Korean J. Chem. Eng., **16**(2), 202-207 (1999)

A LIFE-CYCLE ASSESSMENT (LCA) STUDY ON THE VARIOUS RECYCLE ROUTES OF PET BOTTLES

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(*Received 27 July 1998 • accepted 11 February 1999*)

Abstract–A life-cycle assessment (LCA) study on various recycle routes of plastic materials has been conducted using the case of polyethylene terephthalate (PET) bottles as an example. The energy consumed and the emissions released during the entire life-cycle of the plastic material were accounted for using the energy and material balances on each stage of the life-cycle. A mathematical model including a simple nonlinear relation for the collection process of the bottles was derived for the system which encompasses all possible recycle alternatives. This model contains several adjustable parameters representing each alternative step of the recycle routes. Then through parameter sensitivity analysis and optimization analysis we could both identify environmentally favorable recycle routes and determine the optimal conditions for the best one. The methodology of this study can be easily applied to the comparison of the general waste management alternatives determining their relative advantages and disadvantages viewed from the associated environmental burdens. Those results will be reported elsewhere.

Key words : Life-Cycle Assessment (LCA), Nonlinear Programming (NLP), Multi-Objective Optimization, PET Bottles, Plastics Recycling Routes, Sensitivity Analysis

INTRODUCTION

Significant technological advances in plastics manufacturing made by the related industries over the past several decades have contributed to the production of a large amount of plastics worldwide every year but at the same time, they have resulted in an equally large amount of plastic waste produced as well, causing many serious environmental problems [Boettcher, 1992]. Plastics constitutes a major portion, especially on the volume basis, of the solid waste generated by municipalities throughout the world [Fletcher and Mackay, 1996]. Although most of the plastic wastes are being dumped into landfills at the moment, this kind of disposal will be forbidden in the future due to the ensuing environmental problems like leachate hazards, groundwater pollution, gaseous emissions, and to the lack of dumping space. Instead, we are required to find environmentally favorable alternatives to landfill for the effective management of plastic wastes [Brown, 1993].

In order to evaluate and compare various waste management methods of plastics hitherto known on a comprehensive and objective basis, we need to consider overall environmental burdens brought by plastics during their entire life-cycle, namely, from the cradle to the grave, which includes such different stages of the plastic products as the extraction and processing of raw materials, manufacturing, transportation, distribution, use/reuse, maintenance, recycling, and the final disposal of plastics. The concept of the life-cycle assessment (LCA) has been developed for this purpose and widely used in recent years in many different situations [SETAC, 1991]. The LCA is defined as an objective process evaluating the environmental burdens associated with certain products, processes or activities, which includes the identification and quantification of energy and materials consumed and of wastes produced therefrom. Generally, the LCA study is performed following the four stages: (1) goal definition and scoping, (2) inventory analysis, (3) impact assessment, and (4) interpretation. Among these four stages the inventory analysis has been most developed, and the impact assessment and interpretation stages are still being developed [Curran, 1996].

Many research efforts on LCA to date have been made using a spread sheet type of model to compare different alternatives for the same end use or application [Curran, 1996; Sauer et al., 1994]. However, it is believed more desirable to perform LCA studies on plastic materials using a systematically derived mathematical model because of the many possible recycle alternatives existing for the disposal of plastics.

The present study thus deals with the mathematical modeling and subsequent optimization related to the plastics waste management problem with focus on the inventory analysis of the LCA study, using the case of polyethylene terephthalate (PET) bottles as an example. The relationships between various recycle operations and their associated environmental burdens involved in the chosen system are considered linear except for the collection process of the plastic bottles which is believed to have a nonlinear relationship between the environmental burdens and the collection ratio of the total bottles consumed [Boustead, 1995b]. A simple model for the collection process is chosen to reflect this nonlinear nature of the functional relationship, i.e., the energy required for the collection becomes infinite as the collection approaches 100 %.

The final model of the system then becomes a nonlinear

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multi-variable functional relation from which we perform two analyses, i.e., parameter sensitivity analysis and optimization analysis. The former leads us to find which recycle route is environmentally favorable, while the latter allows us to get optimal solutions for the given waste management situations. The Jacobian matrix is the tool for the parameter sensitivity analysis to find the best recycle route while the objective function formulated using various environmental burden variables is the key concept in the optimization analysis

MATHEMATICAL MODELING

1. Block Diagram of the Alternative Recycle Routes

For the PET bottles which we have chosen for our study as an example, the following alternative recycle routes are considered possible [Westerhout, 1998; Paszun and Spychaj, 1997; Hensen, 1995]. (1) Mechanical recycling where the waste PET bottles are recycled through the reprocessing steps of melt extrusion and filtration as polymer input either to the bottle production process (closed-loop recycling), or (2) to a carpet production process (open-loop recycling), (3) chemical recycling where the waste PET bottles are recycled either through depolymerization by solvolysis (e.g., hydrolysis) as chemical input, i.e., terephthalic acid (TPA) and ethylene glycol (EG) as raw materials, (4) thermal recycling where the waste PET bottles are recycled through degradation or pyrolysis as fuels or raw materials, or (5) through incineration as heat energy, and finally, (6) the dumping where the waste PET bottles are discarded in landfills.

Fig. 1 shows the diagram illustrating the whole system of the above alternative recycle routes for PET bottles from the production stage of raw materials for PET to the final disposal stage (The operations involved in the individual stages are explained at the bottom in Fig. 1). The functional units in this system are 60 kg of PET bottles and 60 kg of PET carpets. The above-mentioned six alternative recycle routes or any combinations of them can be easily recovered by properly adjusting the values of the five parameters representing the individual recycle operations. Some of the results of these alternative routes are shown in Table 1.

Table 1. Various recycle alternatives set by different parameter values

Alternatives	c	r	λ	f	w
L	0	*	*	*	*
I	0<c<1	0	*	*	1
P	0<c<1	0	*	*	0
D	0<c<1	1	0	0	*
R	0<c<1	1	0	1	*
O	0<c<1	1	1	*	*

where L=landfill, I=incineration+landfill, P=pyrolysis+landfill, D=depolymerization+landfill, R=reprocessing+landfill, O=open-loop recycle+landfill, *=not applicable

2. Mathematical Modeling

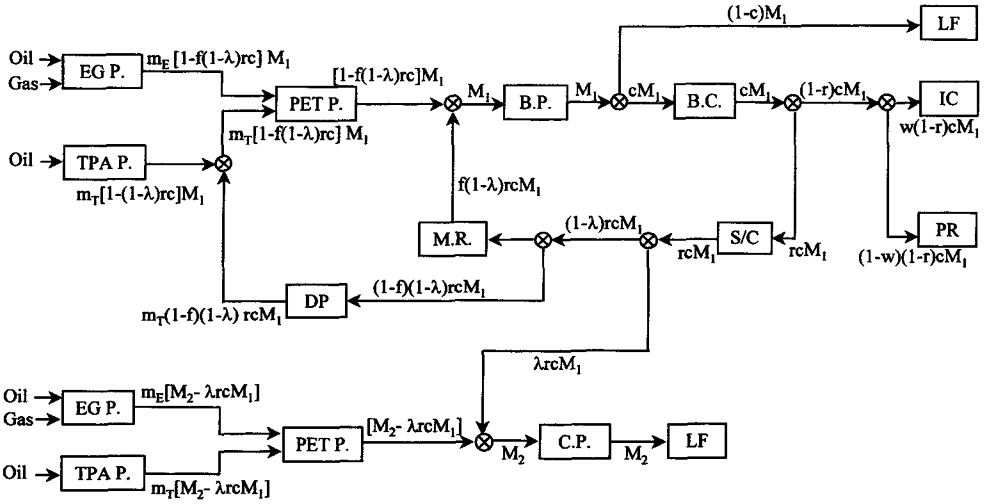
Now that the overall flow diagram showing the alternatives is established, we proceed to obtain the energy consumed and the emissions released by the individual process. All the necessary values for the energy and emissions have been taken from the open literature [PRé Consultants, 1997; BUWAL, 1996; PIRA, 1995; Boustead, 1993, 1995].

The energy needed for the collection process of PET bottles is assumed to have the following functional form :

$$E_C[\text{MJ/kg PET Bottle}] = P_1 + P_2\frac{c^m}{1-c} \tag{1}$$

where E_C and c denote the collection energy required for unit kg of the bottles, and the collection ratio, respectively, while P_1, P_2, and m are the adjustable parameters making the model fit the data.

The model of Eq. (1) thus shows that the limiting case of



where EG P. = EG production, TPA P. = TPA production, PET P. = PET production, B.P. = bottles production, B.C. = bottles collection, S/C = sorting and cleaning, M.R. = melt reprocessing, DP = depolymerization, C.P. = carpet production, LF = landfill, IC = incineration, PR = pyrolysis

Fig. 1. Schematic diagram showing the recycle routes of PET bottles.

hypothetical 100 % collection, i.e., c approaching 1, incurs an infinite amount of collection energy, whereas in the case of moderate collection, e.g., $c<0.6$, the collection energy per kg of bottles, E_C, remains almost constant and equal to P_1, meaning that the total collection energy increases linearly with the amount of the collected bottles [Boustead, 1995b]. The parameters P_2 and m explain the nonlinear character of the model in that P_2 represents at what value of the collection ratio (c) the collection energy curve starts to increase fast with respect to c, and m represents how fast that curve increases.

As described above, the parameters of the model of Eq. (1) can be determined if the experimental collection data are available over the entire range of the collection ratio, i.e., $0<c<1$. It is unfortunately not the case in Korea at the present time: the collection ratio is only around 10 %. Thus what we did was to determine the linear parameter P_1, from the available data for a limited range of c and then estimate the other nonlinear parameters P_2 and m best as we can invoking reasonable assumptions.

In the particular example of this study, we thus found $P_1=0.12$ from the data [Moon, 1997] and chose $P_2=1$ and m=5 (As seen from Fig. 2, the curve with $P_2=1$ and m=5 is judged reasonable for the collection energy curve).

After choosing the appropriate model for the collection process of the bottles, we proceed to derive the overall mathematical model for the total energy consumed and the total emissions released by the functional units of the system, i.e., 60 kg of PET bottles and 60 kg of PET carpets, during the entire life-cycle of PET bottles as illustrated by Fig. 1. The appendix explains the detailed procedure of the derivation of the energy consumed over the entire life-cycle, counting all the involved steps in Fig. 1.

The final functional form of the resulting model equations of the system can be written as follows:

$$\begin{aligned} F &= F(c,r,\lambda,f,w) \\ &= A_0+A_1c+A_2rc+A_3\lambda rc+A_4f(1-\lambda)rc+A_5w(1-r)c \end{aligned} \quad (2)$$

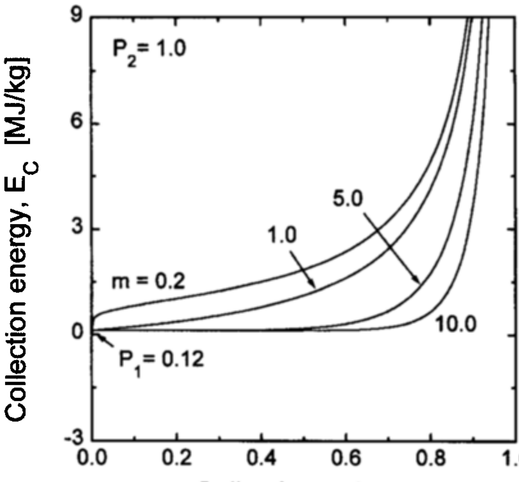


Fig. 2. Example curves of the energy for collection.

where the function F represents any of five variables like energy (E), CO_2 (C), NO_x (N), SO_x (S), or solid wastes (W), while parameters, c, r, λ, f, and w denote collection ratio, recycle ratio, open-loop recycle ratio, recycle ratio as polymer and incineration/pyrolysis ratio, respectively, and A_i's are the coefficients.

Eq. (2) can be made to represent any recycle alternatives or any combinations of them by simply setting appropriate values for the five parameters. Table 1 shows some examples of such results.

PARAMETER SENSITIVITY ANALYSIS

In the block diagram of Fig. 1 explaining the entire life-cycle of PET bottles, there are eight junctions where more than three streams of materials are involved. Of these, five junctions have one input and two output streams whereas the other three have two input and one output streams, respectively. Depending on the values that the five parameters c, r, λ, f, and w take on, all possible recycle routes can be identified.

One obvious utility of this diagram is the fact that the effect of different recycle operations on the final environmental burdens can be easily determined. In other words, by computing the sensitivity of the environmental burdens of energy, CO_2, NO_x, SO_x, or solid wastes to the different recycle operations, we can answer questions like which route is better in what category of environmental burdens, and so on. This sensitivity is nothing more than the partial derivatives of function F of Eq. (2) with respect to the five parameters c, r, λ, f, and w, i.e.,

$$\frac{\partial F}{\partial c}, \frac{\partial F}{\partial r}, \frac{\partial F}{\partial \lambda}, \frac{\partial F}{\partial f}, \text{ and } \frac{\partial F}{\partial w} \quad (3)$$

Since F here stands for any of the five different functions, i.e., E (energy), C (CO_2), N (NO_x), S (SO_x), and W (solid wastes), the above partial derivatives can form a Jacobian matrix as shown below which represents all the sensitivities of the environmental burdens to the different recycle operations. This Jacobian matrix thus contains the information about the individual recycle route as to how beneficial the particular route is against the environmental burdens in question.

$$M_J \equiv \begin{bmatrix} \frac{\partial E}{\partial c} & \frac{\partial E}{\partial r} & \frac{\partial E}{\partial \lambda} & \frac{\partial E}{\partial f} & \frac{\partial E}{\partial w} \\ \frac{\partial C}{\partial c} & \frac{\partial C}{\partial r} & \frac{\partial C}{\partial \lambda} & \frac{\partial C}{\partial f} & \frac{\partial C}{\partial w} \\ \frac{\partial N}{\partial c} & \frac{\partial N}{\partial r} & \frac{\partial N}{\partial \lambda} & \frac{\partial N}{\partial f} & \frac{\partial N}{\partial w} \\ \frac{\partial S}{\partial c} & \frac{\partial S}{\partial r} & \frac{\partial S}{\partial \lambda} & \frac{\partial S}{\partial f} & \frac{\partial S}{\partial w} \\ \frac{\partial W}{\partial c} & \frac{\partial W}{\partial r} & \frac{\partial W}{\partial \lambda} & \frac{\partial W}{\partial f} & \frac{\partial W}{\partial w} \end{bmatrix} \quad (4)$$

Let's consider, as an example, the case where we would like to know the effect of the particular recycle route on the CO_2 emissions. We then compute the values of the elements in the second row of the above Jacobian matrix. Fig. 3 shows the results of one example case, i.e., the recycle route having $r=\lambda=f=w=0.5$ and $0<c<1$. From Fig. 1 we know that this case involves (1) a 50 % out of all the collected bottles is

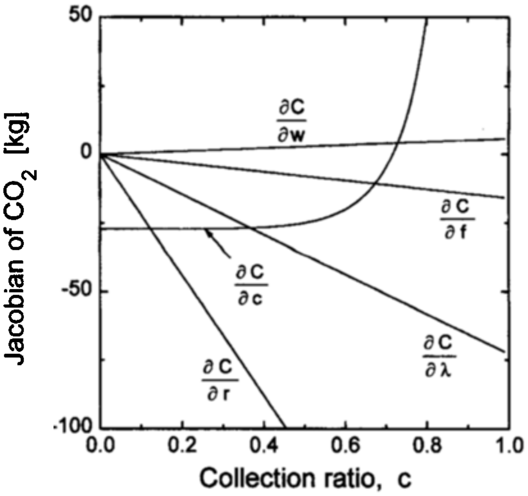


Fig. 3. Sensitivities of CO_2 emissions to different recycle operations.

recycled, i.e., r=0.5, (2) a 50 % out of the recycled is fed to the closed-loop route, i.e., (1–λ)=0.5, (3) a 50 % out of the closed-loop feedback is for the polymer reprocessing route, i.e., f=0.5, (4) a 50 % out of the unrecycled bottles is for incineration route, i.e., w=0.5. From the curves in Fig. 3, we can immediately find that the CO_2 emission is decreased by increasing any of r, f or λ, and increased by increasing w. As for the effect of the collection ratio (c), we can see that more collection is good in terms of reducing the overall CO_2 emission only when c is below 72 %.

We can compute the values of the elements of other rows or columns in the Jacobian matrix of Eq. (4) to determine any particular effects of any particular recycle operations shown in Fig. 1. In other words, we can always determine the direction we have to go in choosing the best recycle route in order to reduce the particular environmental burdens for the given waste management system.

OPTIMIZATION ANALYSIS

The optimization analysis of the system has the following format.

Minimize the objective function

$$J=J(E, C, N, S, W) \tag{5}$$

subject to the constraints

$$0 \le c < 1$$
$$0 \le r, \lambda, f, w \le 1 \tag{6}$$

The simplest functional form of the objective function of Eq. (5) is a weighted linear combination as shown below.

$$J=w_1E+w_2C+w_3N+w_4S+w_5W \tag{7}$$

where the weighting functions w_i's can take on any values including zero.

The above optimization analysis in general constitutes an unconstrained nonlinear optimization problem for which nonlinear programming techniques like DFP (Davidon-Fletcher-Powell) or BFGS (Broyden-Fletcher-Goldfarb-Shanno) methods can be used to obtain solutions [Rao, 1996; Reklaitis et al., 1983], whereas for linear problems linear programming tools are also available [Azapagiz, 1995]. Table 2 shows the results of this optimization problem when the objective function takes on single environmental burden variable with the remaining four variables set to zero. Here we can notice that except for 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 has a nonlinear relationship between the collection parameter (collection ratio c) and the environmental burden variable as shown in Eq. (1), whereas all the other recycle operations have linear relationships with respect to their corresponding parameters (r, λ, f, w).

Table 2. Best environmental results by the particular recycle route

	Optimum values				
J	c	r	λ	f	w
E=9,936 [MJ]	0.896	1.0	1.0	*	*
C=456.6 [kg]	0.862	1.0	1.0	*	*
N=1.12 [kg]	0.715	1.0	1.0	*	*
S=2.25 [kg]	0.919	1.0	1.0	*	*
W=75.13 [kg]	0.999	0.0	*	*	1.0

where *=not applicable

There are two possible ways to solve the optimization problem having an objective function like the one of Eq. (7). One is to find suitable weightings for each environmental burden variable using the results of the impact assessment of the LCA methodology, which is currently developed [Curran, 1996]. The other way of solving the general optimization problem is to choose a single environmental variable for the objective function of Eq. (7) while the other variables are treated as constraints. The following illustrates one such example.

Minimize

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

subject to

$$C \le C_{SET},\ N \le N_{SET},\ S \le S_{SET},\ W \le W_{SET},$$
$$0 \le c < 1, \text{ and } 0 \le r, \lambda, f, w \le 1 \tag{9}$$

where the values of C_{SET}, N_{SET}, S_{SET} and W_{SET} could be given by external conditions like the governmental regulations or the impact assessment analysis of the LCA.

CONCLUSIONS

Using the case of PET bottles as an example, a life-cycle assessment (LCA) study on various possible recycle routes of plastic materials has been conducted. Mathematical models for the overall waste recycle system, including a nonlinear relationship for the collection process of the PET bottles, have been developed using the energy and material balances on each recycle operation involved. Based on this model, we have performed parameter sensitivity analysis and optimization analysis to determine both the most favorable recycle route in terms of the environmental burdens in question, and the best possible environmental results when the optimal conditions are met. The Jacobian matrix of partial derivatives representing the sensitivity of each environmental burden to the particular recycle operation is used for the former analysis whereas the properly formulated objective function is minimized for the latter analysis. The methodology adopted in this study can be easily applied to other waste management problems.

ACKNOWLEDGMENT

We are grateful for the financial support to this study given by Korea Science and Engineering Foundation (KOSEF) under Grant 96-0502-07-01-3.

APPENDIX

The derivation of the model for the total energy consumed during the entire life-cycle of PET bottles as shown in Fig. 1 is illustrated below. First, we enumerate all the operations which involve energy as process requirements in the following.

Total energy consumed=
(EG production for PET bottles)+(TPA production for PET bottles)+(PET polymerization for bottles)+(bottles production and filling)+(collection of waste bottles)+(sorting/cleaning/shredding)+(reprocessing of flakes)+(depolymerization of waste bottles)+(landfill of waste bottles)+(incineration of waste bottles)+(pyrolysis of bottles to fuels)+(EG production for carpets)+(TPA production for carpets)+(PET polymerization for carpets) +(carpets production)+(landfill of waste carpets) (A1)

Next we express each item above as the product of the mass term and the required energy term for that unit mass. For example, the first item above is expressed as
(Energy required for EG production for PET bottles)=
{the EG mass term}×{required energy term for the production of unit mass of EG}={(mass of EG for 1 kg of PET bottle)×(60)×$[1-f(1-\lambda)rc]$}×{(energy equivalent for required crude oil)+(energy equivalent for required natural gas)+(process energy for EG production)}={(numerical value)×(60)×$[1-f(1-\lambda)rc]$}×{(numerical value)+(numerical value)+(numerical value)}=(constant)+(constant)×$[f(1-\lambda)rc]$ (A2)

All the other items in Eq. (A1) can also be obtained in a similar fashion with the numerical values obtained from the open literature like BUWAL, APME, PEMS, SimaPro, etc. When we add up all of them, we will have the following expression for the total energy consumed having the same functional as of Eq. (2).

$$E=A_{E,0}+A_{E,1}c+A_{E,2}rc+A_{E,3}\lambda rc+A_{E,4}f(1-\lambda)rc+A_{E,5}w(1-r)c \qquad (A3)$$

where the cofficients $A_{E,i}$'s are the sums of the contributions by the individual recycle operations involved as shown below.

$A_{E,0}$=[(Oil for 1 kg EG)+(Gas for 1 kg EG)+(Energy for 1 kg EG)](EG mass for 1 kg PET)(60)+[(Oil for 1 kg TPA)+(Energy for 1 kg TPA)](TPA mass for 1 kg PET)(60)+(Energy for 1 kg PET resin for bottles)(60)+(Energy for 1 kg PET bottles)(60)+(Energy for landfilling of 1 kg PET)(60)+[(Oil for 1 kg EG)+(Gas for 1 kg EG)+(Energy for 1 kg EG)](EG mass for 1 kg PET)(60)+[(Oil for 1 kg TPA)+(Energy for 1 kg TPA)](TPA mass for 1 kg PET)(60)+(Energy for 1 kg PET resin for carpets)(60)+(Energy for 1 kg PET carpets)(60)+(Energy for landfilling 1 kg PET)(60)=13971.7

$A_{E,1}$=(Energy for collecting 1 kg PET bottles)(60)−(Energy for landfilling of 1 kg PET)(60)+(Energy for pyrolysis of 1 kg PET)(60)=−801.6

$A_{E,2}$=−[(Oil for 1 kg TPA)+(Energy for 1 kg TPA)](TPA mass for 1 kg PET)(60)+(Energy for sorting & shredding of 1 kg PET bottles)(60)+(Energy for depolymerization of 1 kg PET)(60)−(Energy for pyrolysis of 1 kg PET)(60)=−958.7

$A_{E,3}$=[(Oil for 1 kg TPA)+(Energy for 1 kg TPA)](TPA mass for 1 kg PET)(60)−(Energy for depolymerization of 1 kg PET)(60)−[(Oil for 1 kg EG)+(Gas for 1 kg EG)+(Energy for 1 kg EG)](EG mass for 1 kg PET)(60)−[(Oil for 1 kg TPA)+(Energy for 1 kg TPA)](TPA mass for 1 kg PET)(60)−(Energy for 1 kg PET resin for carpets)(60)=−3077.2

$A_{E,4}$=−[(Oil for 1 kg EG)+(Gas for 1 kg EG)+(Energy for 1 kg EG)](EG mass for 1 kg PET)(60)−(Energy for 1 kg PET resin for bottles)(60)+(Energy for reprocessing 1 kg PET flakes) (60)−(Energy for depolymerization of 1 kg PET)(60)=−595.6

$A_{E,5}$=(Energy for incineration of 1 kg PET)(60)−(Energy for pyrolysis of 1 kg PET)(60)=−400.8 (A4)

The expressions for the emissions of CO_2, NO_x, SO_x, or solid wastes can also be similarly obtained following the same procedure as for the energy consumed in the above, i.e., Eqs. (A1)-(A4).

NOMENCLATURE

A_i's	: coefficients of environmental burden variables of Eq. (2)
C	: total amount of CO_2 emissions during the life-cycle of 60 kg of PET bottle [kg]
c	: collection ratio [-]
E	: total amount of energy consumed during the life-cycle of 60 kg of PET bottles [MJ]
E_C	: process energy required for collecting 1 kg of PET bottles [MJ/kg]
f	: recycle ratio as polymer [-]
J	: objective function
m	: parameter of the nonlinear collection model [-]
$\mathbf{M}_J$	: Jacobian matrix of sensitivity functions
N	: total amount of NO_x emission during the life-cycle of 60 kg of PET bottles [kg]
P_1, P_2	: parameters of the nonlinear collection model [MJ/kg]
r	: recycle ratio [-]
S	: total amount of SO_x emission during the life-cycle of 60

kg of PET bottles [kg]
w : ratio of incineration of pyrolysis [-]
w_i : weighting factors [i=1-5]
W : total solid wastes generated during the life-cycle of 60 kg of PET bottles [kg]

Greek Letter
λ : open-loop recycle ratio [-]

Substript
SET : upper limits of the variables set by external conditions

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