The Exergy of Materials With Application to Societal Exergy Analysis

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Abstract

A single paragraph of about 200 words maximum. For research articles, abstracts should give a pertinent overview of the work. We strongly encourage authors to use the following style of structured abstracts, but without headings: (1) Background: place the question addressed in a broad context and highlight the purpose of the study; (2) Methods: describe briefly the main methods or treatments applied; (3) Results: summarize the article's main findings; (4) Conclusions: indicate the main conclusions or interpretations. The abstract should be an objective representation of the article, it must not contain results which are not presented and substantiated in the main text and should not exaggerate the main conclusions.

Keywords: keyword 1; keyword 2; keyword 3 (List three to ten pertinent keywords specific to the article; yet reasonably common within the subject discipline.)

1. Introduction

The study of raw material extraction and processing is growing in importance at the societal level for at least three interconnected reasons [1]. The first reason is related to *climate change*. The drive to reduce CO_2 and other greenhouse gas emissions is leading to adoption of renewable generation technolgies, electrified end uses, and energy storage. Furthermore, declining ore quality can lead to increased energy consumption (and CO_2 emissions) to extract and process raw materials [2]. These changes require increasing levels of material extraction, especially for copper ore and rare earth minerals. In short, the energy transition will also be a materials transition, and depletion of key material resources may become a long-term concern.

Second, continued *economic growth* implies increasing rates of ore extraction and toxic outflows from mining and processing of minerals such as iron ore, bauxite, manganese, and rare earth metals to support fabrication of products and construction of roads, buildings, and other infrastructure. Expanded mining and processing of materials within the economy requires growing energy consumption and CO_2 emissions associated with those activities.

Third, and in response to the above reasons, many countries maintain lists of *critical materials* that are important, especially but not exclusively, for renewable energy technologies [3,4]. Many critical materials are produced by supply chains whose disruption would

threaten economic or national security. Materials on critical lists focus the attention of governments and researchers.

1.1. Material and energy conversion chains (MCCs and ECCs)

Extracted raw materials are converted to products and infrastructure via supply chains that we call *material conversion chains* (MCCs). Although all processes in societal MCCs consume energy, some processes exhibit high energy- and carbon-intensity, such as steel-making, concrete production, aluminum smelting, and chemical manufacturing.

The energy for material transformation processes is delivered via energy conversion chains (ECCs) that describe the extraction and conversion of energy carriers throughout the economy. An example ECC follows coal from extraction through beneficiation and finally to dissipation as heat in the iron and steel sector.

High-intensity processes like steel-making consume energy for the purpose of upgrading material quality. Iron ore is upgraded to pig iron and later steel with the aid of heat from coal combustion. Aggregate and limestone are combined with cement to make concrete with the aid of heat from fossil fuel combustion. Bauxite is upgraded to aluminum via electricity for electrolysis. Industrial chemicals are produced using heat from methane combustion. In all cases, the quality of material is upgraded (e.g., from ore to steel) while the quality of energy is downgraded (e.g., from coal to heat). Societies trade energy quality for material quality at many points in the economy.

1.2. The exergy of materials and energy

One way to address concerns about critical materials in high-intensity processes is to increase the efficiency of energy-consuming material processing stages. The "efficiency" of a material conversion process is often quantified by material output (in mass units) per unit of energy input (in energy units), e.g. tonnes of iron produced per MJ of coal consumed or tonnes of cement produced per MJ of heat required.[1] Strictly speaking, such efficiencies are *efficacies*, because they are quantified in units of tonnes/MJ and are not unitless. Because different materials are involved (iron and cement), the above two efficacies are not comparable in the thermodynamic sense. To obtain a unitless and comparable efficiency for such processes, both inputs and outputs must be quantified in the same meaningful units. One approach is to quantify both inputs and outputs as exergy.

Exergy is a work quantification of materials and energy expressed in energy units (joules). For materials, exergy is defined as the maximum work that could be obtained from thermodynamic processes that bring a material into equilibrium with a reference environment. Material exergy has four components, each accounting for a different disequilibration relative to the reference environment. Physical exergy accounts for differences in temperature and pressure, with the reference environment typically defined as $T_0 = 298.15$ K and $P_0 = 1$ atm. Chemical exergy accounts for differences in chemical species, with the reference environment characterized by reference substances at reference partial pressures (in the atmosphere) and reference concentrations (in seawater or the crust of the Earth). Concentration (or mixing) exergy accounts for differences in relative abundance compared to the reference environment and represents the minimum work required to separate substances from a mixture. Concentration exergy can be especially relevant at the beginning and end of an MCC for ores and complex products, respectively. Finally, comminution exergy accounts for differences in molecular structure. **** Is "molecular structure" correct? —MKH ****. For energy, exergy is defined as the maximum work that

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[1] A related concept is material productivity in units of \$/tonne (or its inverse material intensity in units of tonne/\$) where \$ are GDP at the national level. See **** add references from Nicolas here ****.

could be obtained from thermodynamic processes that bring the energy into equilibrium with its surroundings.

An important aspect of both the exergy of materials and the exergy of energy is defining the reference environment, a non-trivial task for the calculation of chemical exergy for minerals due to the inhomogeinity of the Earth's crust. To that end, Valero Capilla and Valero Delgado [5] defined *Thanatia*, a theoretical model of the Earth with all minerals and materials dispersed in their most degraded and homogeneously mixed form.

With both materials and energy quantified as exergy (in work units, joules), thermodynamically meaningful and unitless efficiencies can be calculated for intensive processes that trade the exergy of energy for the exergy of materials. For example, the pig iron output of a blast furnace can be quantified as exergy instead of mass, thereby enabling calculation of a unitless exergy efficiency in joules (of pig iron) per joule (of coal).

Quantifying materials and energy as exergy enables calculation of comparable efficiencies of all processes in societal MCCs. With such efficiencies available, hot-spots of inefficiency can be identified and actions taken to improve processes.

1.3. Previous exergy analyses of materials and energy

In recent years, researchers have developed databases of material flows in MCCs at the world and societal levels [6–10]. These MCCs are in mass terms, not in exergy terms.

Members of the Exergy Economics community [11] have assembled datasets of energy-only conversion chains (ECCs) and exergy conversion chains (XCCs) at the societal level in both energy and exergy quantifications going as far back as 1800 [12–15]. Data for these ECCs and XCCs are organized in the **RUVY** matrices of the physical supply-use table (PSUT) framework to describe the movement of energy through society from primary to final to useful stages via energy transformation processes [16,17].

The unified exergy analysis of materials and energy has been applied to the analysis and design of chemical [18], steel [19,20], cement [21], and energy plants [22] to quantify resource efficiency and exergy destruction. At the sectoral level, a unified exergy analysis of materials and energy has been applied to the UK transport sector [23]. Covering the period from 1960–2015, the study quantifies resource productivity by tracking improvements in passenger-kilometres per megajoule (pkm/MJ), which increased from approximately 0.42 to 0.61 pkm/MJ across the period of study.

At the societal level, there are several examples of unified exergy analysis of materials and energy. Carmona et al. [24] quantified the exergy of products (defined as mixtures of substances) as a mean weighted average of the chemical exergies of minerals and metals that compose each product. Carmona et al. ignored concentration exergy (i.e., the exergy of mixing).

Wall and coauthors [25–27] applied a unified exergy-based analysis to assess resource use in Sweden, Japan, and Italy, tracing flows from primary inputs to end-use applications, excluding the exergy flows of non-metals and precious metals. The studies reveal low overall exergy efficiencies (around 20% for Sweden, 21% for Japan, and 23% for Italy) and highlight substantial losses across the material and energy conversion chains. Carmona et al. [24] quantified global resource flows and stocks from 1900 to 2010, from extraction to end-use, including the exergy flows of non-metals, precious metals, and products. During this period, primary exergy use increased from 115 to 903 EJ/year, while useful exergy rose from 9 to 148 EJ/year, with 47% embedded in material goods by 2010. Resource conversion efficiency improved from 8% to 16%. Previous unified exergy analyses of materials and energy at the societal level have lacked process-level detail in characterizing material and energy transformations.

To our knowledge, no previous studies of material conversion chains at the societal level include the concentration exergy (b_c) of inputs and outputs of material and energy transformations. Furthermore, no previous studies have demonstrated application of the PSUT framework to unified exergy analysis of material and energy conversion chains.

1.4. Question, contributions, and structure

All of which raises the question addressed by this paper: *how should unified energy and material conversion chains that extend to products with process-level detail be represented for unified exergy analysis of materials and energy at the societal level?* The answer to this question will inform future efforts to develop datasets for unified exergy analysis of material and energy conversion chains that extend to products with process-level detail at the societal level.

Our approach to answering the question builds upon and improves previous efforts and provides three contributions to the literature. For the first time, we

1. demonstrate a consistent exergy analysis approach for ECCs and MCCs, including chemical and concentration exergies;
2. perform exergy analysis with an example MCC (production of pig iron) using PSUT matrices; and
3. illustrate the interactions between MCCs and ECCs using the **RUVY** matrices of the PSUT framework in a manner amenable to use with existing XCC datasets.

The remainder of this paper is organized as follows: Section 2 documents data sources and methods. Section 3 shows selected results of applying methods to data. Section 4 discusses the results, and Section 5 concludes.

2. Data and methods

Our method for demonstrating a consistent approach for societal exergy analysis along unified conversion chains (BXCCs) is to elucidate mathematical expressions and example calculations in full detail. The mathematical expressions are shown in Section 2.2.2 below. We apply that approach to a unified material and energy conversion chain, following material from natural resource extraction to pig iron production. Data for the example MCC, whose basis is 1000 kg of iron ore, are discussed in Section 2.1 below. Finally, we demonstrate interactions between material and energy conversion chains by developing Physical Supply-Use Table (PSUT) matrices that are amenable to existing energy conversion chain datasets. The process for assembling the PSUT matrices is discussed in Section 2.2.4 below.

We begin by discussing data sources for the example MCC developed in this paper.

2.1. Data

2.1.1. Material Data

Mass ratios and composition for each statepoint in the example MCC come from a variety of sources. Iron ore and coal compositions are representative of pig iron production in South Africa. The exergy of coal is calculated as shown in Kotas [28, Equation C.3]. Coal composition is determined by the coke oven output compositions, given by Kölling [29, Tables 2, 5, 8, and 9], Apicella et al. [30], and Sarna [31, Table 2]. The coke oven mass balance is modeled after Ergul and Selimli [32, Figure 4].

Limestone production compositions and energy inputs are taken from Saidur et al. [33] and Sarna [34, para.3].

2.1.2. Material conversion chain energy requirements

Processes in the example MCC include extraction, hauling, and beneficiaion of iron ore, limestone, and coal; a rotary kiln to convert limestone into quicklime; a coke oven to produce both anthracite and coke oven gas from beneficiated coal; coke oven gas treatment and distribution; and a blast furnace to make pig iron. All of the processes in the example MCC require energy inputs.

For example, limestone and coal beneficiation processes use electricity for grinders and separating machines such as crushers, screens, and pelletizers. Coal and natural gas are used by the coke oven. Gasoline, fuel oil, and diesel are consumed by iron, limestone, and coal ore extraction and the blast furnace.

Information on the direct energy requirements for extraction and beneficiation processes was taken from the Energy and Environmental Profile of the U.S. Mining Industry Ore [35, Tables 4.3-4, 9.2-3, and 2.7] and Jamison et al. [36, Table A3.4]. Information for energy requirements of iron ore hauling was obtained from the University of Cape Town Energy Research Institute [37, Table 8]. Energy inputs to the coke oven and coke oven gas treatment were taken from Carmona et al. [20, Fig. 3] and Kandanevia INOVA [38].

Note that most energy inputs to the example MCC can also be considered as material inputs, including coal, gasoline, diesel, natural gas, and coke oven gas. We treat all energy inputs to the example MCC to be materials, the exception being electricity which we assume to be massless.

2.1.3. Energy conversion chain to supply energy requirements

The direct energy requirements for the example material conversion chain (MCC) are supplied by an energy conversion chain that starts at energy extraction and delivers electricity, natural gas, gasoline, fuel oil, and diesel to material conversion processes. Data for the energy conversion chain is obtained from the Country-Level Primary-Final-Useful (CL-PFU) database, which includes energy and exergy flows for 1960–2020 covering "152 individual countries and 3 rest of world regions, 7 aggregate and 46 detailed sub-sectors, 68 final energy products, and 85 final-to-useful (FU) energy conversion devices" [15, p. 1]. We extract energy conversion chain data for South Africa, one of the countries in the CL-PFU database and for 2013, because a consistent energy conversion chain can be used from the year.

The energy conversion chain is quantified as exergy (XCC) to match the exergy version of the material conversion chain (BCC).

2.2. Methods

The methods used to create the example MCC are given below. We begin by discussing the material hierarchy that organizes information at any statepoint.

2.2.1. Material hierarchy

We define a statepoint (k) as a material stream with a known pressure, temperature, and composition as a mixture of compounds and or elements Ting [39, p.19-33]. To analyze each statepoint of the example MCC, we employ the material hierarchy shown in Table 2. This hierarchy enables later expansion to include components (a configuration of mixtures) and products (an assembly of components) between mixture and statepoint in our hierarchy.

For this paper, we adopt subscript symbols for the hierarchy as shown in Table 2 adapted from Remmen [40, p. 10]. For example, $B_{m,k}$ gives the material exergy (B) of a mixture (subscript m) of materials at statepoint k. Our choices of subscript j (for elements) and subscript i (for compounds) follow Valero Capilla and Valero Delgado [5].

Table 1. Components of material exergy.

Name	Subscript	From	To	Constraint
physical exergy	b_{ph}	T and P	T_0 and P_0	without changes in the chemical composition
chemical exergy	b_{ch}	Chemical composition	Reference chemical composition	while the system remains at T_0 and P_0
concentration exergy	b_c	Concentration at the statepoint	Entirely concentrated	NA
comminution exergy	b_{com}	Dispersed state	Cohesive state	NA

Table 2. Material hierarchy.

Name	Subscript	Definition
mixture	m	a combination of compounds and/or elements that exist at a statepoint
compound	i	a combination of elements
element	j	a combination of atoms

2.2.2. The exergy of materials

In this section, we carefully elucidate concepts and equations for consistent exergy analysis approach for ECCs and MCCs, including chemical and concentration exergies (contribution 1 of Section 1.4). Material exergy (B) is the exergy of a mixture of compounds that exist at a statepoint (B_k). Material exergy is the maximum amount of work that could be extracted by a process that brings the mixture into equilibrium with the reference environment, defined by its temperature (T_0), pressure (P_0), and chemical composition. Thus, the total exergy of a material (B) is the sum of the work of four reversible processes.

We assume that all statepoints in the example MCC are at T_0 and P_0; thus, physical exergy (b_{ph}) is zero. (The exception is Appendix E, which for illustration purposes assumes material temperature to be different from T_0.) Natural resources have a positive material exergy (b in kJ/mol) because they have a chemical composition different from their Environment. Comminution exergy is minimal[5, p. 280] and ignored for the analysis of conversion chains herein. (The exception, again, is Appendix E, which for illustration purposes demonstrates communition exergy calculations.)

Reference environments can include the atmosphere, the ocean, or the Earth's crust. Species in reference environments are characterized by partial pressure ($P_i = y_i P_0$) in the atmosphere, by concentrations (C_i) in the ocean, and by mole fraction (y_i) in the Earth's crust. We take reference environments from Valero Capilla and Valero Delgado [5, Tables 11.1–11.7].

Mixture (m)

The total material exergy of a mixture at a statepoint (B_m) is

$$B_m = N_m b_m \,, \tag{1}$$

where B_m is the total exergy of the mixture (in units of kJ_m), N_m is the amount of the mixture (in units of mol_m), and b_m is the molar intensive material exergy of the mixture (in units of kJ_m/mol_m).

The material exergy of a mixture may be calculated from compounds (i) in the mixture with

$$B_m = \sum_i N_i b_i = N_m \sum_i y_i b_i \,, \tag{2}$$

where N_i is the number of moles of compound i (in mol_i), b_i is the molar intensive material exergy of compound i (in kJ_i / mol_i), and y_i is the mole fraction of compound i in its mixture (in mol_i / mol_m).

Compound (i)

In general, the molar intensive material exergy of compound i (b_i) is defined as

$$b_i = b_{ph,i} + b_{ch,i} + b_{c,i} + b_{com,i} \, , \tag{3}$$

where $b_{ph,i}$ is physical exergy, $b_{ch,i}$ is chemical exergy, $b_{c,i}$ is concentration exergy, and $b_{com,i}$ is communition exergy. (See Valero Capilla and Valero Delgado [5, p. 276].) All terms are in units of kJ_i / mol_i. As discussed above, physical exergy ($b_{ch,i}$) is zero for all statepoints in the example MCC of this paper, because all statepoints are assumed to be at T_0 and P_0. Comminution exergy ($b_{com,i}$) is assumed small and neglected. (See Appendix E for confirmation of this assumption.) Thus, for this paper the molar intensive material exergy of a compound is given by

$$b_i = b_{ch,i} + b_{c,i} \, . \tag{4}$$

The molar intensive material exergy of a statepoint is given by

$$b_m = \sum_i b_i \, . \tag{5}$$

Chemical exergy(b_{ch})

The chemical exergy of a compound ($b_{ch,i}$) existing in the reference environment is the potential amount of work obtainable by decomposing the compound to compounds and elements in their environmentally stable forms. If compound i does not exist in the reference environment, its chemical exergy is the amount of work obtained in the reversible chemical reactions that decompose the pure compound to the set of compounds in equilibrium with the environment.

This process can be decomposed into two steps: decomposition of compound in the environment to its most stable form of compounds and elements including the formation of a compound from stable compounds and elements, which is captured by Gibbs free energy. The reversible work produced from the first process is the chemical exergy of the compound.

**** Perhaps we can cite this paper: Michalakakis et al. [41]. —MKH ****

The chemical exergy of a compound ($b_{ch,i}$) is given by

$$b_{ch,i} = \Delta G_{f,i} + \sum_i n_j b_{ch,j} \, , \tag{6}$$

where $b_{ch,i}$ is in units of kJ_i / mol_i, n_j is the number of moles of an element (in units of mol_i), and Gibbs energy of formation (ΔG_f) is in units of kJ_i / mol_i. ΔG_f values are taken from Dean [42, pp. 9.4–9.94], Vaxa Software [43, Table 2], and Tro [44, Appendix II B].

The chemical exergy of a mixture ($b_{ch,m}$) is

$$b_{ch,m} = \sum_i N_m b_{ch,i} \, . \tag{7}$$

Concentration exergy (b_c)

The concentration exergy of a mixture ($b_{c,m}$) is the the minimum work required to separate the mixture into pure compounds. The definition of concentration exergy is

derived from the entropy of mixing. The entropy of a mixture (ΔS_m) is the increase in entropy that occurs when different substances are mixed reversibly and isothermally and is given by

$$\Delta S_m = -RN_m(y_1 \ln y_1 + y_2 \ln y_2 + y_3 \ln y_3 + \ldots) = -RN_m \sum_i y_i \ln y_i \,, \tag{8}$$

where ΔS_m is in units of $\text{kJ/mol}_m \cdot \text{K}$, and R is the universal gas constant (in units of $\text{kJ/mol} \cdot \text{K}$), and y_i are in $\text{mol}_i/\text{mol}_m$.

The reference points for concentrations (y_i) are species as pure substances, so $y_{i,0} \equiv 1$.

The concentration exergy of a compound (as defined above) is the reversible work needed to concentrate it to the pure state. Valero Capilla and Valero Delgado [5] **** Include page number. —MKH **** define concentration exergy of a compound ($b_{c,i}$) as

$$b_{c,i} = RT_0[\ln(y_i) - \ln(y_{i,0})] \,. \tag{9}$$

Simplifying Equation (9) with $y_{i,0} = 1$ gives

$$b_{c,i} = RT_0 \ln(y_i) \,. \tag{10}$$

The concentration exergy of a compound in a mixture is always negative because the pure substance in the reference environment becomes less concentrated at any statepoint.

The minimum work required to separate a mixture reversibly at constant temperature and pressure is given by

$$W_{min} = -T_0 \Delta S_m = RT_0 N_m \sum_i (y_i \ln y_i) \,, \tag{11}$$

where W_{min} is in units of kJ/mol_m. The minimum work is negative because the environment puts work into the mixture.

Elements (j)

We take chemical exergies of elements ($b_{ch,j}$) from the crepuscular earth model of Valero Capilla and Valero Delgado [5, Table 9.1].
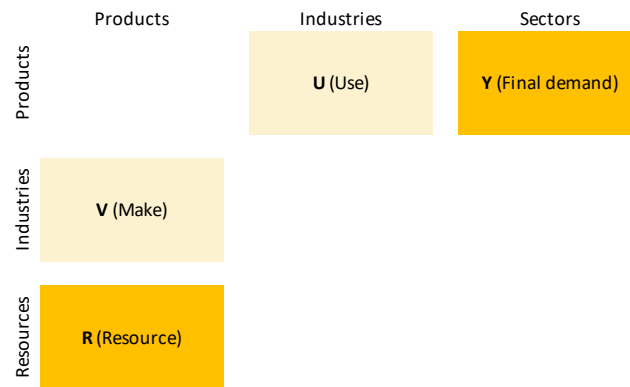
2.2.3. The exergy of energy

The example MCC has both material and energy inputs to processes. We calculate the exergy of energy as shown in Equation (4) for all energy sources with mass (e.g., coal, oil, and natural gas). The exergy of energy inputs are determined by Equation (6) when the Gibbs energy of formation (ΔG_f) is available. Otherwise (such as for coal and fuel oil), we calculate material exergy by

$$\varepsilon_i = [LHV_i + wh_{fg}]\phi_i + (9417 \text{ kJ/kg}) s \tag{12}$$

where ε_i is the exergy of energy (in units of kJ), LHV_i is the lower heating value of the fuel (in units of kJ/kg), w is the fuel's mass fraction of moisture (in units of kg/kg), h_{fg} is the enthalpy of evaporation of H_2O (in units of kJ/kg), ϕ_i is the ratio of exergy to energy (in units of kJ/kJ), the constant 9417 kJ/kg is the difference in rhombic sulfur's chemical exergy and it's lower heating value, and s is the mass fraction of sulfur in the fuel (in units of kg/kg). (See Kotas [28, Eq. C.5a].) We obtain ϕ values from Kotas [28, Appendix C]. (See Appendix C for solid and liquid fuel exergy equations.)

All other energy sources in the example MCC are electricity. The exergy of energy at any statepoint is given by

Figure 1. Matrices of the PSUT framework. After Aramendia et al. [17, Figure 1].

$$X_i = \phi_i E_i \,, \tag{13}$$

where X_i is the exergy of energy of a species (in units of kJ), ϕ_i is the exergy to energy ratio (unitless), and E_i is the energy of a species (in units of kJ). Note $\phi_{electricity} \equiv 1$, by definition.

2.2.4. PSUT framework and **RUVY** matrices

The native data format for the ECCs and XCCs of the CL-PFU database [15] is the **RUVY** matrices[2] of the Physical Supply-Use Table (PSUT) framework [16,17]. Although the PSUT framework has been applied to analysis of energy conversion chains (both ECCs and XCCs) [45,46], this paper represents its first application to material conversion chains (MCCs and BCCs) and to unified exergy analysis of material and energy conversion chains (BXCCs).

One benefit of the PSUT framework is that it provides a natural structure for data in material conversion chains (MCCs in mass units), energy conversion chains (ECCs in energy units), and exergy conversion chains (BCCs for material, XCCs for energy, and BXCCs for unified, all in exergy units). We apply that structure to the conversion chains developed in Section 3 below. The four matrices of the PSUT framework are the resource matrix (**R**), which contains exogenous inputs to a conversion chain; the use matrix (**U**), which includes the consumption of materials and energy; the make matrix (**V**), which describes the production of materials and energy by processes in conversion chains; and the final demand matrix (**Y**), which contains consumption of materials and energy by economic sectors. See Figure 1.

In the PSUT framework, processing stages are generically called "industries," and flows of mass, energy, or exergy between processing stages are generically called "products." In a flow diagram, industries are represented visually by boxes. Products are represented visually by arrows that indicate the direction of product flow from one industry to another.

2.2.5. Material and energy conversion chains

To illustrate application of the exergy of materials to societal exergy analysis, we develop several material and energy conversion chains using the the **RUVY** matrices of the PSUT framework. First, we develop a direct energy input and material flow model (DEIMFM). The DEIMFM includes all material flows and *direct* energy inputs.[3]

2　Note that matrices are represented by capital letters in bold, non-italic font. Vectors are represented by lower-case or script letters in bold, non-italic font.

3　Direct energy inputs are consumed directly by a machine, such as electricity consumed by crushers. Indirect energy inputs include upstream resources to create the direct energy inputs, such as coal used to make electricity.

Table 3. Characteristics of the independent material (MCC and BCC) and energy (ECC and XCC) conversion chains used to build the integrated material and energy conversion chain (BXCC). Non-energy materials include limestone, iron ore, and combustion air. Energy materials are fuels considered as mass and later converted to exergy, including coal, natural gas, diesel, and coke oven gas. Massless energy is electricity and heat.

	DEIMFM	MCC & BCC	ECC & XCC	BXCC
Non-energy materials	✓	✓		✓
Energy materials (direct)	✓	✓	✓	✓
Massless energy (direct)	✓	✓	✓	✓
Energy materials (indirect)			✓	✓
Massless energy (indirect)			✓	✓

Next, we develop two matrix representations of the mass flows of the DEIMFM. (a) A mass-only version (MCC) that quantifies material flows in mass units from extraction through a blast furnace to the Iron and steel industry (Section 2.1.1). (b) An exergy version (BCC) that quantifies material flows in exergy units. Each statepoint in the MCC is converted to exergy to form the BCC in accordance with the methods discussed in Section 2.2.2.

Then, we develop two versions of an independent energy conversion chain to supply the DEIMFM's energy requirements: (c) an independent energy conversion chain (ECC) obtained from the CL-PFU database where all flows are in energy terms as described in Sections 2.1.2 and 2.1.3 and (d) an independent exergy version of the energy conversion chain (XCC), also extracted from the CL-PFU database. To obtain the ECC and XCC, we perform an "upstream swim" from a new final demand (**Y**) matrix populated with the energy requirements of the BCC, as discussed in Heun et al. [16, Section 2.2.5].

Finally, we develop (e) a matrix representation of a unified conversion chain (BXCC) that brings the exergy of materials and energy together, as described in Section 2.2.6 below. The benefit of unifying the independent material and energy conversion chains is that all upstream activities for the MCC and ECC are accounted in the BXCC.

Table 3 shows the characteristics of the DEIMFM and various conversion chains.

2.2.6. Creating the unified conversion chain (BXCC)

The method for creating a unified material and energy conversion chain (BXCC) involves three steps. The beginning and end points of the process to create the BXCC are flow diagrams depicting the movement of exergy from resources to final demand. In the middle, we generate and manipulate the **RUVY** matrices of the PSUT framework. The process is illustrated by Figures 2–5 which show an illustrative portion of the blast furnace example developed elsewhere in this paper. The basis for the partial example is 100 kJ of electricity delivered to the blast furnace. Despite not including all exergy flows of the full example developed in this paper, the partial example is sufficient to demonstrate the steps for creating a BXCC.

We start with independent exergy quantifications of material and energy conversion chains (BCC and XCC) as described in Section 2.2.5. (See Figure 2 for the independent conversion chains for the partial example.) The independent BCC and XCC are based upon (a) the material conversion chain expressed in mass units (MCC) and (b) an energy conversion chain expressed in energy units (ECC). The MCC contains only the direct energy requirements for material transformations and does not contain upstream energy-production processes. The ECC does not contain any material transformation information. The ECC contains only the energy supplied to material conversion processes (industries) in the MCC.
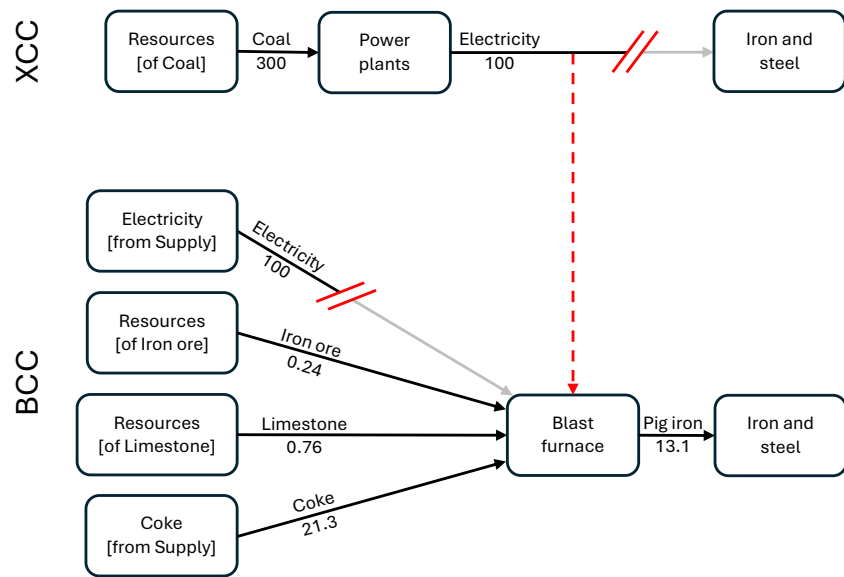
Figure 2. Example independent material (BCC) and energy (XCC) conversion chains. All values are exergy in kJ.

In the independent XCC of Figure 2, electricity produced by the XCC is delivered to the "Iron and steel" sector, consistent with existing ECC and XCC datasets [13,15]. In the independent BCC of Figure 2, electricity consumed by the blast furnace is supplied by "Electricity [from Supply]", indicating that the electricity supply is exogenous to the BCC.

The goal of creating a unified BXCC is endogenizing the exogenous energy inputs to the independent BCC, as illustrated by the red cut-lines, the gray lines, and the red dashed line in Figure 2. Electricity entering the "Iron and steel" sector of the independent XCC will be re-routed to the "Blast furnace" in the independent BCC, as shown by the red dashed line. In the BXCC, electricity formerly provided by "Electricity [from Supply]" will come from the "Power plants" industry instead.

The first step is to convert the flow diagrams for the independent BCC and XCC into the **RUVY** matrices of the PSUT framework. Figure 3 shows **RUVY** matrices consistent with the independent material and energy conversion chains of the partial example in Figure 2. Note that the red "X"s in Figure 3 indicate matrix entries to be removed according to the red cut-lines in Figure 2.

The second step involves three actions: (a) removing entries from the final demand matrix (**Y**) of the XCC, (b) removing selected entries from the resource matrix (**R**) of the BCC, and (c) summing corresponding matrices in the BCC and XCC, respecting row and column names. The result for the partial example is the unified conversion chain (BXCC) shown in Figure 4.

The third and final step is to translate the **RUVY** matrices for the unified conversion chain (BXCC) (Figure 4) into a flow diagram. The result for the partial example is shown in Figure 5.

2.2.7. Inter-industry balances

When constructing the **RUVY** matrices of the PSUT framework, we perform an important consistency check via balances of inter-industry product flows. The matrix equation for inter-industry product balances is

$$(\mathbf{iR})^{\mathrm{T}} + (\mathbf{iV})^{\mathrm{T}} - \mathbf{Ui} - \mathbf{y} \overset{?}{=} \mathbf{0}, \tag{14}$$
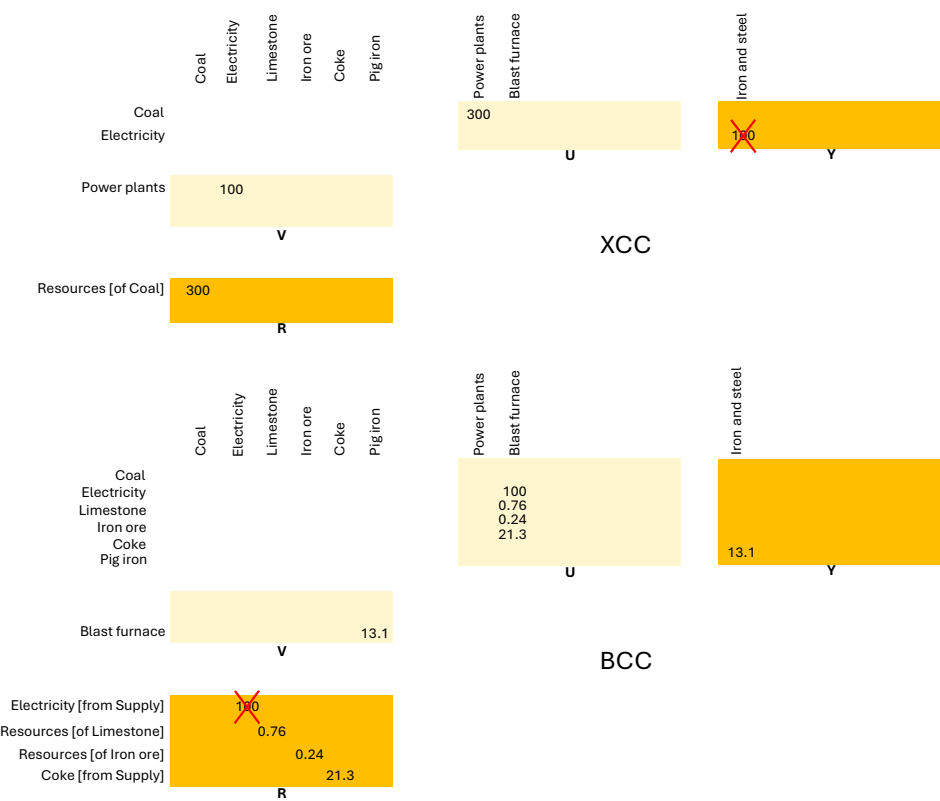
Figure 3. Resource (**R**), use (**U**), make (**V**), and final demand (**Y**) matrices for the independent material (BCC) and energy (XCC) conversion chains of the partial example. All values are exergy in kJ.
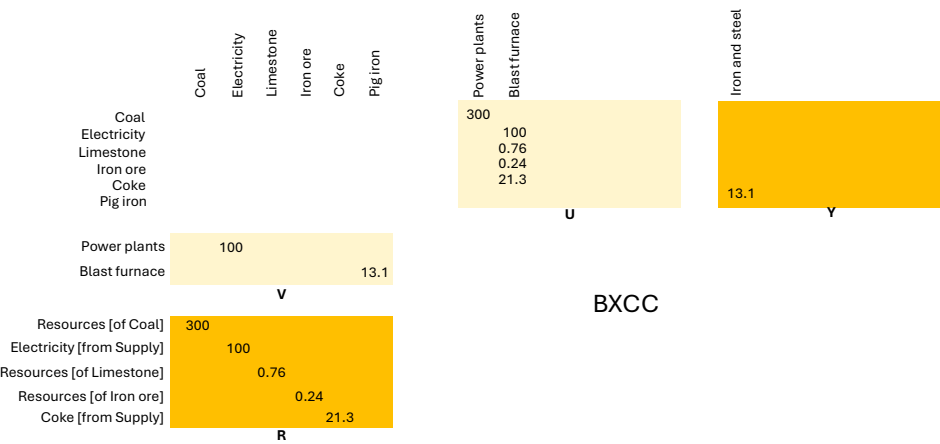
Figure 4. Resource (**R**), use (**U**), make (**V**), and final demand (**Y**) matrices for the unified material and energy conversion chains (BXCC) of the partial example. All values are exergy in kJ.
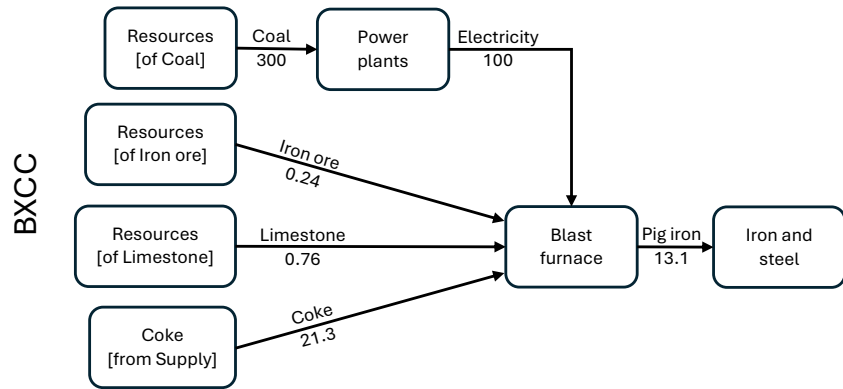
Figure 5. An example unified material and exergy conversion chain (BXCC). All values are exergy in kJ.
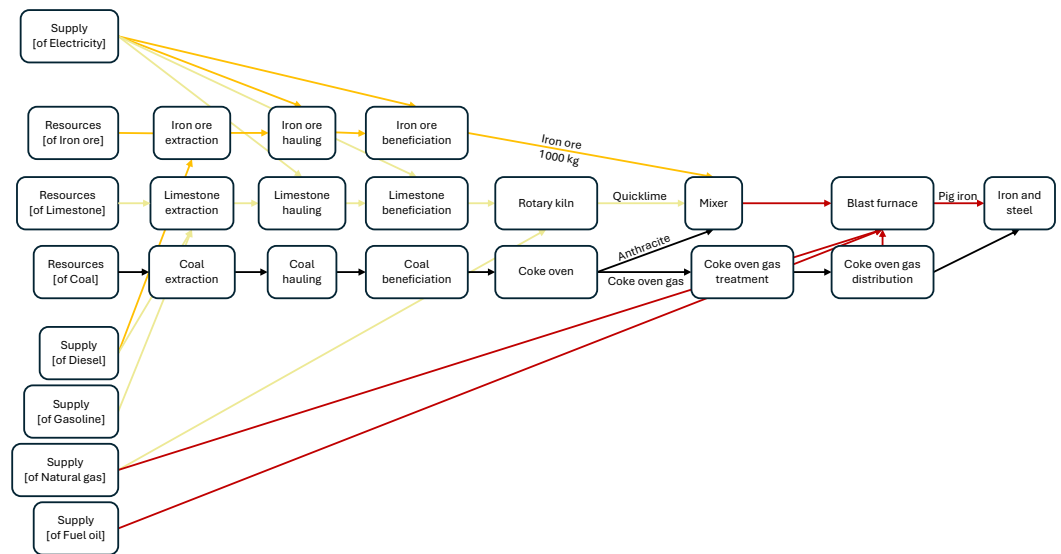
Figure 6. Simplified version of the example MCC.

where **i** is a unity row or column vector of appropriate length, **iR** gives column sums of the resource matrix (a row vector), ^{T} is the transpose operator, **iV** gives column sums of the make matrix (a row vector), **Ui** gives row sums of the use matrix (a column vector), and $\mathbf{y} \equiv \mathbf{Yi}$ is the row sums of the final demand matrix (a column vector). The result is a column vector with products in rows.

Regardless of the type of conversion chain (MCC, BCC, ECC, XCC, BXCC), Equation (14) tests whether all products extracted from resources (**R**) or produced by industries (**V**) become inputs to industries (**U**) or final demand sectors (**Y**). When Equation (14) is true (i.e., when the calculation on the left side produces the **0** vector), the conversion chain is internally consistent.

All matrix representations of conversion chains developed for this paper pass the inter-industry consistency check.

3. Results

This section shows results corresponding to contributions 2 and 3 of Section 1.4. Section 3.1 below addresses contribution 2 and Section 3.3 below addresses contribution 3.

3.1. Material conversion chain

Using the methods of Section 2.2, we compiled an example independent material conversion chain (MCC) for the production of pig iron (contribution 2 of Section 1.4). The

example independent material conversion chain contains 46 material statepoints, 9 energy statepoints, and 14 material conversion processes (industries). **** We need to double-check these numbers. Be sure to include heat loss statepoints. We made a few changes. —MKH **** Figure 6 shows a representation of the MCC. (For simplicity, heat loss and waste streams are not shown in Figure 6.) Full details of the example independent MCC, the example independent ECC from the CL-PFU database, and the example unified BXCC, including magnitudes for all flows, are available in the supplementary information.

3.2. Material Exergies

Equations (1) and (2) are the basis for material exergy accounting along the independent material conversion chain. At each statepoint, we calculate mixture material exergies (B_m), including chemical (b_c) and concentration (b_{ch}) exergies and all components thereof. Table 4 shows the solid material inputs to the blast furnace: iron ore (Fe_2O_3 with SiO_2 impurities), quicklime (CaO), and coking coal. Table 5 shows the pig iron output. Table 6 gives details of the waste slag from the blast furnace. See the supplementary information for details of the gaseous inputs and outputs of the blast furnace.

Using Table 4 as the example, the lower-right value (B for the mixture) is calculated by Equation (1) or (2). The values in the middle rows of the $b_{ch,i}$ column are calculated by Equation (6). The values in the middle rows of the $b_{c,i}$ column are calculated by Equation (10). The values in the middle rows of the b_i column are calculated by Equation (4). The values in the middle rows of the b_m column are calculated by Equation **??**. The values in the middle rows of the B_m column are calculated by Equation 1. Fully-detailed calculations for exergies at the inlet to the rotary kiln can be found in Appendix E.

Table 4. Material exergy details for iron ore (Fe_2O_3 and SiO_2), quicklime (CaO), and coking coal at the inlet to the blast furnace.

	m_i [kg_i]	x_i [kg_i/kg_m]	MW_i [kg_i/mol_i]	N_i [mol_i]	h_i [kJ_i/kg_i]	$b_{ch,i}$ [kJ_i/mol_i]	y_i [mol_i/mol_m]	$\ln(y_i)$ [$-$]	$b_{c,i}$ [kJ_i/mol_i]	b_i [kJ_i/mol_i]	b_m [kJ_i/mol_m]	B_m [kJ_i]
Fe_2O_3	881.1	0.67	0.160	5,517.38	-824.2	17.36	0.212	-1.551	-3.843	13.515	2.865	74,567.1
SiO_2	118.9	0.09	0.060	1,979.55	-910.7	1.53	0.076	-2.576	-6.383	-4.857	-0.369	-9,614.7
CaO	111.0	0.08	0.056	1,979.55	-634.9	122.26	0.076	-2.576	-6.383	115.875	8.813	229,380.5
Coking Coal	203.3	0.15	0.012	16,552.13	369.4	387.16	0.636	-0.453	-1.122	386.036	245.488	6,389,724.6
Mixture	1,314.3	1.00	0.050	26,028.61	-57.3	259.30	1.000		-2.499	256.797	256.797	6,684,057.5

Table 5. Material exergy details for pig iron at the output of the blast furnace.

	m_i [kg_i]	x_i [kg_i/kg_m]	MW_i [kg_i/mol_i]	N_i [mol_i]	h_i [kJ_i/kg_i]	$b_{ch,i}$ [kJ_i/mol_i]	y_i [mol_i/mol_m]	$\ln(y_i)$ [$-$]	$b_{c,i}$ [kJ_i/mol_i]	b_i [kJ_i/mol_i]	b_m [kJ_i/mol_m]	B_m [kJ_i]
Fe	616.2	1.00	0.056	11,034.75	0.0	376.80	1.000	0.000	0.000	376.800	376.800	4,157,895.3
Mixture	616.2	1.00	0.056	11,034.75	0.0	376.80	1.000		0.000	376.800	376.800	4,157,895.3

Table 6. Material exergy details for slag at the output of the blast furnace.

	m_i [kg_i]	x_i [kg_i/kg_m]	MW_i [kg_i/mol_i]	N_i [mol_i]	h_i [kJ_i/kg_i]	$b_{ch,i}$ [kJ_i/mol_i]	y_i [mol_i/mol_m]	$\ln(y_i)$ [$-$]	$b_{c,i}$ [kJ_i/mol_i]	b_i [kJ_i/mol_i]	b_m [kJ_i/mol_m]	B_m [kJ_i]
$CaSiO_3$	229.9	1.00	0.116	1,979.55	-89.6	34.29	1.000	0.000	0.000	34.288	34.288	67,875.4
Mixture	229.9	1.00	0.116	1,979.55	-89.6	34.29	1.000		0.000	34.288	34.288	67,875.4

The material exergy of the iron ore, quicklime, and coking coal inputs to the blast furnace in the example independent BCC is 6,684.1 MJ. The material exergy of the pig iron output is 4,157.9 MJ. The material exergy of the solid waste (slag) output is 67.9 MJ. Material exergies for all statepoints in the example MCC can be found in supplementary information.

3.3. PSUT matrices

We created a representation of the example unified material and energy conversion chain in the **RUVY** matrix format of the PSUT framework using the methods of Section 2.2.6 (contribution 3 of Section 1.4). Appendix F contains **RUVY** matrices for the example unified material and energy conversion chain (BXCC).

4. Discussion

Arranging material and energy conversion chain data in the **RUVY** matrices of the PSUT framework provides many benefits to analysts. This section discusses further applications beyond the contributions shown in Section 3 above. In particular, without the PSUT framework, analyses of all transformation processes (industries) involve repetitive calculations, once for each process. With the PSUT framework, the repetitive calculations can be expressed as a single matrix equation that performs the analyses for all industries in a conversion chain. The interpretation of the results varies, depending on the type of conversion chain under consideration. We demonstrate below the benefits of the PSUT framework by discussing across-industry balances (Section 4.1) and industry efficiencies (Section 4.2).

4.1. Across-industry balances

In contrast to the inter-industry balances of Equation (14), across-industry balances do not and should not always calculate to the **0** vector. Instead, across-industry balances calculate important quantities depending on the information contained in the **RUVY** matrices, possibly mass flows, energy flows, or exergy flows. Across-industry balances for every industry in a conversion chain are given by the matrix equation

$$(\mathbf{iU})^{\mathrm{T}} - \mathbf{Vi},\tag{15}$$

where **iU** gives column sums of the use matrix, $^{\mathrm{T}}$ indicates the transpose, and **Vi** gives row sums of the make matrix. The result of Equation (15) is a column vector with industries in rows.

In the following subsections, we discuss calculations using across-industry balances for mass, heat loss, and irreversibility.

4.1.1. Across-industry mass balances: mass losses

For an MCC, the across-industry balance of Equation (15) becomes

$$\mathbf{m}_{loss} = (\mathbf{iU}_{MCC})^{\mathrm{T}} - \mathbf{V}_{MCC}\mathbf{i},\tag{16}$$

where $\mathbf{m}_{loss}$ is a vector of mass losses in which rownames are processing stages and the subscript "MCC" indicates mass versions of the **U** and **V** matrices.

For an MCC with all waste flows included (as in the example in this paper), the across-industry balance of Equation (16) becomes

$$\mathbf{m}_{loss} = (\mathbf{iU}_{MCC})^{\mathrm{T}} - \mathbf{V}_{MCC}\mathbf{i} = \mathbf{0},\tag{17}$$

Table 7. Mass losses (m_{loss}) in the example material conversion chain.

	m_{loss} [kg]
Iron ore extraction	0.000
Limestone extraction	0.000
Coal extraction	0.000
Iron ore hauling	0.000
Limestone hauling	0.000
Coal hauling	0.000
Iron ore beneficiation	0.000
Limestone beneficiation	0.000
Coal beneficiation	0.000
Rotary kiln	0.000
Coke oven	0.000
COG treatment	0.000
COG distribution	0.000
Mixer	0.000
Blast furnace	0.000

Table 8. Process heat losses (Q_{loss}) in the example material conversion chain.

	Q_{loss} [kJ]
Iron ore extraction	180,961
Limestone extraction	519
Coal extraction	125,419
Iron ore hauling	609,792
Limestone hauling	2,825
Coal hauling	282
Iron ore beneficiation	46,560
Limestone beneficiation	35
Coal beneficiation	50
Rotary kiln	1,515,160
Coke oven	14,519,667
COG treatment	99,018
COG distribution	0
Mixer	0
Blast furnace	11,186,112

where the **0** vector on the right side of Equation (17) indicates that mass is conserved. The example MCC of Section 3 is mass-balanced across industries, as shown in Table 7.

4.1.2. Across-industry energy balances: heat losses

For an ECC with no heat losses included (as in the example of Section 3), the across-industry balance of Equation (15) calculates heat loss from each industry:

$$\mathbf{Q}_{loss} = (\mathbf{i}\mathbf{U}_{ECC})^{\mathrm{T}} - \mathbf{V}_{ECC}\mathbf{i}, \tag{18}$$

where the subscript "*ECC*" indicates energy versions of the **U** and **V** matrices obtained by

$$\mathbf{U}_{ECC} = (\mathbf{U}_{MCC} \circ \mathbf{U}_h) + \mathbf{U}_{elect} \tag{19}$$

and

$$\mathbf{V}_{ECC} = (\mathbf{V}_{MCC} \circ \mathbf{V}_h) + \mathbf{V}_{elect}, \tag{20}$$

with ∘ indicating the Hadamard (element-wise) product, subscript "*h*" indicating **U** and **V** matrices containing enthalpy values, and subscript "*elect*" indicating indicating **U** and **V** matrices containing only (massless) electricity inputs. See the supplementary information for the $\mathbf{U}_{MCC}$, $\mathbf{V}_{MCC}$, $\mathbf{U}_h$, $\mathbf{V}_h$, $\mathbf{U}_{elect}$, $\mathbf{V}_{elect}$, $\mathbf{U}_{ECC}$, and $\mathbf{V}_{ECC}$ matrices for the example of Section 3. Table 8 shows the heat loss vector ($\mathbf{Q}_{loss}$) for the example in Section 3.

For industries that simply transport mass (e.g., hauling), Q_{loss} is equal to the energy input.

Table 9. Irreversibilities ($\mathcal{I}_{BXCC}$) in the example unified material and energy conversion chain.

	I_{BXCC} [kJ]
Iron ore extraction	0
Limestone extraction	0
Coal extraction	0
Iron ore hauling	0
Limestone hauling	0
Coal hauling	0
Iron ore beneficiation	36,862
Limestone beneficiation	0
Coal beneficiation	0
Rotary kiln	1,130,284
Coke oven	11,769,224
COG treatment	86,584
COG distribution	0
Mixer	0
Blast furnace	8,272,912
Blast furnaces	0
Charcoal production plants	-0
Coal liquefaction plants	64,084
Coal mines	5,821
Coke ovens	0
Gas works	-0
Gas-to-liquids (GTL) plants	4,754
Main activity producer electricity plants	2,251,368
Manufacture [of Hydro]	0
Manufacture [of Nuclear]	0
Manufacture [of Primary solid biofuels]	0
Manufacture [of Solar photovoltaics]	0
Manufacture [of Solar thermal]	0
Manufacture [of Wind]	0
Natural gas extraction	0
Nuclear industry	123,740
Oil extraction	0
Oil refineries	7,801
Transfers	-1,525

For an ECC that includes heat losses, the across-industry balance of Equation (15) should calculate the **0** vector.

4.1.3. Across-industry exergy balances: exergy losses and irreversibility

For an exergy conversion chain (BCC, XCC, or BXCC) that includes waste heat and mass flows, the across-industry balance calculates the thermodynamic irreversibility ($\mathcal{I}$) of (or exergy destruction by) an industry. For exergy conversion chains that include waste mass flows and exclude heat loss terms (as in the example unified material and energy conversion chain of this paper), the across-exergy balance of Equation (15) calculates the sum of irreversibility and exergy loss due to heat dissipation ($\mathcal{I}$). Equation (15) becomes

$$\mathcal{I}_{BXCC} = (\mathbf{i}\mathbf{U}_{BXCC})^{\mathrm{T}} - \mathbf{V}_{BXCC}\mathbf{i} \,, \tag{21}$$

where $\mathcal{I}$ is a column vector of the sum of irreversibility (or exergy destruction) and exergy loss due to heat dissipation with industries in rows. Table 9 shows irreversibilities for the example conversion chains of Section 3. Exergy is destroyed across all industries, unless the process is trivial (e.g., coke oven gas distribution).

The irreversibilities and loss of exergy at a process is determined by the exergy inputs and outputs to the process,

$$\mathcal{I} = \sum_{in} B_m + I_m - \sum_{out} B_m + I_m \,, \tag{22}$$

where $\mathcal{I}$ is the irreversibility (or exergy destruction) of the process, $B_{in,m}$ is the exergy of a mixture going into a process, and $B_{out,m}$ is the exergy of a mixture leaving a process (all in
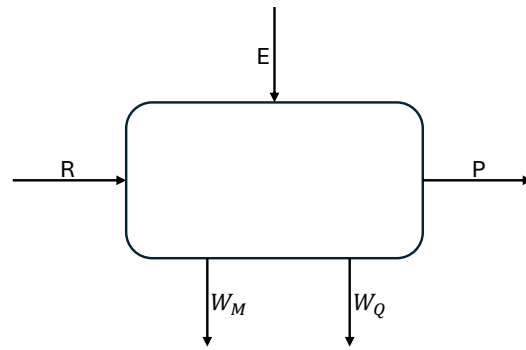
Figure 7. An example process for efficiency methods.

units of kJ). *I* should never be a negative value because exergy can not be generated, only destroyed.

The exergy lost (B_{lost}) from a process is given by

$$B_{lost} = \sum_{out} B_{k,m,waste} \tag{23}$$

where $B_{k,m,waste}$ is the exergy of a waste stream from a process (in units of kJ). The embodied exergy is the exergy loss in a supply chain, give by

$$B_{em} = \sum B_{lost} \tag{24}$$

where B_{em} is the embodied exergy (in units of kJ).

4.2. Efficiencies

We illustrate the application of material exergy to societal exergy analysis within the PSUT framework by calculating process efficiencies throughout the unified conversion chain (BXCC). There are many ways to calculate the efficiencies of industries in a material or energy conversion chain. We demonstrate two methods here: the rational efficiency and the resource efficiency.

Irreversibility arises from thermodynamic inefficiencies. Exergy loss arises from unused outputs, i.e., wastes, including mass and heat.

To illustrate calculations for the rational and resource efficiencies, we employ Figure 7 which shows an example process (industry) within a conversion chain. Inputs R and E represent material resources and energy inputs, respectively. Output P represents beneficial products, output W_M represents material waste products. and output W_Q represents heat waste. Note that additional resource, energy input, product, or waste streams can be present in real processes.

4.2.1. Rational efficiencies

The rational efficiency method accounts for all process outputs in the numerator and all process inputs in the denominator. With reference to Figure 7, Dincer and Rosen [47, Equation (2.45)] define the rational efficiency efficiency as

$$\eta_{rational} = \frac{B_P + B_{W,M}}{X_{elect} + B_R} . \tag{25}$$

where X_{elect} is the exergy of energy input E. Equation (25) must be applied separately to each process in a conversion chain.

In the PSUT framework, Equation (25) can be re-cast as a matrix equation that applies to all processes in a conversion chain.

Table 10. Process efficiencies in example material conversion chain.

	$\eta_{rational}$ [%]	$\eta_{resource}$ [%]
Iron ore extraction	54.5	45.1
Limestone extraction	98.9	86.0
Coal extraction	98.9	98.8
Iron ore hauling	15.1	12.7
Limestone hauling	90.0	78.2
Coal hauling	100.0	99.9
Iron ore beneficiation	90.9	75.8
Limestone beneficiation	99.9	86.8
Coal beneficiation	100.0	99.9
Rotary kiln	17.0	12.2
Coke oven	60.2	32.9
COG treatment	99.6	18.2
COG distribution	100.0	100.0
Mixer	99.2	99.2
Blast furnace	37.9	34.1

$$\boldsymbol{\eta}_{rational} = (\widehat{\mathbf{i}\mathbf{U}}_{BXCC})^{-1}(\mathbf{V}_{BXCC}\mathbf{i})\,, \tag{26}$$

where $\boldsymbol{\eta}_{rational}$ is a column vector of rational efficiencies for transformation processs with industries in rows, the $\widehat{}$ symbol indicates diagonalization of the $\mathbf{iU}$ vector into a square matrix, and $^{-1}$ indicates matrix inversion. Table 10 shows rational efficiencies for the example BXCC in Section 3.

The rational efficiencies of iron ore processes, in Table 10, are lower than the limestone and coal efficiencies. **** Need to add explanation for the lower efficiencies. **** The rational efficiency for iron ore extraction is 54.5 %. The rational efficiencies for limestone and coal extraction are 98.9 % and 98.9 %. Refer to Table 10 to see similar results for hauling and beneficiation efficiencies. The rational efficiencies for the mixer and blast furnace are 99.2 % and 37.9 %, respectively.

4.2.2. Resource efficiencies

The resource approach quantifies how efficiently a process converts resources (all inputs) into the desired product of the process. The resource efficiency removes wastes and accounts only for beneficial exergy outputs in the numerator of the efficiency calculation. Similar to the rational efficiency, the resource efficiency includes all exergy inputs in the denominator of the efficiency calculation. With reference to Figure 7, Dincer and Rosen [47, Equation (2.44)] define the resource efficiency efficiency as

$$\eta_{resource} = \frac{B_P}{X_{elect} + B_R}\,. \tag{27}$$

Similar to Equation (25), Equation (27) must be applied separately to each process in a conversion chain.

In the PSUT framework, Equation (27) can be re-cast as a matrix equation that applies to all process in a conversion chain.

$$\boldsymbol{\eta}_{resource} = (\widehat{\mathbf{i}\mathbf{U}}_{BXCC})^{-1}(\mathbf{V}_{BXCC}\mathbf{i}_P) \tag{28}$$

Equation (28) is identical to Equation (26) except that the make matrix ($\mathbf{V}_{BXCC}$) is post-multiplied by $\mathbf{i}_P$ instead of by $\mathbf{i}$. $\mathbf{i}_P$ is a product selection vector containing "1" for beneficial outputs and "0" for wastes. Table 10 shows resource efficiencies for the example BXCC of Section 3.

In Table 10, resource efficiencies are equal to or less than rational efficiencies in all cases, as expected. The greatest difference between rational and resource efficiencies are observed for the COG treatment.

The resource efficiency of the COG treatment process is much lower than its rational efficiency, because the beneficial product of COG treatment is methane, which is only 6% of the output (by mole).

4.3. Relative magnitude of concentration exergy

Concentration exergy has a relatively low magnitude in comparison to chemical exergy when calculated for a single statepoint.

At the unified conversion chain level, concentration exergy increases in magnitude and represents the destruction of work at a statepoint. Iron, for example, is concentrated from hematite ore to pig iron with energy inputs to several processes. The total concentration exergy across the change of iron from ore to pig iron is significant in comparison to the concentration exergy of a single process such as iron ore beneficiation.

As ore qualities degrade, concentration exergy will grow increasingly important as more critical materials take more work to extract due to lower concentrations within the earth's crust.

5. Conclusion

**** Note to Laura and Jorge: We need to write the conclusion and complete the sections prior to the appendix. ****

5.1. Summary
5.2. Future work

**** Add a note here about embodied exergy (exergy cost) being enabled by the PSUT framework. The reference should be Heun et al. [16, Section 3.3] —MKH ****

6. Patents

This section is not mandatory, but may be added if there are patents resulting from the work reported in this manuscript.

NAME OF INSTITUTE (protocol code XXX and date of approval)." for studies involving animals. OR "Ethical review and approval were waived for this study due to REASON (please provide a detailed justification)." OR "Not applicable" for studies not involving humans or animals.

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Abbreviations

The following abbreviations are used in this manuscript:

MDPI	Multidisciplinary Digital Publishing Institute
DOAJ	Directory of open access journals
TLA	Three letter acronym
LD	Linear dichroism

Appendix A Nomenclature

Appendix A.1

The appendix is an optional section that can contain details and data supplemental to the main text—for example, explanations of experimental details that would disrupt the flow of the main text but nonetheless remain crucial to understanding and reproducing the research shown; figures of replicates for experiments of which representative data are shown in the main text can be added here if brief, or as Supplementary Data. Mathematical proofs of results not central to the paper can be added as an appendix.

Table A1. Nomenclature table

Symbol	Description
T_0	ambient temperature [K]
P_0	ambient pressure [atm]
y_i	molar fraction of a species [mol/mol mixture]
b	material exergy [kJ/mol]
b_{ch}	chemical exergy [kJ/mol]
b_c	concentration exergy [kJ/mol]
b_{com}	comminution exergy [kJ/mol]
$\Delta G_{f,i}$	Gibbs free energy of formation [kJ/mol]
i	compound [NA]
j	element [NA]
m	mixture [NA]
S_m	entropy of mixing [kJ/mol-K]
R	universal gas constant [kJ/mol-K]
N	number of moles [mol]
B	molar intensive exergy [kJ]
X	energy exergy [kJ]
E	energy [kJ]
ϕ	exergy to energy ratio [kJ/kJ]
η	efficiency [kJ/kJ]
W_{min}	minimum work [kJ]
ε	exergy of a fuel [kJ]
LHV	lower heating value [kJ/kg]
w	mass fraction of moisture in a fuel [kg/kg]
h_{fg}	enthalpy of evaporation of H_2O [kJ/kg]
s	mass fraction of sulphur in a fuel [kg/kg]
I	irreversibility [kJ]
B_{lost}	exergy destroyed in a process [kJ]
B_{em}	sum B_{lost} across a MCC [kJ]

Appendix B

All appendix sections must be cited in the main text. In the appendices, Figures, Tables, etc. should be labeled, starting with "A"—e.g., Figure A1, Figure A2, etc.

See Kotas [28, Eq. C.5a].

Appendix C Exergy to energy ratios, ϕ

The exergy-to-energy ratio is given by ϕ. A table of ϕ constants are given by Kotas [28, Table C.1].

Fuels such as fuel oil, diesel, and gasoline do not have consistent chemical compositions. Kotas [28, Appendix C, Equation C.3,6] provides equations to calculate the ϕ values for these fuels. The value of ϕ for dry solid fuels is given by

$$\phi_{dry} = 1.0437 + 0.1882\frac{h}{c} + 0.0610\frac{o}{n} + 0.0404\frac{n}{c}, \tag{A1}$$

where h, c, n, and o are mass fractions of hydrogen, carbon, nitrogen, and oxygen (in units of kg/kg).

The value of ϕ for liquid fuels is given by

$$\phi = 1.0401 + 0.1728\frac{h}{c} + 0.0432\frac{o}{c} + 0.2169\frac{s}{c}\left(1 - 2.0628\frac{h}{c}\right), \tag{A2}$$

where s is the mass fraction of sulfur (in units of kg/kg).

Appendix D Chemical Formulas for MCC

Processes within the material conversion chain cause chemical change. The following sections give the chemical formulas for certain processes.

Appendix D.1 Rotary Kiln 670

$$1\,CaCO_3 + MgCO_3 \longrightarrow 1\,CaO + 2\,CO_2 + 1\,MgO \,. \tag{A3}$$
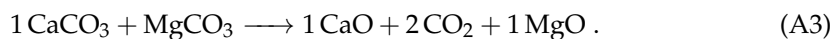
Appendix D.2 Coke Oven 671

Coal becomes coke oven gas and coke. 672

$$C_c\,H_h\,N_n\,O_o \longrightarrow C + H_2 + C_2H_4 + CO + CO_2 + N_2 + CH_4 \,. \tag{A4}$$

The coke oven gas is treated to create methane (CH_4). 673

$$H_2 + C_2H_4 + CO + CO_2 + N_2 + CH_4 \longrightarrow H_2 + CH_4 + O_2 + N_2 \,. \tag{A5}$$
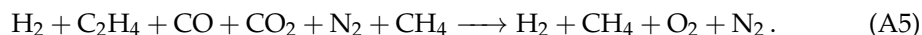
Appendix D.3 Blast Furnace 674

$$1.5\,C + 1.5\,O_2 \longrightarrow 1.5\,CO_2 + 5.64\,N_2$$
$$1.5\,CO_2 + 1.5\,C \longrightarrow 3\,CO$$
$$1\,Fe_2O_3 + 3\,CO \longrightarrow 2\,Fe + 3\,CO_2$$
$$1\,CaO + 1\,SiO_2 \longrightarrow 1\,CaSiO_3$$
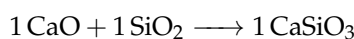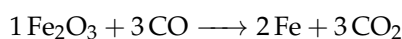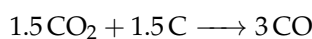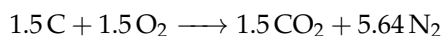
$$\tag{A6}$$

Appendix D.4 Fuel Combustion 675

Methane complete combustion: 676

$$1\,CH_4 + 2\,(O_2 + 3.76\,N_2) \longrightarrow 1\,CO_2 + 2\,H_2O + 7.52\,N_2 \,. \tag{A7}$$
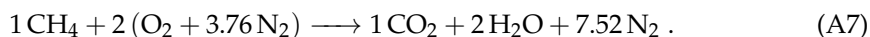
Diesel complete combustion: 677

$$1\,C_{12}\,H_{23} + 17.75\,(O_2 + 3.76\,N_2) \longrightarrow 12\,CO_2 + 11.5\,H_2O + 66.74\,N_2 \,. \tag{A8}$$
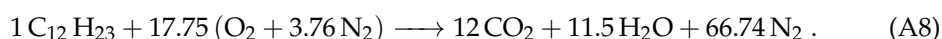
Gasoline complete combustion: 678

$$1\,C_8\,H_{18} + 12.5\,(O_2 + 3.76\,N_2) \longrightarrow 8\,CO_2 + 9\,H_2O + 47\,N_2 \,. \tag{A9}$$
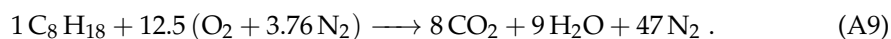
Fuel oil complete combustion: 679

$$C_{10}\,H_{20} + 15\,(O_2 + 3.76\,N_2) \longrightarrow 10\,CO_2 + 10\,H_2O + 56.4\,N_2 \,. \tag{A10}$$

Appendix E MCC exergy calculations 680

In the 2.2.2 section of this paper, four reversible processes are used to describe each 681
component of material exergy. 682

To demonstrate material exergy component calculations, the values given by A2 are 683
used to determine the exergy of limestone entering a rotary kiln. 684

Table A2 shows details of material exergy calculations for limestone, a mixture of 685
calcium carbonate ($CaCO_3$) and magnesium carbonate ($MgCO_3$), at the inlet to the rotary 686
kiln. 687

Table A2. Material exergy details for limestone at the inlet to the rotary kiln.

	m_i [kg$_i$]	x_i [kg$_i$/kg$_m$]	MW_i [kg$_i$/mol$_i$]	N_i [mol$_i$]	h_i [kJ$_i$/kg$_i$]	$b_{ch,i}$ [kJ$_i$/mol$_i$]	y_i [mol$_i$/mol$_m$]	$\ln(y_i)$ [$-$]	$b_{c,i}$ [kJ$_i$/mol$_i$]	b_i [kJ$_i$/mol$_i$]	b_m [kJ$_i$/mol$_m$]	B_m [kJ$_i$]
CaCO3	198.1	0.95	0.100	1,979.55	-1,207.6	11.26	0.941	-0.061	-0.150	11.107	10.454	21,986.2
MgCO3	10.4	0.05	0.084	123.68	-1,095.8	33.79	0.059	-2.834	-7.020	26.770	1.574	3,310.9
Mixture	208.6	1.00	0.099	2,103.23	-1,201.0		1.000				12.028	25,297.1

Appendix E.1 Physical exergy of $CaCO_3$

Physical exergy is given by

$$b_{ph,i} = \Delta h_{k,i} - T_0 \Delta s_{k,i} \tag{A11}$$

where $\Delta h_{k,i}$ is the change in enthalpy of a compound from a temperature or pressure at a statepoint to another (in units of kJ$_i$/mol$_i$) and $\Delta s_{k,i}$ is the change in entropy of a compound from a temperature or pressure at a statepoint to another (in units of kJ$_i$/mol$_i$K).

An estimate for the enthalpy of a compound is

$$\Delta h_i = c_{p,i} \Delta T \tag{A12}$$

where $c_{p,i}$ is the specific heat capacity of a compound (in units of kJ$_i$/mol$_i$K).

An estimate for the entropy of a compound is

$$\Delta s_i = c_{p,i} \ln \frac{T_k}{T_0} . \tag{A13}$$

where T_k is the temperature at a statepoint (in units of K) Sarna [34, Fig.1].

The temperature of limestone at the rotary kiln is ambient and changes to 1,173.15 K K in the kiln.

The change in enthalpy of $CaCO_3$ is

$$66.56940 \, kJ/mol = 0.07607 \, kJ/mol \cdot K (1,173.15 \, K - 298.00 \, K) . \tag{A14}$$

See Chase [48, p.1-1951] for cp_{CaCO_3} value . The change in entropy is

$$0.10424 \, kJ/mol \cdot K = 0.07607 \, kJ/mol \cdot K \ln \frac{1,173.15 \, K}{298.00 \, K} . \tag{A15}$$

Therefore, the physical exergy of calcium carbonate ($CaCO_3$) is

$$35.50655 \, kJ/mol = 66.56940 \, kJ/mol - (298.00 \, K)(0.10424 \, kJ/mol \cdot K) . \tag{A16}$$

Appendix E.2 Chemical exergy of $CaCO_3$

Unlike physical exergy, chemical exergy is independent of temperature and pressure. Chemical exergy is notable when a process changes the chemical composition of a mixture.

In 2.2.2.3, Eqn. 6 is used to define chemical exergy.

$$b_{ch,i} = \Delta G_{f,i} + \sum_i n_j b_{ch,j} . \tag{6}$$

For $CaCO_3$ the chemical exergy is

$$b_{ch,CaCO_3} = -1,012.10960 \, kJ/mol + ((1\left(\frac{mol_{Ca}}{mol_{CaCO_3}}\right))723.8 \, kJ/mol)$$
$$+ ((1\left(\frac{mol_C}{mol_{CaCO_3}}\right))410.3 \, kJ/mol$$
$$+ ((\frac{3}{2}\left(\frac{mol_{O_2}}{mol_{CaCO_3}}\right))4.0 \, kJ/mol$$
$$= 33.7904 \, kJ/mol \,.$$

Appendix E.3 Concentration exergy of $CaCO_3$

In 2.2.2.4, Eqn. 10 is used to define concentration exergy.

$$b_{c,i} = RT_0 \ln(y_i) \,. \tag{10}$$

The value for (y_{CaCO_3}) is obtained from A2 which represents the molar fraction of $CaCO_3$ in the limestone mixture. If mass fractions are known instead, then convert the mass fraction (x_i) to molar fractions (y_i) with the molecular weight of each compound (MW_i).

$$-0.12708 \, kJ/mol = 2.47757 \, kJ/mol(\ln(0.94120 \, mol_{CaCO_3}/mol_{limestone})) \,. \tag{A17}$$

Appendix E.4 Comminution exergy of $CaCO_3$

Comminution exergy (b_{com}) is defined by Valero Capilla and Valero Delgado [5, p.279] as, " the minimum energy required to bind solids from a given dispersed state to a more cohesive one ". The work required increases as the solid's particles decrease.

We calculate comminution exergy using Valero Capilla and Valero Delgado [5, Eqn.9.31]:

$$b_{com} = \Delta A_v \cdot \frac{\gamma}{\rho} = 6F_r \cdot [\frac{1}{d_M} - \frac{1}{d_\Theta}] \approx \frac{6F_r}{d_M} \,, \tag{A18}$$

where ΔA_v is undefined, but assumed to be the change in surface are (in units of m^3), γ is the surface energy (in units of $\frac{J}{m^{-2}}$), ρ is the solids density (in units of $\frac{g}{cm^3}$), the constant 6 has units of $\frac{J}{m^2}$, F_r is the surface roughness factor (unitless), d_M is the geometrical mean size (in units of m), and d_Θ is " the size of the barerock composing Thantia " (in units of m) Valero Capilla and Valero Delgado [5, p.279]. For certain materials, ρ, F_r, and γ are given by Valero Capilla and Valero Delgado [5, Tab. D.2, D.3, and D.4]. F_r for limstone is 1.373 Valero Capilla and Valero Delgado [5, Tab.D.4]. The comminution exergy for $CaCO_3$ is

$$0.03298 \, kJ/mol = \frac{6.00000 \, J/m^2(1.373)}{0.000025 \, m^3}(0.001\text{m}^3/\text{kg})(0.001\text{kJ/J}) \,. \tag{A19}$$

d_M for $CaCO_3$ is from Archbold [49, Tab.6].

add cp citations

Appendix E.5 Material exergy of $MgCO_3$

The second compound in limestone is magnesium carbonate ($MgCO_3$). The same equations used to calculate the exergy of $CaCO_3$ can be applied to $MgCO_3$ as follows:

- With equations A11, A12, and A13, the physical exergy of MgCO$_3$ ($b_{ph,MgCO_3}$) is determined by the change in enthalpy:

$$b_{ph,\text{MgCO}_3} = 0.00642 \, kJ/mol \cdot K[kJ/mol \cdot K](1,173.15 \, K - 298.00 \, K) \tag{A20}$$

$$= 5.62188 \, kJ/mol \,, \tag{A21}$$

  minus the change in entropy:

$$0.00880 \, kJ/mol \cdot K = 0.00642 \, kJ/mol \cdot K \left(\ln \left(\frac{1,173.15 \, K}{298.00 \, K} \right) \right), \tag{A22}$$

  when entropy is multiplied by the ambient temperature:

$$2.99858 \, kJ/mol = 5.62188 \, kJ/mol - 298.00 \, K(0.00880 \, kJ/mol \cdot K)\,. \tag{A23}$$

- The chemical exergy of MgCO$_3$ ($b_{ch,MgCO_3}$) is calculated with Eqn. 6.

$$b_{ch,\text{MgCO}_3} = \Delta G_{f,\text{MgCO}_3} + \sum_j n_j b_{ch,j} \tag{6}$$

$$= -1,012.10960 \, kJ/mol + \left(\left(1 \left(\frac{mol_{Mg}}{mol_{MgCO_3}} \right) \right) 629.6 \, kJ/mol \right)$$

$$+ \left(\left(1 \left(\frac{mol_C}{mol_{MgCO_3}} \right) \right) 410.3 \, kJ/mol \right.$$

$$+ \left(\left(\frac{3}{2} \left(\frac{mol_{O_2}}{mol_{MgCO_3}} \right) \right) 4.0 \, kJ/mol \right.$$

$$= 33.7904 \, kJ/mol \,.$$

- The concentration exergy of MgCO$_3$ ($b_{c,MgCO_3}$) is given by Eqn. 10 where the molar fraction (y_{MgCO_3}) is from A2.

$$-7.42214 \, kJ/mol = 2.47757 \, kJ/mol \ln(0.05880 \, mol_{MgCO_3}/mol_{limestone})\,. \tag{A24}$$

- The comminution exergy of MgCO$_3$ ($b_{com,MgCO_3}$) is

$$b_{com,\text{MgCO}_3} = \frac{6.00000 \, J/m^2(1.373)}{0.001548 \, m^3}(0.001 \text{m}^3/\text{kg})(0.001\text{kJ/J})$$

$$= 0.00045 \, kJ/mol \,,$$

$$\tag{A25}$$

Appendix E.6 Material exergy of the statepoint

The total exergy at the statepoint is the exergy of the mixture. See **??**.
The total exergy of CaCO$_3$ is

$$b_{\text{CaCO}_3} = b_{ph,\text{CaCO}_3} + b_{ch,\text{CaCO}_3} + b_{c,\text{CaCO}_3} + b_{com,\text{CaCO}_3}$$

$$= 35.50655 \, kJ/mol + 11.2568 \, kJ/mol + -0.12708 \, kJ/mol + 0.03298 \, kJ/mol$$

$$= 43.92493 \, kJ/mol \,.$$

$$\tag{A26}$$

The total exergy of $MgCO_3$ is

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$$
\begin{aligned}
b_{MgCO_3} &= b_{ph,MgCO_3} + b_{ch,MgCO_3} + b_{c,MgCO_3} + b_{com,MgCO_3} \\
&= 2.99858 \; kJ/mol + 33.7904 \; kJ/mol + -7.42214 \; kJ/mol + 0.03298 \; kJ/mol \\
&= 3.63849 \; kJ/mol \, .
\end{aligned}
$$

(A27)

The total exergy of the statepoint includes the molar intensity of each compound by including the molar fraction of each compound.

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$$
\begin{aligned}
b_{statepoint} &= y_{CaCO_3} b_{CaCO_3} + y_{MgCO_3} b_{MgCO_3} \\
&= 0.94120 \; mol_{CaCO_3}/mol_{limestone}(43.92493 \; kJ/mol) \quad + 0.05880 \; mol_{MgCO_3}/mol_{limestone}(3.63 \\
&= 47.56342 \; kJ/mol
\end{aligned}
$$

(A28)

Note that the comminution exergy is small compared to the total value.

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$$
\begin{aligned}
\frac{b_{com}}{b_{total}} &= \frac{b_{com,CaCO_3} y_{CaCO_3} + b_{com,MgCO_3} y_{MgCO_3}}{b_{total}} \\
&= \frac{0.03298 \; kJ/mol(0.94120 \; mol_{CaCO_3}/mol_{limestone}) + 0.00045 \; kJ/mol(0.05880 \; mol_{MgCO_3}/mol_{li}}{47.56342 \; kJ/mol} \\
&= \frac{0.03107 \; kJ/mol}{47.56342 \; kJ/mol} \\
&= 0.00065 \; kJ/mol
\end{aligned}
$$

(A29)

Thus, we ignore comminution exergy when analyzing large material conversion chains.

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Appendix F RUVY matrices for unified material and energy conversion chain

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This appendix contains the **RUVY** matrices for the example presented in this paper, including (a) the independent material conversion chain (BCC), (b) the independent energy conversion chain (XCC), and (c) the unified material and energy conversion chain (BXCC). The basis for the conversion chains is 1000 kg of beneficiated iron ore. All matrices in Figures A1–A12 contain exergy values in MJ. Rows and columns are removed if all values are 0. Entries of 0.0 indicate non-zero values that round to 0.0 MJ. See the Supplemental Information for an Excel file containing these matrices.

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Appendix F.1 Independent material conversion chain (BCC)

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For the independent material conversion chain (BCC), Figure A1 shows the resource (**R**) matrix, Figure A2 shows the use (**U**) matrix, Figure A3 shows the make (**V**) matrix, and Figure A4 shows the final demand (**Y**) matrix.

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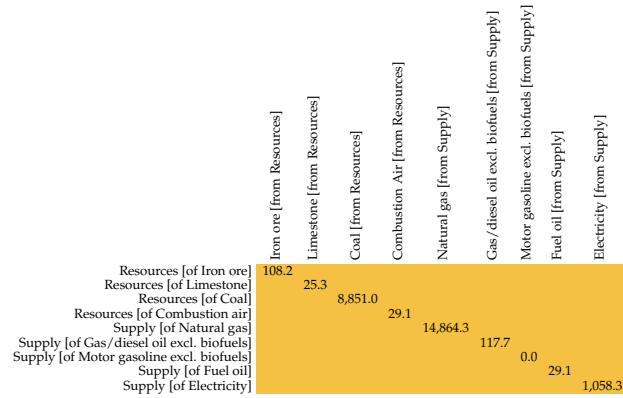
Figure A1. Resource (**R**) matrix for the example material conversion chain (BCC). All values are exergies in MJ.

Figure A2. Use (**U**) matrix for the example material conversion chain (BCC). All values are exergies in MJ.

	Iron ore [from Iron ore extraction]	Combustion emissions [from Iron ore extraction]	Limestone [from Limestone extraction]	Combustion emissions [from Limestone extraction]	Coal [from Coal extraction]	Combustion emissions [from Coal extraction]	Iron ore [from Iron ore hauling]	Limestone [from Limestone hauling]	Coal [from Coal hauling]	Iron ore [from Iron ore beneficiation]	Iron ore impurities [from Iron ore beneficiation]	Limestone [from Limestone beneficiation]	Coal [from Coal beneficiation]	Quicklime [from Rotary kiln]	Magnesium oxide [from Rotary kiln]	Kiln emissions [from Rotary kiln]	Anthracite [from Coke oven]	Coke oven gas [from Coke oven]	Tar [from Coke oven]	Ash [from Coke oven]	Combustion emissions [from Coke oven]	Treated coke oven gas [from COG treatment]	Treated coke oven gas [from COG distribution]	Blast furnace mixture [from Mixer]	Pig iron [from Blast furnace]	Blast furnace gas [from Blast furnace]	Pig iron slag [from Blast furnace]
Iron ore extraction	108.2	2.2																									
Limestone extraction			25.3	0.0																							
Coal extraction					8,855.8	0.6																					
Iron ore hauling							108.2																				
Limestone hauling								25.3																			
Coal hauling									8,855.8																		
Iron ore beneficiation										88.1	21.7																
Limestone beneficiation												25.3															
Coal beneficiation													8,855.8														
Rotary kiln														242.0	7.7	87.2											
Coke oven																	6,408.3	4,026.2	955.4	9.0	303.8						
COG treatment																						4,043.4					
COG distribution																							4,043.4				
Mixer																								6,684.1			
Blast furnace																									4,157.9	404.2	67.9

Figure A3. Make (**V**) matrix for the example material conversion chain (BCC). All values are exergies in MJ.

Figure A4. Final demand (**Y**) matrix for the example material conversion chain (BCC). All values are exergies in MJ.

Appendix F.2 Independent energy conversion chain (XCC)

For the independent energy conversion chain (XCC), Figure A5 shows the resource (**R**) matrix, Figure A6 shows the use (**U**) matrix, Figure A7 shows the make (**V**) matrix, and Figure A8 shows the final demand (**Y**) matrix.

Appendix F.3 Unified material and energy conversion chain (BXCC)

The unified material and energy conversion chain (BXCC) was created using the process discussed in Section 2.2.6. Figure A9 shows the resource (**R**) matrix. Figure A10 shows the use (**U**) matrix. Figure A11 shows the make (**V**) matrix. Figure A12 shows the final demand (**Y**) matrix.
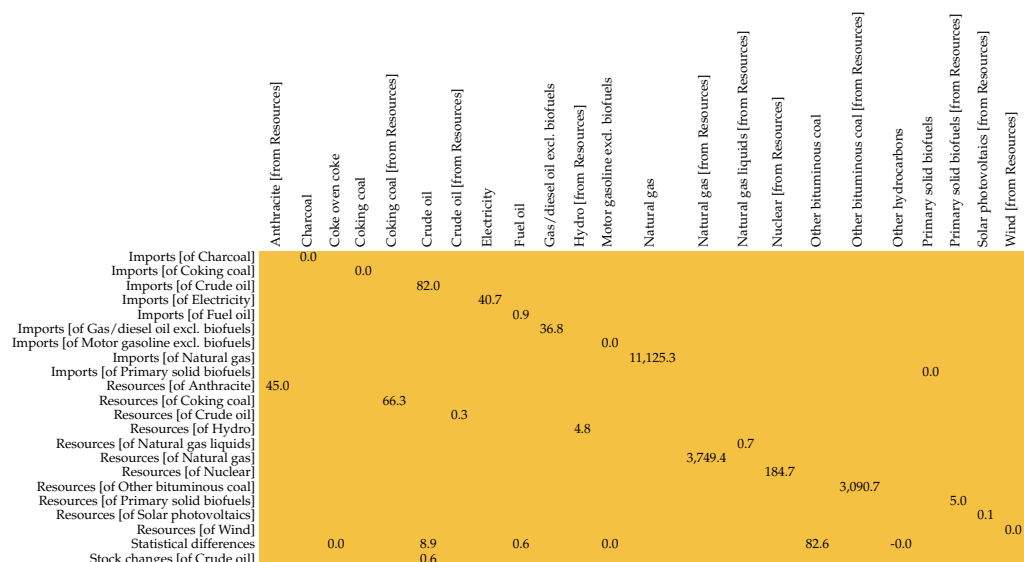
Figure A5. Resource (**R**) matrix for the example energy conversion chain (XCC). All values are exergies in MJ.
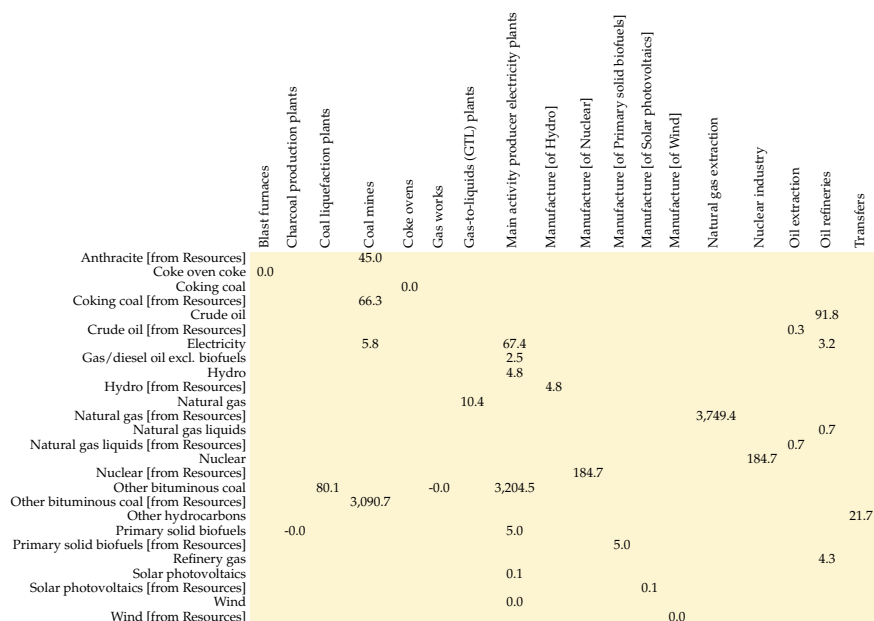
Figure A6. Use (**U**) matrix for the example energy conversion chain (XCC). All values are exergies in MJ.
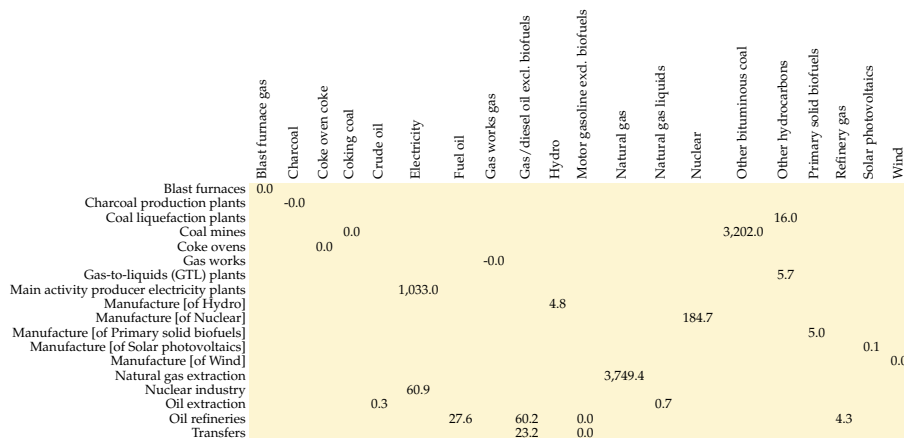
Figure A7. make (**V**) matrix for the example energy conversion chain (XCC). All values are exergies in MJ.

Figure A8. Final demand (**Y**) matrix for the example energy conversion chain (XCC). All values are exergies in MJ.

	Iron and steel
Electricity	1,058.3
Fuel oil	29.1
Gas/diesel oil excl. biofuels	117.7
Motor gasoline excl. biofuels	0.0
Natural gas	14,864.3
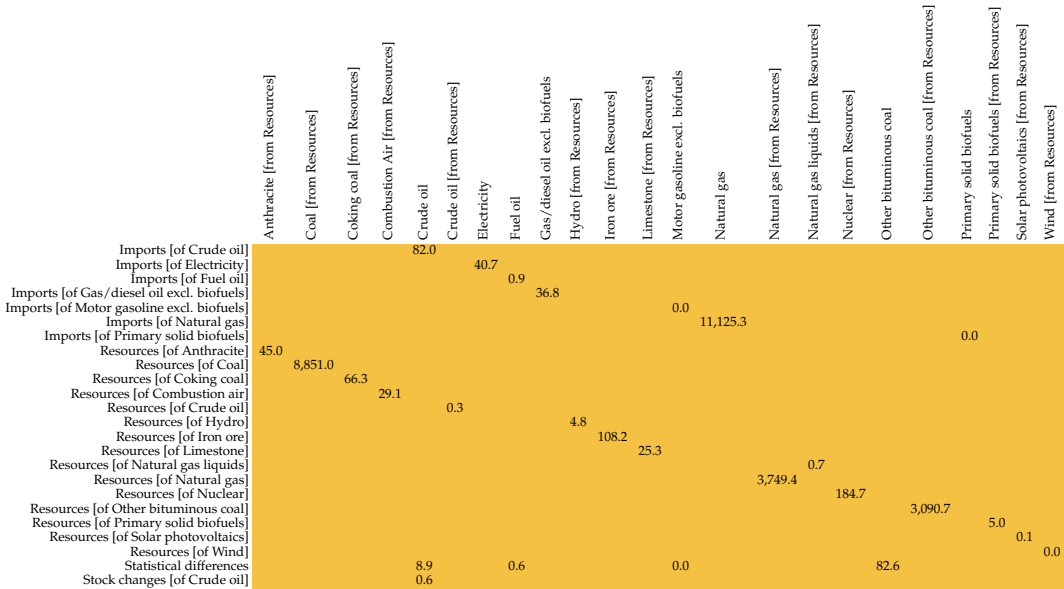
Figure A9. Resource (**R**) matrix for the example unified material and energy conversion chain (BXCC). All values are exergies in MJ.

	Crude oil	Electricity	Fuel oil	Gas/diesel oil excl. biofuels	Natural gas	Motor gasoline excl. biofuels
Imports [of Crude oil]	82.0					
Imports [of Electricity]		40.7				
Imports [of Fuel oil]			0.9			
Imports [of Gas/diesel oil excl. biofuels]				36.8		
Imports [of Motor gasoline excl. biofuels]						0.0
Imports [of Natural gas]					11,125.3	

	Anthracite	Coal	Coking coal	Combustion Air	Crude oil [from Res.]	Hydro	Iron ore	Limestone	Natural gas liquids	Natural gas [from Res.]	Nuclear	Other bituminous coal [from Res.]	Primary solid biofuels [from Res.]	Solar photovoltaics	Wind
Imports [of Primary solid biofuels]													0.0		
Resources [of Anthracite]	45.0														
Resources [of Coal]		8,851.0													
Resources [of Coking coal]			66.3												
Resources [of Combustion air]				29.1											
Resources [of Crude oil]					0.3										
Resources [of Hydro]						4.8									
Resources [of Iron ore]							108.2								
Resources [of Limestone]								25.3							
Resources [of Natural gas liquids]									0.7						
Resources [of Natural gas]										3,749.4					
Resources [of Nuclear]											184.7				
Resources [of Other bituminous coal]												3,090.7			
Resources [of Primary solid biofuels]													5.0		
Resources [of Solar photovoltaics]														0.1	
Resources [of Wind]															0.0

	Crude oil	Gas/diesel oil excl. biofuels	Natural gas	Other bituminous coal [from Res.]
Statistical differences	8.9	0.6	0.0	82.6
Stock changes [of Crude oil]	0.6			

Use (**U**) matrix table for the example unified material and energy conversion chain (BXCC):

Commodity	Blast furnace	Coal beneficiation	Coal extraction	Coal hauling	Coal liquefaction plants	Coal mines	COG distribution	COG treatment	Coke oven	Gas-to-liquids (GTL) plants	Iron ore beneficiation	Iron ore extraction	Iron ore hauling	Limestone beneficiation	Limestone extraction	Limestone hauling	Main activity producer electricity plants	Manufacture [of Hydro]	Manufacture [of Nuclear]	Manufacture [of Primary solid biofuels]	Manufacture [of Solar photovoltaics]	Manufacture [of Wind]	Mixer	Natural gas extraction	Nuclear industry	Oil extraction	Oil refineries	Rotary kiln	Transfers
Anthracite [from Coke oven]																							6,408.3						
Anthracite [from Resources]						45.0																							
Blast furnace mixture [from Mixer]	6,684.1																												
Coal [from Coal beneficiation]									8,855.8																				
Coal [from Coal extraction]				8,855.8																									
Coal [from Coal hauling]		8,855.8																											
Coal [from Resources]			8,851.0																										
Coke oven gas [from Coke oven]					66.3																								
Coking coal [from Resources]									4,026.2																				
Combustion Air [from Resources]	11.8		0.0						14.5			0.1			0.0														2.7
Crude oil																										0.3	91.8		
Crude oil [from Resources]																													
Electricity	318.9	0.1	80.6	0.3		5.8		33.2				12.6		609.8	0.0	2.8	67.4											3.2	
Fuel oil	29.1																												
Gas/diesel oil excl. biofuels			23.3										94.1			0.3	2.5												
Hydro																	4.8												
Hydro [from Resources]																		4.8											
Iron ore [from Iron ore beneficiation]																								88.1					
Iron ore [from Iron ore extraction]													108.2																
Iron ore [from Iron ore hauling]											108.2																		
Iron ore [from Resources]												108.2																	
Limestone [from Limestone beneficiation]																												25.3	
Limestone [from Limestone extraction]																25.3													
Limestone [from Limestone hauling]														25.3															
Limestone [from Resources]															0.0														
Motor gasoline excl. biofuels																													
Natural gas	2,329.4									10,583.8	10.4																		1,951.1
Natural gas [from Resources]																								3,749.4					
Natural gas liquids																											0.7		
Natural gas liquids [from Resources]																								0.7		0.7			
Nuclear																									184.7				
Nuclear [from Resources]																			184.7										
Other bituminous coal				80.1													3,204.5												
Other bituminous coal [from Resources]					3,090.7																								
Other hydrocarbons																													21.7
Primary solid biofuels																	5.0												
Primary solid biofuels [from Resources]																				5.0									
Quicklime [from Rotary kiln]																								242.0					
Refinery gas																												4.3	
Solar photovoltaics																	0.1												
Solar photovoltaics [from Resources]																					0.1								
Treated coke oven gas [from COG distribution]	2,830.4																												
Treated coke oven gas [from COG treatment]							4,043.4																						
Wind																	0.0												
Wind [from Resources]																						0.0							

Figure A10. Use (**U**) matrix for the example unified material and energy conversion chain (BXCC). All values are exergies in MJ.
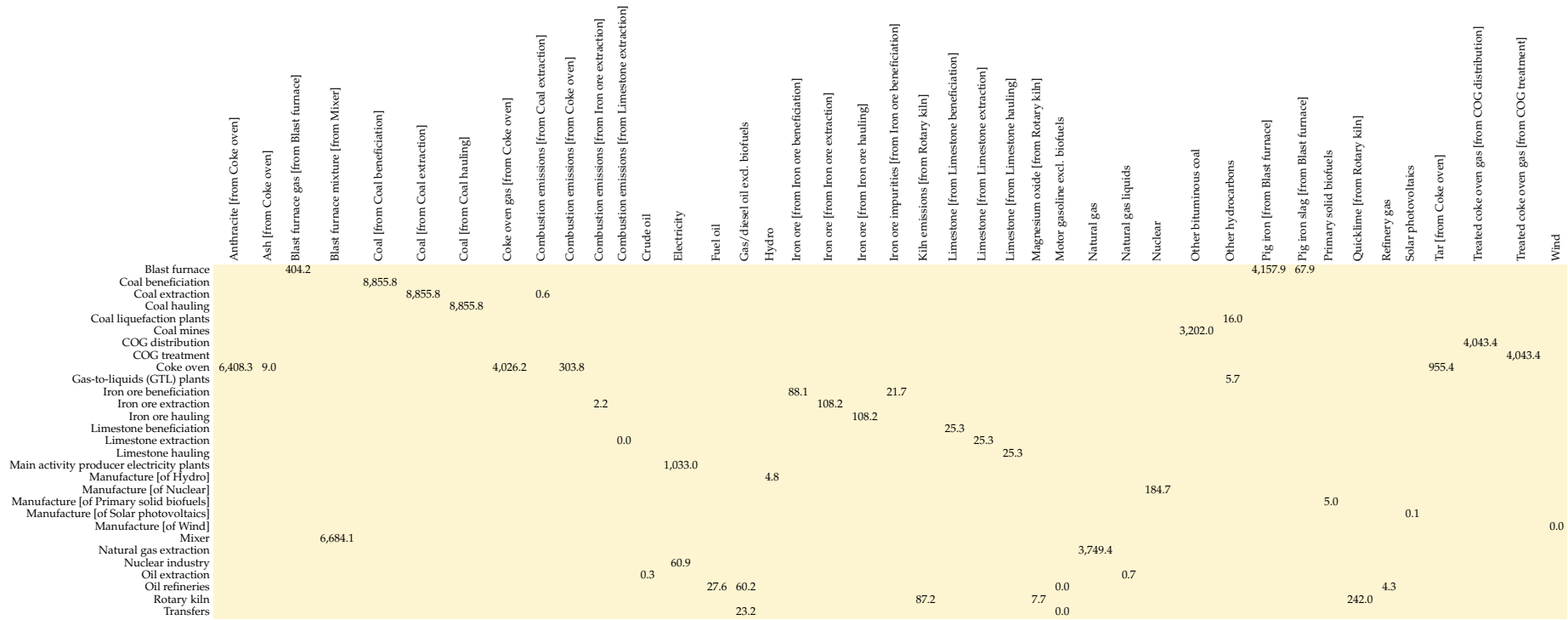
Figure A11. Make (**V**) matrix for the example unified material and energy conversion chain (BXCC). All values are exergies in MJ.

Make (**V**) matrix entries (producing process → commodity [source], value in MJ):

Process (row)	Commodity (column)	Value
Blast furnace	Blast furnace gas [from Blast furnace]	404.2
Blast furnace	Pig iron [from Blast furnace]	4,157.9
Blast furnace	Pig iron slag [from Blast furnace]	67.9
Coal beneficiation	Coal [from Coal beneficiation]	8,855.8
Coal extraction	Coal [from Coal extraction]	8,855.8
Coal extraction	Combustion emissions [from Coal extraction]	0.6
Coal hauling	Coal [from Coal hauling]	8,855.8
Coal liquefaction plants	Other bituminous coal	16.0
Coal mines	Other bituminous coal	3,202.0
COG distribution	Treated coke oven gas [from COG distribution]	4,043.4
COG treatment	Treated coke oven gas [from COG treatment]	4,043.4
Coke oven	Anthracite [from Coke oven]	6,408.3
Coke oven	Ash [from Coke oven]	9.0
Coke oven	Coke oven gas [from Coke oven]	4,026.2
Coke oven	Combustion emissions [from Coke oven]	303.8
Coke oven	Tar [from Coke oven]	955.4
Gas-to-liquids (GTL) plants	Other hydrocarbons	5.7
Iron ore beneficiation	Iron ore [from Iron ore beneficiation]	88.1
Iron ore beneficiation	Iron ore impurities [from Iron ore beneficiation]	21.7
Iron ore extraction	Combustion emissions [from Iron ore extraction]	2.2
Iron ore extraction	Iron ore [from Iron ore extraction]	108.2
Iron ore hauling	Iron ore [from Iron ore hauling]	108.2
Limestone beneficiation	Limestone [from Limestone beneficiation]	25.3
Limestone extraction	Combustion emissions [from Limestone extraction]	0.0
Limestone extraction	Limestone [from Limestone extraction]	25.3
Limestone hauling	Limestone [from Limestone hauling]	25.3
Main activity producer electricity plants	Electricity	1,033.0
Manufacture [of Hydro]	Hydro	4.8
Manufacture [of Nuclear]	Nuclear	184.7
Manufacture [of Primary solid biofuels]	Primary solid biofuels	5.0
Manufacture [of Solar photovoltaics]	Solar photovoltaics	0.1
Manufacture [of Wind]	Wind	0.0
Mixer	Blast furnace mixture [from Mixer]	6,684.1
Natural gas extraction	Natural gas	3,749.4
Nuclear industry	Electricity	60.9
Oil extraction	Crude oil	0.3
Oil extraction	Natural gas liquids	0.7
Oil refineries	Fuel oil	27.6
Oil refineries	Gas/diesel oil excl. biofuels	60.2
Oil refineries	Motor gasoline excl. biofuels	0.0
Oil refineries	Refinery gas	4.3
Rotary kiln	Kiln emissions [from Rotary kiln]	87.2
Rotary kiln	Magnesium oxide [from Rotary kiln]	7.7
Rotary kiln	Quicklime [from Rotary kiln]	242.0
Transfers	Electricity	23.2
Transfers	Magnesium oxide [from Rotary kiln]	0.0

Figure A12. Final demand (**Y**) matrix for the example unified material and energy conversion chain (BXCC). All values are exergies in MJ.

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