed using the Aspen Energy Analyzer v12.1. Conversion, selectivity, and operating conditions for the reactions were based on literature.[7]

Table S1 | Inputs and outputs of the one-step and five-step production routes per kg N_2O produced. For both pathways, these values were extracted from the Aspen Plus v12.1 simulation (**Figs. S1,S2**).

Stream	One-step	Five-step
Feedstock		
Ammonia / kg	0.818	0.894
Utilities		
Electricity / kWh	0.050	0.547
Cooling water / MJ	4.521	12.943
Heating (natural gas) / MJ	-	0.281
Emissions to air		
Nitrogen / kg	-	5.581
Nitrogen oxides / kg	-	0.068
Nitric acid / kg	-	0.001

Table S2 | Inputs and outputs of the AO production route per kg H_2O_2 produced. These values were extracted from the Aspen Plus v12.1 simulation (**Fig. S3**). Conversion, selectivity, and operating conditions for the reactions were based on literature.[5]

Stream	AO process
Feedstock	
Hydrogen / kg	0.066
2-Ethylanthraquinone / kg	0.003
Benzene / kg	0.002
Utilities	
Electricity / kWh	0.089
Cooling water / MJ	2.800
Heating (natural gas) / MJ	1.925
Emissions to air	
Hydrogen / kg	0.007
Carbon dioxide, fossil / kg	0.009
Water / kg	0.001

Table S3 | Inputs and outputs of the direct benzene oxidation routes per kg phenol produced using N_2O or H_2O_2. For both pathways, these values were extracted from the Aspen Plus v12.1 simulation (**Figs. S4,S5**). Conversion, selectivity, and operating conditions for the reactions were based on literature values for the direct oxidation of benzene to phenol with N_2O[6] and H_2O_2,[7] respectively.

Stream	Using N_2O	Using H_2O_2
Feedstock		
Benzene / kg	0.829	0.922
Nitrous oxide / kg	0.475	-
Hydrogen peroxide / kg	-	0.479
Utilities		
Cooling water / MJ	0.979	4.947
Heating (natural gas) / MJ	12.784	6.923
Emissions to air		
Benzene / kg	0.001	-
Nitrogen / kg	0.302	-

2. Techno-economic analysis methodology

The process flowsheet for the N_2O, H_2O_2, and phenol production technologies (**Figs. S1-S5**) were modelled using standard process models in Aspen Plus v12.1. Simulation results, including input-output mass and energy flows and process unit sizes, were employed in the techno-economic analysis (TEA). **Tables S1-S3** present the mass and energy balance in the process simulations. The TEA considers operational and capital expenditures (OPEX and CAPEX, respectively) for the reference year 2022. For all the routes, the OPEX was calculated following Ioannou *et al.*,[9] while the CAPEX was estimated using correlations from Sinnott and Towler,[10] accounting for installation factors of each equipment unit, and the annual capital charge ratio was used to annualise the CAPEX. **Table S4** provides feedstock and utility prices used in the OPEX calculations for all the production pathways.

Furthermore, to estimate the costs for the year 2050, we performed a prospective TEA analysis. Such an analysis is inherently challenging due to the significant uncertainty and volatility of future prices, which are influenced by geopolitical factors and technological advancements. **Table S5** outlines the feedstock and utility prices used in the OPEX calculations for all production pathways. Only the costs of NH_3 (for N_2O), H_2 (for H_2O_2), and N_2O or H_2O_2 (for phenol) were assumed to change by 2050, as these were identified as the main cost drivers. The 2022 costs of fossil-derived NH_3 and H_2 were projected to 2050 using the average historical inflation rate from 2010 to 2020, and later discounted to 2022 nominal dollars using a 2% discount rate.

Table S4 | Cost parameters used to calculate the unitary production cost of N_2O, H_2O_2, and phenol, with all costs reported using 2022 as the reference year.

Flow	Average	Low	High	Source
Fossil ammonia / USD kg^{-1}	0.728	0.668	0.790	11
Green ammonia (wind-based electrolysis) / USD kg^{-1}	1.366	1.025	1.742	11
Fossil hydrogen / USD kg^{-1}	1.847	1.509	3.166	12
Green hydrogen (wind-based electrolysis) / USD kg^{-1}	6.210	5.190	7.290	11
2-Ethylanthraquinone / USD kg^{-1}	472.000	-	-	Merck
Benzene / USD kg^{-1}	0.800	-	-	13
Fossil nitrous oxide / USD kg^{-1}	0.636	0.587	0.686	This work
Green nitrous oxide / USD kg^{-1}	1.158	0.879	1.465	This work
Fossil hydrogen peroxide / USD kg^{-1}	1.639	1.617	1.726	This work
Green hydrogen peroxide / USD kg^{-1}	1.926	1.859	1.997	This work
Heating (natural gas) / USD GJ^{-1}	6.120	-	-	14
Cooling water / USD GJ^{-1}	0.510	-	-	9
Grid electricity / USD kWh^{-1}	0.093	-	-	9

Table S5 | Cost parameters used to calculate the unitary production cost of N_2O, H_2O_2, and phenol in 2050.

Flow	**Average**	**Low**	**High**	**Source**
Fossil ammonia / USD kg^{-1}	0.510	0.433	0.586	-
Green ammonia (wind-based electrolysis) / USD kg^{-1}	0.925	0.659	1.192	15
Fossil hydrogen / USD kg^{-1}	1.293	1.057	2.216	-
Green hydrogen (wind-based electrolysis) / USD kg^{-1}	3.500	2.400	4.600	15
Fossil nitrous oxide / USD kg^{-1}	0.795	0.682	0.909	This work
Green nitrous oxide / USD kg^{-1}	0.797	0.579	1.015	This work
Fossil hydrogen peroxide / USD kg^{-1}	1.672	1.643	1.782	This work
Green hydrogen peroxide / USD kg^{-1}	1.748	1.675	1.820	This work

3. Life cycle assessment methodology

For the life cycle assessment (LCA), the global average climate change impacts are quantified using an attributional LCA in accordance with ISO 14044/14040 standards.[16,17] We consider 1 kg N_2O, H_2O_2, or phenol produced as the functional unit, following a cradle-to-gate approach that encompasses all activities from raw material acquisition to the production of the chemical. The end-use phase is assumed to remain the same across all cases, regardless of the production route. The mass and energy flows for the chemical production routes (**Table S1-S3**) were obtained from simulations (**Figs. S1-S5**). These data enable us to model the foreground system (production of N_2O, H_2O_2, or phenol), while data for the background system (activities supplying inputs to the production facility) were primarily sourced from the Ecoinvent v3.10 database.[8] The 100-year average global warming potentials (GWPs) as outlined by the IPCC in 2021 were used to calculate the climate change impacts.[18] Additionally, the ReCiPe 2016 v1.03 method was employed to assess human health, ecosystem quality, and natural resources endpoints.[19] The inventories used to calculate impacts for all production technologies and chemicals are presented in **Table S6** for N_2O, **Table S7** for H_2O_2, and **Table S8** for phenol production technologies. An uncertainty assessment for all production scenarios was conducted using Monte Carlo sampling with 1,000 iterations. Such scenarios were generated using the default values provided by the Ecoinvent pedigree matrix approach. Uncertainty in the foreground system was modeled using a normal distribution with a standard deviation of 10% of the mean, while uncertainty in the background system was modeled using a lognormal distribution, consistent with Ecoinvent's default approach for life cycle inventory parameters.

Furthermore, to calculate the impacts for the year 2050, we conducted a prospective LCA. In this context, we considered an optimistic future scenario aligned with the 2 °C climate target. To update the background system, we utilised future projections derived from Integrated Assessment Models (IAMs). IAMs, such as IMAGE (Integrated Model to Assess the Global Environment), model the interactions among the biosphere, society, and climate.[20] We used the *premise* v2.1.3[21] framework to construct future background data consistent with the results from the IMAGE model. Additionally, the IMAGE model assumes specific Shared Socioeconomic Pathways (SSPs) that describe the relationship between challenges for adaptation and mitigation. In our study, we assumed the SSP2 scenario ("middle-of-the-road"). For the mitigation scenario, we considered the Representative Concentration Pathway (RCP) aimed at limiting the global mean surface temperature to 2 °C (RCP26 from *premise*). All calculations for the environmental assessment were conducted using the Brightway2.5 framework.[22] Notably, we did not perform an uncertainty assessment for the prospective 2050 scenarios due to lack of available uncertainty data, i.e., the corresponding pedigree matrix values.

Table S6 | Inventories used in the LCA to calculate the impacts of all N_2O production technologies.

Flow	Activity	Source
Fossil ammonia	market for ammonia, anhydrous, liquid	Ecoinvent v3.10
Green ammonia	ammonia production, from nitrogen and hydrogen, green	D'Angelo *et al.*[23]
Green hydrogen (wind-based electrolysis)	hydrogen production, PEM electrolysis, green	D'Angelo *et al.*[23]
Wastewater treatment	market for wastewater, average	Ecoinvent v3.10
Grid electricity	market group for electricity, high voltage	Ecoinvent v3.10
Wind electricity	electricity production, wind, >3MW turbine, onshore	Ecoinvent v3.10
Cooling water	cooling water	Ioannou *et al.*[9]
Heating (natural gas)	heat production, natural gas, at boiler condensing modulating >100kW	Ecoinvent v3.10

Table S7 | Inventories used in the life cycle assessment (LCA) to calculate the impacts of all H_2O_2 production technologies.

Flow	Activity	Source
Fossil hydrogen	market for hydrogen, gaseous, medium pressure, merchant	Ecoinvent v3.10
Green hydrogen (wind-based electrolysis)	hydrogen production, PEM electrolysis, green	D'Angelo *et al.*[23]
2-Ethylanthraquinone	market for anthraquinone	Ecoinvent v3.10
Benzene	market for benzene	Ecoinvent v3.10
Wastewater treatment	market for wastewater, average	Ecoinvent v3.10
Grid electricity	market group for electricity, high voltage	Ecoinvent v3.10
Wind electricity	electricity production, wind, >3MW turbine, onshore	Ecoinvent v3.10
Cooling water	cooling water	Ioannou *et al.*[9]
Heating (natural gas)	heat production, natural gas, at boiler condensing modulating >100kW	Ecoinvent v3.10

Table S8 | Inventories used in the life cycle assessment (LCA) to calculate the impacts of all phenol production technologies.

Flow	Activity	Source
Phenol from cumene oxidation	phenol production, cumene oxidation	Ecoinvent v3.10
Benzene	market for benzene	Ecoinvent v3.10
Fossil nitrous oxide	Nitrous oxide production using fossil ammonia	This work
Green nitrous oxide	Nitrous oxide production using green ammonia	This work
Fossil hydrogen peroxide	Hydrogen peroxide production using fossil hydrogen	This work
Green hydrogen peroxide	Hydrogen peroxide production using green hydrogen	This work
Grid electricity	market group for electricity, high voltage	Ecoinvent v3.10
Cooling water	cooling water	Ioannou *et al.*[9]
Heating (natural gas)	heat production, natural gas, at boiler condensing modulating >100kW	Ecoinvent v3.10

4. Assessment of safety metrics

First, we evaluate the Dow Fire and Explosion Index (F&EI)[24] for all N_2O and H_2O_2 production technologies. The Dow F&EI is a widely used hazard analysis tool to quantify the potential fire and explosion risks in chemical process units. The methodology involves a step-by-step evaluation of process units, focusing on material properties, process conditions, and equipment characteristics. **Table S9** shows the various parameters calculated using these guidelines. The final F&EI value categorises the process into hazard levels (e.g., light, moderate, severe) and informs safety management and insurance decisions. Next, another set of safety metrics is evaluated using the trinitrotoluene (TNT) equivalency framework proposed by Crowl.[25] This framework simplifies the comparison by expressing the energy of a combustible fuel using the equivalent mass of TNT.

Notably, this TNT-based estimate reflects a conservative worst-case, ideal detonation scenario that does not account for preventive and mitigative measures and therefore provides an upper-bound estimate of the inherent explosion potential. Such preventive and mitigative measures are instead incorporated via the Dow F&EI loss control credit factors, which account for process control, material isolation and fire protection, covering measures such as emergency power, cooling, explosion control, emergency shutdown, computer control, inert gas, operating instructions, reactive chemical review, other process hazard analysis, remote control valves, dump/blowdown, drainage, interlocks, leak detection, structural steel, fire water supply, special systems, sprinkler systems, water curtains, foam, hand extinguishers/monitors and cable protection.

Table S9 | Safety metrics for N_2O and H_2O_2 production technologies, calculated using the Dow F&EI framework.[24]

Metric	Five-step N_2O	One-step N_2O	H_2O_2
Material factor	**29.0**	**10.0**	**21.0**
General process hazards			
Base factor	1.0	1.0	1.0
Exothermic chemical reactions	1.0	0.5	0.5
Endothermic processes	0.4	0.0	0.0
Material handling and transfer	0.0	0.0	0.0
Enclosed or indoor process units	0.0	0.0	0.0
Access	0.0	0.0	0.0
Drainage and spill control	0.0	0.0	0.0
Total	**2.4**	**2.4**	**1.5**
Special process hazards			
Base factor	1.0	1.0	1.0
Toxic materials	0.0	0.6	0.0
Sub-atmospheric pressure	0.0	0.0	0.0
Operation in or near flammable range	0.0	0.0	0.0
Dust explosion	0.0	0.0	0.0
Pressure	0.0	0.0	0.0
Low temperature	0.0	0.0	0.0
Quantity of flammable/unstable material	1.9	1.1	2.0
Corrosion and erosion	0.0	0.0	0.0
Leakage–joints and packing	0.0	0.0	0.0
Use of fired equipment	0.0	0.0	0.0
Hot oil heat exchange system	0.0	0.0	0.0
Rotating equipment	0.5	0.5	0.5
Total	**3.4**	**3.2**	**3.5**
Process unit hazards factor	**8.2**	**4.8**	**5.3**
Fire & Explosion Index	**238.1**	**47.5**	**111.2**
Radius of Exposure / m	**61.0**	**12.2**	**28.5**
Area of Exposure / m^2	**11,678.4**	**464.1**	**2,546.2**
Original Cost / million USD	41.7	9.8	10.9
Replacement Value / million USD	34.2	8.1	9.0
Damage Factor	1.0	0.2	0.2
Base Maximum Probable Property Damage / million USD	32.5	1.6	1.8
Loss control credit factor	0.6	0.6	0.6
Actual Maximum Probable Property Damage / million USD	18.9	0.9	1.0
Maximum Probable Days Outage	**120.8**	**20.4**	**21.7**
Business Interruption / million USD	**64.4**	**10.9**	**11.6**

Table S10 | Safety metrics for N_2O and H_2O_2 production technologies, calculated using the TNT equivalency framework.[25]

Description	**Unit**	**One-step N_2O**	**Five-step N_2O**	**H_2O_2**
TNT equivalency of ammonium nitrate	-	0.1	0.4	0.1
Molar mass of ammonium nitrate	kg kmol^{-1}	17.0	80.0	2.0
Mass of fuel used	kg hr^{-1}	30,690.5	76,817.0	2,469.4
Heat of combustion	kJ kg^{-1}	18,346.0	1,447.7	4,008.8
Energy of explosion of TNT	kJ kg^{-1}	4,686.0	4,686.0	4,686.0
Equivalent mass of TNT	kg hr^{-1}	6,007.8	30,727.8	70,747.6
Distance from ground-zero point of the explosion	m	100.0	100.0	100.0
Scaled distance	m kg$^{-1/3}$	5.5	3.2	2.4
Overpressure	kPa	48.7	141.9	264.4
Number of deaths due to lung haemorrhage	-	0	5	9
Number of eardrum ruptures	-	1	3	4
Maximum distance at which projectiles can land	m	1,920.5	2,736.7	3,279.6

5. Assumptions and limitations of the study

- The findings in this study are influenced by the assumptions embedded within the IMAGE IAM, which generated the background inventories. Our study uses the *premise*[21] Python package to generate prospective background inventories.
- Data trends indicate that while recycling at the end of their lifecycle could reduce the carbon intensity of onshore wind turbines, projections suggest that these reductions would be minimal.[26] Therefore, no efficiency improvements are assumed for onshore wind turbines.
- Inventory data were sourced from Ecoinvent v3.10, utilising a cut-off system model.[8] Global inventories were prioritised, and when these were not available, inventories for the rest of the world were used.
- Life cycle assessments were conducted for the production of 1 kg of chemicals, namely N_2O, H_2O_2, and phenol, employing various impact assessment methods. A cradle-to-gate assessment was performed for all categories, avoiding assumptions about the use phase of these platform chemicals and thereby reducing uncertainties.
- In the analysis of all production pathways, we assumed the continuous operation of compressors and pumps powered by grid electricity. In contrast, H_2 production via the water electrolysis process was assumed to be powered by onshore wind electricity. The study does not account for potential energy storage requirements for wind electricity. Additionally, all environmental burdens are allocated to H_2, as the current market cannot absorb the excess oxygen generated as a by-product of water electrolysis.[23]
- For green H_2 production, we considered only proton exchange membrane (PEM) water electrolysis powered by onshore wind electricity due to its high potential for large-scale deployment.
- Conducting a prospective LCA based on IAMs has certain limitations. First, premise is currently focused on power generation, cement and steel production, transport, and fuels, omitting potential improvements in other sectors.
- We assess region-specific impacts by incorporating regional variability across the technosphere flows, such as electricity mixes. The datasets most consistent with the regional scope of our analysis are selected, with particular emphasis on the United States, China, and Europe. When country- or region-specific data are unavailable, global or "rest of the world (RoW)" inventories are used as substitutes.

6. Breakdown of costs and climate change impacts in 2050

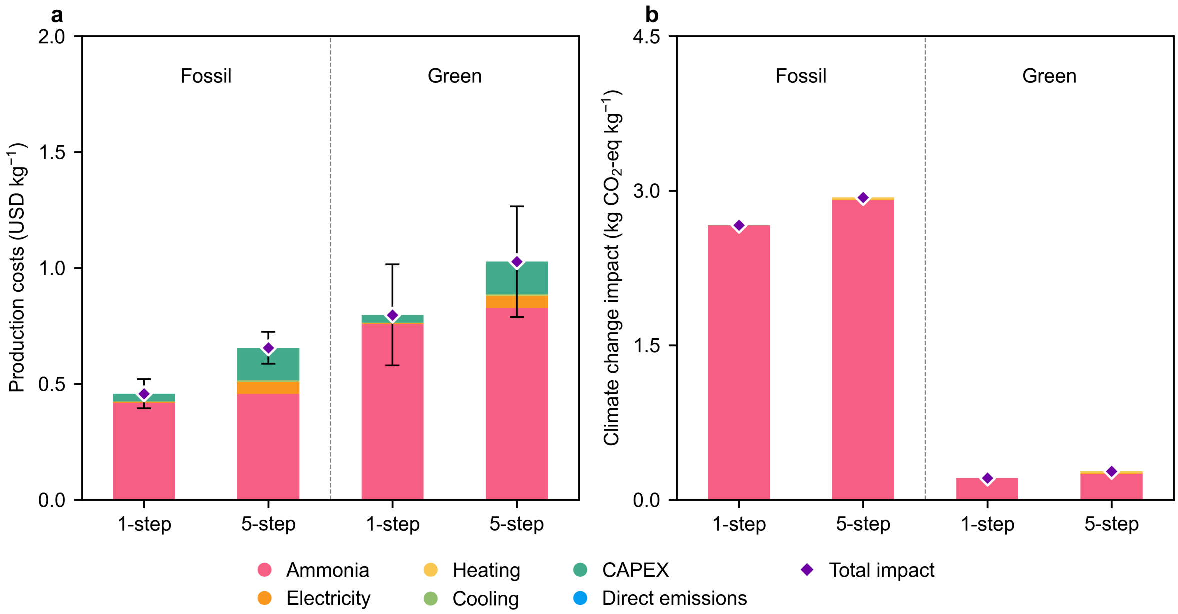

Fig. S6 | (a) Production costs and **(b)** climate change impacts by 2050, per kg of N_2O produced, using two technologies: one-step NH_3 oxidation and five-step thermal decomposition of NH_4NO_3. The analysis includes N_2O production via both fossil-based NH_3 (derived from natural gas) and green NH_3 (produced via the electrolytic H_2-based Haber-Bosch process). Error bars for the climate change impacts are omitted due to insufficient data points in the *premise* database (**Section 3** of the SI).

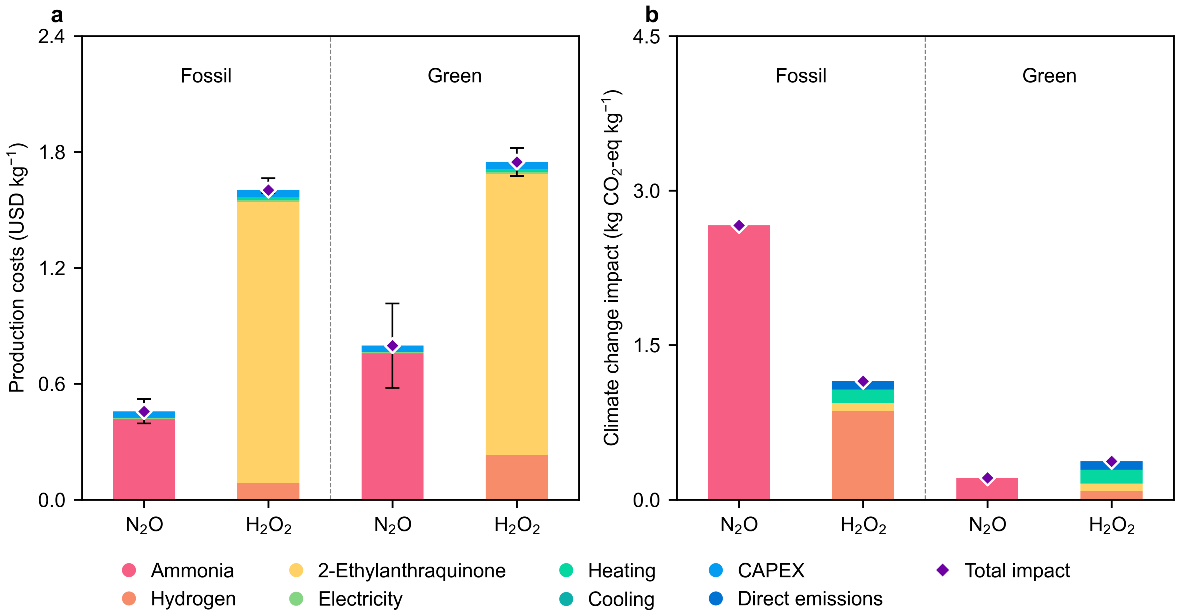

Fig. S7 | (a) Production costs and **(b)** climate change impacts by 2050, per kg of N_2O and H_2O_2. For N_2O production, the one-step process using NH_3 derived from either natural gas (fossil-based) or the electrolytic H_2-based Haber-Bosch process (green) is shown. Similarly, the anthraquinone process for H_2O_2 production, utilising H_2 from either natural gas reforming or electrolytic sources, is presented. Error bars for climate change impacts are not included due to a lack of sufficient data points in the *premise* database (**Section 3** of the SI).

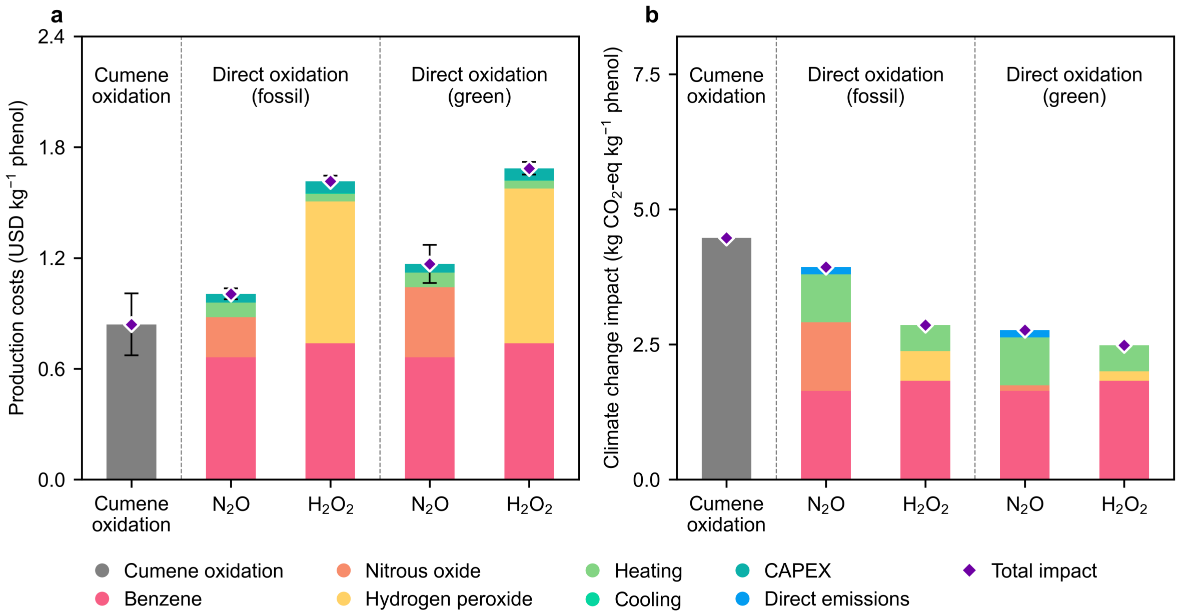

Fig. S8 | (a) Production costs and **(b)** climate change impacts by 2050, per kg of phenol production using the business-as-usual cumene oxidation process, and the direct oxidation of benzene to phenol using N_2O and H_2O_2. For N_2O contributions, the one-step process using NH_3 derived from either natural gas (fossil-based) or the electrolytic H_2-based Haber-Bosch process (green) is shown. Similarly, the anthraquinone process for H_2O_2 contributions, utilising H_2 from either natural gas reforming or electrolytic sources, is presented. Error bars for climate change impacts are omitted because the *premise* database lacks sufficient data points (**Section 3** of the SI).

7. Additional impact categories

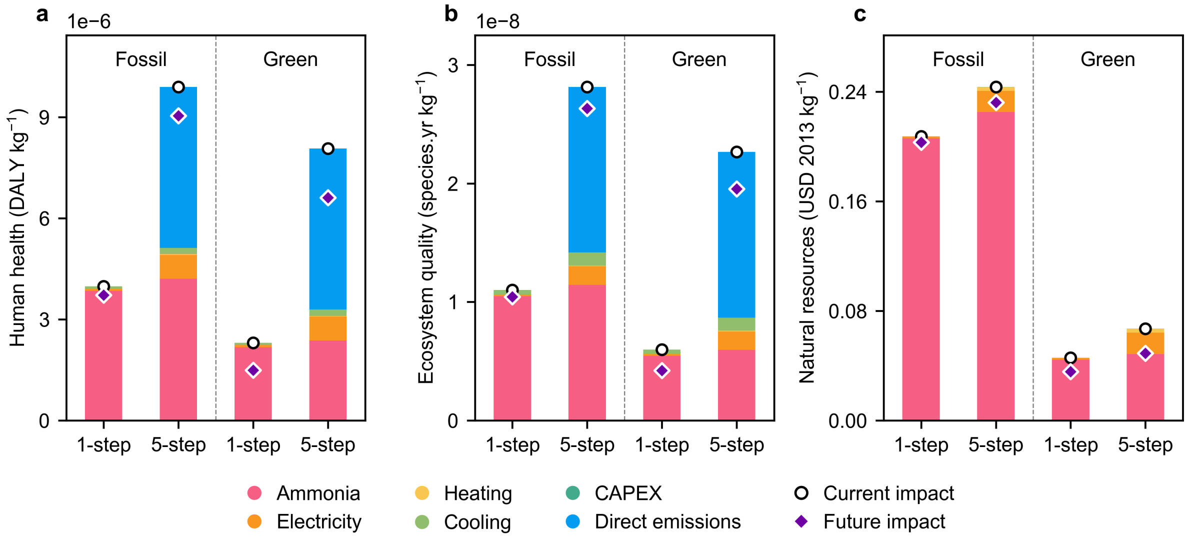

Fig. S9 | (a) Human health, **(b)** ecosystems quality, and **(c)** natural resource impacts per kg of N_2O produced using two technologies: one-step NH_3 oxidation and five-step thermal decomposition of NH_4NO_3. The analysis includes N_2O production via both fossil-based NH_3 (derived from natural gas) and green NH_3 (produced via the electrolytic H_2-based Haber-Bosch process). Future projections for 2050 are highlighted for all impact categories across all technologies.

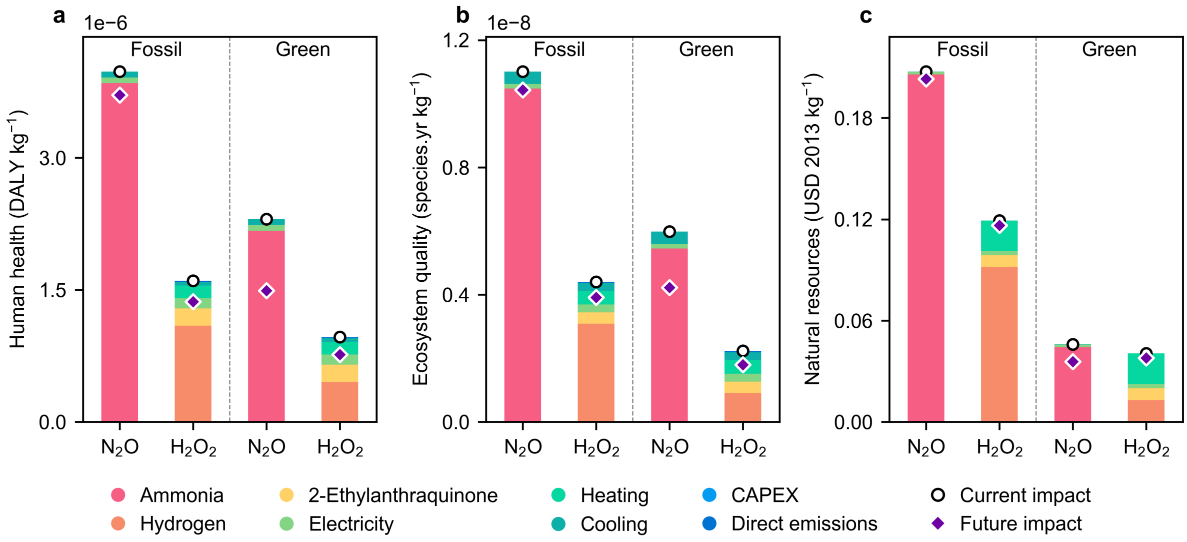

Fig. S10 | (a) Human health, **(b)** ecosystems quality, and **(c)** natural resource impacts per kg of N_2O and H_2O_2. For N_2O production, the one-step process using NH_3 derived from either natural gas (fossil-based) or the electrolytic H_2-based Haber-Bosch process (green) is shown. Similarly, the anthraquinone process for H_2O_2 production, utilising H_2 from either natural gas reforming or electrolytic sources, is presented. Future projections by 2050 for all impact categories across all technologies are highlighted.

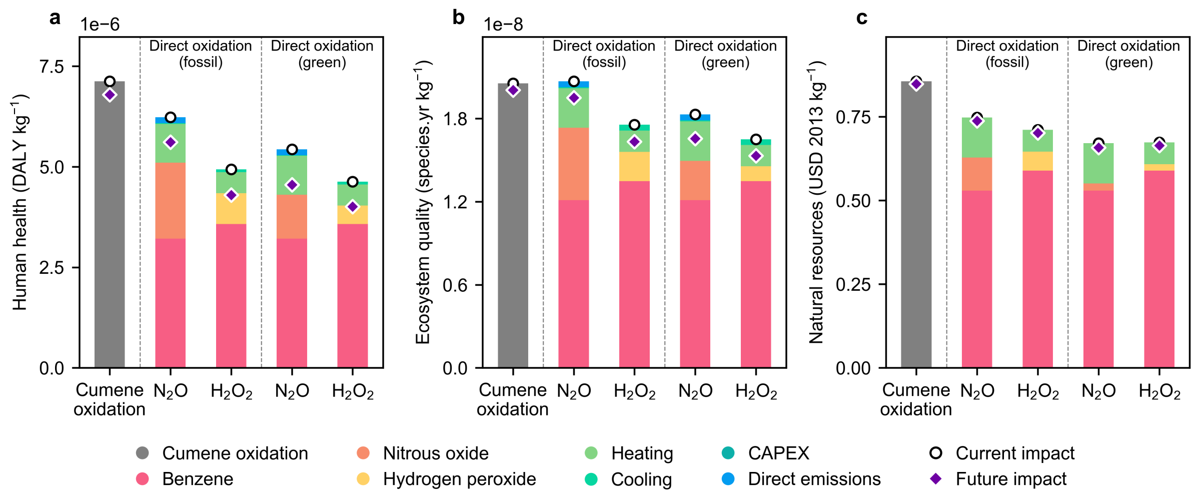

Fig. S11 | (a) Human health, **(b)** ecosystems quality, and **(c)** natural resource impacts per kg of phenol production using the business-as-usual cumene oxidation process, and the direct oxidation of benzene to phenol using N_2O and H_2O_2. For N_2O contributions, the one-step process using NH_3 derived from either natural gas (fossil-based) or the electrolytic H_2-based Haber-Bosch process (green) is shown. Similarly, the anthraquinone process for H_2O_2 contributions, utilising H_2 from either natural gas reforming or electrolytic sources, is presented. Projections for 2050 highlight potential reductions in all impact categories across all technologies.

8. Uncertainty analysis

The uncertainty assessment was conducted using Monte Carlo sampling based on the Ecoinvent pedigree matrix values, which contains uncertainty data for the LCI values of the background system. This matrix considers diverse qualitative criteria, including geographical and temporal aspects, to model the uncertainty distribution of the LCI parameters in the Ecoinvent database. The results from the uncertainty assessment and the probability of burden shifting are shown in **Figs. S12-S15**.

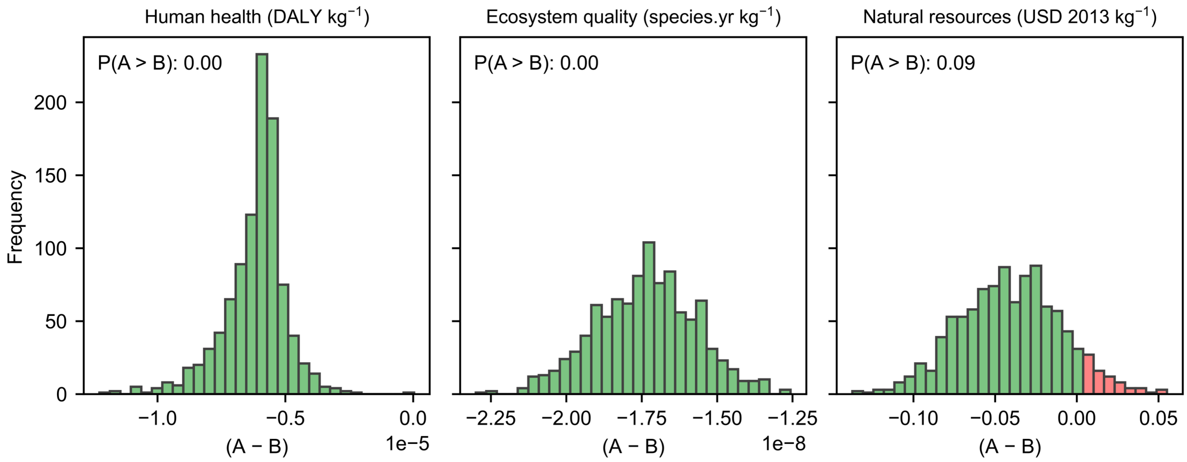

Fig. S12 | Probability of burden-shifting (A > B) for N_2O production technologies across the three endpoint categories of the ReCiPe 2016 v1.03 method. Here, A represents the fossil one-step NH_3 oxidation, and B represents the fossil five-step thermal decomposition of NH_4NO_3. Green bars indicate cases where the environmental footprint of the one-step process is lower than that of the five-step process, while red bars indicate cases where the environmental footprint of the one-step process is higher. Burden shifting is considered to occur when $P(A > B) \geq 0.75$, whereas no burden shifting is observed when $P(A > B) < 0.25$.

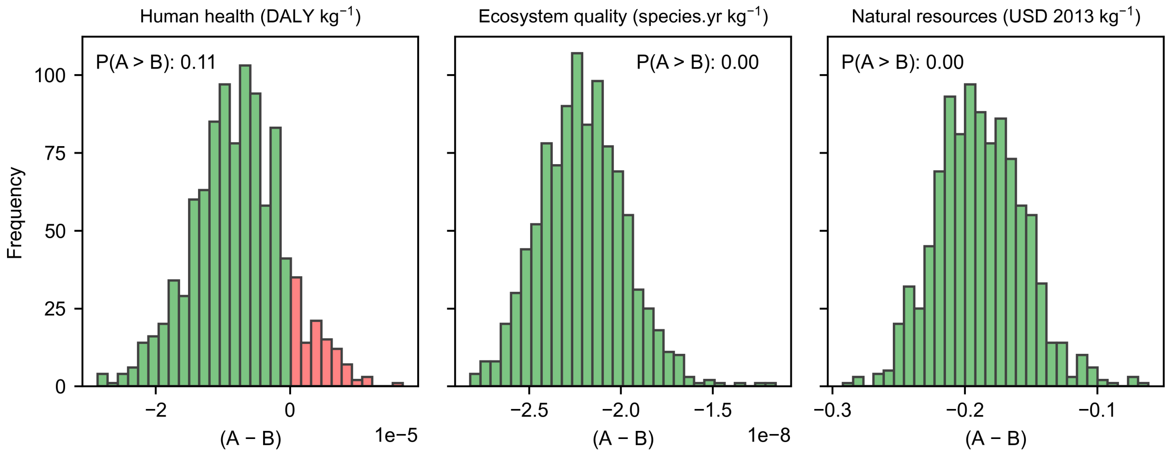

Fig. S13 | Probability of burden-shifting (A > B) for N_2O production technologies across the three endpoint categories of the ReCiPe 2016 v1.03 method. Here, A represents the green one-step NH_3 oxidation, and B represents the fossil five-step thermal decomposition of NH_4NO_3. Green bars indicate cases where the environmental footprint of the one-step process is lower than that of the five-step process, while red bars indicate cases where the environmental footprint of the one-step process is higher. Burden shifting is considered to occur when P(A > B) ≥ 0.75, whereas no burden shifting is observed when P(A > B) < 0.25.

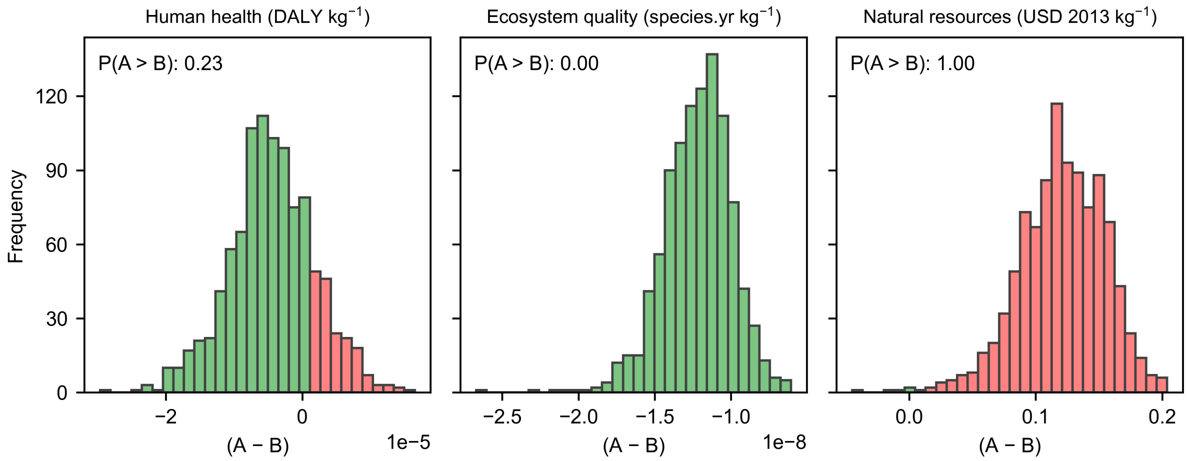

Fig. S14 | Probability of burden-shifting (A > B) for N_2O production technologies across the three endpoint categories of the ReCiPe 2016 v1.03 method. Here, A represents the fossil one-step NH_3 oxidation, and B represents the green five-step thermal decomposition of NH_4NO_3. Green bars indicate cases where the environmental footprint of the one-step process is lower than that of the five-step process, while red bars indicate cases where the environmental footprint of the one-step process is higher. Burden shifting is considered to occur when $P(A > B) \geq 0.75$, whereas no burden shifting is observed when $P(A > B) < 0.25$.

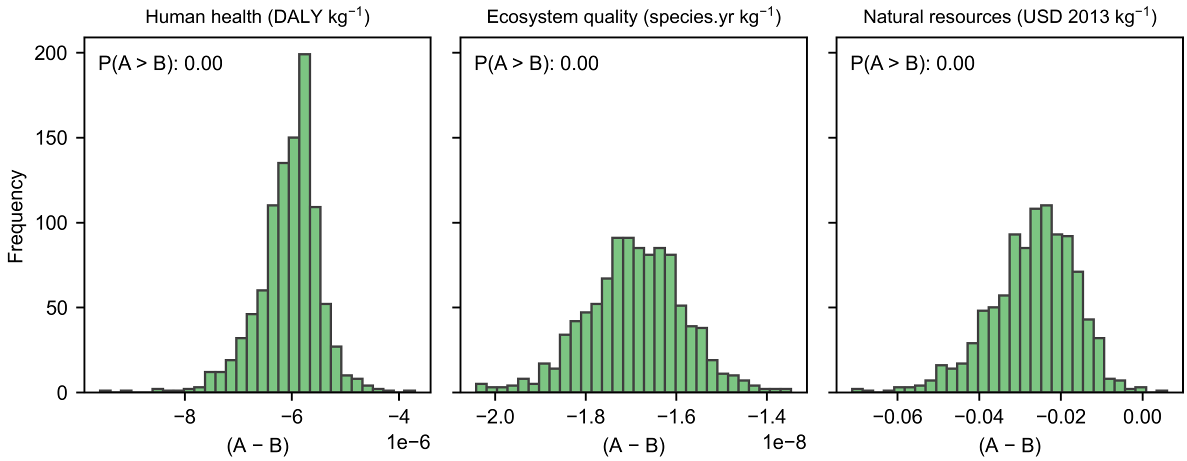

Fig. S15 | Probability of burden-shifting (A > B) for N_2O production technologies across the three endpoint categories of the ReCiPe 2016 v1.03 method. Here, A represents the green one-step NH_3 oxidation, and B represents the green five-step thermal decomposition of NH_4NO_3. Green bars indicate cases where the environmental footprint of the one-step process is lower than that of the five-step process, while red bars indicate cases where the environmental footprint of the one-step process is higher. Burden shifting is considered to occur when P(A > B) ≥ 0.75, whereas no burden shifting is observed when P(A > B) < 0.25.

9. Regional climate change impacts

We evaluate region-specific climate change impacts by accounting for regional variability in technosphere flows, such as electricity mixes. Datasets best aligned with the regional scope of our analysis are selected, with particular focus on the United States, China, and Europe. Regional analysis is carried out only for regions and countries that together account for more than 50% of global GDP. When data for a specific country or region are unavailable, global or "rest of the world (RoW)" inventories are used as substitutes. The corresponding results are presented in **Table S11**.

Table S11 | Regional climate change impacts (kg CO_2-eq kg^{-1} N_2O or H_2O_2) for one- and five-step N_2O production from fossil-based NH_3 and green NH_3 (produced via an electrolytic H_2-based Haber-Bosch process), and for H_2O_2 via the AO process using H_2 from natural gas reforming or electrolytic sources.

Region	Five-step N_2O	One-step N_2O	H_2O_2
Fossil scenario			
Global average	3.440	2.821	1.286
United States	3.356	2.813	1.103
China	5.351	4.479	1.304
Europe	2.805	2.390	1.098
Green scenario			
Global average	1.125	0.703	0.492
United States	0.965	0.625	0.479
China	1.337	0.805	0.510
Europe	0.776	0.533	0.462

10. Safety metrics for storage, transport, and use

Quantifying safety metrics across the storage, transportation, and application stages of N_2O and H_2O_2 is essential for a comprehensive assessment. To this end, we apply the Dow F&EI beyond the production stage to explicitly include the storage, transportation, and application of N_2O. In the case of H_2O_2, we do not report separate F&EI values for storage or transport, as concentrated H_2O_2 is typically produced and consumed in situ. This practice aligns with safety and regulatory constraints, given that H_2O_2 is a highly reactive oxidant that decomposes exothermically when contaminated or confined, rendering bulk storage and long-distance transport impractical. The Dow F&EI values for N_2O storage and transportation are reported in **Table S12**. Similarly, for the use phase, we evaluated the Dow F&EI for phenol production via benzene oxidation using N_2O and H_2O_2 as oxidants, in comparison to the business-as-usual cumene oxidation route, as shown in **Table S13**.

Table S12 | Safety metrics for N_2O storage and transport, calculated using the Dow F&EI framework.[24]

Metric	Storage	Transport
Material factor	**14.0**	**14.0**
General process hazards		
Base factor	1.0	1.0
Exothermic chemical reactions	0.0	0.0
Endothermic processes	0.0	0.0
Material handling and transfer	0.0	0.0
Enclosed or indoor process units	0.0	0.0
Access	0.0	0.0
Drainage and spill control	0.0	0.0
Total	**1.0**	**1.0**
Special process hazards		
Base factor	1.0	1.0
Toxic materials	0.2	0.2
Sub-atmospheric pressure	0.0	0.0
Operation in or near flammable range	0.0	0.0
Dust explosion	0.0	0.0
Pressure	0.9	0.9
Low temperature	0.0	0.0
Quantity of flammable/unstable material	0.0	0.0
Corrosion and erosion	0.0	0.0
Leakage–joints and packing	0.1	0.3
Use of fired equipment	0.0	0.0
Hot oil heat exchange system	0.0	0.0
Rotating equipment	0.0	0.0
Total	**2.2**	**2.4**
Process unit hazards factor	**2.2**	**2.4**
Fire & Explosion Index	**30.8**	**33.6**
Radius of Exposure / m	**7.9**	**8.6**
Area of Exposure / m^2	**195.4**	**232.5**

Table S13 | Safety metrics for phenol production technologies, calculated using the Dow F&EI framework.[24]

Metric	Cumene oxidation	Benzene oxidation via N_2O	Benzene oxidation via H_2O_2
Material factor	**40.0**	**16.0**	**16.0**
General process hazards			
Base factor	1.0	1.0	1.0
Exothermic chemical reactions	0.5	1.0	1.0
Endothermic processes	0.0	0.0	0.0
Material handling and transfer	0.0	0.0	0.0
Enclosed or indoor process units	0.0	0.0	0.0
Access	0.0	0.0	0.0
Drainage and spill control	0.0	0.0	0.0
Total	**1.5**	**2.0**	**2.0**
Special process hazards			
Base factor	1.0	1.0	1.0
Toxic materials	0.4	0.4	0.4
Sub-atmospheric pressure	0.0	0.0	0.0
Operation in or near flammable range	0.8	0.8	0.8
Dust explosion	0.0	0.0	0.0
Pressure	0.2	0.2	0.2
Low temperature	0.0	0.0	0.0
Quantity of flammable/unstable material	2.0	1.9	2.2
Corrosion and erosion	0.1	0.1	0.1
Leakage–joints and packing	0.1	0.1	0.1
Use of fired equipment	0.0	0.0	0.0
Hot oil heat exchange system	0.0	0.0	0.0
Rotating equipment	0.5	0.5	0.5
Total	**5.1**	**5.0**	**5.3**
Process unit hazards factor	**7.6**	**10.0**	**10.6**
Fire & Explosion Index	**303.2**	**159.2**	**169.0**
Radius of Exposure / m	**77.6**	**40.8**	**43.3**
Area of Exposure / m^2	**18,929.5**	**5,222.4**	**5,879.5**

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