EHT Environmental Health and Toxicology

Open Access

Volume: 30 Suppl, Article ID: s2015002, 11 pages
http://dx.doi.org/10.5620/eht.e2015002

• Original Article

eISSN: 2233-6567

Research on the development of green chemistry technology assessment techniques: a material reutilization case

Seokpyo Hong, Kilsoo Ahn, Sungjune Kim, Sungyong Gong

Department of Environmental Economy and Policy Research, Korea Environment Institute, Sejong, Korea

Objectives This study presents a methodology that enables a quantitative assessment of green chemistry technologies.

Methods The study carries out a quantitative evaluation of a particular case of material reutilization by calculating the level of "greenness" i.e., the level of compliance with the principles of green chemistry that was achieved by implementing a green chemistry technology.

Results The results indicate that the greenness level was enhanced by 42% compared to the pre-improvement level, thus demonstrating the economic feasibility of green chemistry.

Conclusions The assessment technique established in this study will serve as a useful reference for setting the direction of industry-level and government-level technological R&D and for evaluating newly developed technologies, which can greatly contribute toward gaining a competitive advantage in the global market.

Keywords Degree of green assessment, Economics assessment, Environmental assessment, Exhaustion of resources assessment, Green chemistry technology assessment techniques

Correspondence: Sungyong Gong
370 Sicheong-daero, Sejong 339-007, Korea
Tel: +82-44-415-7618
Fax: +82-44-415-7764
E-mail: sgong@kei.re.kr

Received: January 8, 2015
Accepted: April 13, 2015
Published online: June 12, 2015

This article is available from: http://e-eht.org/

Introduction

Rapid advancements in the chemical industry have helped in maintaining the high quality of life of the modern society. Unfortunately, the excessive abuse and misuse of harmful chemical materials, such as nylon, plastic, and phthalate, under the pretext of "modern society's convenience" has given rise to various human health and environmental problems. To address such problems, leading countries/regions that dominate the chemical sector, such as the US and the European Union (EU), have been advocating green chemistry through collaborative efforts between their governments and the industry; this approach has been labeled "sustainable development." The general idea behind green chemistry is promoting the design and use of zero- or low-toxic chemical materials and minimizing the production and emission of hazardous chemical substances by means of ecofriendly production process management.

In 1998, Anastas and Warner [1] defined "green chemistry" as the totality of activities that reduce or eliminate the generation and use of substances harmful to human health and environment in the design and production process, and application of chemical products. They presented 12 principles of green chemistry [1]: minimizing waste generation, maximizing synthetic production efficacy, using less hazardous chemical synthesis methods, using low-toxicity chemical product design, minimizing the use of auxiliary substances such as solvents, minimizing energy consumption, maximizing the use of renewable raw material, minimizing the use of derivatives, using catalysts with high selectivity, designing products degradable into innocuous materials at the end of their function, preventing the formation of hazardous substances through real-time monitoring, and selecting materials with low risk for accidents.

In response to international regulations associated with chemical products along with increasingly stringent safety requirements, South Korea (hereafter Korea) has also been striving to apply green chemistry principles and develop green chemistry technologies. However, the evaluation of the level of compliance with the principles of green chemistry (hereafter greenness) has been carried out only at a qualitative level, exposing the limitations in quantifying the greenness compared to the state prior to the implementation of green chemistry technologies.

Against this backdrop, this study was conducted to develop an evaluation technique that enables a quantitative assessment of the greenness of green chemistry technologies. The study also tests the validity of the assessment technique by quantitatively assessing the greenness achieved in a case of material reutilization through the application of green chemistry.

Materials and Methods

We performed a preliminary analysis of various foreign cases for quantitative assessment of green chemistry and presented supplementary features by evaluating the suitability of indices and their respective proxy variables in an additional expert panel. The selected indices are 1) environment: ecological footprint, thereby classifying the substances generated during production and use of chemical products into greenhouse gases (GHGs) as an international issue and hazardous substances affecting residents' health and living environment as a domestic issue; 2) safety: industrial chemical accidents such as explosion and fire; 3) resource: energy consumption as a social factor, and 4) economy: economic feasibility of green chemistry technologies [2]. Table S1 presents the proxy variables of each index. Each of these four indices is extracted as a value, allowing a quantitative assessment of greenness using equation (1) (Figure 1).

$$\text{Greenness} = \alpha \cdot \Sigma\text{environment} + \beta \cdot \Sigma\text{safety} + \gamma \cdot \Sigma\text{resource} \ (+\delta \cdot \Sigma\text{economy}) \quad (1)$$

where α, β, γ, and δ are the results of analytic hierarchy process (AHP) analysis derived via an expert questionnaire survey and denote weights for respective weights.

Environment

Environment is defined as the sum of GHGs and hazardous substances reflecting the international and local factors, respectively, and expressed by equation (2).

$$\Sigma\text{Environment} = \alpha_a \cdot \Sigma\text{GHGs} + \alpha_b \cdot \Sigma\text{hazardous substances} \quad (2)$$

Greenhouse gases

GHGs are defined as the total amount of GHG reduction, and their sum total is calculated in equation (3) in compliance with the Intergovernmental Panel on Climate Change method.

$$\Sigma\text{GHGs} = \text{t}CO_2 \text{ reduction} \quad (3)$$

- Energy consumption and GHGs are calculated after converting them into toe and tCO_2, respectively.
- GHG emissions during the production process are calculated after converting them into tCO_2.

Hazardous Substances

Hazardous substances are defined as the sum total of the health hazard factors (HHFs) and environmental hazard factors (EHFs) for assessing the harmful effects on humans and environment; their sum total is calculated in equation (4).

$$\Sigma\text{Hazardous substances} = \alpha_{a1} \cdot \Sigma\text{HHFs} + \alpha_{a2} \cdot \Sigma\text{EHFs} \quad (4)$$

Hazardous substances include the impact of raw materials, products/by-products, and emissions of each substance. Figure S1 presents these impact factors in a mimetic diagram.

The raw material in Figure S1 comprises the main ingredients, adjuncts, and catalysts. Products mean the final products of the production process, and by-products are concurrently generated

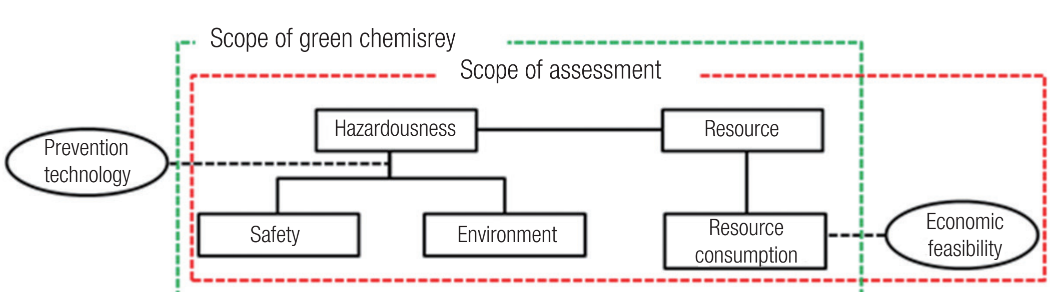


Figure 1. Scope of assessment of the green chemistry technology applied in this study.

secondary products usable without further process. If a by-product can be used for the production process, it is classified as resource, and if it is discharged to the living environment, it is classified as emission, such as the substances released to the environment after waste treatment, including the waste itself.

Health Hazard Factor

The HHF, i.e., the impact of a hazardous substance on the human body, is calculated with equation (5). To implement a quantitative assessment of the HHF, carcinogenicity expressed as Integrated Risk Information System (IRIS) categories, permissible exposure limit (PEL), and risk phrase (R-Phrase) for all hazardous components involved in the production process (raw material, products/by-products, and emissions) should be determined and quantified with respect to a reference scale.

$$\Sigma \text{HHF} = x_1 \cdot \Sigma \text{raw material} + y_1 \cdot \Sigma \text{products/bi-products} + z_1 \cdot \Sigma \text{emissions} \quad (5)$$

· IRIS categories: evaluation and quantification of carcinogenicity of chemicals, the IRIS categories offered by the US Environmental Protection Agency (EPA) are used (Table S2).

· PEL: for airborne chemicals, we referred to the Occupational Safety and Health Act (OSHA) as legal standard reference values. Equation (6) represents the reference scale of PEL:

$$\text{Reference scale PEL} = \log\left(\frac{10^4}{\text{PEL}}\right) \quad (6)$$

· R-Phrase: the risk phrase of each hazard component is determined according to the classification of and standard for dangerous substances as set out in the EU Directive 67/548/EEC.

Environmental Hazard Factor

EHF, i.e., the impact of a hazardous substance on environment, is calculated with equation (7). To implement a quantitative assessment of the EHF, the median effective concentration (EC_{50}) and R-Phrase for all hazardous components involved in the production process (raw material, products/by-products, and emissions) should be determined and quantified with respect to the reference scale.

$$\Sigma \text{EHF} = x_1 \cdot \Sigma \text{raw materials} + y_1 \cdot \Sigma \text{products/by-products} + z_1 \cdot \Sigma \text{emissions} \quad (7)$$

· EC_{50}: the reference scale for the median or half maximal effective concentration is set out using the classification labeling of GHS after measuring the acute toxicity to arthropods (Table S3).

· R-Phrase: The risk phrase of a hazard component is determined according to the hazardous substance classification and standard, as set out in EU Directive 67/548/EEC.

Safety

Safety can be quantified by checking the R-Phrase of each chemical substance involved in the production process (raw material, products/by-products, and emissions) against the reference scale using equation (8).

$$\Sigma \text{Safety} = x_2 \cdot \Sigma \text{raw materials} + y_2 \cdot \Sigma \text{products/by-products} + z_2 \cdot \Sigma \text{emissions} \quad (8)$$

Resource

Improvement of resource consumption means efficacious production of chemical products by minimizing the depleting resources, i.e., reduction in waste generation. To calculate the improvement in resource consumption, we selected raw materials with a high resource value and materials that reflect well the characteristics of the raw materials as a reference scale. For example, the consumption improvement rates for organic chemical compounds and precious or rare metals are calculated in terms of carbon efficiency and content, respectively, and expressed by equation (9).

$$\text{Resource} = 1 - \frac{\text{(after the improvement) (raw materials, adjuncts, catalysts)}}{\text{(before the improvement) (raw materials, adjuncts, catalysts)}} \quad (9)$$

Economy

Although not included in the 12 principles of green chemistry, it is considered essential to include the economic aspect in the green chemistry technology assessment technique in order to make green economy more attractive to the industry. Additionally, the market share of the technology concerned can serve as a reliable yardstick for gauging its impact on the market , and expressed by equation (10).

$$\text{Economic feasibility} = \frac{\text{production cost reduction}\left[\frac{\text{w}}{\text{t}}\right]}{\text{baselin expenditures}\left[\frac{\text{w}}{\text{t}}\right]} + \frac{\text{consumer price reduction}\left[\frac{\text{w}}{\text{t}}\right]}{\text{baselin retail price}\left[\frac{\text{w}}{\text{t}}\right]} \quad (10)$$

Summary of Greenness Calculation

Table S4 gives an overview of the greenness calculation methods by index as described above in order to perform a quantitative assessment of green chemistry technologies.

Results

Equipment Improvement Case

The example presented in this study is a case of reutilization of waste acid from the pickling process of electronic parts. By installing cooling equipment to address the problem posed by excessive use of nitrogen chemicals and ensuing increase in costs for purchasing chemicals and treating waste, the acid solution could be used three times instead of discarding it after the first use, thus achieving reduction in the use of chemicals and waste treatment volume [3]. Figure 2 illustrates the simplified production process of the example case and "pre and post" comparison of economic and ecological impacts.

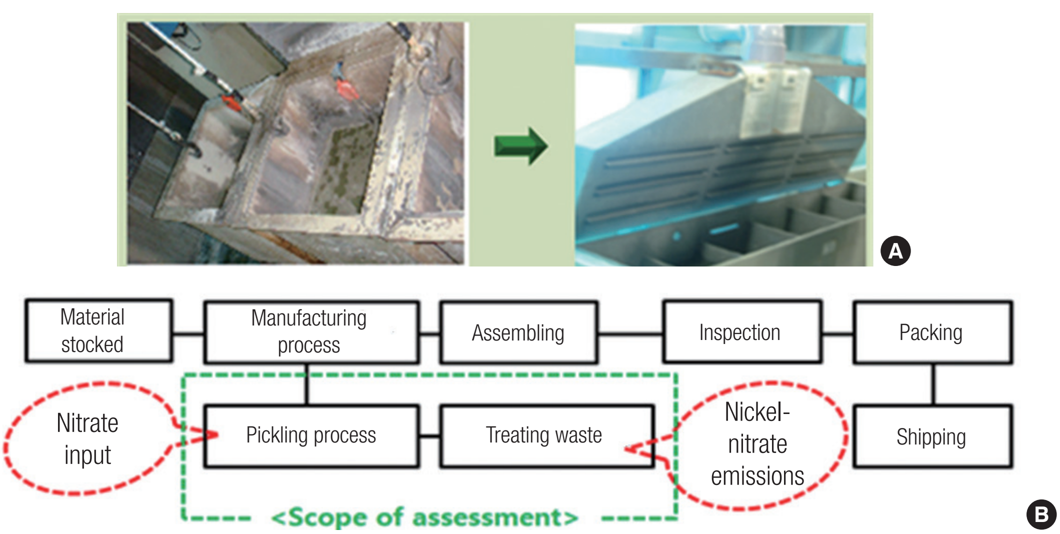
Green Chemistry Technology Assessment

Based on the above-described procedure, we could quantify

Table 1. Assessment results for nitric acid by index before the improvement [4-6]

Category		Before the improvement				After the improvement			
Substance		Nitric acid							
CAS no.		71-55-6							
Consumption during 5 yr (L)		389232				194616			
R-Phrase		R8, R35							
Category		Raw info	N	TPI	Max TPI	Raw info	N	TPI	Max TPI
Health hazard factor	IRIS category	-	-	-	0.80	-	-	-	0.80
	PEL	5	3.30	0.80		5	3.30	0.80	
	R-Phrase	-	-	-		-	-	-	
Environmental hazard factor	EC_{50}	-	-	-	0.00	-	-	-	-
	R-Phrase	-	-	-		-	-	-	
Safety	R-Phrase	R8, R35	5.00	4.48	4.48	R8, R35	5.00	4.48	4.48
Pollutant emissions (tonne/yr)		30.04				8.72			
Pollutant treatment cost during 5 yr (10^6 KRW)		458.53				133.31			
Expenditure during 5 yr (10^6 KRW)		237.04				120.62[a]			

R-Phrase, risk phrase; Raw info, information of each index; N, reference scale of each index; TPI, toxic potensial indicator; IRIS, Integrated Risk Information System; PEL, permissible exposure limit; EC_{50}, median effective concentration; KRW, Korean won.
[a]This amount includes the investment cost amounting to 2.1×10^6 KRW.



Category	Before improvement	After improvement
Investment (10^6 KRW)	-	2.0
Chemical use (L/d)	5.1	2.55
Treatment cost (10^6 KRW/yr)	91.71	26.62

C

Figure 2. Production process design of the reutilization of waste acid from the acid pickling process. (A) Improvement compare before and after of process. By installing cooling equipment to address the problem posed by excessive use of nitrogen chemicals and ensuing increase in costs for purchasing chemicals and treating waste, the acid solution could be used three times instead of discarding it after the first use. (B) The whole process and scope of assessment. (C) Economic improvement. Data from Korea Institute of Industrial Technology. Regional eco-innovation program success casebook. Cheonan: Korea Institute of Industrial Technology; 2011 [3]. KRW, Korean won.

Table 2. Assessment results for nickel nitrate by index after the improvement [4-6]

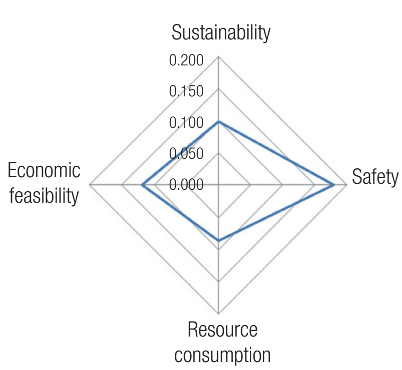
Category		Before the improvement: waste data				After the improvement: waste data			
Substance		Nickel nitrate							
CAS no.		13138-45-9							
R-Phrase		R49, R61, R8, R20/22, R38, R41, R42/43, R48/23, R68, R50/53							
Category		Raw info	N	TPI	Max TPI	Raw info	N	TPI	Max TPI
Health hazard factor	IRIS category	-	-	-	13.81	-	-	-	13.81
	PEL	-	-	-		-	-	-	
	R-Phrase	All except R8	6.12	13.81		All except R8	6.12	13.81	
Environmental hazard factor	EC_{50}	0.466	7.00	33.33	33.33	0.466	7.00	33.33	33.33
	R-Phrase	-	-	-		-	-	-	
Safety	R-Phrase	R8	1.00	0.05	0.05	R8	1.00	0.05	0.05
Pollutant emissions (tonne)			30.04				8.72		

R-Phrase, risk phrase; Raw info, information of each index; N, reference scale of each index; TPI, toxic potensial indicator; IRIS, Integrated Risk Information System; PEL, permissible exposure limit; EC_{50}, median effective concentration.
[a]This amount includes the investment cost amounting to $2.1x10^6$ Korean won.

Table 3. Green chemistry technology assessment results

Category				Weight[a]	Improvement factor	Greenness
Environment	Greenhouse gas			0.078	0.000	0.000
	Hazardous substances	Health hazard factor	Raw material	0.037	0.500	0.019
			Products	0.044	0.000	0.000
			Emissions	0.061	0.710	0.043
		Environmental hazard factor	Raw material	0.017	1.000	0.017
			Products	0.020	0.000	0.000
			Emissions	0.028	0.710	0.020
Total (environment)				0.286	2.919	0.099
Safety			Raw material	0.101	0.000	0.000
			Products	0.136	0.500	0.068
			Emissions	0.157	0.710	0.111
Total (safety)				0.393	1.210	0.179
Resource consumption				0.172	0.500	0.086
Economic feasibility				0.148	0.800	0.118
Total				1.000	-	0.483

[a]Rounding off at the 5th decimal place.



Category	Weight	Greenness
Environment	0.286	0.099
Safety	0.393	0.179
Resource consumption	0.172	0.086
Economic feasibility	0.148	0.118
Sum total	1.000	0.483

Greenness=weight×improvement factor

Figure 3. Green chemistry technology assessment results. The values of greenness and improvement factor indicated in the table reflect the guarantee period of 5 years for the cooling equipment.

the hazard factors, safety factors, resource consumption, and economic feasibility of nitrogen used as input substance for the pickling process (Table 1), and nickel nitrate emitted as output substance from the pickling process (Table 2). Table 3 and Figure 3 show the results of quantitative assessments of the green chemistry technology applied to the specimen equipment.

Raw information on nitrogen and nickel nitrate was sourced from the IRIS categories provided by the US EPA and their respective material safety data sheets (R-Phase: EU Directive 67/548/EEC; PEL: OSHA; EC_{50}: EPA). The costs for pollutant treatment and expenditure for a 5-year period were taken from the regional eco-innovation program success casebook.

The application of the green chemistry assessment technique developed in this study revealed a 48% improvement in greenness compared to the state before the improvement. Breaking down 48% into individual indices, safety was found to occupy the highest portion with 17.9%, followed by economic feasibility (17.9%), environment (9.9%), and resource (8.6%). The weights used for the calculation were derived from the AHP analysis performed through an expert questionnaire survey.

Discussion

We proposed a novel technique for quantitative assessment of green chemistry technologies and calculated the improvement in an example case of material reutilization by quantifying the level of greenness that was achieved by implementing a green chemistry technology. The calculation results revealed an enhancement of the greenness level by 42% compared to the level before the improvement, including economic benefits. This study will serve as a basis for establishing a useful tool for evaluating the greenness of technologies from a strategic perspective for businesses to use it for setting the directions of their R&D plans and for the governments to perform objective evaluations of technologies. In particular, it is expected to greatly aid businesses in gaining competitive advantage in the global markets.

Acknowledgements

This subject is supported by Korea Ministry of Environment (MOE) as "MOE's R&D Program on environmental technology development" (no. 412-111-007), and by Korea Environment Institute (KEI, 2014-025).

Conflict of Interest

The authors have no conflicts of interest with material presented in this paper.

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Table S1. Weight of each indicator

Category				Weighta
Environment	Greenhouse gas			0.078
	Hazardous substances	Health hazard factor	Raw material	0.037
			Products	0.044
			Emissions	0.061
		Environmental hazard factor	Raw material	0.017
			Products	0.020
			Emissions	0.028
Total (environment)				0.286
Safety			Raw material	0.101
			Products	0.136
			Emissions	0.157
Total (safety)				0.393
Resource consumption				0.172
Economic feasibility				0.148
Total				1.000

[a]Rounding off at the 5th decimal place.

Table S2. Integrated Risk Information System (IRIS) carcinogen classification criteria

IRIS category	Description	Reference scale
Group A	Human carcinogen	7
Group B	Probable human carcinogen	7
Group B1	Indicative of a limited causal relationship in epidemiological research	7
Group B2	Indicative of a sufficient causal relationship in animals, with little or no human data	7
Group C	Possible human carcinogen	7
Group D	Not classifiable as to human carcinogen	6
Group E	Evidence of non-carcinogen for human	4

Table S3. Classification table of the median effective concentration (EC_{50})

Category	Acute category 1	Acute category 2	Acute category 3
EC_{50} range (mg/L)	$EC_{50} \leq 1.00$	$1.00 < EC_{50} \leq 10.0$	$10.0 < EC_{50} < 100$
Reference scale	7	5	3

Table S4. Green chemistry technology assessment index/proxy variable with related data

Index	Proxy variable		Related data
Environment	GHG	GHG emissions	- kg-CO_2 conversion
		IRIS category	- IRIS (US EPA)
	Hazardous substances	PEL	- PEL (OSHA)
		R-Phrase	- EU Directive 67/548/EEC
		EC_{50}	- EC_{50} (US EPA_ECOTOX)
Safety	Risk for explosion/fire	R-Phrase	- EU Directive 67/548/EEC
Resource	Depleting resource	Resource consumption	- Material balance (GHG, metal)
Economy	Production cost/retail price	Market share	- Production cost: actual or estimated
		Production cost	- Retail price: actual or estimated
		Retail price	

GHG, greenhouse gas; IRIS, Integrated Risk Information System; EPA, Environmental Protection Agency; PEL, permissible exposure limit; OSHA, Occupational Safety and Health Administration; EU, European Union; EC50, median effective concentration; R-Phrase, risk phrase.

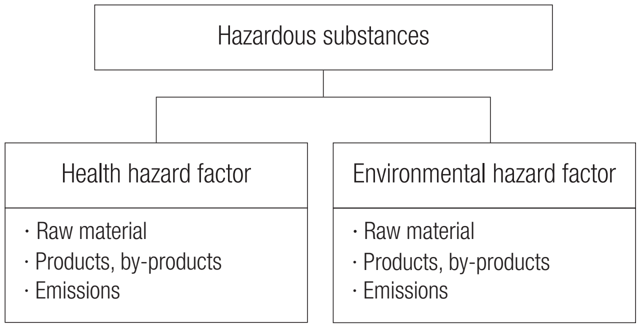

Figure S1. Mimetic diagram for the hazard factors of hazardous substances for human body and environment.