A Generalized Mathematical Model for Sustainability

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Abstract

At the 2005 Spring Meeting of the AIChE, we discussed sustainability in a broad context and proposed that the limitations imposed by the second law of thermodynamics and by process rates be considered as well as the conservation of energy, matter, species, and ecosystems; and furthermore that more care be taken in identifying the system, that is the location of the physical or conceptual envelope. That analysis suggested that the choice of that envelope is the primary source of the contradictory conclusions that pervade the current literature relative to the sustainability of different sources of energy and raw materials.

Herein, we propose a mathematical model for the quantitative description and comparison of various fuels, processes, infrastructures, and schemes to determine their relative degrees of sustainability, thereby providing a basis for technological and political choices. This model is intended to be dynamic and independent of scale. It includes both stationary and dynamic behavior and extends beyond the conservation of species and energy. So-doing permits the inclusion of sustainability in the cost-benefit analysis of engineering processes and technologies. Even so, our approach is handicapped by the difficulty of describing quantities such as the quality of life in mathematical terms.

Introduction

Sustainability is usually examined only in terms of the first law of thermodynamics, that is, in terms of the conservation of mass and energy. This approach is inadequate in two senses. First the environment cannot be defined in terms of mass and energy only. Other qualities that are more difficult to quantify, are also essential to the current well-being of mankind, both locally and globally, as well as to the long-term survival of mankind and other biological species and indeed of the earth itself. In addition, the second law of thermodynamics reveals that sustainability is not possible in an exact sense and can only be considered to be a goal to be approached. That is, the entropy of any limited system increases with time due to irreversibilities, and the *exergy* (or *availability*), which is a quantitative measure of the ability to do work in a thermodynamic sense decreases. These irreversibilities are, for example, an unavoidable consequence of a chemical reaction, of heat exchange, and of the separation of species.

When widespread public agreement to clean up and protect the environment emerged in the 1960's the most commonly proposed model of action with respect to the chemical industry was simply to reduce or prevent end-of-the-pipe pollution. A much broader concept has since evolved that incorporates the concept of sustainability. Sustainability is essential in the long run because all resources are subject to the first and second laws of thermodynamics. The first law reveals that all resource are finite and that their exploitation invokes inexorable tradeoffs. The second law reveals limitations on and consequences of these tradeoffs. Both laws require the careful choice of an envelope or system, for example, a single apparatus, a single processing unit, an entire plant, a city, a geographical region, the entire earth and its atmosphere, or the universe.

All choices for the exploitation of resources invoke the rate at which they can be carried out, and thereby introduce restrictions in terms of space and/or time. In general, sustainable development is the result of the design of a human environment that is adapted to its surroundings without exceeding the capacity of the surroundings to support that development and to absorb its impacts, both in space and time, and both now and in the future.

Social, political, religious, and short-term economic factors may outweigh scientific and technical ones in terms of sustainability - for example, the choice of fuels and engines, the allowable exploitation of natural resources, zoning restrictions, and building restrictions. Chemical engineers are generally aware of what must occur both within and outside an envelope to accomplish a desirable end, and of the consequences of technical choices, but the public and policy makers generally are not. For example, although the choice of alternative fuels such as hydrogen and its use in fuel cells or engines, and of alcohol as obtained from biomass for use in engines, may be a primarily a political one, at least in the short run, chemical engineers have the professional responsibility to provide evaluations in terms that are understandable to the technically illiterate, and to refocus attention on those fuels and processes whose use is more sustainable. Of course, it must be recognized that individuals chemical engineers may be strongly influenced by the immediate economic interests of their employer.

Although there is general agreement about fundamental precepts such as balancing environment and development, as well as mediating social, economic, and ecological concerns with an eye toward future generations, each discipline has its own theories, methods, and vocabulary. What has been missing in science and policy is a rigorous definition of sustainability and a theory to conceptualize and measure it that encompasses all disciplines. That is the long-range objective of which this a first step. Although both of the authors are chemical engineers, one (SWC) has spent his career in design and research on thermal and reactive processes, while the other (MN) has focused on urban planning and landscape architecture. This unusual collaboration was undertaken with the prospect and hope of providing new and broader insights into this pqrticular subject.

There is a widespread consensus in the technical community about the need for sustainability with respect to energy and raw materials in the long term. On the other hand, there is no consensus on the definition of sustainability, or on what needs to be done in the short term. When drastically differing conclusions on the thermal, economic, and ecological consequences of using fuels such as hydrogen and biomass are asserted by reputable engineers, the first reaction is that these differences may reflect self-interest. However, our conclusion in earlier work was that at the technical level the differences are more likely to result from incomplete application of thermodynamic criteria or, even more likely, different choices of the envelope for the process.

Sustainability and irreversibility are often confused. For example, the growth, combustion, and fermentation of biomass are all highly irreversible processes in a thermodynamic sense but in combination are generally considered to be sustainable or nearly so because the solar flux to the surface of the earth is exempted from consideration. That exemption is based on the recognition that, if it were not used for photosynthesis, the solar flux would be almost wholly absorbed by the ground and thereby degraded to the ambient temperature with a total loss of its exergy.

The limited objective of the work reported herein has been to devise a mathematical model that is applicable to sustainability in a broad sense. Past modeling has been restricted almost wholly to the application of the first law of thermodynamics, that is to the conservation of energy and chemical species. The limitations imposed by the second law of thermodynamics and by rates (length and time scales) have largely been ignored. The modeling herein attempts to undo that omission.

One, as yet unresolved, difficulty has been to incorporate quantities such as the quality of life, and one, as yet only partially resolved, difficulty has been to define the model in terms that are consistent with past work in different technical and political frameworks.

Definitions

Sustainability. The common definition of a sustainable process is one that restores energy and materials to their original state insofar as realistically possible. The concept of extended sustainability considered herein incorporates the additional constraint that the rates of regeneration equal or exceed the rates of depletion plus extraction plus consumption, and that the rate of production of wastes and by-products is less than the rate at which the environs of the process can absorb them and remain healthy and viable over the long term. One characteristic of a truly sustainable process is the elimination of wastes.

Reversability. Sustainability does not imply reversibility. For example, the extraction of energy from a river may be interpreted as sustainable in spite of the irreversibilities in both the turboelectric generator and in the convective recycling of the water through the atmosphere. These irreversibilities may be ignored in this particular context because they would have occurred without the diversion of the water through a turbine.

Renewable Sources. Petroleum, natural gas, coal, oil shale, and uranium are generally thought of as non-renewable resources and of limited extent. Geothermal energy is clearly not renewable but it is so vast in extent and so inaccessible that its depletion is beyond our vision. Solar energy is inexhaustible time-wise within our vision although finite in scale. The secondary sources of energy created continuously by solar radiation such as rivers, winds, oceanic temperature-differences, and biomass are generally considered renewable but are certainly limited in scale and location . Tides, which are a consequence of the combined gravitational vector of the moon and sun, are also generally considered to be a renewable but severely limited source of energy.

The removal of oil, coal, shale, and natural gas from the ground and their combustion to generate power in the form of electricity might be considered sustainable if a sufficiently long time frame were chosen and the proper climatic conditions established for the growth, deposit, and consolidation of carbonaceous materials, but such a long time frame and such conditions are not meaningful to mankind.

Over-looked Limitations on Sustainability

The sustainability of energy is generally treated in terms of the first law of thermodynamics as applied to mass, that is, in terms of replacement or renewal of all materials. For example, the growth and combustion of a tree is to generate heat or electricity are often asserted to constitute a sustainable process in that the carbon, hydrogen, and minerals taken from the environment are returned to it, although admittedly not in the same exact physical and chemical forms and not in the same locations.

The limitations imposed by the second law of thermodynamics on the use of biomass as a source of energy or raw material are almost universally ignored. In the instance of biomass, the loss of exergy in the photosynthesis is excused on the grounds that the exergy of the solar radiation would otherwise have been totally lost by degradation to the ambient temperature. The further losses of exergy in combustion, in heat exchange, and in the generation of electricity go unmentioned on the same grounds. The limitations imposed by rate of absorption of the incident solar flux by the leaves, the delivery of water through the roots, trunk, and limbs to the leaves by osmosis, and photosynthesis itself go unmentioned in the context of sustainability just as do the expenditures of energy, raw materials, and manpower to make fertilizer. On the other hand these factors are generally accounted for in design and in economic analyses.

First-law, second-law, and rate analyses are all three critically dependent on the choice of a system. Any conclusions concerning sustainability are thereby also critically dependent on this choice. The system may be a fixed space, such as a piece of equipment, an entire chemical plant, a region, or the entire planet. On the other hand the system may be a process such as a single chemical reaction or the synthesis of complex compound.

As mentioned in the subsection on definitions, sustainability does not require reversibility in a thermodynamic sense. An example is the generation of electricity by diverting water from Niagara river above the Falls through a turbine driven by the difference in hydraulic head between the Niagara river above the Falls and that in the Niagara Gorge below. Insofar as the water, after passage through the Niagara Gorge, Lake Ontario, and the St. Lawrence River to the Atlantic Ocean is recycled by solar-driven evaporation, solar-driven winds, and the eventual rainfall of an equivalent mass of water on the region of the Great Lakes, the overall process might be considered sustainable in that the irreversibilities in the piping, turbine generator, and in the atmosphere are compensated for by the solar flux that evaporates, lifts, and transports the water back to Lakes Superior, Michigan, Huron, St. Clair, and Erie. If the water were not diverted through a turbine, the hydraulic head would simply be dissipated thermally, thereby heating the water about 0.12 K. The temperature rise due to the irreversibilities in the diversion through the turbine is even less. Over a short enough period of time such that the solar flux to the earth is not changed significantly by the man-made addition of greenhouse and ozone-depleting chemicals to the atmosphere, this process can be considered as essentially a steady-state one, as well as reversible and sustainable except for the transport of suspended and dissolved materials in the water and the periodic replacement of the machinery. The rate of generation of electricity is controlled by the rate of flow of water through the Niagara River itself, and the tolerable diversion by considerations of tourism. The rate of flow of the Niagara River is dependent on climatic conditions in that region and subject to some control by virtue of diversion of water from Lake Michigan to the Mississippi River. The rainfall that controls the rate of flow of the Niagara River is dependent on seemingly unrelated processes all over the globe and is not directly related to the diversion of water to generate electricity. This process has a higher potential degree of sustainability than biomass because of the greater complexity of the processes of photosynthesis and combustion inherent in the latter.

Even within the restricted concept of sustainability as represented by the first law of thermodynamics, secondary elements such manpower, cooling water, and materials of construction are often not taken into account. As an example, in the ‘70s almost every house in Japan had a solar water-heater on the roof. The water was used each day for the united family bath. These collectors have now largely disappeared because the cost of replacing the polymeric materials, which rapidly decay chemically due to the solar radiation, has become excessive due to the greater availability and lesser cost of imported hydrocarbon fuels. Thus this usage proved to be sustainable only insofar as the replacement of the material of construction and the water were overlooked.

Sustainability is only one factor in evaluating either the short-term or the long-term feasibility of a process. Technical, economic, and social considerations are also essential factors. As an example, changing life-styles in Japan may also have contributed to the demise of the individual solar water-heaters. As a further related example of social considerations, one of the authors (SWC) in 1974 imported a typical solar water-heater from Japan to study its behavior and applicability in the USA. He was promptly forced to remove it from the roof of his house because “it downgraded the appearance of the neighborhood”.

A Mathematical Model for Rates of Change in Terms of Rate Mechanisms

The primary objective of this analysis has been to devise and present a mathematical model for sustainability. The first and second laws of thermodynamics, as generalized for open a well as closed systems and for dynamic (time-dependent) as well as stationary conditions, constitute a necessary constraint. The rate process concept (see Churchill, 1974, 1979) provides a necessary complement. Expressions for the rate of change of energy, mass and chemical species can be derived from the first law of thermodynamics but not for rate processes in general.

The first and second laws of thermodynamics and the concepts of entropy and exergy (availability) are well known and well understood by most of the scientific and technical community and therefore need not be elaborated upon here. However, in order to apply thermodynamics to either a closed or an open system it is necessary to define the boundaries of the system. Different choices of a boundary are the major source of disagreement over the sustainability of various processes. A secondary source of disagreement is the failure to account for all the inputs and outputs through the boundary. To compare the sustainability of two processes their boundaries, all of the inputs and outputs through these boundaries, and all net changes within the boundaries must be identified. Thermodynamics indicates the limits of what can be done within any framework of space. On the other hand, the rate processes such as fluid flow, heat transfer, mass transfer, chemical reactions, and bulk transport determine the time and/or space required to carry out the transformations. Such times and space also limit sustainability in a practical sense.

The generalized treatment of rates is not so well or so widely known, and hence will be described briefly. The rate process concept was developed by Churchill (1974, 1979) in the context of process design and was generalized with respect to chemical reactions, fluid flow, heat transfer, mass transfer, and bulk transport. For example, for a batch (confined, unsteady-state) process

$$\frac{1}{L}\frac{dx}{dt} = \sum r_i \qquad (1)$$

Here, x represents some extensive quantity such as mass, t time, and L is a measure of the extent of the system, while r_i represents various rate mechanisms, which may be positive (inputs) or negative (outputs). A positive value for the right-hand side of Eq. 1 namely $(dx/dt)/L$, represents the rate of accumulation of the quantity x and a negative value its rate of depletion, in both cases by the sum of the rate mechanisms r_i. In either event a finite value of $(dx/dt)/L$ indicates a deviation from sustainability that must be compensated for by some other rate mechanisms. Thus, Eq.1 is only one component of an expression for sustainability.

As a simple example of a rate of change in a closed system consider the decrease in the number of moles of species *A* in a batch reactor due to first-order forward and reverse reactions. Equation 1 then becomes

$$-\frac{1}{V}\frac{dN_A}{dt} = k_1 C_A - kC_B \tag{2}$$

Here, N_A is the number of moles of species *A*, *V* is the volume of the reactor, C_A and C_B are molar concentrations, and k_1 and k_2 are forward and reverse rate constants, respectively, for the disappearance of species *A*. As an aside, chemists usually postulate implicitly an invariant density and replace $-\frac{1}{V}\left(\frac{dN_A}{dt}\right) \text{with} -\frac{dC_A}{dt}$.

The analogue of Eq. 1 for a process carried out in continuous flow through a tube of cross-sectional area *a* is

$$\frac{d(wX)}{adz} = \sum r_i \tag{3}$$

Here *z* is the distance along the tube, w is the mass rate of flow through the tube, and *X* is the quantity of interest per unit mass. Thus *az* is the volume swept out by the flow.

For a continuous but stationary process, the Eulerian equivalent of Eq. 2 for the same reactions carried out in flow through a tube may be symbolized by

$$-\frac{d(mX_A)}{adz} = k_f C_A - k_r C_B \tag{4}$$

Here *m* represents the rate of flow in moles per unit time and X_A the mole fraction of species *A*. Again in a generic sense the term on the left-hand side represents the deviation from sustainability resulting from this process when considered in isolation.

One of the contributions of the rate process concept as introduced by Churchill (1974, 1979) was the distinction between rates of change (as represented by the left-hand-side of Eqs. 1 and 3) and process rates (as represented by the terms on the right-hand-side of Eqs. 2 and 4). (See, for example, Kabel, 1981, 1992). The rate of change is still confused with rate mechanisms in many textbooks on chemistry.

Equations 2 and 4 may also be derived by reducing the general partial differential equation for the conservation of a species (See, for example, Bird, et al. (2001) in accordance with the many restrictions imposed. That is, Eqs. 2 and 4 are special cases of the first law of thermodynamics. However, the direct formulations are conceptually simpler than their derivation by specialization and reduction of the general equation of conservation for species.

Application of the Rate Process Concept to Sustainability

The several simple equations presented above provide a basis for more complete modeling of sustainability, particularly in particular

The rate process concept has the advantage of being applicable to problems of complex ecological and social complexity. And to a wide range of the factors that determine whether a process is sustainable or not. Moreover, it is a scale-independent theory that answers what until now has been the most intractable barrier in the search for a general theory of sustainability – what are we trying to sustain, where are we trying to sustain it, and over what time span?

The rate process concept combined with thermodynamics is applicable to dynamic, non-linear, non-equilibrium systems as well as to equilibrium systems. It is applicable to complex urban, social and ecological phenomena such as cities, organizations, and ecosystems as well as to single, simple processes such as a chemical reactor.

The rate process concept is an essential component of sustainability because the innate and “natural” limitations of the surroundings to support processes must be taken into account. This concept goes beyond existing formulations in terms of the carrying-capacity, which are popular in the field of urban and environmental planning and which were pioneered in the sixties and seventies by Ian McHarg and by Donella Meadows and her colleagues in The Club of Rome report (McHarg 1969, Meadows, et al. 1972). These traditional views of carrying capacity dealt with a specific place at a specific point in time. Neither was process oriented. They did not account fully for the dynamic nature of the systems and did they consider the co-evolutionary character of human interaction with ecosystems. Another flaw in the applications of these two carrying-capacity approaches and their derivatives is that they did not pay close attention to the surrounding environment and the definition of the boundary between the activity system under study and its surroundings. The rate process theory adds the dimension of time to the dimensions of space that the carrying-capacity approaches employed..

It is proposed to apply the rate concept to sustainability in five different categories: consumption, production, accumulation, depletion, and assimilation. The theory can be applied to any factor within these categories. For example, the rate of consumption can be expressed in terms of energy and materials, the rate of production in terms of goods, services, and wastes, and the rate of accumulation in terms of wealth and poverty, and debt and profit – whether personal, corporate, or governmental, as well as to such natural processes such as nitrogen fixation, the formation and release of atmospheric carbon dioxide and nitrogen oxides, global changes in climate, and the contamination of aquifers. The rate of depletion can be applied to atmospheric ozone, aquifer recharge, desertification, biological diversity, habitat loss, language and cultural loss, and the like. The rate of assimilation is applicable to water quality, atmospheric fluorocarbons, the introduction of invasive and exotic species into a new environment,

Illustrations of the Role of Rates in Sustainability

As a simple, specific example of the role of rates in sustainability, the usage of water may be described quantitatively in terms of the difference between the volumetric rates of withdrawal from and recharging into an aquifer per unit of population per unit of time, or alternately per unit of area per unit of time.

The maintenance of the temperature inside a building provides a slightly more complex system involving rates. The change in enthalpy of the air with time (the accumulation term) can be equated to the sum of the inputs by the occupants and equipment and the inputs and outputs by the heating and cooling systems, by flow through the doors, windows and other openings to the surroundings, and by heat exchange with the surroundings through the walls and windows by conduction, convection, and radiation in parallel and in series. Insofar as a constant temperature can be maintained the accumulation term may be equated to zero. A broader, coupled problem is posed by consideration of the humidity and other components of the air, and a more complicated one by consideration of the temperature of each individual room. The exchanges of energy and air with the surroundings couple the behavior inside the building with the varying temperature and humidity of the surroundings as as well with the varying solar flux. Their diurnal and day-to-day variation make the consideration of rates mandatory. One convenient measure which allows comparability across buildings, locations, and seasons is the rate of heat loss or gain in units of energy per building unit volume per degree-day.

As one more step upward in complexity, irreversibility, sustainability, and the role of rate mechanisms may be examined for the production of useful energy by means of growing and burning biomass, as illustrated for simplicity by a single tree. The leaves of the tree absorb the solar flux, and by means of photosynthesis produce cellulose from CO_2 and H_2O, the former from the surrounding air and the latter from the soil. The tree grows because of the formation of this cellulose. If the tree and its roots are cut up and burned some of the energy in the hot burned gas can be transferred to a working fluid. The partially cooled gas composed of CO_2, H_2O, N_2, excess air, and pollutants such as NO_x, is released to the atmosphere and the ashes are returned to the soil. The water vapor eventually condenses from the atmosphere and returns to the soil, although not necessarily in the same location. A more serious deviation from sustainability is the difference in the chemical composition of the ashes as compared to that of the minerals taken into the tree with the water absorbed by the roots. In the long run, fertilizer must be added to the soil, and the energy and raw materials that its manufacture and transport entails must be accounted for.

The biochemical conversion of radiant energy to chemically stored energy and the combustion and heat exchange are each highly irreversible, and the exergy increase of the working fluid is far less than that of the solar flux.

Complete sustainability in terms of the solar system would require return of the energy obtained from the solar flux back to the sun. However, in the more practical framework of a tree-farm the irreversibilities in the growth of the tree, in its combustion, and in the ensuing heat exchange need not be accounted for in terms of sustainability because the same ultimate degradation of the exergy of the solar flux would occur if the tree was simply allowed to decay away or was not even grown.

The rate of this process is limited by the combinations of many different mechanisms such as the solar flux, osmosis, photosynthesis, combustion. and heat exchange, none of which are accounted for by static energy and material balances.

This gross description could be expanded almost endlessly by considering such processes as the original growth of the tree from a seed, the imperfect absorption of the radiation by the chlorophyll in the leaves, the complex series of reactions to synthesize chlorophyll and cellulose, the transfer of O_2 from the leaves to the atmosphere, the growth of the roots and their penetration of the soil, their absorption of water, and the flow of the water and essential dissolved elements through the capillaries by osmosis, the evaporation of water from the leaves, and all of the the associated thermal effects.
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Implications

The general theory of sustainability presented here has manifold implications for sustainable development in related fields such as economics, and urban and environmental planning, as well as in energetic and chemical processes. An important implication is the use of indicators. Insofar as possible, measures of the environmental, of economics, of the quality-of-life, and of sustainability should be should be expressed in quantitative terms so as to conform to the rate-process model. On the other hand, these indicators should also be broadened to include all human and economic activities, not just natural factors, as represented by the laws of physical science and of environmental accounting.

Other implications concern the design and management of productive and consumptive processes, and the design and management of infrastructural and social-service delivery systems. The general nature of the theory enables it to be applied to the life-cycle of all these processes - that is, for their assessment, planning, design, construction, management, maintenance, operation, repair, replacement, and funding. Indeed, the theory is consonant with and provides a theoretical foundation for the multitude of life-cycle methods that are being instituted in realms as diverse as industrial ecology, social service delivery, infrastructure provision, building design and construction, and in the public sector the fiscal management of ecosystems and natural resources.

Summary and Conclusions

Thermodynamics and the rate process concept have been combined and adapted to develop a general mathematical model for sustainability. The model permits the quantitative calculation of the sustainability of any process, whether chemical, biological, ecological, economic, or social. It is a dynamic and scale-independent model that takes into consideration the spatial and temporal factors of processes, thus permitting empirical applications that correspond to actual (dynamic, complex, evolving) conditions.

The contributions of the model include the following:

1. It enables the mathematical calculation of the degree to which any process is sustainable over the long term, using the methodology of thermodynamics and rate processes.

2. It enables consideration of the relevant factors that impinge upon sustainability - economically, ecologically, technically, and socially..

3. It facilitates the determination of where in geographic space to draw the boundaries of the system.

4. It enables a quantitative comparison of several processes to determine their relative degrees of sustainability and thereby inform technological and political choices.

5. It places long-term sustainability alongside short-term efficiency in the cost-benefit calculus of choosing processes, technologies, and materials.