Practical Optimization Methods for Finding Best Recycling Pathways of Plastic Materials

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요 약

ABSTRACT : Optimization methodologies have been proposed to find the best environment-friendly recycling pathways of plastic materials based on life-cycle assessment (LCA) methodology. The main difficulty in conducting this optimization study is that multiple environmental burdens have to be considered simultaneously as the cost functions. Instead of generating conservative Pareto or noninferior solutions following multi-objective optimization approaches, we have proposed some practical criteria on how to combine the different environmental burdens into a single measure. The obtained single objective optimization problem can then be solved by conventional nonlinear programming techniques or, more effectively, by a tree search method based on decision flows. The latter method reduces multi-dimensional optimization problems to a set of one-dimensional problems in series. It is expected the suggested tree search approach can be applied to many LCA studies as a new promising optimization tool.

1. INTRODUCTION

In the face of the increasingly serious problems of plastic wastes management, various approaches for developing effective disposal or recycling solutions have actively been attempted in industry, government, and academic institute [1]. The waste management strategies in plastics may encompass diverse recycle pathways, i.e., mechanical, thermal, chemical recycling, etc. [2]. In order to evaluate and compare these various alternatives, or to find an optimum combination of them, it is not sufficient to limit out attention to the recycling process itself because the efforts for reducing the environmental burdens of one process may increase the burdens elsewhere in the life cycle, so that overall environmental impacts may be increased. In this regard, a life-cycle assessment (LCA) is a useful tool for quantitatively evaluating the environmental burdens considering the whole life cycle of the products[3].

It would be more effective to use an analytic mathematical model in an LCA study rather than to rely on simple calculations using spreadsheet software. The necessity of the utilization of mathematical models are much more felt for the case that a product has a large number of recycle alternatives like plastic materials being discussed here. In our previous paper, a comprehensive life-cycle model of plastic materials was derived adopting polyethylene terephthalate (PET) bottles as an example [4]. The developed model has been applied for comparing the environmental performance of various waste management scenarios as well as for identifying the most effective decisions for recycling through parameter sensitivity analysis[4]. As an extension of usages of the mathematical model in LCA, we here treat the optimization problems for finding optimum waste management policies of plastic materials.

One difficulty for conducting this optimization study is the multi-objective nature of the problem. There can be a number of environmental burdens or impacts of interests, which are often in conflict. Two options can be made for treating this situation. Firstly, we can simply combine the individual objective functions into a single measure by introducing weighting parameters and then solve conventional single-objective optimization problems. Otherwise, we could generate somewhat conservative Pareto solutions (i.e., noninferior solutions) using multi-objective optimization techniques, leaving the final trade-offs to the decision-makers. This paper is mainly concerned with the first approach. PET bottles were also chosen here as an example material as before. The latter topic will be treated in detail elsewhere in the near future.

2. MATHEMATICAL MODELING

A simple schematic diagram of life cycle of PET bottles is presented in Fig. 1. The life-cycle model of PET bottles encompass various possible recycle pathways and disposal, i.e., to recycle the collected plastic wastes as polymers (to the bottles or carpets production) by mechanical treatment, as a raw material by solvolysis, or as fuels by pyrolysis while to send the uncollected ones to the landfill or to the incineration. We have introduced five parameters in the model for describing the relative ratio of two output material (or energy) flows at the junctions. The implications of the model parameters can be more clearly understood from the decision flow diagram shown in Fig. 2.

From the overall material and energy balance for the life cycle of PET bottles with 60 kg PET bottles and the same amount of PET carpets chosen as a functional unit, the final functional form of the resulting model equations of the system can

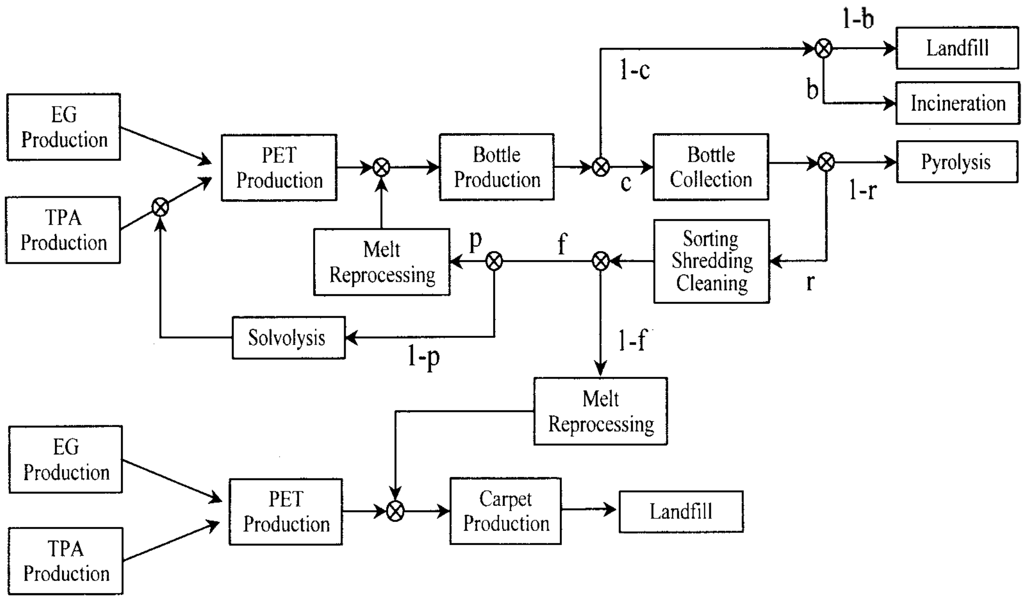

Figure 1: Schematic diagram showing the recycle pathways of PET bottles

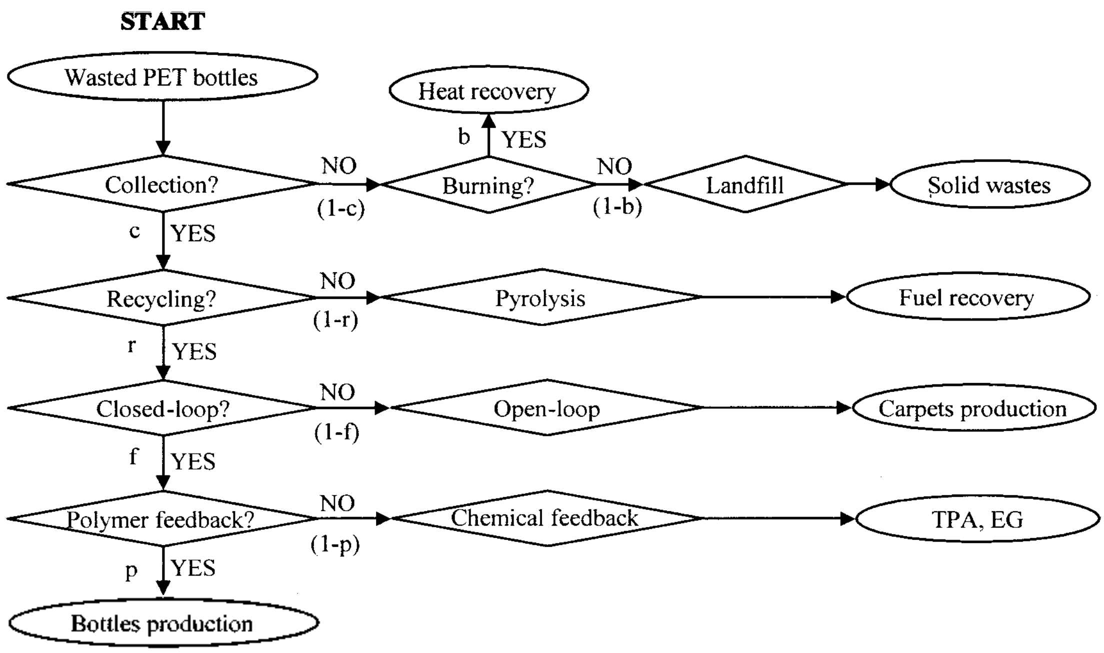

Figure 2: Decision hierarchy diagram

be written as follows:

$$F = A_0 + A_1c + A_2rc + A_3frc + A_4pfrc + A_5b(1-c) \quad (1)$$

where the function F can represents environmental burdens such as energy (E), CO_2 (C), NO_x (N), SO_x (S), or solid wastes (W) while the parameters, c, r, f, p and b denote the collection ratio, recycle ratio, closed-loop (feedback) recycle ratio, recycle ratio as polymer input, and incineration (burning) ratio, respectively. It should be noted that the coefficient A_0, A_2-A_5 are constant while A_1 is a nonlinear function of collection ratio c, i.e.,

$$A_1 = A_{1,L} + A_{1,N}c^5/(1-c) \quad (2)$$

which is due to our nonlinear modeling for the collection process[4-5]. Unlike the conventional linear models adopted in most LCA studies which is amenable to linear analysis[6-7], our nonlinear model needs more complex nonlinear tools for analysis as will be explained in the later sections. By assigning appropriate numerical values between 0 to 1 in the parameters (c, r, f, p and b), we can make Eq. (1) flexibly represent any waste management routes shown in Fig. 1 or any combinations of them. The detailed procedure for the derivation of the model equation, invoked assumptions and premises therein are found in our previous studies[4-8].

3. OPTIMIZATION METHODOLOGIES

3.1 Formulation of optimization problems

The objective function to be minimized in this study are five different environmental burdens, i.e., E, C, N, S and W. This vector minimization problem is formulated as a general multi-objective optimization format as follows[8-9]:

Minimize the objective function

$$J = J\ (E,C,N,S,W) \quad (3)$$

subject to the constraints

$$0 \le c < 1 \text{ and } 0 \le r,f,p,b \le 1 \quad (4)$$

The above optimization analysis in general constitutes an unconstrained nonlinear optimization problem for which, once the objective function of Eq. (3) is defined, optimum solutions can be readily obtained using conventional nonlinear programming (NLP) techniques like Davidson-Fletcher-Powell (DFP) or Broyden-Fletcher-Goldfarb-Shanno (BFGS) methods [10-11]. One of the simplest functional forms of Eq. (3) may be a linear combination of individual environmental variables, i.e.,

$$J = \alpha_1 E + \alpha_2 C + \alpha_3 N + \alpha_4 S + \alpha_5 W \tag{5}$$

where the weighting functions α_i's can take any nonnegative values including zero.

The difficulty in the use of Eq. (5) is that there are no general criteria on how to assign the appropriate weighting functions to the each environmental variable. Under this difficult situation, we first consider the simplest case that only the one environmental burden among the five variables is chosen as an objective function. Table 1 shows the results of this optimization problem where only one weighting factor is set to unity with other four weightings zeros in Eq. (5). Here we can notice that except for the parameter c, all the other parameters turn out to have the values of either zero or unity as their optimal values in the solutions. This is because, in our model, only the collection operation is assumed to have a nonlinear relationship between the collection parameter (collection ratio c) and the environmental burden variable, whereas all the other recycle operations have linear relationships with respect to their corresponding parameters (r, f, p and b).

Table 1

	Optimum values				
J	c	r	f	p	b
E = 11,923[MJ]	0.8193	1.0	1.0	1.0	1.0
C = 551.92[kg]	0.8097	1.0	1.0	1.0	0.0
N = 0.972[kg]	0.0	-	-	-	1.0
S = 2.437[kg]	0.0	-	-	-	1.0
W = 75.05[kg]	0.0	-	-	-	1.0

where, (-)=not applicable

3.2. Tree search method based on decision flows

Besides relying on NLP techniques, we propose, here, another interesting method to easily find the optimum solutions using the decision flow diagram shown in Fig. 2. From the parameter sensitivity analysis conducted in our previous study[4], it has been proved that the earlier decision makes a more significant effect on the overall results than the later ones, i.e., the collection ratio (c) is the most sensitive parameter affecting the environmental performance while the polymer feedback ratio (p) the least. It is worth noting that it is impossible to determine the optimum value for the earlier decision until the subsequently following parameters are fixed. For example, we cannot say anything about whether closed-loop feedback (f) is an environmentally favorable action until we can have information about what would be the next recycle pathway, i.e., polymer feedback (p) or chemical feedback (1-p). Thus, for the determination of the optimum parameter set, we should backtrack from the latest decision to the earlier one.

This fact can be also verified by analyzing the model equation. Consider the case that we want to find an optimum parameter set minimizing only energy consumption during the life cycle of PET bottles (in that case, α_1=1, and the others are zero), then the objective function becomes

$$J = E = A_{E0} + A_{E1}c + A_{E2}rc + A_{E3}frc + A_{E4}pfrc + A_{E5}b(1-c) \tag{6}$$

where A_{E0} = 13971.7, A_1 = - 0.801.6 + $60c^5/(1-c)$, A_{E2} = -1386.6, A_{E3} = 428.8, A_{E4} = -595.6 and A_{E5} =

- 1209.6[4-8]. It is evident that the optimum values for the parameters p and b can easily be determined only by checking the sign of their coefficients, i.e., $A_{E4}frc$ and $A_{E5}(1-c)$. Since the coefficients of p and b are all negative, the optimum values for two parameters should be their allowable maximum limits, i.e., $p_{opt}=b_{opt}=1$ (100% polymer feedback and 100% burning). Now that the optimum polymer feedback ratio is determined, we can in turn proceed to the next decision, i.e., the determination of f. Because the coefficient of the parameter f, $(A_{E3}+A_{E4}p_{opt})rc$, is also negative in this case, we have also 100% closed-loop feedback ($f_{opt}=1$) as the best value. For the determination of the parameter r, the same method can be applied, resulting in $r_{opt}=1$. Finally the optimum collection ratio, c_{opt}, can be calculated with the already determined p_{opt}, f_{opt}, r_{opt}, and b_{opt}. There is no significant difference in calculating the optimum value of the parameter c except that we should solve a one-dimensional nonlinear optimization problem unlike the case of the linear parameters of which the optimum values exist as a corner point. This concept is called as a tree search method[12] and the procedure for determining the optimum parameter values is illustrated in Fig. 3. As expected, the final results obtained by this tree search method are the exactly same as the ones by the nonlinear programming techniques in Table 1. The proposed method has a strong advantage in that the multi-dimensional optimization problems can be reduced to one-dimensional search problems in series. If the parameters are linear, we just need to examine the sign of the corresponding coefficient of the parameter to determine its optimum value, and if the parameters are nonlinear, their optimum values can be easily found just using a one-dimensional search method. Besides this simplicity of the tree search method, it is provides a deeper insight on the optimization results than the general multi-dimensional optimization analysis does.

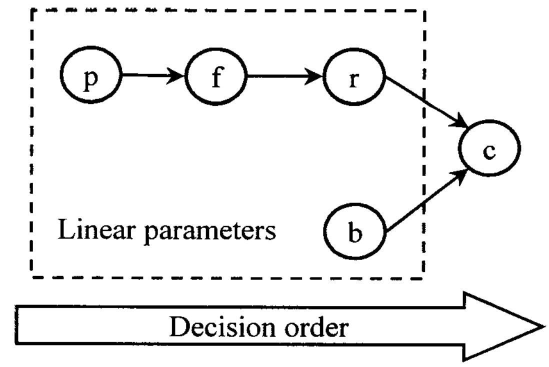

Figure 3: Parameter decision order in a tree search method

3.3 Combination of multiple objective functions

As we can see in Table 1, the optimum parameter sets obtained in the above single objective optimization problems are quite different depending on the environmental variable chosen as an objective function. To combine these results in a reasonable way, we consider some more advanced methodologies, which will be discussed now[8].

As mentioned before, although a general methodology for assigning the proper weighting factors of Eq. (5) has not been developed yet, transformation of the different environmental burdens into economic value can be one of the most promising methods applicable for those purposes. To estimate the cost for the gaseous emissions, the damage done by specific gaseous emissions can be considered. Acc-

Table 2

Items	Raw data	Transformed results
Energy	1.74 \$/B	2.57 won/MJ ($=\alpha_1$)
CO_2	0.4 pence/kg	8 won/kg ($=\alpha_2$)
NO_x	127.0 pence/kg	2,540 won/kg ($=\alpha_3$)
SO_x	258.4 pence/kg	5,168 won/kg ($=\alpha_4$)
Solid wastes	255 won/kg	255 won/kg ($=\alpha_5$)

where, the raw data have been transformed assuming
1 barrel = 158.985 liter
density of crude oil = 0.9 kg/liter
heat of combustion (crude oil) = 45 MJ/kg
1 dollar = 1,300 wo
1 pound = 2,000 won

ording to the reported European methodology, we have considered the physical impacts of gaseous emissions derived from dose-response functions of damage to crops and forest and the damage value for human health based on the value of lost productivity, medical costs, the value of a statistical life and willingness to pay to avoid symptoms [13-14]. The economic value of the energy is roughly estimated from the average price of imported crude oils in Korea [15] and that of the solid wastes are obtained from the landfill costs of PET in Korea [16]. The units for the economic costs are all transformed into Korea monetary unit (i.e., won) (Table 2). Then the multiple objective functions can be aggregated using the calculated economic costs for each environmental burden as weighting factors. The optimum solutions found in such a way is r=f=p=b=1.0 and c=0.8153.

As another way to combine the multiple objectives into a singular measure, it is possible to use some externally-provided criteria like the results of the impact assessment of the LCA methodology. For this case, the objective function is reformulated as follows:

$$J = k_1EDP + k_2GWP + k_3AP + k_4HT + k5NP + k_6SW \tag{7}$$

where EDP = energy depletion potential, GWP = global warming potential, AP = acidification potential, HT = human toxicity, NP = nutrition potential, SW = solid waste, and k_i's (i=1-6) are the weights. Here, all the scores for each environmental theme used in Eq. (7) was normalized to an inhabitant equivalent of Korea. In the weighting of environmental profiles, every environmental theme gets a weight, representing the relative seriousness of that theme. Now that the weighting factors except k_1 and k_6 are available from the open literatures [17-18], we have shown the optimization results with various values for k_1 and k_6 in Table 3. There are four

Table 3

Cases	k_1	k_6	c	r	f	p	b	J
I	2.5	2.5	0	-	-	-	-	1.005
II	2.5	10	0	-	-	-	-	1.526
III	10	2.5	0.603	1	1	1	1	1.584
IV	10	10	0	-	-	-	-	2.117

where, $J = k_1EDP + k_2GWP + k_3AP + k_4HT + k_5NP + k_6SW$
and
$k_2 = 2.5$, $k_3 = 10$, $k_4 = 5$, $k_5 = 5$

cases where the relative priorities of EDP and SW are set to be different. The Case I, for example, consider EDP and SW serious to the same extent as GWP (i.e., k_1=k_6=k_2=2.5) while in the Case IV their environmental seriousness is treated the same as AT (i.e., k_1=k_6=k_3=10). When the relative weight for EDP is low compared to other items, the optimum parameter values are in tune with the results of N, S, W in Table 1, i.e., no collection is the most favorable activity for environments. But, when we feel that energy depletion is the most serious problem, i.e., the weighing is set relatively large, the situation becomes different (the Case III in Table 3). However, we have to admit the limitations to these results. The weighting factors chosen here, to a large extent, have a subjective nature and, until now, no consensus has been reached regarding a preferred approach.

Finally, we propose another way for solving the multi-objective optimization given by Eqs. (3) and (4) where a single environmental variable is chosen as a objective function while the other four variables are treated as constraints [9]. This method is called bounded objective function method in optimization theory [19]. One simple example is illustrated below,

Minimize

$$J = E \tag{8}$$

subject to

$$C \le C_{SET},\ N \le N_{SET},\ S \le S_{SET},\ W \le W_{SET},\ 0 \le c < 1, \text{ and } 0 \le p,f,r,b \le 1 \quad (9)$$

where the values of C_{SET}, N_{SET}, S_{SET}, and W_{SET} could be given by external conditions like the government regulations or by the impact assessment analysis of the LCA. The above constrained nonlinear optimization problem can be solved using constrained nonlinear programming techniques like successive quadratic programming (SQP) or generalized reduced gradient (GRG) method [19]. Table 4 shows the various results of this optimization method where various constraints for the C, N, S and W are imposed on each case. In Case II, for example, all the emissions and solid wastes are limited to be below the landfill level. But, these constraints are too strict to have a solution. Thus, these constrains are a little bit relaxed to obtain a feasible solution in Case III. Such obtained optimum collection ratio (i.e., c_{opt}=0.8085) is slightly different from the unconstrained optimization problems of Case I (i.e, c_{opt}=0.8193), but the minimum energy consumption obtained in each case is not affected by this small changes. The similar results are found in Cases III and IV, where the constrains imposed on Case IV are more strict than Case III.

Table 4

Cases	CSET [kg]	NSET [kg]	SSET [kg]	WSET [kg]	Emin [MJ]	c	r	F	p	b
I	∞	∞	∞	∞	11,923	0.819	1	1	1	1
II	616.3	1.416	3.133	135.1	-	-	-	-	-	-
III	647.1	1.487	3.290	141.9	11,923	0.809	1	1	1	1
IV	644.4	1.287	2.989	95.15	11,923	0.812	1	1	1	1
V	612.2	1.223	2.840	90.39	-	-	-	-	-	-

where, (-)=no solutions are found satisfying the imposed constraints.
Case I: no constraints.
Case II: landfill level
Case III: 105% level of Case II.
Case IV: A specific situation level (e.g., c=r=f=p=b=0.5, here)
Case V: 95% level of Case IV.

4. CONCLUSIONS

Some practical optimization methodologies have been proposed for finding optimum waste management scenarios of PET bottles. The objective functions chosen in this paper are energy consumption, gas emissions and solid waste generation during a life cycle of PET bottles. These multi-objective optimization problems could be converted into single objective optimization problems based on various combining criteria suggested in this paper. The resulting single objective function can be solved by conventional nonlinear programming techniques or, more effectively, by a tree search method. The latter method is based on the decision hierarchy for the various recycling options, capable of easily identifying optimum values of linear and nonlinear decision parameters. The methodologies for combining this tree search concept with the multi-objective nonlinear programming techniques are being under investigation, which will be reported elsewhere in the future.

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NOTATION

AP normalized acidification potential [-]
A_i's coefficients of environmental burden variables of Eq. (1)
b burning ratio [-]
C total amount of CO_2 emissions during the

life cycle of 60kg of PET bottle [kg]

c collection ratio [-]

E total amount of energy consumed during the life cycle of 60kg of PET bottle [MJ]

EDP normalized energy depletion potential [-]

F general function representing energy, gaseous emissions and solid wastes

f closed-loop feedback ratio [-]

GWP normalized global warming potential [-]

HT normalized human toxicity [-]

k_i's weighting factors for the environmental theme of Eq. (7)

J objective function in the formulated optimization problem

N total amount of NO_x emissions during the life cycle of 60kg of PET bottle [kg]

NP normalized nutrition toxicity [-]

p polymer feedback ratio [-]

r recycle ratio [-]

S total amount of SO_x emissions during the life cycle of 60kg of PET bottle [kg]

SW normalized solid wastes generation [-]

W total amount of solid wastes generated during the life cycle of 60kg of PET bottle [kg]

Greek letter

α_i's weighting factors for the environmental variables of Eq. (5)

Subscript

SET upper limits of the variables set by external conditions

opt optimum value of the decision parameters

E energy function

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