An exergy-based ecosphere-technosphere-ecosphere lifetime model of general productive systems: A Nicholas Georgescu-Roegen-inspired view

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Abstract:

Current and novel production systems projects have required life-cycle assessments to evaluate their environmental impact throughout their lifetime production existence. However, as twin transition (green digital transitions) projects have taken place, different arbitrary midpoint and endpoint environmental and social indicators have misguided with opposite suggestions about their environmental, economic and social viabilities. This paper aims to suggest a novel perspective of a general production system modeling (e.g., raw materials and energy streams, chemicals, minerals) under an exergy-based view over their lifetime. The model encompasses a 9-stage, 3-phase analysis to evaluate a system's overall lifetime performance. Such a model allows comprehensive analysis of macro and micro (global and local) effects in terms of natural resources depletion (cradle-to-grave) and waste generation (grave-to-cradle) through a novel concept called irreversibility backpack. It represents all cumulative irreversibilities associated with the production of a product with full disclosure of all irreversibility sources throughout all resources' supply chain and residues treatment. This physical-based approach allows for the usage of exergy costs/cumulative exergy demand with associations with both natural resources depletion/scarcity creation (and their exergy replacement costs) and irreversibilities linkages with each one of Rockstrom's planetary boundaries (and their exergy abatement costs). We provide a representative example with the lifetime production analysis of green ammonia in an industrial plant. This novel approach focuses on a cradle-to-cradle view from Earth's perspective, emphasizing natural resources depletion and residues generation with respective levelized exergy replacement and remediation costs, and irreversibilities association with planetary boundaries and therefore, to absolute sustainability.

Keywords:

Total sustainability; Exergy; Planetary boundaries; Prospective exergy life cycle analysis; Thermodynamics.

1. Introduction

Nicholas Georgescu-Roegen's concept of irreversibility focuses on the idea that economic processes, like all natural processes, are fundamentally irreversible due to the second law of thermodynamics [1]. This causes an inherent tendency towards entropy (increase in disorder) that makes true reversibility impossible in reality. His work emphasized that economic activity, especially the extraction and transformation of resources, irreversibly degrades the environment, leading to a qualitative degradation of free energy into bound energy.

In parallel to such a view, exergy-based methods apply the second law to evaluate the performance of distinct production systems via exergy evaluation of energy and material streams. The methods directly related to environmental and ecologic analyses (e.g., exergy life-cycle assessment (ELCA), thermoecology, exergoenvironmental analyses, emergy, theory of exergy cost, etc.) [2–7] present interesting fundamentals and robust mathematical basis to evaluate environmental impacts. However,

they present fundamental issues among themselves due to different prioritization criteria (either economic, environmental, physical, social, etc.), limited primary exergy support, static technology representation, and others. For example, Thermoecology [4] express the total expenditure related to the consumption of natural resources and their relation emissions and required exergy remediation, but it only accounts for non-renewable resources and does not account for local environmental changes. ELCA is usually adopted to a more expanded view of exergy analyses with environmental impacts and is available on most LCA tools (e.g., SimaPro, Gabi, openLCA) with their contain extensive databases, but it lacks appropriate mass and energy balances, provides limited exergy support, static technology representation and there is no direct fleet integration. There are also specialized exergy calculator tools, but these focus on single processes or systems, with no life-cycle integration and fleet-level analysis. Additionally, neither of them directly deals with both natural resources depletion [8] and irreversibility disaggregation towards residues and to the planetary boundaries [9].
It is clear that significant gaps remains between several environmental assessment tools available on literature, despite advances in both exergy analysis and energy system modeling. There are no detailed exergy-based life-cycle assessments with unified natural resource + emission vectors. Also, there are no dynamic electricity grid composition and fleet-level capacity evolution (e.g., IEA scenarios) for transition scenarios such as the digitalization scenario we are currently. In order to cover all aforementioned gaps, the authors adopted the theory of exergy cost's systematic mathematical structure and related it with both ELCA and thermoecological cost theory to build as initial method capable of exergy-based supply chain (cradle-to-gate) environmental impact assessments and inventories database buildup, and thermodynamic-based natural resources, environmental impact traceability. Then, linking this mix with industrial ecology and emergy fundamentals, and with the planetary boundaries theory, we obtained the bases of the thermodynamics of sustainability (ToS) framework. The main goal [10] is to present a unified physical-cost accounting framework that measures the thermodynamic cost of any human activity — from resource extraction through production, use, and environmental impact remediation — in a single, physically consistent currency: exergy. Its development should fill the identified gaps of integrating exergy throughout (from elementary flows to fleet-weighted averages and chemical product costs), with different production scales (system life-cycle, fleet dynamics, sub-systems) and dynamics (learning curves, grid evolution, technology improvement, year-dependent operation vectors). All these by tracking down natural resources and emissions explicitly with a 22-dimensional natural resource and a 26-dimensional emission tensors. This chain of information allows us to prepare for future spatiotemporal assessment of local reference environments, natural resources depletion (e.g., ore-grade-dependent concentration exergy and exergy replacement costs) and linkage of irreversibility with the planetary boundaries (e.g., local and global remediation exergy).
The following sections introduce the current state of the thermodynamics of sustainability methodology (Sec. 2.), an applied example of this method and its current potential, limitations, and future work (Sec. 3.).

2. METHODOLOGY

2.1. Thermodynamics of sustainability

In order to present a novel, physics-based method that links both the issues addressed by Georgescu-Roegen's work with those from sustainability and Rockström's planetary boundaries, the authors developed a 17-criteria literature review comparison on methods involving thermodynamics and sustainability [10]. The references adopted for such a review are publicly available on page of our research group [11]. Such a review gave us a contextualized basis to develop the fundamentals of the thermodynamics of sustainability. The current work expands on what is briefly commented on the other paper and develops a novel mathematical modeling of exergy-based lifetime analysis of general production systems. This new framework is capable of tracing back and accounting for both natural resources depletion and irreversibilities generated during a production system lifespan and linking each of them to the 9 planetary boundaries theory [9]. To the best of the authors' knowledge, some exergy-based methods [2–6, 12–17] had briefly included either natural resources depletion or emission abatement aspects presented here, but neither of them considered both of these features together, especially with irreversibility disaggregation for each of the 9 planetary boundaries in the way it is taken here. Thus, besides the new framework detailed next, these are considered our main novelties.

2.2. Fundamentals

Figure 1 presents the schematic diagram of the thermodynamics of sustainability framework. This framework is a physics-based, cradle-to-cradle (cradle-to-grave for the main economic supply chain activities and grave-to-cradle to second-life activities), dynamic, local-based reference environment approach that also includes natural resources exergy reposition and residues remediation costs at local and global scales on the overall balance.

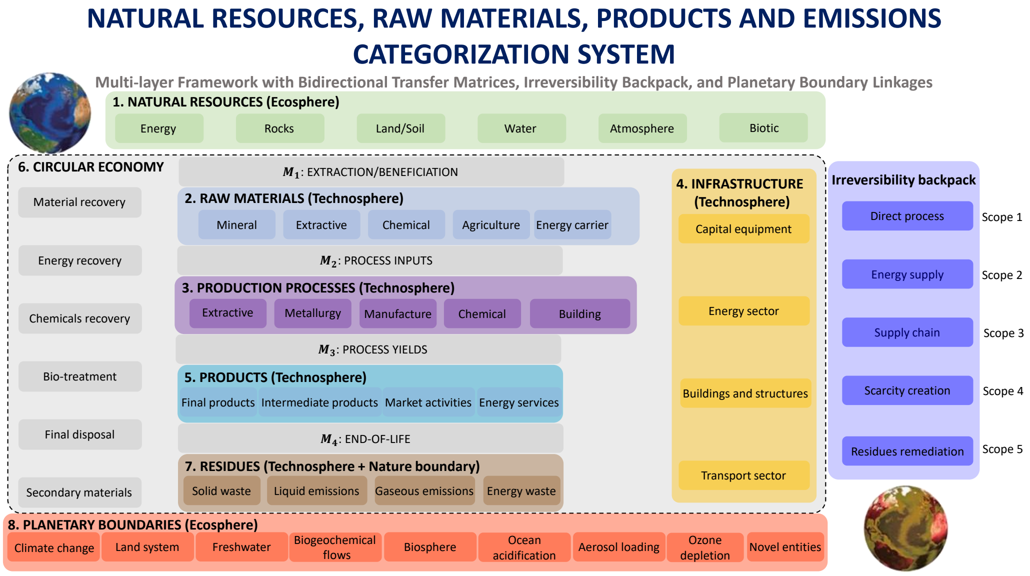

Figure 1: Multi-layer framework for the thermodynamics of sustainability model. The model features bidirectional functional matrices relating the layers among themselves, the irreversibility backpack concept and the exergy-based linkage with Rockström's planetary boundary concept.

Figure 1 also introduces the natural resources, raw materials, products and emissions categorization system adopted in the ToS framework. The global production chain is split in 8 different layers (which differ between either material or process ones): natural resources (from the ecosphere to the technosphere), raw materials, production processes, infrastructure, and products (all inside the technosphere) and residues (from the technosphere to the ecosphere). Second-life routes (represented on the left of the circular economy layer) are also included here. We adopt a multi-layer framework with bidirectional transfer matrices (represented by the matrices M) between each of these layers to create a robust traceability framework using exergy as the variable of interest (and complemented with mass, composition, and cumulative irreversibilities) to split the information data between natural resources, raw materials and products, and emissions with each of the planetary boundaries via the state vector $\vec{B}_p$ of Eq. 1.

In this paper, we introduce a new concept called irreversibility backpack. It is the sum of all irreversibilities associated to a general lifetime product production process are presented under five different scopes: direct process, energy supply, supply chain (these three associated with resources consumption), natural resources scarcity creation (or their depletion) and residues remediation (causing environment degradation); all represented on Fig. 1. We adopt a five-scope viewpoint (as qualitatively described by Fig. 2) based on the fundamentals of exergy cost theory [7] $(B^* = B + \sum_{i=1}^{N_{scopes}} I_i)$

to account for the product's exergy and direct production process irreversibility (scope 1), the supply chain's energy and material footprints (scopes 2 and 3) and, especially, natural resources scarcity reposition and emissions remediation physical costs (scopes 4 and 5). These links are represented by dimensions of the irreversibilities created throughout the supply chain of a product. Therefore, the irreversibility backpack of a product represent all disaggregated cumulative irreversibilities generated during the production of any good (materials or energy streams, infrastructures, human-demanded objects, etc.) and the respective (direct or indirect) environmental harms caused by its production.

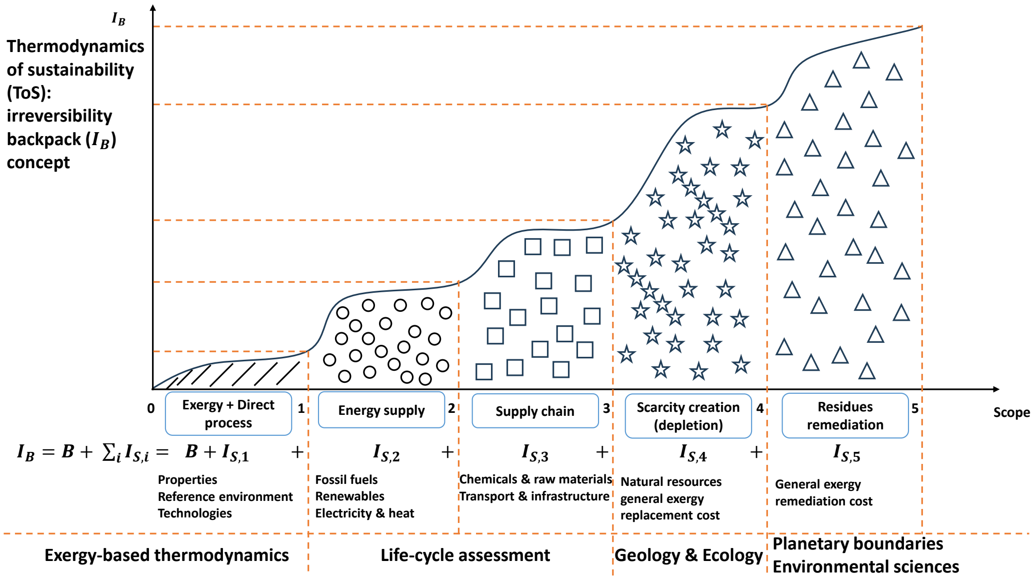

Figure 2: 5-scope thermodynamics of sustainability irreversibility backpack (I_B) concept. Scope 1 refers to exergy-based thermodynamics (stream exergy and direct process irreversibility). Scopes 2 and 3 refer to life-cycle assessments (energy supply sources and the supply chain). Scope 4 refer to geology and ecology (with scarcity creation). Scope 5 refers to the planetary boundaries and environmental sciences (residues remediation).

2.3. Theoretical framework and state vector representation

For any product (p), we define the extended state tensor:

$$\vec{\mathbf{B}}_p = \left[\mathbf{B}_p^{(nr)}\ \mathbf{E}_p^{(em)}\ \mathbf{\Psi}_p^{(pb)}\ \mathbf{W}_p^{(waste)}\right] \in \mathbb{R}^{N+L+M+K} \tag{1}$$

where $\mathbf{B}_p^{(nr)} \in \mathbb{R}^N$ is the natural resource requirement tensor (N = 22), $\mathbf{E}_p^{(em)} \in \mathbb{R}^L$ is the associated residues/ emission tensor (L = 26), $\mathbf{\Psi}_p^{(pb)} \in \mathbb{R}^M$ is the planetary boundary irreversibility tensor, and $\mathbf{W}_p^{(waste)} \in \mathbb{R}^K$ is the waste remediation/treatment tensor.

The state tensor is responsible for keeping the information related to the production history of a good from both upstream (supply chain) and downstream (sub-sequential) processes. The model is capable With this traceability feature to differentiate the same product (e.g., hydrogen) obtained from different production routes, its overall irreversibility and footprints (material, energy, water, environmental), renewability and circularity, technological advancement, criticality, local and global availability, etc. The 22 dimensions of the natural resources tensor is presented by Eq. 2:

$$\begin{aligned}\mathbf{B}^{(nr)} = [&B_{solar}, B_{wind}, B_{hydro}, B_{geo}, B_{coal}, B_{NG}, B_{oil}, B_{nuclear}, B_{biomass}, \cdots \\ &\vec{m}_{metallic}, \vec{m}_{non-metallic}, \vec{m}_{rare,elements}, \vec{m}_{construction,mineral}, \vec{m}_{industrial,mineral}, \vec{m}_{atmosphere,gas}, \cdots \\ &\vec{m}_{water,fresh}, \vec{m}_{water,sea}, \vec{S}_{land,occupation}, \vec{S}_{land,transformation}, \vec{B}_{soil}]^T\end{aligned} \tag{2}$$

Currently, we account for 9 different primary energy sources (PES); each one of these contain structures that indicate their exergy, natural resources state (e.g., solar radiation energy converted for solar and crude oil for oil) and most adopted unit, etc. The material resources are represented by the vectors of metallic-based materials (Fe,Cu,Pb, etc.), non-metallic materials (limestone, clay, sand, gravel, etc.), rare elements (REEs, PGMs, Li, Co, etc.), construction minerals (aggregated materials for construction, e.g., concrete, steel types, high-grade silicon electronic parts, etc.), industrial minerals (feldspar, talc, kaolin, etc.), and atmospheric gases (N_2,O_2,Ar, CO_2, etc.). Water, land and soil resources are similarly represented and categorized. The topsoil exergy [18] is included here to assess the non-renewable exergy lost whenever healthy soils are replaced for any production process activity. The emissions tensor is represented by Eq. 3:

$$\begin{gathered}\mathbf{E}^{(em)} = [\vec{m}_{\mathrm{CO_2}}, \vec{m}_{\mathrm{CH_4}}, \vec{m}_{\mathrm{N_2O}}, \vec{m}_{Acidifying}, \vec{m}_{Photochemical}, \vec{m}_{Particulate}, \vec{m}_{Ozone,Depleting}, \cdots \\ B_{Radioactive,air}, \vec{m}_{Eutrophying,N}, \vec{m}_{Eutrophying,P}, \vec{m}_{Ecotoxic,water}, \vec{m}_{Heavymetal,water}, \vec{m}_{Organic,water}, \cdots \\ B_{Radioactive,water}, \vec{m}_{Pesticides}, \vec{m}_{Heavymetal,soil}, \vec{m}_{Organic,soil}, \vec{m}_{Acidifying,soil}, \vec{m}_{Salinization}, \cdots. \\ \vec{m}_{Radioactive,soil}, \vec{m}_{Hazardous,waste}, \vec{m}_{Non-hazardous,waste}, \vec{m}_{Radioactive,waste}, \cdots. \\ B_{Heat,waste}, B_{Others,waste}]^T \end{gathered} \tag{3}$$

Air emissions cover the first eight vectors (up to $B_{Radioactive,air}$), water emissions are the next 6 (up to $B_{Radioactive,water}$, soil emissions then come with the next 6 (up to $\vec{m}_{Radioactive,soil}$), and finally general waste cover the last 5 categories. Both natural resources and emission tensors are adopted in similar ways as on Ecoinvent v3.11 database. The last two elements of Eq. 1 are the planetary boundary and waste remediation tensors, who are introduced here, but their scope will be properly presented in future works.

2.4. Life-cycle Stage Framework

The mathematical model evaluates the exergy cost of general production system across its complete life-cycle, from resource extraction to decommissioning. It is designed to be a general-purpose, exergy-based evaluator applicable to any production process. It provides dynamic evaluation of all physical costs required on its pre-operation, operation and post-operation phases (according to the production system' mathematical model capacities). It connects detailed system-level life-cycle assessment with either local individual or global electricity fleet-level capacity evolution. It is also capable of adopting technology learning curves and material intensity reductions for dynamic evolution of physical costs. All of these features enable analyses of how technology improvements affect the exergy efficiency, renewability, footprints, and sustainability of such a system.

For this framework, the life-cycle of a general production system (e.g., thermal plants, chemical plants, mining, manufacturing, electricity production, transmission, and storage, water desalinization and treatment, residue treatment/abatement, agriculture, biomass, and biological activities, data centers, etc.) can be decomposed into nine stages, each with independent resource tracking: extraction (raw material acquisition, e.g. mining, drilling, harvesting), refining (material processing, e.g., smelting, enrichment, purification), manufacturing (component fabrication, e.g., assembly, machining, forming), transport (logistics, e.g., shipping, trucking, pipelines), building (on-site construction, e.g., installation, commissioning), operation (production phase, energy and material conversion), maintenance (repairs and replacements, e.g., component replacement, repairs), waste treatment (operational waste, e.g., emissions control, waste processing), and finally decommissioning (end-of-life, e.g., dismantling, recycling, disposal). For each stage (s), we track the resource consumption tensor ($\mathbf{B}_s^{(nr)} \in \mathbb{R}^{22}$), the emission tensor ($\mathbf{E}_s^{(em)} \in \mathbb{R}^{26}$), material inventory $(\mathbf{m}_s)$ (mass flows), energy flows $(\mathbf{E}_s)$ (input/output), exergy flows $(\mathbf{B}_s)$ (input/output/destroyed), and the lifetime integration $\mathbf{B}_{\text{lifetime}} = \sum_{s=1}^{9} \mathbf{B}_s \cdot f_s(t)$, where $f_s(t)$ is the temporal scaling factor for stage (s) (e.g., operation stage scales with lifetime, maintenance with scheduled events).

By coupling these data for each stage and applying the exergy cost theory [7], the exergy cost to obtain any product can be generally expressed as the total exergy input per unit exergy of product output by proper decomposition into the 22D resource vector showing which natural resources contribute to the cost (Eq. 4). The corresponding levelized form that accounts for temporal degradation, learning curves, and discounting (Eq. 5):

$$\text{ExCoP} = \frac{\sum_{r=1}^{21} \mathbf{B}_r^{(nr)}}{B_{\text{product}}} \quad [\text{MJ}_{\text{ex}}/\text{MJ}_{\text{product}}] \tag{4}$$

$$\text{LExCoP} = \frac{\sum_{t=0}^{T} \frac{B_t}{(1+r)^t}}{\sum_{t=0}^{T} \frac{B_{\text{product}}}{(1+r)^t}} \tag{5}$$

where T is the system lifetime, r is the physical amortization rate of the production process system, B_t is the exergy consumption in year (t), and E_t is the product(s) production in year (t). ExCoP/LExCoP generalize ExCoE/LExCoE to any functional unit [19, 20]. For example, for electricity systems, the product is MJ of electricity. However, with proper traceability, these values can also be represented on different units most commonly used in a sector; for chemical plants, the product would be kg of the target substance (e.g., kg NH_3). Finally, by combining natural resources, efficiency and material improvements:

$$\text{ExCoP}(t, p) = f(\mathbf{B}_p^{nr}(t, p), \eta(t, p), MI(t, p), \text{grid}(t)) \tag{6}$$

The full life-cycle calculation is performed for each (year, primary energy sources, material intensity, scenario) combination, incorporating year-specific parameters.

2.5. Model example and process description

Our model example focuses on a small-scale industrial complex of green hydrogen and ammonia production. Fig. 3 details the process flow diagram (PFD) of our adopted small-scale green ammonia synthesis plant (9.46 kt kt_{NH_3}/year). The authors modeled the presented plant model in Aspen PLUS v14. The adopted Haber-Bosch configuration involves a two-bed reactor loaded with a Fe-C catalyzer) [19] with a recirculation circuit that is used by the control system whenever it needs to regulate the plant load due to intermittent renewable electricity/upstream hydrogen availability. All operation, configuration, modeling and other details of interest are available on [19]. The goal on this paper is to apply this newly introduced approach to this previous study to highlight its new features, and gaps that still need to be covered.

Fig. 4 shows the schematic diagram under the thermodynamic sustainability framework applied for this plant. A regular perspective adopted in classical engineering thermodynamics (i.e., as in 3) is represented by Scope 1, following the criteria presented on Fig. 2. Scopes 2 and 3 provide LCA-perspective data about required energy sources, raw materials, and infrastructure. For this case of study, we adopted an exergy-based, cradle-to-gate, small-scale chemical plant infrastructure inventory to represent the infrastructure equivalent to ”chemical factory, organics” of Ecoinvent v3.11 on a scale of 0.1 units/kg_{NH_3}. Code 1 described on [10] introduces how this exergy-based, cradle-to-gate tiered life-cycle inventory was developed. The auxiliary systems included in our study include an self-sustainable, hybrid renewable wind-solar PV plant (with a 50-50% average capacity factor) used to feed not only the ammonia plant, but also a cryogenic air-separation plant to produce N_2 and O_2, a state-of-the-art alkaline electrolyzer that is replaced to account for membrane degradation to produce H_2, a distilled water pump and an H_2 compressor required to transport and adjust H_2’s pressure to the ammonia’s plant inlet pressure (30 bar$_g$), H_2 storage tank and pipelines.

As mentioned before, scopes 4 and 5 (scarcity creation and residues remediation) will be properly described and evaluated in future works. However, their overall structure is already accounted for the ToS framework.

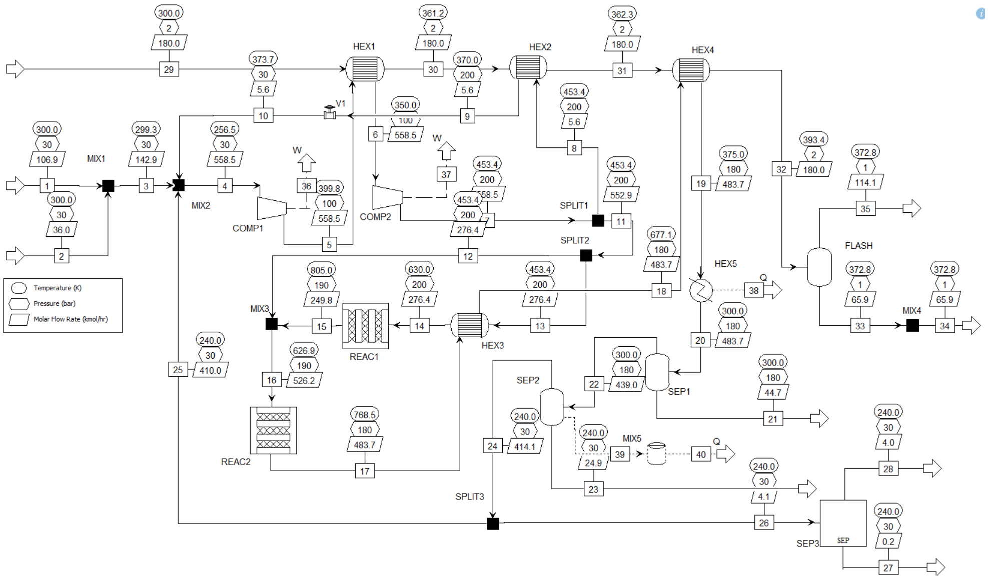

Figure 3: Process flow diagram (PFD) of a small-scale green ammonia plant (GAP) with a recirculation circuit (from streams 8 to 10) to intermittent renewable electricity/hydrogen load control [10].

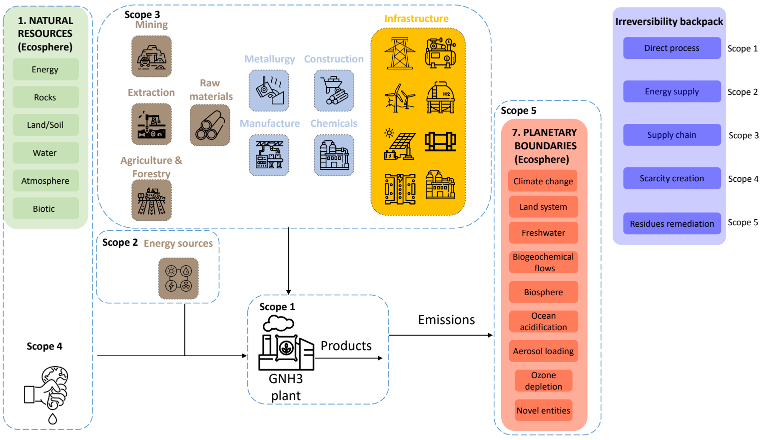

Figure 4: Example of thermodynamics of sustainability framework: green ammonia (NH_3) plant based on [19].

3. RESULTS AND DISCUSSION

3.1. Pre-operation phases - chemical plant infrastructure

Under the thermodynamics of sustainability perspective, the pre-operation phase of any general production system involves the extraction, refining, manufacturing, transport and building phases. These were all lumped here into only one representative phase including all information related to natural resources, raw materials, chemicals, energy sources and emissions from each of them. Besides the electrolyzer material intensity [20] requirement, we adopted a tiered, cradle-to-gate life-cycle inventory (LCI) of the flow ”chemical factory, organics” from Ecoinvent v3.11 as a representative model of the infrastructure required by our production system. We used the tiered exergetic life-cycle inventory aggregator [10] to compile and disaggregate all upstream inputs from such an item to have access to the $\mathbf{B}^{(nr)}_{\text{chemical,factory}}$ and $\mathbf{E}^{(em)}_{\text{chemical,factory}}$. According to our green ammonia plant size and to the chemical engineering six-tenths thumb-of-rule, we adopted a scale factor of 0.1 related to the original size of Ecoinvent’s infrastucture item to appropriately represent our facilities size. Next, by using an iterative adaptative Leontief algorithm to evaluate all required items from ”chemical factory, organics” and its upstream flows, we obtained a list of 580 products required by upstream processes to build such an infrastructure. These involve chemicals, raw materials, fossil fuels, intermediate infrastructures and other item types associated with the supply chain. We used cradle-to-gate inventories of EcoInvent v3.11, CarbonMinds and literature papers to build this dataset and to properly account for circularity issues. Details are left out of the scope of this paper.

3.2. Operation phase - exergy costs disaggregation and irreversibility backpack

Figures 5 show the disaggregated exergy cost of product (ExCoP, ammonia + co-products in this case) values (and its levelized value), that is, the exergy costs divided by resource type for the electricity grid and hybrid solar PV + wind electricity scenarios. These values represent normalized values of exergy consumption from the first 17 natural sources dimensions and the soil exergy (17-D of $\mathbf{B}_r^{(nr)}$ + soil exergy). Such an approach highlights the differences between the exergy costs of the chemical facility obtained from the grid and from 100% renewable sources. The electricity grid is defined by the IEA net-zero emission (NZE) scenario [21] between 2025 and 2050, that is, it assumes there is a hard decarbonization of the global electricity production. This is noticeable by the initial hard cumulative fossil fuel contribution (coal, natural gas, oil, and nuclear) and the renewable energy supply transition (solar, wind, hydro and biomass) on the overall ExCoP. The exergy costs of other materials is low here because the materials are basically used for the chemical facility infrastructure. On the other hand, renewables predominate the both metrics overtime, since the renewable electricity is used over the 25 years during operation stage. Soil exergy has increased importance here due to the land occupation by renewables.

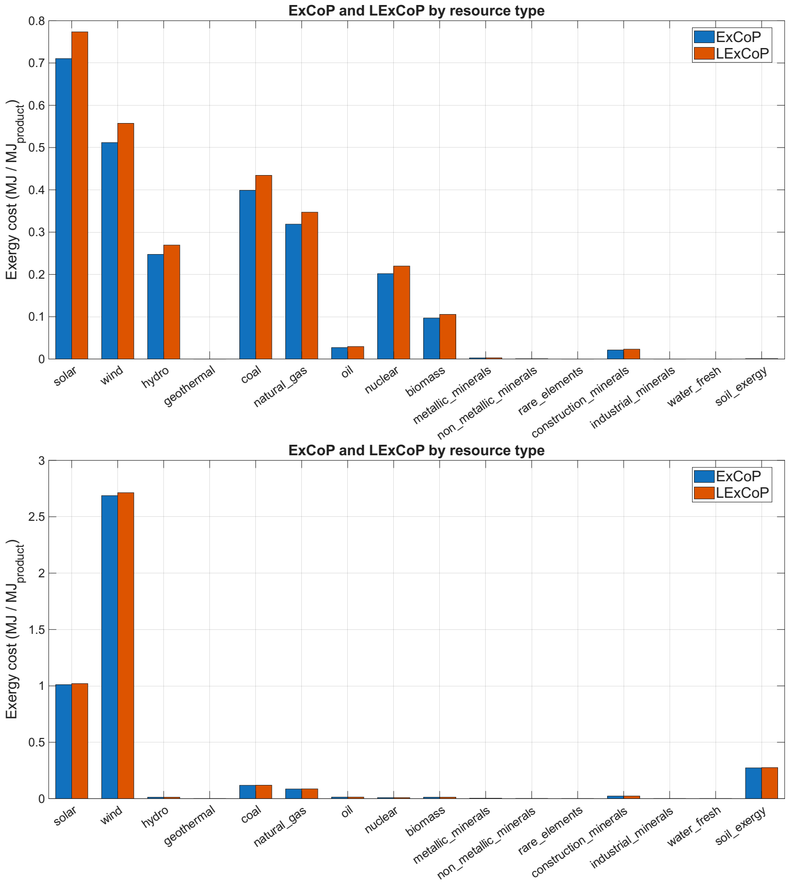

Figure 5: Exergy cost of products of the electricity grid and hybrid renewable electricity-scenarios for the lifetime green ammonia plant in study based on the thermodynamics of sustainability framework.

Figure 6 presents the irreversibility backpack concept for both cases: from a thermodynamic origin (a), (b) by life-cycle stage, and (c) by the 5-scope backpack. By analyzing the thermodynamic origin, fossil fuel origin presents a significant influence on the grid case, whereas soil exergy overcomes the fossil fuel influence by becoming the second most important consumed natural resource on the hybrid's case lifetime. However, topsoil has been mostly disregarded on environmental assessment analyses; especially on exergy-based analyses (they are not even accounted for). Such a result therefore sheds a light on the importance of including topsoil exergy accounting and remediation efforts required for their regeneration. By analyzing the life-cycle stage perspective, the operation phase naturally predominates on both pathways (values over 10^4 TJ), but it is clear the importance of the building/ commissioning phase (close to 10^3 TJ), especially under a world where material scarcity and criticality, energy footprint, and importance of material origins are of fundamental importance in any production process. The maintenance phase comes next (around 10^2 TJ), but its value could be significantly great depending on the complexity of components replacement (we adopted an alkaline electrolyzer, but we could have adopted a proton-exchange membrane eletrolyzer with high CRM dependency). Finally, even though the decommissioning phase represents the lowest value among those discussed here (lower than 10^2 TJ), it is responsible for allowing mostly material recovery for second-life applications, therefore it plays a fundamental role under a circular economy perspective. Finally, by analyzing the 5-scope backpack, even though the grid scenario presents significantly lower irreversibility backpack (12000 versus 20000 TJ), its renewability is lower (the weight of renewable energy sources when compared to the overall exergy requirements, Fig. 5) and its product + scope 1 (direct process) irreversibility back is approximately equivalent to the hybrid scenario. The difference lies on the scope 2 (energy sources) and 3 (raw materials and supply chain) required by the hybrid scenario: it requires more material extraction and energy transformations through the supply chain, whereas the grid case takes advantage of its scalability and assumes a hypothetical, very optimistic energy transition scenario that will mostly turn grid electricity as mainly renewables dependent.

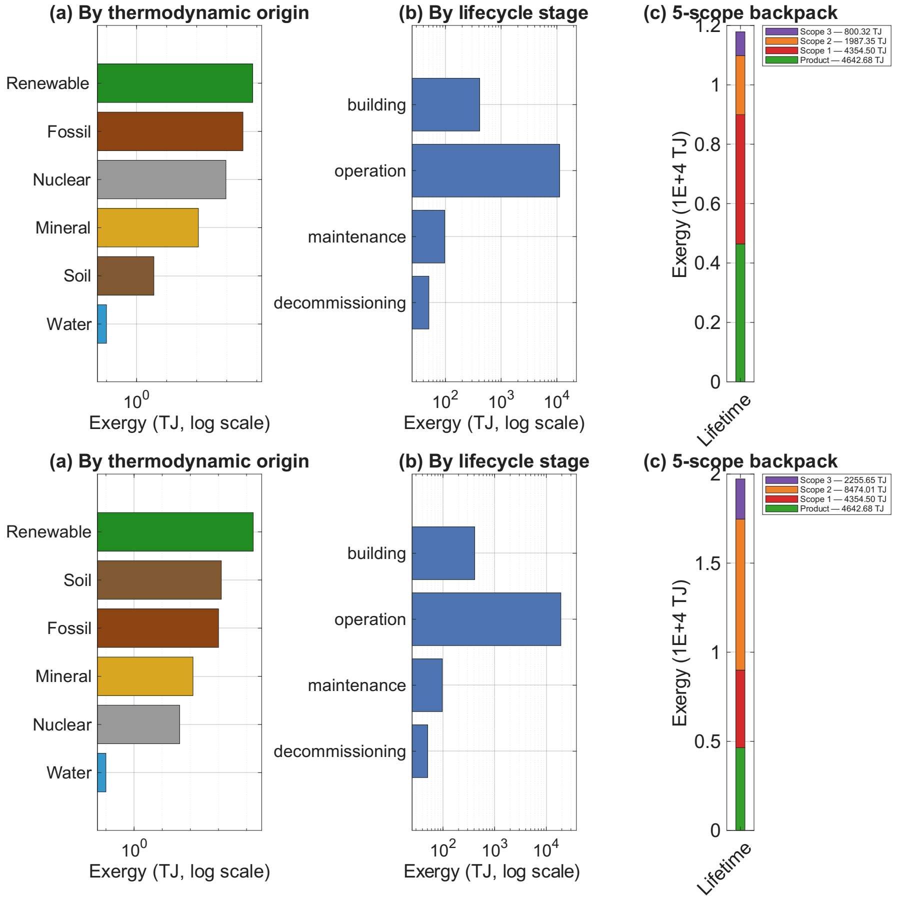

Figure 6: Irreversibility backpacks of electricity grid and Hybrid renewable electricity-scenarios for the lifetime green ammonia plant in study based on the thermodynamics of sustainability framework.

3.3. Grassmann diagrams under a thermodynamics of sustainability perspective

In order to present a more traditional, energy systems-based view of our results, Fig. 7 present Grassmann diagrams from natural resources (L1), life-cycle stages (L2) and destinations (L3). It is clear the exergy flow differences among the product (”useful” exergy under this perspective) and scopes 1-3 (process irreversibilities, upstream energy and material embodied exergy). Scope 1 covers lost topsoil exergy (indirectly related to the operation phase here) and other cumulative process irreversibilities, whereas scope 2 accumulates the process (direct) and supply chain (indirect) energy usage and transformations for all productive processes in study. Scope 3 encompasses the building, maintenance and decommissioning phases.

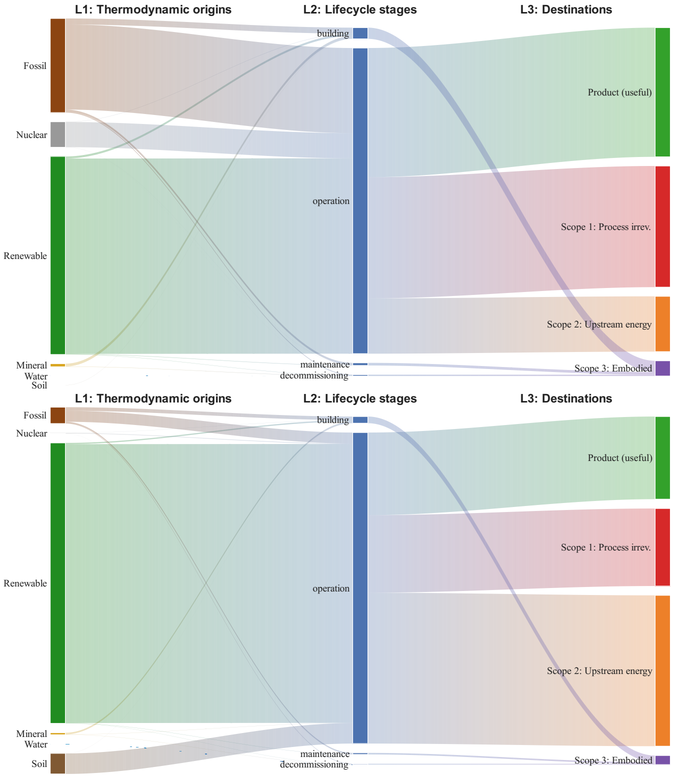

Figure 7: Grassmann diagrams of electricity grid and hybrid renewable electricity-scenarios for the lifetime green ammonia plant in study based on the thermodynamics of sustainability framework.

3.4. Framework’s overall capacity, current limitations and future work

Based on the results previously analyzed, when we adopt a different pathway to the production of such a fundamental chemical as ammonia, we are basically doing a natural resources tradeoff involving land, water, electricity, and materials (environmental burdens) with economic cost. Such a perspective agrees with a previous planetary boundary analysis [22] of different ammonia production systems. Here we highlighted similar conclusions, but with the usage of the irreversibility backpack. This novel concept sheds a light as planetary boundary analyses and ToS have an interesting link and together have a strong potential to become an important second-law based tool to real, multi-criteria problems. In addition, ToS was developed with industrial ecology, second-life production systems, circular economy and industrial symbiosis perspectives in its core: its overall structure and data traceability allows for full disclosure of natural resources, recycled materials and co-products information, thus creating a fair base for comparison of pathways to produce certain products on different locations of economy’s supply chain (e.g., H_2 from natural gas, water electrolysis, natural origins, pyrolysis, and biomass-based).

However, the ToS framework initially presented on this paper and on [10] is still in development;

there are several aspects that need to be covered as future work in order to reach all its aforementioned goals. For example, the 22D resource and 26D emission tensor already link such a framework with scopes-4 and 5 variables (scarcity creation, ore-grade-dependent exergy replacement) and 5 (planetary-boundary-weighted remediation). But these still need proper validation and thorough data collection and therefore will be presented in a future work. Other aspects involve adopting exergy-based Monte Carlo sensitivity analysis across the life-cycle of a product, developing a basis for ToS dynamic analysis (timely analysis accounting for production variability according to the modeler's data availability), proper flexibility for either micro (components, specific processes, industries) or macro (regional, national, global) analyses, according to the required scope, scalability (inclusion of scalar size effects to properly adjust production to systems size). Finally, two fundamental aspects that still need to be addressed by a ToS perspective are: the current processes and residues irreversibilities disassociation with the planetary boundaries and the local-environment exergy evaluation (inclusion of local-based effects on spatiotemporal reference environment evaluation, especially for critical raw materials, water, biodiversity and soils) we should refer to resources for their local availability and categorize those that come from other places.

4. CONCLUSIONS

In this work, the authors presented thermodynamics of sustainability, a novel framework that develops on the works done for more than 40 years of research in the areas of thermodynamics and sustainability/environmental analyses and expands them by linking all supply chain of natural resources, raw materials, products and residues of our society associated with nature under a second-law of thermodynamics viewpoint. Novelties include a dynamic, spatiotemporal approach to evaluate the exergy-based, physical costs of producing any product from any general production system during their life-cycles, besides inclusion of exergy costs of all materials, infrastructure, land and soils, water; anything that is actually required for the production system to operate.

The future inclusion of local-based reference environments, and both natural resources replacement (or scarcity creation) and residues abatement costs naturally moves into the direction of total sustainability, a fundamental aspect for both nature and human's current and future generations.

System-wise, preemptive studies involving load control optimization by dynamic analyses and mixing of hydrogen sources should be further investigated to mitigate significant non-renewable exergy footprint. For a global perspective, alternatives between sustainable agriculture, renewables production (by land occupation and transformation) and biodiversity work should benefit the overall exergy consumption of a renewable ammonia plant without wasting non-renewable natural resources.

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