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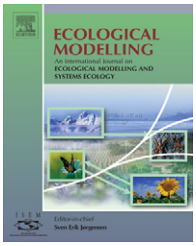

Short communication

Chemical exergy based evaluation of water quality

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ABSTRACT

The thermodynamic concept of chemical exergy is introduced for water quality evaluation, to develop unified objective indicators in contrast to conventional indicators characteristic of subjectivity. While a quantity termed specific standard chemical exergy based on the global reference substances is used to evaluate the standard water quality, an indicator as specific relative chemical exergy with reference to a spectrum of substances associated with some specified water quality standard is developed for practical water quality evaluation, with related concepts of carrying deficit and carrying capacity well embodied in exergy terms. Based on the data collected in the GEMS/WATER project, water qualities of 72 rivers and 24 lakes over the world are evaluated, as a detailed case study to illustrate the adaptability of the chemical exergy based indicators for water quality evaluation.

1. Introduction

The thermodynamic concept of exergy as a unified measure of the deviation of a system from its environment has gained wide acceptance in environmental and ecological fields (Jørgensen, 2001; Szargut, 2001; Chen, 2005, 2006). With a sound scientific foundation in physics, exergy has been adopted as an ecological indicator and goal function (Jørgensen, 1988, 1992a,b,c, 1994, 1995, 2000, 2001, p153; Jørgensen et al., 1995) for environmental evaluation and ecological modeling.

In addition to the conventional application of evaluating the efficiency or efficacy of energy-utilization systems and detecting quantitatively the causes of the thermodynamic imperfection of thermal or chemical processes, exergy attracts escalating interests in environmental resource accounting, environmental impact assessment, ecological cost evaluation, and ecological modeling in recent years (e.g., Jørgensen et al., 1995; Rosen and Dincer, 1997b, 1999, 2001, 2003; Dincer, 2000, 2002; Gong and Wall, 2001; Wall, 2002; Szargut, 2003, 2004; Dincer and Rosen, 1998, 2005; Chen, 2005, 2006).

The resource accounting in terms of exergy has been carried out based on nation or industrial sector scales (e.g., Reistad, 1975; Wall, 1987, 1990; Rosen, 1992; Wall et al., 1994; Rosen and Dincer, 1997a; Ertesvåg and Mielnik, 2000; Hammond and Stapleton, 2001; Ayres et al., 2003; Dincer et al., 2003, 2004a,b,c,d,e; Ji and Chen, 2006; Chen and Chen, 2006, in press-a,b,c,d,e). Rosen and Dincer (Rosen and Dincer, 1997a,b, 1999, 2001, 2003; Dincer, 2000, 2002; Dincer and Rosen, 1998, 2005) paid much attention to the relationship between energy utilization and the environmental impacts, and highlighted the implication of the exergy analysis to the sustainable development. A number of researchers (e.g., Ulgiati et al., 1995; Creyts and Carey, 1997) have tried to devise unified objective measures for environmental impact assessment based upon exergy, via either estimating the chemical

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exergy associated with a waste stream or the total exergy consumption associated with corresponding human helped treatment courses of the waste stream. Hellstörm (1997, 2003) estimated and compared the exergy consumption of physical resources in some wastewater treatment plants and sewerage systems. Finnveden and Östlund (1997), Ayres et al. (1998), and Cornelissen et al. (1999) have developed an Exergy Based Life Cycle Analysis, introducing the concept of exergy into the methodology of environmental life cycle assessment and using it as a uniform indicator of total environmental impact. Sciubba and co-workers (Sciubba, 1999, 2001a,b, 2003a,b; Sciubba and Ulgiati, 2005) discussed a new paradigm for the calculation of the real environmental cost by performing the Extend Exergy Accounting, and provided a novel framework for integrated evaluation of concerned factors of capital, labor and environmental impact, etc. The concept of ecological cost has been defined as the cumulative consumption of non-renewable natural resources measured by exergy in the fabrication of particular products (Szargut et al., 2002). In a framework for systems evaluation based on exergy circuit language, ecological value for a waste stream is defined negative and equal in magnitude to corresponding embodied exergy in terms of the total exergy consumed in human helped treatment or natural degradation of the waste stream (Chen, 2006).

Jørgensen and co-workers (Jørgensen et al., 1995; Bendoricchio and Jørgensen, 1997; Martins et al., 1997; Xu, 1997; Xu et al., 1999, 2001, 2002, 2004; Jørgensen, 2001; Jørgensen et al., 2002a,b,c; Marques et al., 2003; Zhang et al., 2003, 2004) have made much efforts in exergetic modeling for aquatic systems such as lakes and coastal areas, by demonstrating and illustrating the relationships between exergy and biomass, biodiversity, species composition, and other properties of ecosystems. A preliminary resource accounting for river water has been carried out by Zaleta-Aguilar et al. (1998) in terms of the river water availability quantified as the mechanical, thermal and chemical exergy flux with the river flow. A more general approach involving biological and sedimental exergy has been proposed for a unitary objective accounting of water resources, with application to the Yellow River basin (Chen, 2004). An exergy based evaluation of water quality remains to be initiated.

The monitoring of water quality of rivers dates back to around 1890 when some European rivers, such as the Thames and the Seine, highly contaminated due to domestic sewage, were monitored in terms of a few simple parameters of dissolved oxygen, pH, etc. With the rapid industrialization and development of the energy sectors and high-input agriculture, there has been an exponential rise in the number of water quality indicators, corresponding to the increasing diversity of pollutants (Meybeck and Helmer, 1989). These indicators, including the earliest monitored simple indicators, major irons, organic, and inorganic matters, and toxic pollutants, etc., cover a broad range of water quality. In order to comprehensively evaluate the water quality, a variety of evaluation methods such as the single index, fuzzy mathematics, principal factor analysis, specialist evaluation, gray correlation, radial basis function, artificial neural network, and comprehensive index evaluation, etc. have been established (Cater, 1996, pp. 56–99, 122–143). Common to all those models is the unavoidable subjectivity, of the weighting factor for each involved indicator, mathematical models or corresponding parameters. Due to the subjective weighted factors out of so-called specialist inquiry, contradictory evaluations may be resulted for the same water quality data with different specialist groups. For reasonable and consistent water resource exploitation and management, it is essential to pursue a unified objective assessment of water quality.

In the present paper, the chemical exergy based evaluation method is developed for a unified objective assessment of water quality. While a quantity termed specific standard chemical exergy based on the global reference substances might be adopted, an indicator as specific relative chemical exergy with reference to a spectrum of substances associated with the specified water quality standard is proposed for water quality evaluation with more practical implications, resulting in unified objective quantifiers for the carrying capacity and carrying deficit of water resources. With the data collected in the GEMS/WATER project, water qualities of 72 rivers and 24 lakes over the world are evaluated as a detailed case study to illustrate the adaptability of the chemical exergy based indicators for water quality evaluation.

2. Chemical exergy and water quality

Standard chemical exergy of a substance is defined as the minimum amount of available energy or work necessary to produce the substance under consideration from environmental substances in the sense of Szargut's global averaged model and associated with standard environment with temperature T_0 of 298.15 K and pressure P_0 of 1 atm, i.e., 101.325 kPa (Riekert, 1974; Morris and Szargut, 1986).

To assess the chemical exergy of a substance, the properties of the chemical elements comprising the substance must be referred to the properties of some corresponding reasonably selected substances in the environment (Kotas, 1985, p. 44). The reference substances selected are the most abundant substances in the natural environment, and in equilibrium with the rest of the environment. Obviously, the most suitable reference substance for the chemical element in question is the one not only containing the chemical element but also with the lowest chemical potential among all the corresponding environmental substances. For instance, what qualifies to be a suitable reference substance in the global environment for the solid S is SO_4^{2+} in the hydrosphere rather than SO_3^{2+}, and what for C is CO_2 in the atmosphere rather than CO rarely found in the environment as a whole. Na^+, K^+, Cl^-, Ca^+, etc. in the hydrosphere, N_2, O_2, CO_2, etc. in the atmosphere, and S_iO_2, Fe_2O_3, etc. in the external layer of the earth crust have been adopted as the reference substances (Morris and Szargut, 1986).

For a general case the standard chemical exergy (SCE) comprises two parts as the standard standard mixing exergy (SME) and reaction exergy (SRE).

The standard mixing exergy for the concentration effect of the reference substances is calculated as

$$\mathrm{SME_i} = RT_0 \ln \frac{C_0}{C_{i00}}, \qquad (1)$$