# A Thermodynamic Framework for Ecologically Conscious Process Systems Engineering

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*(to appear in Computers and Chemical Engg., special issue on "Selected Papers from PSE 2000")*

**Abstract:** Long term growth and well being of the chemical industry requires economically and ecologically conscious process engineering. Traditional process engineering methods fall short of meeting this need due to their treating the environment as being secondary to economic objectives. Life cycle assessment and design methods broaden the scope of traditional methods, but focus primarily on the environmental impact of emissions while ignoring the contribution of ecological products and services. Taking nature for granted could provide misleading results since natural products and processes are a significant contributor to all industrial products and processes. Methods from systems ecology do account for ecological inputs, but ignore the impact of emissions. This paper presents an original approach for the joint analysis of industrial and ecological systems. This approach considers inputs from both ecological and economic resources, as well as the impact of emissions. It uses thermodynamics to exploit the synergy between methods from process systems engineering, systems ecology, and life cycle assessment to overcome the shortcomings of methods from each field. The approach is based on the fact that growth and sustenance of both industrial and ecological processes are limited by the available energy and its conversion to useful work. Thus, the embodied energy (emergy), that is, the energy used directly or indirectly to make a product or service is a thermodynamic measure of ecological investment or cost, while exergy loss provides a holistic measure of the impact of emissions. Together, emergy and exergy analysis can provide insight into the environmental performance and sustainability of the industrial process or product. The proposed framework is broadly applicable to assist decision making in chemical and other engineering tasks. Challenges and research opportunities for making this framework practical are identified.

**Keywords:** Life Cycle Assessment, Ecosystem Services, Exergy, Emergy, Embodied energy.

## 1. Introduction

Increasing awareness of the impact of chemical and process engineering decisions on the environment has motivated the development of methods for environmentally conscious process engineering. Techniques have been developed for incorporating environmental considerations in all the process engineering tasks (Pistikopoulos, 1999; El-Halwagi and Petrides, 1994) including, process design and synthesis (Douglas, 1992; Ciric and Huchette, 1993; Linninger et al., 1997; Stefanis et al., 1997; Cabezas et al., 1999); process integration (Manousiothakis and Allen, 1995; El-Halwagi, 1997); process operation; product design and assessment (Hostrup et al., 1999). Most of these approaches have focused on reducing environmental impact at the scale of the equipment or process. Furthermore, many approaches have focused on maximizing the economic potential of a process while posing environmental and safety regulations or cost of waste treatment as constraints (Ciric and Huchette, 1993; Manousiothakis and Allen, 1995; Pistikopoulos et al., 1994). These approaches have been successful in modifying processes to prevent pollution and minimize waste at the scale of the process. Unfortunately, such an approach of minimizing waste only at the equipment or process scale, and of considering the environment to be ancillary to economic objectives is too narrow in scope, and often causes the environmental impact to shift from one domain or process to another without truly reducing or eliminating it (Cano-Ruiz and McRae, 1998; Allenby, 1998). For example, at the process scale, replacing lead-based solders by bismuth-based ones in electronics manufacturing may seem appropriate since bismuth is likely to be less toxic than lead. At a broader scale, the benefits of this change become questionable since bismuth is usually a by product of lead mining, and increasing use of bismuth is likely to cause increasing availability of lead (Allenby, 1998). Such examples and experiences highlight the need for a broader analysis for environmentally conscious decision making.

In response to this need for broader analysis, the technique of life cycle assessment (LCA) (Heijungs et al., 1996; Curran, 1996; Hofstetter, 1998) considers the impact of all the industrial processes in the life cycle of a product from extracting the natural resources to using and disposing the product. The steps in LCA have been standardized and widely applied to many products and processes. Life cycle methods for process design have posed the life cycle impact considerations as a constraint while maximizing the economic potential, or as part of the objective function (Azapagic and Clift, 1995). If life cycle impact is posed as a constraint, the resulting solution of the optimization problem gives greater importance to the economic objective function, and cannot do better than the constraint. Including both economic and environmental considerations in the objective function results in a multiobjective optimization problem, whose solution requires decisions about the relative trade-off between various objectives. Similar valuation based decisions are required in any life cycle assessment and several approaches have been proposed (Hofstetter, 1998). Excellent reviews on the topic of environmentally conscious process design are provided by Cano-Ruiz and McRae (1998) and Azapagic (1999).

Despite it's many benefits and popularity, LCA suffers from several shortcomings. It focuses primarily on the environmental impact of emissions and nonrenewable and energy inputs, while ignoring ecosystem services and products. Ignoring these inputs can cause significant error in the analysis and misleading results. Furthermore, LCA does not consider environmental sustainability of products or processes.

Thermodynamic techniques for waste minimization and environmentally conscious decision making have also been developed. These methods have been quite popular in chemical and mechanical engineering applications, and include process integration (El-Halwagi, 1997), and exergy analysis (Szargut et al., 1988). They are based on applying the first and second laws of thermodynamics to design thermodynamically optimal processes. Thus, heat integration methods integrate hot and cold process streams to maximize the feasible exchange of energy. Exergy or availability analysis focuses on the amount of energy that is available for conversion to useful work from any product or process. Since according to the second law of thermodynamics, exergy is always lost in any process, exergy analysis aims to design, retrofit and operate equipment and processes to reduce the amount of exergy lost.

Exergy analysis has also been used for assessing the environmental aspects of a process at a life cycle scale. The cumulative exergy consumed in all processes starting from natural resources such as minerals, wood, and water has been suggested as a measure of the ecological cost of any process (Szargut, 1986). Thus, analysis of the cumulative exergy consumption may be used for incorporating environmental considerations in engineering decision making (Morris, 1991; Mozes et al., 1998). Furthermore, the exergy content of emissions with respect to the natural environment may be related to their potential for harming the environment (Szargut et al., 1988) and has been suggested for use in LCA (Ayres et al., 1998). Despite these developments, the thermodynamic approach is still not adequate for incorporating ecological aspects in process engineering tasks, and for the combined analysis of industrial and ecological systems. Cumulative exergy consumption is a good but incomplete measure of the ecological cost of any product or service, since it does not consider the fact that natural resources require different amounts of ecological effort in their production. For example, the ecological effort required in making more concentrated sources of energy such as, coal and petroleum is significantly more than that required in making dilute forms such as, sunlight and wood.

A common deficiency of the existing methods for environmentally conscious engineering decision making is that they ignore the contribution of ecological products and services that sustain every industrial activity. Examples of such products and services include coal, petroleum, wood, water, wind, rain, pollination, and photosynthesis. This attitude of considering nature's products and services to be free and unlimited has resulted in their widespread deterioration as indicated by recent studies (WRI, 2000; WWF, 2000). These studies show a broad global decline in the ability of ecosystems to provide products and services such as, absorbing industrial emissions and providing fresh water and clean air. Since ecosystem products and services lack a traditional market value, several attempts have also been made to quantify their importance in monetary terms. For example, Costanza et al. (1997) have estimated the value of nature's products and services to be approximately twice that of the global gross national product. While these estimates are controversial, no one argues against the critical importance of natural processes to human well being and economic growth (Arrow et al., 1995; Pearce, 1998; Bockstael et al., 2000). Consequently, ecologically conscious decision making must consider the contribution of nature's services and products in the analysis of industrial systems.

Over the last several decades, systems ecologists have developed significant insight into the development and growth of ecological systems, and have formulated thermodynamic methods for measuring the ecological contribution to nature's products and services. These techniques are based on considering ecosystems to be networks of energy flow, and on the fact that the development and sustenance of natural systems is limited by the available energy and their ability to use the energy for themselves and other systems that they depend on. Since solar energy is the main source of energy for the planet, the ecological input in any product or service may be measured by the equivalent solar energy embodied in it (Odum, 1988, 1996). Methods based on analyzing thermodynamic properties such as the embodied solar energy and the exergy content provide information about the health and sustainability of ecosystems (Jorgensen, 1997). However, systems ecology methods ignore the impact of emissions, making them incomplete for analyzing the environmental aspects of industrial processes and products.

This paper proposes a thermodynamic framework for ecologically conscious process systems engineering that overcomes the shortcomings of existing methods in process engineering, life cycle assessment and systems ecology. The framework exploits the complementary nature of existing methods in these fields with the common link provided via thermodynamics. It permits the inclusion of ecological and economic factors, along with the impact of emissions in engineering decision making. The approach is based on considering ecological and industrial systems to be networks of energy flow. Since all materials and services in this network are transformed and stored forms of solar energy, the amount of solar energy used directly or indirectly to make any product or service can be used as a measure of the ecological input or investment in that product or service. Thus, solar embodied energy or solar emergy is used as a common currency for the analysis of industrial and ecological systems (Odum, 1988). Techniques are suggested for representing the impact of emissions in terms of the exergy loss or emergy change of the system perturbed by the emissions. The proposed approach extends the engineering approach of exergy and cumulative exergy analysis to include ecological processes and the impact emissions. It extends the systems ecology approach of emergy analysis to include the impact of emissions and links it with exergy analysis. The resulting energy flow diagram of an industrial process with its ecological and economic inputs and outputs can be analyzed by common metrics such as, return on investment and yield, as well as other metrics such as environmental loading and sustainability, to assist decision making.

The rest of this paper is structured as follows. A brief introduction to the principles of life cycle assessment and design along with the shortcomings of existing methods is provided in Section 2. This is followed in Section 3 by a short introduction to the principles of systems ecology, and the thermodynamic concepts of energy, exergy and emergy. The thermodynamic framework for the joint analysis of industrial and ecological systems is discussed in Section 4. The practical challenges for applying the proposed framework and methods for addressing them are discussed in Section 5 along with the preliminary results of the thermodynamic LCA of soybean growth.

## 2. Life Cycle Assessment and Design

LCA is a systematic approach for considering the environmental impact of a product or process throughout its life cycle from the extraction of materials from the environment to the use and disposal of the products (Curran, 1996; Heijungs et al., 1996). The steps in LCA have been standardized and include goal definition and scope, inventory analysis, impact assessment, and improvement assessment. The first step defines the goal of the LCA and determines the processes in the life cycle to be assessed. This is an important decision since if the LCA boundary is too narrow, important processes may be ignored, or if the boundary is too broad, the assessment may become less tractable. Inventory analysis collects information about the inputs and emissions in each stage of the life cycle. These data are usually representative of the process at a regional or national scale, as opposed to a specific plant or manufacturer, and large data bases have been compiled for obtaining this information (Vigon, 1996). Impact assessment is quite challenging and often controversial due to the variety of impacts of emissions, and the high degree of uncertainty due to a lack of knowledge and understanding. One of the important contributions of LCA is the standardization of impact assessment of a broad variety of emissions. Life cycle impact assessment (LCIA) involves classification of the emissions into various impact categories such as, abiotic depletion potential, energy depletion potential, global warming, ozone depletion, human toxicity, ecotoxicity, etc. Different emissions are converted into equivalents of selected reference substances such as, equivalents of $CO_2$ for global warming, and equivalents of $SO_2$ for acidification. The quantified contribution in each impact category is then normalized by the size of the local or global problem. The next step requires determining the relative importance of various impact categories, that is, the importance of global warming versus eutrophication versus human toxicity versus depletion of nonrenewable resources. This step is particularly controversial and difficult due to the need for human valuation, and many approaches have been suggested (Giegrich and Schmitz, 1996; Hofstetter, 1998).

A recently developed LCIA method is the eco-indicator 99 (Goedkoop and Spriensma, 2000). This approach considers LCIA to be the analysis of three related spheres, the technosphere, ecosphere, and valuesphere (Hofstetter et al., 2000; Hofstetter, 1998). The technosphere or anthroposphere is the domain of technological processes and systems developed by human beings, including industrial systems. The ecosphere is the domain of ecological processes and systems, and subsumes the technosphere. Finally, the valuesphere is the domain of societal or human valuation, and includes both the ecosphere and technosphere. Impact on human beings is quantified by measures such as, disability adjusted life years, while that on the environment in terms of the potentially affected and potentially disappeared fractions of species. Finally, a single indicator is obtained according to the selected valuation approach.

Life cycle approaches have also been used for process systems engineering tasks such as process design, and optimization. Life cycle process design incorporates environmental considerations as constraints or as a part of the objective function. If environmental concerns are posed as inequality constraints, the bounds for these constraints are determined from regulatory requirements, or from life-cycle considerations (Pistikopoulos et al., 1994). Environmental considerations have been included in the objective function as the cost of waste treatment and disposal, or by combining the economic objective with life cycle impact considerations (Cabezas et al., 1999; Azapagic, 1999). Solving the resulting multiobjective optimization problem requires decisions about the relative importance of the economic objective versus various environmental impacts. This trade-off may be addressed by assigning weights to the economic and environmental objectives by human valuation or other criteria.

The systematic consideration of emissions and environmental impact beyond the scale of the process via the life cycle approach is an important advance in environmentally conscious process engineering. In spite of these developments, existing approaches for environmentally conscious process engineering still face many shortcomings. The most significant deficiency, as mentioned in Section 1, is that existing methods ignore the critical need for ecological products and services for making the desired industrial products by the selected processes. These products and services are also not included in economic analysis, since they are not directly valued by the economy, that is, the economy does not pay a price to the environment for these products and services. There is no doubt that these products and services are of critical importance since they constitute the life-support system for the planet (Daily, 1997; Costanza et al., 1997; Arrow et al., 1995; WRI, 2000).

Current LCA methods do account for ecosystem services that are affected by the process or product that is being analyzed. For example, LCA does consider the depletion of non-renewable resources, as well as effects of impact categories such as, ecotoxicity and acidification. As shown by the preliminary results in Section 5.4 of this paper, LCA still ignores a significant portion of ecosystem services.

Existing life cycle and environmentally conscious systems engineering methods lack a systematic and quantitative framework that can be used for assessing both industrial and ecological processes and the impact of their emissions together. The lack of such a framework also does not allow quantitative comparison of the environmental sustainability of processes. Such a framework is developed in this paper based on extending the principles of systems ecology to process systems engineering.

## 3. Systems Ecology and Thermodynamics

Systems ecologists have developed methods for assessing, analyzing and modeling the behavior of ecological systems. Like many techniques in process systems engineering, many techniques in systems ecology are also based on principles of thermodynamics. This common link between systems engineering and systems ecology permits the development of the proposed framework for the combined analysis of industrial and ecological systems. This section introduces some basic principles of systems ecology that are relevant to the framework proposed in this paper.

### 3.1 Energy Flow Diagrams

Ecological systems use flows of energy and mass to remain in a self-organized state that is far from equilibrium. The ultimate driving force for the development of ecosystems is solar energy. Even materials such as nutrients in soil, water and oxygen, are generated directly or indirectly by the capture and transformation of solar energy. Thus, ecosystems may be considered to be networks of energy flow, and all ecological products and services are transformed and stored forms of solar energy (Odum, 1988). Ecologists have developed an energy flow chart language and many techniques for analyzing these charts. This language is better suited for the analysis of ecological and industrial systems together than a similar language developed for energy flow analysis of industrial systems (IFIAS, 1974). The energy flow in a simple food chain is represented in Figure 1. As energy moves through the food chain, its quantity decreases, as required by the second law of thermodynamics, but its quality and concentration increase. Thus, higher organisms such as, predators, require more resources per unit of energy available than lower organisms such as, plants. Higher organisms also contain a higher quality of energy since they are able to perform more types of work and can control the lower organisms. Analysis of energy flow diagrams requires the concepts of eNergy, eXergy and eMergy.

### 3.2 Energy, Exergy, and Emergy

*Energy* is a state variable that is easy to calculate, and satisfies the law of conservation. It is commonly, but mistakenly used as a measure of the ability to do work. In fact, energy is not really a measure of the ability to do work, since according to the second law of thermodynamics, not all the energy can be converted to useful work. Cumulative energy is defined as the sum of the energy content of the fuels used directly or indirectly to make a product. Energy analysis and cumulative energy analysis have been used for the analysis of industrial systems (Boustead and Hancock, 1979) but are of limited use since they do not consider non-fuel materials and the amount of energy actually available to do useful work.

*Exergy* is the energy that can be converted to work when the system is brought to equilibrium with its environment or reference state. Thus, exergy is the entropy-free energy, and is a true measure of the ability to do work. It may be calculated as (Tester and Modell, 1997),

$$B = \left(U - T_0 S + PV + \sum \mu_i N_i + v^2/2 + zg\right) - \left(U - T_0 S + PV + \sum \mu_i N_i + v^2/2 + zg\right)_0 \qquad (1)$$

where, $U$, $T$, $P$, $\mu_i$, $N_i$, $v$, $z$, $g$ denote the internal energy, temperature, pressure, chemical potential, number of moles, velocity, height, and gravitational acceleration, respectively. The subscript, *0* denotes the reference state. Under certain conditions, exergy becomes equivalent to Gibbs free energy, Helmhotz free energy or enthalpy. Exergy is a state variable, since its value depends on the selected reference state. The reference state may be selected to be that of the system at equilibrium or of the natural environment, which is far from equilibrium (Szargut et al., 1988). The value of exergy is independent of the path taken to produce the product. Typical exergy flow in a food chain is shown in Figure 1.

Exergy analysis has been used extensively for identifying inefficiencies and opportunities for saving energy in industrial systems (Szargut et al., 1988; Morris, 1991; Mozes et al., 1998). These efforts aim to minimize the cumulative exergy consumption of a process starting with natural resources as inputs. Thus, cumulative exergy consumption considers the total exergy consumed of all natural resources including non-energetic ones, making it more useful than cumulative energy consumption. Since exergy is a measure of the distance of a product or process from equilibrium, it has also been suggested to be a measure of the potential for emissions to cause environmental degradation (Ayres et al., 1998).

Although exergy is a more useful concept than energy, it only provides information about the current state of the system, and its future ability to do work. It does not provide any information about the quality of the available energy. Thus, the concept of exergy does not indicate that electrical exergy can do more types of work than the same amount of solar exergy. Furthermore, exergy or cumulative exergy provide no information about the thermodynamic or energy history of the product or service in terms of ecological inputs. These shortcomings are overcome by the concept of emergy.

*Emergy* is the embodied energy or energy memory in any product or service. It is defined as the total amount of energy needed directly or indirectly to make any product or service (Odum, 1988). The emergy content of a product or process is the investment made by the ecosystem in that product or service. Consequently, emergy can be used as a measure of ecological cost. Since the ability to do work can be different for different kinds of energy, it is essential to convert all types of energies into a common unit before combining them. For convenience, units of solar energy are usually selected as the common unit. Thus, solar emergy is the amount of solar energy used directly or indirectly to make a service or product. Solar emergy is measured in solar emergy Joules or solar emjoules (sej). For the energy flow diagram shown in Figure 1, the emergy of each product remains unchanged. As depicted in Figure 1, as solar energy moves to higher quality or more concentrated forms, the actual exergy content decreases. The relationship between emergy, $\mathcal{M}$, and the exergy contained in an item is given via the transformity, $\tau$, as,

$$\mathcal{M} = \tau B \tag{2}$$

The units of solar transformity are sej/J. The transformity of solar energy is defined to be unity. For the process in Figure 1, the transformity increases as the energy becomes more concentrated and of higher quality. Thus, transformity is a measure of energy quality.

The values of emergy and transformity depend on the path taken to reach the state. This path dependence makes it more challenging to determine these variables, since their values may change with the efficiency of the transformation processes. Fortunately, the transformities of ecological products and services vary over a very narrow range since these processes have evolved to become very efficient. These transformities have been computed by Odum (1996). In contrast, the transformity of industrial products and services varies according to the selected raw materials and the production efficiency, making them more challenging to determine.

The properties of energy, exergy and emergy are compared in Table 1. Among the three, energy is the only quantity that is conserved. Exergy and emergy complement each other, since emergy is a measure of the energy used in the past to get to the current state, while exergy is a measure of the energy available to do work in the future. Furthermore, emergy is a measure of the environmental inputs to the product or service, while exergy is a measure of the potential output from the product or service to the environment.

Emergy is quite different from cumulative energy since non-fuel materials are included in emergy. Cumulative exergy consumption considers the total amount of exergy consumed starting with natural resources such as, water, petroleum, and minerals (Szargut et al., 1988; Morris, 1991; Mozes et al., 1998). However, unlike emergy, cumulative exergy consumption ignores the ecological processes and services required for creating the natural resources. Systems ecologists have shown that the ecological effort required for producing different natural resources can vary significantly. For example, the solar emergy Joules required per Joule of available energy in resources such as, plantation pine wood, coal and limestone is 6,700 sej/J, 40,000 sej/J, and 1,620,000 sej/J respectively (Odum, 1996). Consequently, the cumulative exergy consumption can be very different from emergy for the same process or product. If a common basis, such as solar energy, is used for determining the cumulative exergy consumption by multiplying the exergy of natural resources by their transformity, then the cumulative exergy consumption can become equivalent to emergy of the product. Additional details about the relationship between emergy and exergy are provided by Hau and Bakshi (2001).

### 3.3 Characteristics of Ecological Systems

Understanding the behavior and functioning of ecological systems is crucial for determining their response to perturbation and importance to society. Since ecosystems are networks of energy flow, thermodynamic methods have been popular for their analysis and modeling. These studies indicate that ecosystems use the flow of energy to self-organize and remain far from equilibrium. Since the three laws of thermodynamics do not explain the behavior of ecosystems and other self-organized systems, significant research has focused on determining the thermodynamic goal functions or organizing principles that determine the development and growth of such systems. In 1905, Ludwig Boltzmann (1974) indicated that “life is a struggle for the ability to perform work”. In 1944, Erwin Schrödinger (1992) said that living systems maintain themselves stationary at a fairly high level of orderliness by “sucking orderliness from the environment”. Alfred Lotka (1925) formulated the maximum power principle which states that systems prevail that develop designs that maximize the flow of useful energy. This principle has been extended by Odum to explain the structure of ecosystems in terms of the rate of emergy flow. Other more recent suggestions for goal functions include maximization of entropy production (Prigogine and Stengers, 1984), maximization of energy dissipation (Schneider and Kay, 1994), and maximization of exergy storage (Jorgensen, 1999). These goal functions indicate that ecological and other self-organized systems create order by maximizing disorder (entropy production) in the surroundings. This is consistent with ecosystems maximizing exergy dissipation in response to an exergy gradient, that is, ecosystems try to degrade any available energy. Maximizing entropy production and exergy dissipation are consistent with maximizing exergy storage since increasing self-organization also increases stored exergy. These and other goal functions are shown to consistent with each other and represent different stages of ecosystem development (Fath et al., 2001).

The effect of perturbation on an ecosystem has also been studied in similar thermodynamic terms. In general, a harmful perturbation brings the system closer to equilibrium and causes the goal functions to change in a direction opposite to that required for ecosystem development and sustenance. Any input to an ecosystem may be represented by the amount of emergy contained in the input, while the resulting perturbation may be represented as the change in stored exergy of the ecosystem. Thus, increasing the flow of a harmful pollutant increases the emergy content of the ecosystem, but decreases its stored exergy, while decreasing this flow increases the stored exergy. The ratio of the change in emergy of inputs to the resulting change in stored exergy of the ecosystem may be used to quantify the effect of pollutants (Bastianoni, 1998). A harmful perturbation has a negative ratio of emergy input to exergy change of the system, indicating a loss (gain) of ecosystem exergy due to the addition (removal) of the perturbing factors. This insight indicates that exergy loss or corresponding emergy change can provide a holistic measure of the impact on a self-organized system. The emergy change due to perturbation may be determined as the product of the exergy loss and transformity of the affected processes and products. Unlike exergy, emergy is never lost, but can be recycled or moved to another system, as shown in Figure 2. Such a measure is used in the proposed framework to represent the impact of emissions.

## 4. Thermodynamic Analysis of Industrial and Ecological Systems

Both, ecological and economic systems are examples of self-organized systems (Jorgensen, 1997; Krugman, 1996), and are governed by the same laws of thermodynamics (Ayres, 1994). Furthermore, industrial and ecological systems may be represented jointly as networks of energy flow, and may be analyzed by thermodynamic methods. Such an approach provides a thermodynamic framework for the combined analysis of both systems. Although thermodynamic methods have been popular in many fields including, process systems engineering, systems ecology, and life cycle assessment, there has been virtually no interaction between these fields. Consequently, thermodynamic methods for the joint analysis of industrial and ecological systems have not been developed to date. Existing thermodynamic methods in systems ecology, process systems engineering, and life cycle assessment are not comprehensive enough. For example, thermodynamic methods in engineering such as, exergy and cumulative exergy analysis ignore the impact of emissions and the contribution of ecological inputs. Systems ecologists have extended their methods to include economic and industrial processes along with ecological systems. For example, joint analysis of agricultural and ecological systems using emergy has been presented by Lagerberg and Brown (1999) and Bastianoni and Marchettini (1996). However, these methods ignore the impact of emissions.

This paper presents a comprehensive thermodynamic approach that overcomes the shortcomings of existing methods in process systems engineering, life cycle assessment, and systems ecology. The resulting approach exploits the synergy between life cycle impact assessment, exergy and emergy analysis to include the ecological and economic inputs as well as impact of emissions in the analysis. This approach is new and is the first thermodynamics-based method of its kind. Additional details are provided in the rest of this section.

### 4.1 Energy Flow in Industrial and Ecological Systems

The energy flow diagram of Figure 1 may also represent flow in industrial and ecological systems with plants being converted to coal and coal to electricity. In general, a typical energy flow diagram for an industrial process may be represented as shown in Figure 2. This diagram uses the language for energy flow analysis developed by Odum (1996), and shows the flow of energy, exergy and emergy through renewable and nonrenewable resources, the ecosystem, the industrial systems being studied, and the economy. For simplification, all the ecological and industrial processes are lumped together in their respective blocks. The industrial processes include all the relevant manufacturing and waste treatment processes. In general, the direct inputs to the industrial processes include local nonrenewable resources, $N$, local renewable ecosystem services and products, $R_1$, and inputs from the economy, $F_1$. The economic inputs represent things that are valued by the economy and involve a monetary transaction. The outputs include the main products that are sold in the market, $Y$, and emissions that return to the environment, $W$. These emissions may require ecosystem services for their dissipation, and may harm the ecological or economic systems. The ecosystem outputs, $R_2$ and $R_3$ represent nature's services needed to dissipate the emissions, and the ecological impact due to the emissions, respectively. Similarly, the economic input, $F_2$, denotes the economic impact of the emissions.

The relationship between existing methods and the proposed approach may be understood based on which streams from Figure 2 are included in the analysis, as summarized in Table 2. Traditional economics only considers streams to and from the economy. It does not account for ecological products and services, since the economy does not pay money for environmental services and products. The renewable and local nonrenewable inputs are economically free, and are often readily available in the ecosystem.

Life cycle assessment methods focus mainly on emissions to the environment and depletion of resources. Thus, as shown in Table 2, LCA accounts for streams $N$, $W$, $R_2$, and $F_1$. Like economic methods, LCA also tends to overlook most ecological products and services. For ecologically and economically conscious decision making it is important to account for all the inputs to the selected industrial processes.

Most applications of emergy analysis ignore the impact of emissions on the environment and economy (Odum, 1996; Brown and Ulgiati, 1997; Lagerberg and Brown, 1999). Thus, emergy analysis accounts for streams, $R_1$, $N$, $F_1$, and $Y$. This results in the implicit assumption that the emissions are benign. Such an assumption is okay for the analysis of ecological systems, but can cause serious errors in the analysis of industrial systems. Recent work by Ulgiati and Brown (1999) accounts for the ecosystem services required for diluting pollutants, $R_2$, but still ignores the impact of the emissions, $R_3$, which can be very significant for many industrial processes. In contrast to existing methods, the approach proposed in this paper accounts for all the streams in Figure 2, as shown in Table 2, making it the most comprehensive and complete approach for ecologically conscious decision making.

## 4.2 Metrics for Assessing Industrial and Ecological Systems

The energy flow chart shown in Figure 2 may be analyzed to assess the ecological and economic viability of industrial processes, and to compare different products and processes. A product or process with lower emergy is not necessarily better than one with a higher emergy. Consequently, metrics similar to those used in economic analysis can be defined to determine the ecological feasibility, environmental loading and sustainability of a product or process. The net emergy is the emergy gained by the economy in exchange for providing its services. It is defined as (Odum, 1996),

$$\mathcal{M}_{net} = Y - F_1 \qquad (3)$$

and is analogous to the economic potential or profit from a process, but in terms of emergy. For any process to be “thermodynamically profitable” for the economy, the net emergy must be positive. That is, the product must contribute more emergy to the economy than the emergy in the economic inputs needed to make it. The emergy yield ratio,

$$\mathrm{EYR} = Y/F_1 \qquad (4)$$

is the emergetic return on investment. Since money is an incomplete measure of ecological goods and services, the net emergy and emergy yield ratio provide a more complete estimate of whether the process is feasible. Alternatively, the net emergy and emergy yield ratio in Equations (3) and (4) may be computed by replacing $F_1$ by $F_1+F_2$ to include the economic impact of emissions.

Other emergy-based metrics have also been defined to assess the environmental loading and sustainability of the process (Brown and Ulgiati, 1997). The environmental loading ratio may be defined as,

$$\text{ELR} = \frac{\left(N + F_1 + F_2 + R_2 + R_3\right)}{R_1} \tag{5}$$

The ELR is an indicator of the stress on the local environment. Since it is desirable to have a higher emergy yield per unit of environmental loading, the sustainability index is defined as,

$$\text{SI} = \text{EYR/ELR} \tag{6}$$

Determining the ELR and SI requires information about the emergy flow from renewable and nonrenewable sources. This information is not required for determining the net emergy and EYR.

## 4.3 Illustrative Example

A simple energy flowchart is shown in Figure 3. The energy and money flows are purely for illustrative purposes and do not represent any real process. The numbers in bold and italics represent the emergy content of each stream. The energy or money flows are indicated by the number in regular font below the emergy value. The loss of energy in each process is denoted by the thin lines going to the sink. The emergy and exergy content of these dissipative streams is zero. The thicker lines denote the flow of emergy and exergy. The emergy values are determined based on conservation or assumed transformities or emergy to money ratio, as discussed in the next section. The emergy content of multiple streams leaving a process may be determined according to the split of exergy between the streams. The emergy under various situations in the energy flow diagram is determined by the emergy network algebra discussed by Odum (1996).

For this energy flow diagram, the net emergy and emergy yield ratio may be computed by Equations (3) and (4) to be 2500 sej and 2 respectively. Including the economic impact of emissions reduces the net emergy and EYR to 1500 sej and 1.43 respectively. The environmental loading ratio and sustainability index may be computed by Equations (5) and (6) to be 1.31 and 1.09, respectively.

Most of the energy flows may be determined from information about inputs to the industrial processes and material and energy balances. Such information about natural resources and economic inputs is available for many processes (Boustead and Hancock, 1979; Szargut et al., 1988). The emergy content of each stream may be determined if the transformities of the inputs are available. The practical challenges and potential approaches for determining the emergy flow rates of each stream are discussed next.

## 5. Practical Challenges

Using the proposed thermodynamic framework for ecologically and economically responsible decision making requires methods for determining the flow rates of each of the input and output streams shown in Figure 2. This section identifies the challenges in determining the value of each stream, and discusses some potential approaches. The success of the proposed framework hinges on meeting these challenges, and is an area of active research.

### 5.1 Economic inputs

Economic inputs are transformed forms of solar energy that have a monetary value. Their emergy content can be determined easily if their quantity or exergy content and corresponding transformity are available. Unfortunately, such information may not be readily available. Consequently, determining the emergy content of economic inputs requires accounting for all the direct and indirect natural resources and services used to make that input. Such accounting is also required in the inventory analysis step of life cycle assessment. Consequently, the databases and techniques devised for inventory analysis in LCA may be used to obtain information about all the inputs within the defined boundary for the selected processes. The emergy content of inputs that are in the form of natural resources may then be determined based on knowledge about the transformity of these resources. Transformities of natural resources and services are available from the systems ecology literature (Odum, 1996).

If the natural resource requirements are not known, transformities are not available, or life cycle inventory data are not available, the emergy content of economic inputs may be assumed to be proportional to its monetary value. In such cases, the emergy content may be approximated as,

$$\mathcal{M} = \mathcal{M}_{region} \times \frac{\$}{\$_{region}} \tag{7}$$

where, \$ is the amount of money to be converted to emergy, $\mathcal{M}_{region}$ is the total emergy of the regional or national system including natural and economic inputs, and $\$_{region}$ is the region or nation’s gross economic product. This approach is commonly used in emergy analysis of ecological and economic systems (Odum, 1996; Bastianoni and Marchettini, 1996; Lagerberg and Brown, 1999).

### 5.2 Ecological inputs

Ecological inputs, $N$ and $R_1$ represent the local ecological resources used by the processes being analyzed. These inputs lie outside the market and are not valued by the economy. Their flow rates may be determined based on knowledge about the processes being analyzed. Ecological services,

$R_2$ are also required for dissipating and diluting emissions such as, wind for emissions to air, river or ocean currents for emissions to water, and photosynthesis for absorbing carbon dioxide. The emergy content of the required ecological services may be determined based on knowledge of the quantity of required ecological service and its transformity. For example, the emergy of wind required to dissipate emissions may be determined as (Ulgiati and Brown, 1999),

$$\mathcal{M}_{wind} = E_{kinetic}\tau_{wind}$$

where, $E_{kinetic}$ is the kinetic energy of the mass of wind required for the necessary dilution, and $\tau_{wind}$ is the transformity of wind. Calculating the kinetic energy of wind requires information about the concentration of the emissions, the acceptable dilute concentration, and average wind velocity. Unlike transformities of industrial products, transformities of ecological products and services tend to remain relatively constant since natural processes have become quite efficient due to evolutionary pressures.

### 5.3 Impact of Emissions

Emissions from industrial processes can harm the ecosystem, people, and the economy. The framework presented in this paper can be used to consider a variety of impacts, if they can be converted into energy flows. As discussed in Section 3.3, the loss of exergy stored in the ecosystem can provide a holistic measure of the impact of emissions. Using this measure requires methods for determining the exergy loss for each type of impact. Although many methods have been developed for impact assessment, they do not represent the impact in terms of exergy loss. The rest of this section discusses potential approaches for quantifying the impact of emissions in thermodynamic terms.

Life cycle impact assessment (Heijungs et al., 1996) classifies the emissions into various impact categories. The results of such a study are measures such as the global warming potential, ozone depletion potential etc., as illustrated in Section 5.4. Converting such outputs into an exergy loss requires knowledge about the mechanism and extent of the effect of the emissions on human well being and the environment. The recently developed eco-indicator99 approach is a step in this direction since it assesses the impact of emissions to human beings and ecosystems (Goedkoop and Spriensma, 2000). The impact on human well being is measured by Disability Adjusted Life Years (DALY). This represents the years of life lost and years lived disabled due to the impact of emissions, and is based on an approach developed by the World Health Organization. Ecological impact is represented by the Potentially Affected Fraction (PAF) or Potentially Disappeared Fraction (PDF) of species in the affected ecosystem. This analysis uses ecological models, which are currently restricted to the Netherlands or Europe. The output of a LCIA approach such as eco-indicator99 may be converted to a corresponding exergy loss, or emergy input, $R_3$. This is an area of active research, and additional knowledge and integration with ecological models is expected to improve the quality of the thermodynamic analysis.

The economic impact is often easier to quantify since many studies have estimated the monetary loss due to emissions. This monetary loss can be converted to emergy via Equation (7). For example, the economic impact of global warming by 3˚C due to $CO_2$ doubling by 2090 from pre-industrial levels is estimated to be $\$ 50.3 \times 10^9$ for the U.S. in 1988 U.S. dollars (Nordhaus, 1994). Using the emergy to money ratio for 1988 U.S. dollars of $1.75 \times 10^{12}$ sej/\$ (Odum, 1996), the emergy cost of global warming is $88 \times 10^{21}$ sej. Dividing this emergy cost by the total kilograms of $CO_2$ equivalent emitted that is, 590 billion metric tons of C equivalent results in a transformity of $1.5 \times 10^8$ sej/kg of C equivalent emitted in the U.S.

## 5.4 Example - Thermodynamic Life Cycle Assessment of Soy Bean Growth

The framework presented in this paper can be used for incorporating ecological considerations in any process systems engineering task. This section discusses the application of the proposed framework to life cycle assessment, and illustrates the complementary nature of LCA and emergy analysis. This example is based on preliminary and approximate data, and is presented only for illustrative purposes. The complete example with more accurate data will be presented in the future.

Traditional LCA focuses on the most significant processes in the life cycle of the product. For LCA of soybean oil, Heijungs et al. (1996) select the following processes: soybean production, steam production, transport by road, electricity production, and soybean oil production. Other processes such as, fertilizer production, insecticide and herbicide production, and hexane production are not included in this LCA boundary. Further discussion about defining the LCA boundary is available in the LCA literature (Curran, 1996; Heijungs et al., 1996).

The data considered by traditional LCA for the soybean growth phase is shown in Table 3. The inputs considered for growing soybeans include the seeds, fertilizers, insecticides, herbicides and fuel. The outputs are determined based on a worst case assumption that all the fertilizers, insecticides and herbicides go to water as emissions. The emissions data are classified into several impact categories and characterized in common units for each category based on equivalency factors. The results of these steps are summarized in Table 4. These results are normalized by the global outputs in each category and then combined by a valuation step. Several valuation methods are discussed by Heijungs et al. (1996), Curran (1996), and Hofstetter (1998).

Traditional LCA focuses mainly on resource depletion, emissions, and their impact, while ignoring ecological products and services required as inputs and to dissipate and absorb the emissions. The thermodynamic framework proposed in this paper can overcome these shortcomings. Since data about ecological inputs for soybean growth are not readily available, this example uses sunlight, rain, water, soil erosion, and labor data for sugarcane growth (Bastianoni and Marchettini, 1996) as a crude approximation. Transformities for these inputs are obtained from Bastianoni and Marchettini (1996) and Odum (1996). The emergy content of other non-renewable inputs such as, fertilizers and insecticides is calculated based on transformities provided by Odum (1996). The only impact considered in this analysis is the economic impact due to the global warming potential (GWP). The other impact categories shown in Table 4 also need to be converted into thermodynamic measures, and included in Table 5. Methods for this task are discussed in Section 5.3 and are a part of on-going research.

While the numbers in Table 5 are incomplete for a full thermodynamic LCA of soybean growth, they do indicate that the emergy content of ecological inputs is at least as important as that of economic inputs. These numbers also show that ignoring the ecological and economic inputs, as done by conventional LCA, is incomplete and can provide misleading results. The emergy analysis (Table 5) focuses mainly on the ecological and economic inputs required for soybean growth, while LCA (Table 4) focuses mainly on the impact of emissions. Thus, emergy analysis and traditional LCA complement each other, which justifies their combination as proposed in this paper.

## 6. Conclusions

A new approach for ecologically conscious process systems engineering is described. This approach combines techniques from process systems engineering with those from systems ecology and life cycle assessment to include the contribution of ecological products and services along with economic inputs and impact of emissions in process analysis. Examples of ecological products and services include, sunlight, rain, and soil formation. These inputs are at least as important as the economic inputs, but are usually not measured by money, and are ignored by most existing environmentally conscious engineering methods including, life cycle assessment and design, energy analysis and exergy analysis. Such an approach of taking nature for granted has resulted in significant deterioration of ecological products and services.

The approach for ecologically conscious PSE is based on considering energy to be the common driving resource for the development and sustenance of both industrial and ecological systems. Since renewable and nonrenewable resources as well as products and services are created directly or indirectly from solar energy, the approach developed in this paper analyzes processes and products based on the embodied solar energy. This embodied energy is called emergy, and has been used by systems ecologists for analyzing, assessing and modeling ecological systems (Odum, 1996). Emergy based metrics may be used to assess the economic and ecological feasibility and sustainability of processes. Emergy complements exergy since emergy measures the energy history of a product or service, while exergy measures the ability to do work in the future. The cumulative exergy consumed considers the exergy consumed in all processes up to the natural resources. Emergy extends cumulative exergy consumption all the way to solar energy and ecological processes.

Practical application of the proposed framework requires methods for determining the emergy content of ecological and industrial products and services and of the impact of emissions. Some potential approaches for meeting these challenges are identified. For example, the data bases developed for the inventory analysis step of LCA may be useful for estimating the emergy content of industrial products, and impact assessment methods such as eco-indicator 99 may permit thermodynamic analysis of impact. The proposed thermodynamic approach is illustrated via a preliminary LCA of the growth phase of soybeans.

This paper has focused on only two of the three components of the "triple bottom line" consisting of economic, environmental, and social factors. The important issue of human valuation has also not been discussed. Many corporations are recognizing and acknowledging the critical importance of considering these three aspects together in any decision making (DeSimone and Popoff, 1997). In response to this realization, organizations such as the Center for Waste Reduction Technologies (http://www.aiche.org/cwrt/) and the World Business Council on Sustainable Development (http://www.wbcsd.org/) are developing methods for incorporating environmental and social considerations in engineering tasks. The proposed framework is expected to be a step towards a systematic and rigorous approach for evaluating and satisfying this triple bottom line in all engineering decisions and tasks.

**Acknowledgments.** Discussions with Dr. Joseph Fiksel and the life cycle management group at Battelle, and financial support from the NSF/EPA program on Technology for a Sustainable Environment through grant BES 9985554, are gratefully acknowledged.

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Table 1.  Properties of energy, exergy and emergy

| | **Energy** | **Exergy** | **Emergy** |
|---|---|---|---|
| 1 | Satisfies law of conservation | Does not satisfy law of conservation | Does not satisfy law of conservation |
| 2 | Depends on state of matter under consideration. | Depends on state of matter under consideration and reference state | Depends on state of matter under consideration |
| 3 | Independent of path taken to reach current state | Independent of path taken to reach current state | Depends on path taken to reach current state |

Table 2. Streams from Figure 2 accounted for by various methods

| **Method** | **Streams  Included** | **Comment** |
|---|---|---|
| Traditional Economics | $F_1$, $Y$, $F_2$ | Focuses on “economically valuable” streams |
| Life Cycle Assessment | $N$, $F_1$, $R_3$ | Focuses on resource depletion and impact of emissions |
| Systems Ecology | $N$, $R_1$, $F_1$, $Y$, $R_2$ | Ignores impact of emissions |
| Proposed Approach | All | Most comprehensive |

Table 3.  Traditional LCA data for soy bean growth phase (Heijungs et al., 1996, page 63)

| **INPUTS** (data per tonne of main product) | | **OUTPUTS** (data per tonne of main product) | |
|---|---|---|---|
| **Raw materials from the environment** | | **Main Products** | |
| Soy bean seeds | 30 kg/tonne | Soy Beans | 1 tonne |
| **Raw materials brought in** | | **Environmental Emissions to AIR** | |
| Nitrogen fertilizer | 99 kg/tonne | $CO_2$ | 45.3 kg/tonne |
| Phosphates | 28 kg/tonne | CO | 0.01 kg/tonne |
| Potassium Oxide | 56 kg/tonne | Hydrocarbons | 0.0046 kg/tonne |
| Calcium Oxide | 21 kg/tonne | $NO_x$ | 0.071 kg/tonne |
| Magnesium Oxide | 17 kg/tonne | $SO_2$ | 0.32 kg/tonne |
| Insecticides | 12 kg/tonne | Particles | 0.015 kg/tonne |
| Herbicides | 1.65 kg/tonne | **Environmental Emissions to WATER** | |
| **Energy** | | Nitrogen | 99 kg/tonne |
| Diesel Fuel | 0.58 GJ/tonne | Phosphates | 28 kg/tonne |
| | | Potassium Oxide | 56 kg/tonne |
| | | Calcium Oxide | 21 kg/tonne |
| | | Magnesium Oxide | 17 kg/tonne |
| | | Insecticides | 12 kg/tonne |
| | | Herbicides | 1.65 kg/tonne |

Table 4.   Impact of emissions in traditional LCA of soybean growth phase

| **Impact Category** | **Units** | **Quantity** |
|---|---|---|
| Energy Depletion Potential | GJ/tonne | 5.8E-01 |
| Global Warming Potential | kg/kg $CO_2$ | 4.53E+01 |
| Photochemical Oxidant Formation | kg/kg Ethylene | 1.734E-03 |
| Acidification Potential | kg/kg $SO_2$ | 3.697E-01 |
| Human Toxicity | kg/kg | 1.478E+01 |
| Ecotoxicity, Aquatic | $m^3$/kg | 9.6E+01 |
| Nutrification Potential | kg/kg Phosphate | 4.159E+01 |

Table 5. Selected Emergies for Thermodynamic LCA of Soy Bean Growth

| # | **Item** | **Amount** | **Transformity** | **Emergy**(sej) |
|---|---|---|---|---|
| 1 | Sunlight | 5.0E+13 J | 1 sej/J | 5.0E+13 |
| 2 | Rain | 4.5E+10 J | 1.05E+04 sej/J | 4.7E+14 |
| 3 | Surface water | 2.3E+10 J | 4.85E+04 sej/J | 1.1E+15 |
|  | **Renew. Inputs, $R_1$** |  |  | **1.6E+15** |
| 4 | Soil Erosion | 1.7E+11 J | 7.38E+04 sej/J | 1.3E+16 |
|  | **Non-Ren. Inputs, N** |  |  | **1.3E+16** |
| 5 | Labor | 5.2E+07 J | 8.90E+06 sej/J | 4.6E+14 |
| 6 | Nitrogen fert. | 99 kg | 4.24E+12 sej/kg | 4.2E+14 |
| 7 | Phosphates fert. | 28 kg | 6.88E+12 sej/kg | 1.9E+14 |
| 8 | Potassium Oxide fert. | 56 kg | 2.96E+12 sej/kg | 1.7E+14 |
| 9 | Insecticides | 12 kg | 1.48E+13 sej/kg | 1.8E+14 |
| 10 | Herbicides | 1.65 kg | 1.48E+13 sej/kg | 2.4E+13 |
| 11 | Diesel fuel | 5.8E+08 J | 6.60E+04 sej/J | 3.8E+13 |
|  | **Economic Inputs, $F_1$** |  |  | **1.5E+15** |
| 12 | Impact due to GWP | 45.3 kg C | 1.5E+08 sej/kg | 7.2E+09 |
|  | **Emissions Impact, $F_2$** |  |  | **7.2E+09** |
|  | **Product Emergy, Y** |  |  | **1.6E+16** |

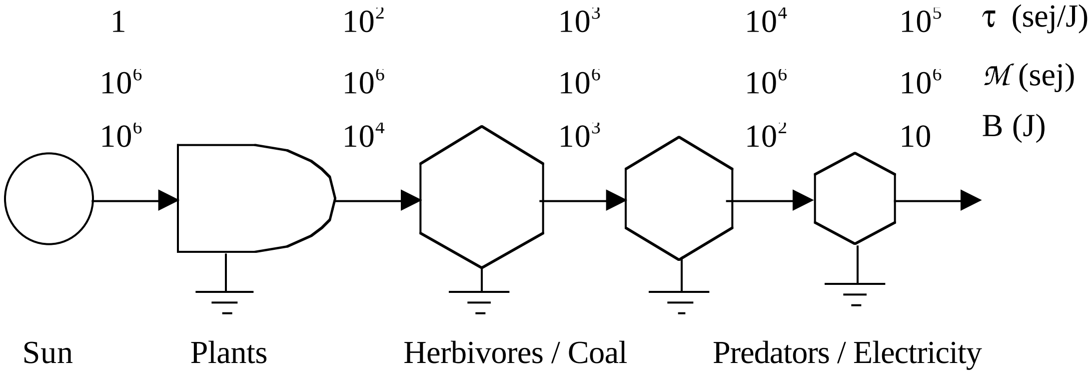

Figure 1. Energy transformation in a food or industrial chain.

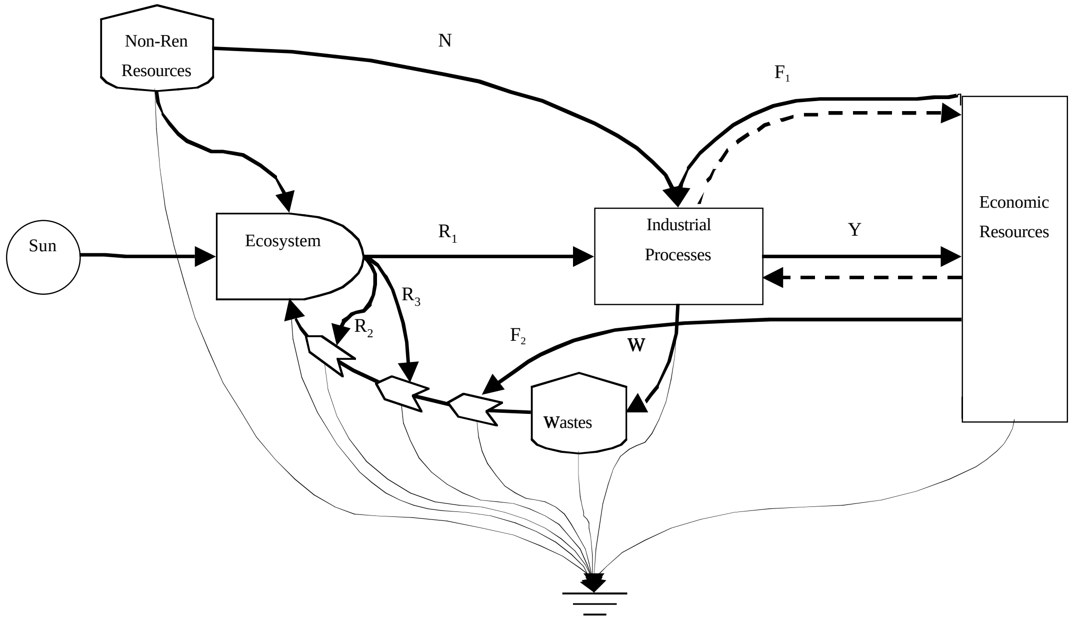

Figure 2. Energy flow diagram for industrial and ecological processes.

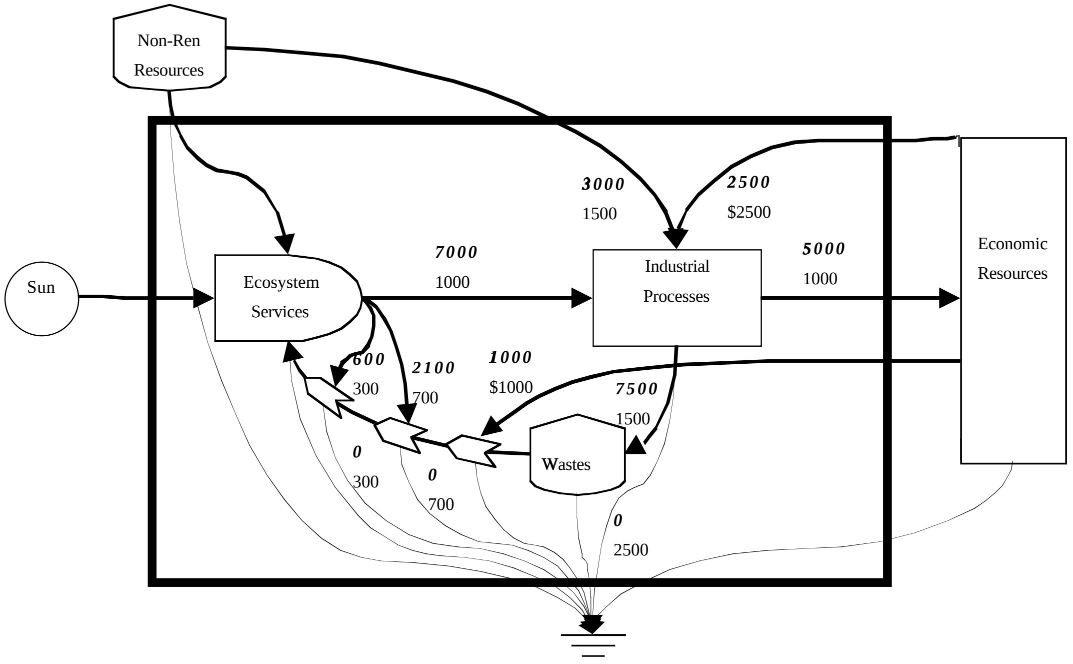

Figure 3. Illustrative example showing energy and emergy flow. Italicized and bold numbers represent emergy. Numbers in regular font below emergy represent energy or money flow.