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Novel flexible-integrated thermodynamic computational tools for advancing the thermodynamics of sustainability framework

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Abstract:

The distinct global transitions the world currently faces present unprecedented challenges in understanding the true physical costs of deploying newer technologies at scale over their lifespans. Renewable energy, hydrogen, sustainable chemicals production are examples of such a problem that requires proper integration of physical, environmental, economic and social perspectives. This poster presents the thermodynamics of sustainability framework, a novel, comprehensive, beta-phase, exergy-based computational framework that integrates exergy analysis with cradle-to-cradle life-cycle assessments (LCA) and other exergy-based methods for general production systems at any stage of the economic supply chain. It was idealized after a thorough literature review on papers related to sustainability, thermodynamics, LCA, material flow analysis, geological, ecological and biological systems, etc. First, the tiered life-cycle inventory (LCI) aggregator program builds and aggregates LCIs at full disclosure using exergy as the unified metric by minimizing losing previous information about all inflows and outflows with automatic handling of multi-output processes and complete natural resources and emission tracking. Then, the life-cycle exergy analysis of general productive systems program features a prospective dynamic (time-based) evaluation of all physical costs required by such a production system during its pre-operation, operation, and end-of-life phases to evaluate its overall lifetime performance; all of which under the ecosphere's perspective. Lastly, the integrated exergy calculator evaluates the overall exergy of complex materials and products in our economy by combining all exergy types with cradle-to-gate cumulative exergy demand for local and global reference environments, levelized exergy replacement and remediation costs for natural resources scarcity creation and environmental harm emitted to a specific reference environment, respectively. This framework presents a first-of-its-kind perspective of integrating exergy-based, system-level LCIs with local and global perspectives, enabling a thermodynamically rigorous comparison of production system technologies under a dynamic viewpoint, with direct association of exergy costs with natural resources depletion/scarcity creation and irreversibilities links with each one of Rockström's planetary boundaries.

Keywords:

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

1. Introduction

The global production system has undergone fundamental transformations via three different transitions: energy, digital and ecological. To deal with the climate change and decarbonization requirements, both the International Energy Agency (IEA) Net Zero Emissions (IEA-NZE) $1.5°C$ energy transition pathways project global renewable electricity generations of 90% by 2050 [2]. However, these require us to change our fossil-fuel, direct consumption energy technology perspective to a material-intensive one, causing great consumption of critical raw materials (CRM). The current digital transition also affects these pathways, with AI insurgence and data centers infrastructure commissioning requiring even more resources, presenting a scenario where this sector will become the highest natural-resource (and electricity) consumer of our society [3,4].

In parallel, both the energy and digital transitions must be in agreement with the most urgent transition of all: the ecological one. The most scientifically accepted and diffused sustainability theory is the planetary boundaries theory [5]; the one that currently presents 9 tipping points that our society should not overcome if we intend to survive in a safe operating space as we have done throughout most of our history (i.e., *pre-anthropocene* period). However, our society has already surpassed 6 of them, named climate change (CC), biosphere integrity (BI), land system change (LSC), freshwater change (FWC), biogeochemical flows (BGC) and novel entities (NE), which has caused irreversible changes in Earth's functionality. Dealing properly with these boundaries while managing our way of living is a very difficult challenge. A representative example is found in the ammonia production sector [6], where even when we adopt state-of-the art, lowest-carbon ammonia production routes, these present natural resources/residues tradeoff issues between some of the planetary boundaries (CC *versus* FWU *versus* BGC *versus* LSC *versus* ocean acidification). Therefore, in order to change this perspective, we need to include on the development of novel production systems' conceptual and detailed plans (theory) and operation (practice) a multidimensional (physical, economical, ecological, social) perspective that covers all their lifetime phases. A significant gap found on the literature, however, is the lack of works using the second law of thermodynamics/exergy analyses to bound irreversibilities (called here the irreversibility backpack) with natural resources, raw materials, products, and residues with all planetary boundaries; all of which under the planet's (ecosphere's) perspective. The methodology presented here is a primary step to reach such a goal.

The aforementioned issues linking nature, economy, human footprint and sustainability are not new. Actually, it had already been conceptually established before early 2000's and even associated with the second law of thermodynamics. Nicholas Georgescu-Roegen's concept of irreversibility [7] focuses on the idea that economic processes, like all natural processes, are fundamentally irreversible due to the laws of thermodynamics. This idea led him to postulate the so-called ”fourth law of thermodynamics”, extending the concept of entropy to materials, since if matter also undergoes qualitative degradation, the consequence is so far-reaching that it imposes absolute limits on economic growth and sustainability. Thus, the inherent tendency towards entropy (increase in disorder) makes true reversibility impossible in reality. Even though this material perspective is actually included on the second law, Georgescu-Roegen's work emphasizes 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 and emphasizing the struggle between circular and spiral economy models of our society.

In order to cover some gaps found on the literature, the authors developed a macro (ecosphere)-micro (productive process, technosphere)-macro (emissions, to ecosphere) viewpoint of the economic process of our planet and society through the lens of the second law of thermodynamics. To the best of our knowledge, no references cover a physics-based, dynamic, local-based reference environment thermodynamic approach that also includes natural resources reposition and residues remediation/abatement physical costs at local and global scales. So, the ”thermodynamics of sustainability” (ToS) framework intends to create a link between a second law-based methodology with natural resources and raw materials supply chain, production processes and their residues, and the current 9 planetary boundaries [8] while accounting for the environmental changes on local environments.

On the next sections, we sequentially present a simplified literature review, the ToS fundamentals and its overall structure. Then, we position it in relation to other methods found on literature through a 17-criteria comparison and propose actions (some already in course) to turn this novel framework already operational.

2. Literature review

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 simplified literature review. The analyzed references, even though do not cover all spectrum of methods available on specialized literature, provided us a starting point to begin establishing the fundamentals of the thermodynamics of sustainability framework. We split them in some clusters (which are not necessarily exclusive) in what their contributions highlight the most: exergy cost theory and thermoeconomics (foundational); exergy history, fundamentals, and reviews; exergy and environmental impact/sustainability link; cumulative exergy methods (cumulative exergy demand (CExD), cumulative exergy extraction from the natural environment (CEENE), cumulative exergy consumption (CExC), thermoecological cost (TEC)); exergetic life-cycle assessment (ELCA/ExLCA); exergoenvironmental analysis; extended exergy accounting (EEA) and societal analysis; mineral sources, thermodynamic rarity and exergy replacement costs (ERC); renewable energy, energy transition and fleet analysis; hydrogen and green fuels; emergy analysis; ecological cumulative exergy (ECEC) and emergy-exergy bridge; eco-exergy and ecosystem thermodynamics; land, water and ecosystem Services in LCA; planetary boundaries and total sustainability; societal exergy analysis and macro-scale; integrated/multi-tool approaches; manufacturing and industrial processes; circular economy and material flows; LCA general methodology and reviews; sustainability indices and general reviews.

The list presented here is not exhaustive; we only present a part of the references related to this topic. All the references adopted for such a comprehensive review are publicly available on page of our research group [9]. The ToS fundamentals are compared to them based on the following criteria: thermodynamic foundation (resource metric, reference environment, substance scope, exergy quality differentiation), system boundaries & dynamics (temporal treatment, spatial differentiation, scale of analysis, technology evolution, material/infrastructure accounting), impact & remediation accounting (environmental impact handling, remediation cost quantification, infrastructure feedback loop, planetary boundary coupling), implementation & applicability (computational implementation), integration level (nE classification, i.e., analytical dimensions integrated, energy, exergy, environmental, economic, ecological, equity/social, evolution).

All papers were then analyzed with a mixed human-AI approach for a structured review and comparison. First, *NotebookLM* collected the following data to build a structured review of each paper in a markdown (.md) format covering following features: citation (authors, year, title, journal), core claim in 1-2 sentences (what is the paper's main argument or contribution?), methodology (what approach do they use?), reference environment (which reference state do they use?), temporal scope (static snapshot or dynamic? What time horizon?), spatial scope (global average, regional, local, site-specific?), key data/results (the 2-3 most important quantitative findings), stated limitations (what do the authors themselves say they could not do?), figures/diagrams of note (briefly describe any key figure that carries essential information not in the text).

Next, another mixed human-AI approach used a combination of AI agents *Cursor 3.0* (AI agent specialized in programming) and *Anthropic Claude Opus 4.6* for building a standalone AI-agent fed with information only from the previously selected papers to build a specialized, thorough literature review analyzer. We combined the structured summaries on the previous step with each full-sized paper to compile thematic-based information about the following: core claims of the field; shared assumptions and clusters categorization; positions and direct contradictions among the papers; citation chain and intellectual lineage; research gaps identification and unanswered questions; supporting pillars.

The thermodynamics of sustainability framework presented next is therefore compared to these consolidated methodologies.

3. Thermodynamics of sustainability fundamentals

Several production systems analysis methods have been developed since the 20th century; each one with its own perspective and priority (physical, technical, economic, environmental, societal, etc.). Figure 1 presents the schematic diagram of the thermodynamics of sustainability framework, whose goal is to establish second law-based, multidimensional links between natural resources and raw materials supply chain, production processes and their residues, and the current 9 planetary boundaries; all of that while accounting for the environmental changes on local environments. This framework is a physics-based, cradle-to-cradle, 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. A novel concept called irreversibility backpack is associated with the three criteria presented below on Fig. 1: natural resources depletion (or scarcity creation), raw materials and energy consumption and residues degradation caused on the environment and associated with each of the planetary boundaries.

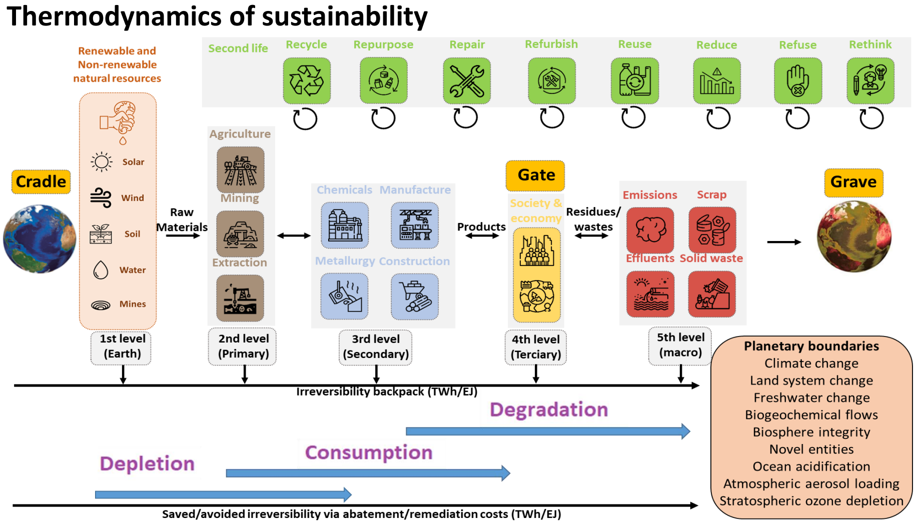

Figure 1: Schematic diagram of the thermodynamics of sustainability framework.

Figure 2 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, named 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 are also accounted here. We adopt a multi-layer framework with bidirectional transfer matrices between each of these layers to create a robust traceability framework using exergy as the variable of interest to split the information line between natural resources, raw materials and products, and emissions with each of the planetary boundaries.

The irreversibilities associated to a product production process are presented under five different scopes: direct process, energy supply, supply chain, natural resources scarcity creation and residues remediation. These links are represented by dimensions of the irreversibilities created throughout the supply chain of a product; when these are grouped up together, they represent the ”irreversibility backpack” of a product, that is, all disaggregated cumulative irreversibilities generated during the production of anything (materials or energy streams, objects, infrastructures, etc.) and the respective environmental harms (either directly or indirectly) caused by it (Fig. 3). Through the irreversibility backpack concept, the proposed ToS framework will allow to answer multidimensional, difficult questions, such as ”How can we fairly compare hydrogen’s different production pathways, each one with its own origin (natural-gas *vs.* coal *vs.* chemical feedstock *vs.* water electrolysis *vs.* biomass *vs.* natural), requiring different natural resources, technosphere products and infrastructures and producing different residues? A possible solution, based on ToS fundamentals, is to adopt an exergy-based,

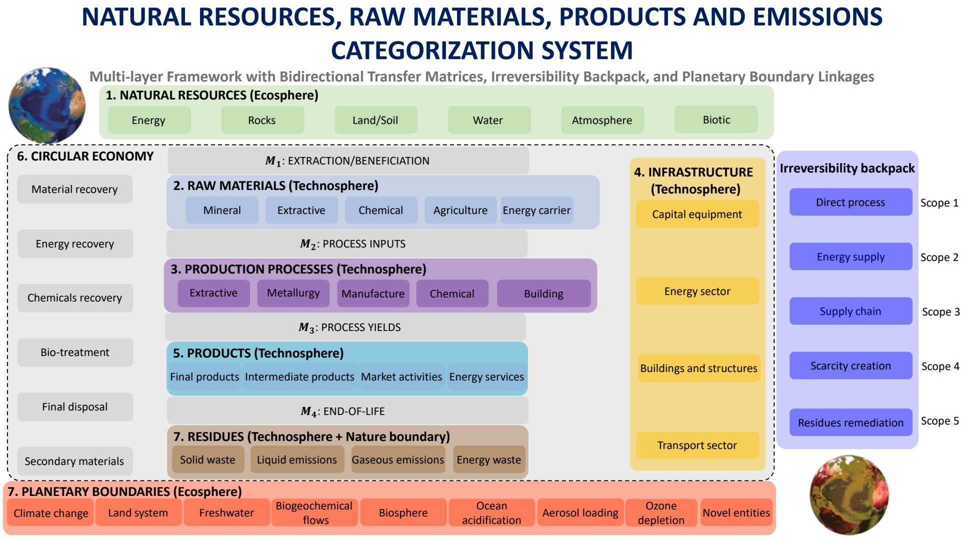

Figure 2: Multi-layer framework for the thermodynamics of sustainability model. The model features bidirectional functional matrices relating the layers among themselves, the irreversibility backpack concept and the exergy-based linkage with Rockström's planetary boundary concept.

five-scope approach (as in Fig. 3) that accounts for H_2's exergy and direct production process irreversibility (scope 1), as well as 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).

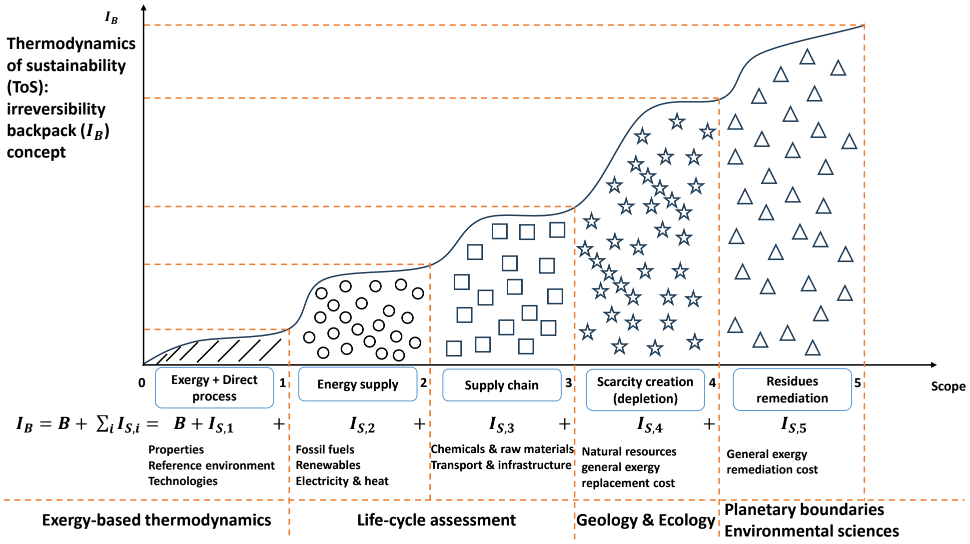

Figure 3: 5-scope thermodynamics of sustainability irreversibility backpack (I_B) concept. Scope 1 refers to exergy-based thermodynamics (stream exergy and direct process irreversibility). Scopes 2 and 3 refer to life-cycle assessments (energy supply sources and the supply chain). Scope 4 refer to geology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

The authors present in this work an initial basis for the fundamentals of the thermodynamics of sustainability.

4. RESULTS AND DISCUSSION

Based on the literature review, some literature gaps between all methods are the following:

- there is no unified framework bridges exergy-based resource accounting with planetary boundary thresholds.

- No dynamic, spatiotemporally resolved exergy cost analysis exists for the full material supply chain of the energy transition.
- Environmental exergy replacement costs have never been systematically computed for non-mineral impacts
- No exergy-based analysis uses geographically varying (local) reference environments for comprehensive resource assessment
- The feedback loop between energy transition, material demand, and resource depletion has not been closed in any exergy-based model

Some references directly highlighted some of these gaps: for example, [12] mentions the central premise that ”sustainability” is a multifaceted concept that requires a multi-dimensional indicator. Earlier, [14] highlights the limitations the limitations of technoeconomics, thermo-economics, ExLCA, thermo-ecological cost, and CEENE methods, emphasizing a need for a better integration among them. Under this context, Tabs. 1-3 summarize the multi-criteria comparison that covers several energy-related methods in literature. Most of the evaluated methods are exergy-based, except those related to the planetary boundaries method.

As noticed, most methods adopt the Szargut reference environment for earth's atmosphere, lithosphere and oceans. Exceptions are ERC with Thanatia, EMG with geobiosphere emergy baseline (GEB) and PBLCA with pre-industrial environmental conditions. However, under the current situation of several planetary boundaries close to (or surpassed) their tipping points, and industrialization on local, abundant natural resources availability (e.g., critical raw materials, water, renewable energy sources, land/soil), issues directly affected by local modifications such as local resources scarcity and residues abatement costs can only be properly evaluated and therefore critically analyzed by exergy if local-based reference environments are adopted. [11] directly mentions the material scarcity and geopolitical limitations of current thermodynamic approaches by not addressing resources criticality. Thus, several methods that adopt global approaches might not represent the whole picture, both physically and environmentally speaking. Without this whole picture, [10] highlights that by not including non-exergetic forms of consumption on the analysis causes exergy blindness to loss of information content, macroscopic structural changes, and geographical distribution changes. Additionally, timely/dynamic analyses are severally restricted by most of the selected methods due to the usage of only static screenshots of production processes - especially when most current processes currently are projected to operate dynamically due to renewable energy sources production variability. Additionally, some methods (LCA, CExD, and ELCA) even consider materials and infrastructures on their evaluations, but lack on including processes and components learning curves and degradation (e.g., electrolyzers), dynamic material footprint timely evolution. [13] sheds a light on the importance of including the critical contribution of ecosystems to industrial activities to not overlook nature's contribution to the exergy supply chain analysis.

Under the presented context, the authors propose the thermodynamics of sustainability mathematical framework under a three-code computational architecture presented next.

4.1. Code 1: Exergy Life Cycle Inventory Aggregator

Code 1 creates aggregated exergy-based natural resources and emission life-cycle inventories for any product in a database. An adaptive Leontief solver input-output model ($\mathbf{x} = (\mathbf{I} - \mathbf{A})^{-1} \cdot \mathbf{e}_j$) works as the mathematical foundation, linking the technology matrix $\mathbf{A}$ of technosphere's supply chain with the unit demand vector $\mathbf{e}_j$ for product j and the resulting activity level vector $\mathbf{x}$ for all processes in the supply chain.

The elementary flows associated with each active process are then mapped to two standardized vectors: a 22-dimensional (22D) natural resource vector and a 26-dimensional (26D) emission vector as presented (more details on [15]). The former vector covers nine primary energy categories, six

Table 1: Master comparison table about methodologies relating thermodynamics with sustainability/sustainable development: **Thermodynamic Foundation, System Boundaries & Dynamics** . Methods: CED, ExA, CExD, CEENE, ELCA, ECT, ERC, TEC, SPECO, ExEnv, EMG, PBLCA, LExC, ToS.

Criterion no.	1	2	3	4	5	6	7	
Method	Resource metric	Reference environment	Substance scope	Exergy quality	Temporal	Spatial	Scale	Te
CED	Energy	N/A	Energy carriers	N/A	Static	Global	Product	
ExA	Exergy	Szargut	Energy carriers	Chem. + phys.	Static	Global	Component	
CExD	Exergy	Szargut	All abiotic	Chem.	Static	Global	Product	
CEENE	Exergy	Szargut	All abiotic	Chem.	Static	Product	Product	
ELCA	Exergy	Szargut	All (incl. land, water)	Chem. + phys.	Static	Product	Product	
ECT	Exergy	Szargut	All abiotic	Chem. + phys.	Static	Global	Plant	
ERC	Exergy	Thanatia	Minerals + fossils	Chem. + conc.	Static	Global	Mineral reserves	
TEC	Exergy	Szargut	All abiotic	Chem. only	Static	National	Product/sector	
SPECO	Exergy	Szargut	Energy carriers	Chem. + phys. + kin	Static	Global	Component	
ExEnv	Exergy	Szargut	Energy carriers	Chem. + phys.	Static	Global	Component	
EEA	Ext. exergy	Szargut	All + labor/capital	Chem. + phys.	Static	Global	Ecosystem	
EMG	Emergy	GEB	All + ecological	Solar equiv.	Static	Global	Ecosystem	
PBLCA	Impact units	Pre-ind.	All (85 flows)	N/A	Static	Regional	Product	
LExC	Exergy	Szargut	All abiotic	Chem. + phys.	Dynamic	Global	Fleet/sector	Le
ToS	Exergy	Local-varying	All	Full (all)	Dynamic	Local	Fleet + product	D

Table 2: Master comparison table about methodologies relating thermodynamics with sustainability/sustainable development: **Infrastructure, Impact & Remediation Accounting**.Methods: CED, ExA, CExD, CEENE, ELCA, ECT, ERC, TEC, SPECO, ExEnv, EMG, PBLCA, LExC, ToS.

Criterion no.	9	10	11	12	13
Method	Material/infrastructure	Env. impact	Remediation cost	Infra. feedback	PB coupling
CED	N/A	N/A	N/A	N/A	N/A
ExA	N/A	N/A	N/A	N/A	N/A
CExD	Static inv.	N/A	N/A	N/A	N/A
CEENE	Static inv.	N/A	N/A	N/A	N/A
ELCA	Static inv.	Zero-ELCA	Conceptual	N/A	N/A
ECT	N/A	N/A	N/A	N/A	N/A
ERC	Mineral only	N/A	Minerals only	N/A	N/A
TEC	Static	Compensation	Conceptual	N/A	N/A
SPECO	N/A	N/A	N/A	N/A	N/A
ExEnv	Construction LCA	Component-allocated	N/A	N/A	N/A
EEA	N/A	Remediation	Fictious process	N/A	N/A
EMG	N/A	N/A	N/A	N/A	N/A
PBLCA	N/A	LCIA CFs	N/A	N/A	Native
LExC	Learning + feedback	25D-emissions	N/A	Partial	N/A
ToS	Dynamic fleet and Self-consistent	Exergy-based	Full (scarcity + environmental impact)	Self-consistent	Integrated

Table 3: Master comparison table about methodologies relating thermodynamics with sustainability/sustainable development: **Implementation, Applicability & Integration Level**. Methods: CED, ExA, CExD, CEENE, ELCA, ECT, ERC, TEC, SPECO, ExEnv, EMG, PBLCA, LExC, ToS..

Criterion no.	14	15	16	17	-
Method	Implementation	Co-products	Ecosystem services	nE class	Dimensions
CED	Ecoinvent	N/A	N/A	1E	E1
ExA	Spreadsheet/code	N/A	N/A	2E	E1,E2
CExD	Ecoinvent	Ecoinvent default	N/A	2E	E1,E2
CEENE	Ecoinvent	Ecoinvent default	Land + water	2E	E1,E2
ELCA	Case-by-base	Single method	N/A	2-3E	E1,E2 (E3)
ECT	Code	Single method	N/A	3E	E1,E2,E3
ERC	Tables	Single method	N/A	3E	E1,E2,E3
TEC	Code	Single method	Natural restoration	3E	E1,E2,E3
SPECO	Comercial (EbS)	SPECO rules	N/A	3E	E1,E2,E4
ExEnv	Case-by-case	Single method	N/A	3E	E1,E2,E3
EEA	Code	Single method	N/A	5E	E1,E2,E3,E4,E6
EMG	Code	Emergy algebra	Full ecological	3E	E1,E2,E5
PBLCA	Prototype	N/A	Land/biosphere	2E	E1,E3
LExC	Code	System exp.	N/A	4E	E1,E2,E3,E7
ToS	Code	Multi-method + sensitivity	NPP-based (planned)	5-6E	E1,E2,E3,E5,E7

material categories and four environmental categories, including conversion to topsoil exergy [16] . The 26D emission vector covers eight air emission categories, six water emission categories and five waste categories.

A key technical challenge is that real LCI systems frequently exhibit spectral radii ($\rho(\mathbf{A}) \geq 1$) due to unit heterogeneity, strongly connected components (circular supply chains), and physical conversion factors exceeding unity. To address this, Code 1 implements an adaptive Leontief solver that automatically selects among direct inversion, truncated power series, and an iterative minimal damping algorithm.

To further manage the complexity of large supply chains, Code 1 implements a tiered aggregation framework. Products are aggregated in phases, bottom-up: raw materials first (e.g., clay, limestone, sand), then basic processed materials (e.g., cement, clinker), then intermediate products (e.g., steel, glass), then energy carriers (e.g., electricity, diesel), and finally target products (e.g., solar panels). Each phase adds up its aggregated 22D+26D vectors into the database, effectively breaking circular dependencies and reducing the spectral radius for subsequent phases. The aggregation pipeline produces, for each product, a complete traceability package including the supply chain composition, per-process resource contributions, an eight-layer process classification such as presented on Fig. 1 (natural resources, raw materials, production, energy/utilities, products, infrastructure, emissions/waste, planetary boundaries), and data for Sankey/Grassmann flow visualization.

4.2. Code 2: Production System Exergy Cost Evaluator

Code 2 evaluates the exergy cost of any production system across its complete lifecycle, from resource extraction to decommissioning. Its main goal is to be applicable to any production process: from traditional systems for thermodynamic analyses, such as thermal or chemical plants, mining, manufacturing, renewable electricity production, transmission and storage, water transport, desalinization and treatment, to uncommon and new applications, such as datacenters, residue treatment and abatement, agriculture and biological systems, biomass systems, etc.

Each lifecycle production system structure is decomposed into nine discrete stages: (1) extraction of raw materials, (2) refining, (3) manufacturing of components, (4) transport, (5) building/construction, (6) operation, (7) maintenance, (8) waste treatment, and (9) decommissioning. Each stage carries a 22D resource array and a 26D emission array using the same shared taxonomy as Code 1. More details about this model are presented on [15].

4.3. Code 3: Total Exergy Calculator

Code 3 is designed to compute the total exergy of any substance from its elemental composition, enabling two capabilities that the current framework lacks: (a) exergy-based allocation in Code 1's multi-output process handling (replacing the current mass-based default with thermodynamically consistent allocation factors), and (b) local and dynamic reference environment computation.

For any substance with known elemental composition, Code 3 will compute the standard chemical exergy using either Szargut's reference environment (298.15 K, 1 atm, specified atmospheric, oceanic, and crustal composition) or a local reference environment. The calculation follows established thermodynamic procedures: standard Gibbs free energy of formation corrected for the chemical potential of each element in the reference environment. A database of 1,400+ pre-computed standard chemical exergy values [17] will provide lookup capability, with proper computation for substances not in the database.

The primary innovation planned for Code 3 is the parameterization of the reference environment as a function of geographic location and time. Rather than assuming a single global dead state, Code 3 will compute how chemical exergy values change under local conditions: temperature T_0, pressure p_0, atmospheric composition (urban vs. rural vs. industrial), crustal composition (geological province) and water availability. Under this generalization, Szargut's standard environment and Valero's Thanatia become special cases — the former corresponding to global average conditions and the latter to a hypothetical fully depleted Earth. This enables spatially resolved exergy cost comparisons: the same product manufactured in different regions will have different exergy costs reflecting genuine differences in local thermodynamic conditions and resource concentrations.

4.4. Limitations and Future Work

The thermodynamics of sustainability is a novel and under-development method that presents a dynamic, multidimensional, flexible, physics-based evaluation of the true thermodynamic costs to the economy and society currently operates, and potential consequences to future generations. The current state of this work naturally presents limitations. Some of these are mentioned next: continuous code architecture improvement for a general, dynamic exergy costs evaluation of natural resources and abatement costs of emissions; local-based reference environments, especially under the context of critical raw materials, renewable energy sources and local environmental impacts, where local availability impacts local exergy of natural resources, scarcity creation and residues environment impact; thorough quantitative comparison for all listed (and complementary) methods for a base-case example or benchmark by checking their multidimensional coverage, advantages and drawbacks for a physics-based total sustainability; method validation with both traditional and modern applications of energy-material-water nexus.

5. Conclusions

Thermodynamics of Sustainability is the first exergy-based framework to simultaneously integrate dynamic fleet analysis, environmental remediation costing with planetary boundary coupling, local reference environments, ecosystem-level resource accounting, and self-consistent infrastructure feedback — achieving a 5E integration where no existing method exceeds 4E with comparable operational comprehensiveness.

The physical reality of increasing extraction costs connects to a deeper-level insight: the spectral radius of the global circular economy represented by the bidirectional functional matrices is a representative proxy of the thermodynamic interconnectedness of all production systems (and naturally, human economy). As resources become scarcer and extraction costs increase, the circular dependencies intensify, thus affecting the possible degree of total sustainability we can achieve with Earth. Therefore, such a novel approach is required to estimate the physical costs of obtaining natural resources, raw materials, chemicals, products and residues, and to highlight possible pathways to be prospected to us to achieve a realistically, physics-based sustainable society. The proposed framework will highlight the following features: renewable x non-renewable energy sources; bio-based x critical raw materials; a second-law based comparison between the same product obtained from different pathways on different stages of the economic supply chain. For example, either directly from the ecosphere (natural H_2), or at intermediate stages of the technosphere (natural-gas-, water-electrolysis and fermentation-based H_2), and at the end boundary of technosphere/ecosphere (MSW-based H_2); 5-scope renewability criteria; circular economy x spiral economy (exergy-based circularity ratio); local (natural resources depletion and scarcity creation) and global environmental effects (planetary boundaries).

In conclusion, in order to see the real impact of a stream categorized as an emission (or a waste) to a local environment, one needs to check not only its cumulative exergy demand/exergy cost (which describes this stream's "history"/origin), current exergy (which describes its potentials regarding the environment), but also the permanent changes it causes to the environment with respect to the original one (before the emission). On the same page, a natural resource extracted from the ecosphere, if it is to be considered available in the future, could not only take into account either its exergy (physical, chemical, concentration, and other properties, e.g., radioactive or electromagnetic) or its increasing cumulative exergy demand/cost, but also its local exergy reposition costs. These fundamentals can guide us to the most sustainable and physically achievable pathway to keep the current supply chains sustainable, safe, and healthy for future generations.

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References

[1] International Energy Agency. *World Energy Outlook Special Report Energy and AI.* International Energy Agency; 2025. Available at: `www.iea.org/terms`.

[2] International Energy Agency. *Global Energy Review 2025.* International Energy Agency; 2025. Available at: `www.iea.org`.

[3] de Vries-Gao A. *Artificial intelligence: Supply chain constraints and energy implications.* Joule 2025:101961.

[4] O'Donell J., Crownhart C. *We did the math on AI's energy footprint. Here's the story you haven't heard.* MIT; 2025.

[5] Richardson K., Steffen W., Lucht W., et al. *Earth beyond six of nine planetary boundaries.* Science Advances 2023;9(37).

[6] D'Angelo S.C., Cobo S., Tulus V., et al. *Planetary Boundaries Analysis of Low-Carbon Ammonia Production Routes.* ACS Sustainable Chemistry and Engineering 2021;9(29):9740-9749.

[7] Georgescu-Roegen N. *The Entropy Law and the Economic Process.* Harvard University Press; 1971.

[8] Ryberg M.W., Owsianiak M., Richardson K., et al. *Development of a life-cycle impact assessment methodology linked to the Planetary Boundaries framework.* Ecological Indicators 2018;88:250-262.

[9] Lima, A, Valero, A., Valero A. *Referencias termodinamica de la sostenibilidad* Research Institute for Energy and Resource Efficiency of Aragón (Institute Energaia); 2026. Available at: `https://energaia.unizar.es/referenciastermodinamicadelasostenibilidad`.

[10] Connelly L., Koshland C.P. *Exergy and industrial ecology—Part 1: An exergy-based definition of consumption and a thermodynamic interpretation of ecosystem evolution.* Exergy, An International Journal 2001;1(3):146-165.

[11] Finnveden G., Arushanyan Y., Brandão M. *Exergy as a Measure of Resource Use in Life Cycle Assessment and Other Sustainability Assessment Tools.* Resources 2016;5(3):23.

[12] Sciubba E. *Exergy and Demography: Present Scenarios and Future Projections.* Energies 2025;18(17):4641.

[13] Hau J.L., Bakshi B.R. *Promise and problems of emergy analysis.* Ecological Modelling 2004;178(1-2):215-225.

[14] Sciubba E. *A possible reconciliation between exergy analysis, thermo-economics and the resource cost of externalities.* Energy 2024;310:132731.

[15] Lima A., Valero A., Valero A. *An exergy-based ecosphere-technosphere-ecosphere lifetime model of general productive systems: A Nicholas Georgescu-Roegen-inspired view.* In: sent to ECOS 2026; 2026.

[16] Valero A., Palacino B., Ascaso S., et al. *Exergy assessment of topsoil fertility.* Ecological Modelling 2022;464:109802.

[17] Michalakakis C., Fouillou J., Lupton R.C., et al. *Calculating the chemical exergy of materials.* Journal of Industrial Ecology 2021;25(2):274-287.