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A study on the comparison of the various waste management scenarios for PET bottles using the life-cycle assessment (LCA) methodology

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Abstract

A comparison study on the various waste management scenarios of polyethylene terephthalate (PET) bottles has been carried out using the life-cycle assessment (LCA) methodology. The energy and material balances were set up to account for all the energy consumed and the emissions released by each stage of the production and waste management phases of the life-cycle of the PET bottles, and then a mathematical model was derived to illustrate these energy and emissions for the various waste management pathways. For the collection process of the bottles, a nonlinear functional relationship was chosen and included in the model. Using the developed model, the environmental burdens of various waste management alternatives were evaluated to yield a ready comparison of each pathway. We can also easily discern through parameter analysis which waste management scenario is deemed best having the least energy consumed and the smallest emissions released with respect to the environmental burdens in question. © 1999 Elsevier Science B.V. All rights reserved.

Keywords: Jacobian matrix; Life-cycle assessment; PET bottles; Plastics waste management scenarios; Parameter sensitivity analysis

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1. Introduction

The phenomenal growth of the plastics industry during the past several decades has resulted in a vast amount of various kinds of plastics produced worldwide every year contributing to the materialistic affluence in human living [1,2]. This abundance of plastic goods in the world, on the other hand, has also created serious environmental problems, for the ever-increasing amount of plastic wastes defies simple conventional waste disposal methods, i.e. land-filling and incineration. The non-biodegradability of most plastics and the toxic gases produced during their simple incineration are among the obvious difficulties for the plastics waste problem.

This is an irony because the said difficulties associated with plastic waste disposal stem directly from the very success of the plastics industry in making their plastic products possess many superb functional properties. Unlike metals or simple organic materials, most plastics will not rust or be disintegrated easily by micro-organisms, although they can be subject to degradation due to photochemical processes, electrolyte corrosion, hydrolysis and the like at a slow pace. Furthermore the technologies of blending, compounding, alloying, etc., have been successfully applied to render many plastics function-specific. However, all these success stories, in turn, have become liabilities or problems for the industry to solve in recent years awakened by the various environmental campaigns since the 1970's.

The task of the industry to solve the plastics waste disposal problems is enormous yet not insurmountable. As a matter of fact, it is rather a welcome challenge for the people who have been involved in the development of plastics materials, since it must be a proud project for them to exercise their vision and insight to make plastics manufacturing technology sustainable in the coming millennia [3].

Plastics constitutes a major portion, especially on a volume basis, of the solid waste generated by municipalities throughout the world [4]. Although much of the plastics waste is being dumped in landfills at the moment, this kind of disposal cannot be continued, or sustained, for too long because of many problems like lack of landfill sites, leachate hazards, groundwater pollution and gaseous emissions [5]. It is thus believed that we have to continue our efforts to upgrade, improve and innovate plastics waste disposal methods to make them environmentally sound and sustainable.

In order to evaluate and compare on a comprehensive and objective basis various plastics waste management methods hitherto known, we need to consider the overall environmental burdens generated by plastics during their entire life-cycle. In other words, the whole process from the cradle to the grave, which includes the different stages of the plastic products such as the extraction and processing of raw materials, manufacturing, transportation, distribution, use and reuse, maintenance, recycling, and the final disposal of plastics, is to be studied. The concept of life-cycle assessment (LCA) has been developed for this purpose and widely used in recent years in many different applications [6,7].

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 in the following four stages: (1) goal definition and scoping, (2) inventory analysis, (3) impact assessment, and (4) interpretation or improvement analysis. Among these four stages the inventory analysis has been most developed and the impact assessment and interpretation stages are still being developed [6,7].

Many research efforts on LCA to date have been made using spread sheet type models to evaluate different effects on the same end use or application. It is more desirable, however, to use a systematically derived mathematical model in performing LCA studies on systems possessing many possible waste management scenarios, such as plastics waste management that we are discussing now.

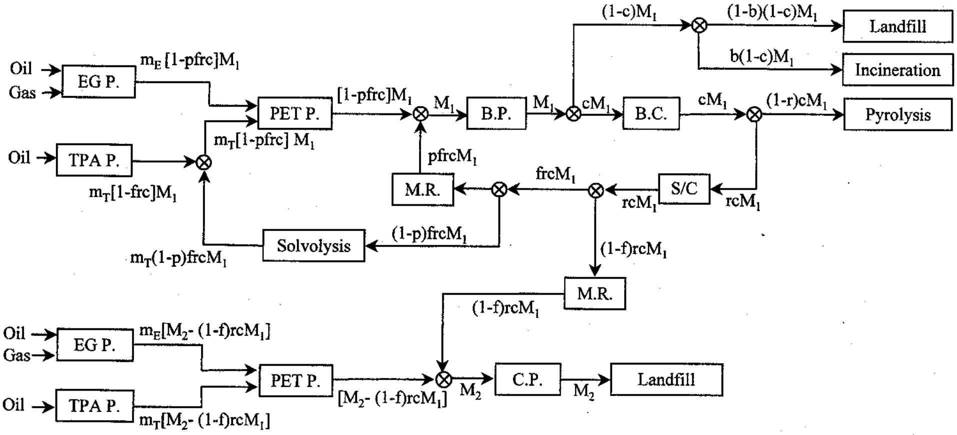
The present study thus deals with the mathematical modeling and the subsequent comparison of various waste management scenarios related to the plastics waste management problem with the focus on the inventory and impact analyses of the LCA study by using the case of polyethylene terephthalate (PET) bottles as an illustrative example. The relationships between various waste management operations and their associated environmental burdens are considered. In parallel with the concept originated by Boustead [8], the collection operation of PET bottles as practised in Korea now where most collected PET bottles are picked up at the community curbsides on scheduled days, is assumed to have a nonlinear relationship between the environmental burdens and the collection ratio of the bottles. This is because any increase in the collection ratio of the bottles above the present level will entail progressively more effort and larger expenditure. A simple model is chosen to reflect this nonlinear nature of the functional relationship, i.e. the energy required for the collection can become unbounded as the collection approaches the theoretical possibility limit of 100%.

The final model of the PET bottles waste management scenarios then becomes a nonlinear multi-variable functional relationship, based on which we perform two analyses in this study, i.e. the comparison of various waste management scenarios and the parameter sensitivity analysis. In the first analysis, the fundamental reasons for the differences in environmental burdens for each pathway are explained, while in the second we find which waste management scenario is environmentally favorable with respect to the environmental burdens in question. Simple algebraic manipulations of the model are what was needed for explaining the differences among the various waste management scenarios, and the Jacobian matrix is what has to be computed for the parameter sensitivity analysis to find the best pathway.

2. Mathematical modeling

The following alternative waste management scenarios are considered possible for the PET bottles chosen as an example for our study [9–11]: (1) mechanical recycling where the waste PET bottles are recycled as a polymer input either to the bottle production process through the reprocessing steps of melt extrusion and filtration (closed-loop feedback recycling), or (2) to other production processes, i.e. the carpet production in this example (open-loop recycling), (3) chemical recycling where the waste PET bottles are recycled through depolymerization or solvolysis (e.g., hydrolysis) as the chemical input of the raw materials of terephthalic acid (TPA) and ethylene glycol (EG), (4) thermal recycling where waste PET bottles are recycled either through degradation or pyrolysis as fuels or raw materials, or (5) through incineration as recovered heat energy, and (6) finally, dumping where the waste PET bottles are discarded in landfills.

Fig. 1 shows the diagram defining and illustrating the whole system along with its system boundary of the above alternative waste management scenarios for PET bottles with mass flows for each individual processing operation. The functional units in this system have been chosen as 1000 units of PET bottles having a volume of 1.5 liter each, which then equals 60 kg total PET. The same amount of 60 kg is also chosen for the PET carpets on the open-loop recycling. The reason for this is that in this study we compare different scenarios for PET waste bottles management, and do not compare PET bottles and PET carpets directly. In other words, PET carpets enter the picture only as an alternative route for the PET waste bottles, not as an independent object of the LCA study on its own merit. So PET bottles and carpets or any other possible open-loop alternatives should be on the same quantity basis of 60 kg to make the study consistent with the same quantity of the material. There are five adjustable parameters of the system representing the individual waste management operations, and the above-mentioned six alternative waste management routes or any combinations of them can be easily identified assigning proper values to these five parameters. The hierarchy diagram in Fig. 2



where EG P. = EG production, TPA P. = TPA production, PET P. = PET production, B.P. = bottles production, B.C. = bottles collection, S/C = sorting, shredding and cleaning, M.R. = melt reprocessing, C.P. = carpet production

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

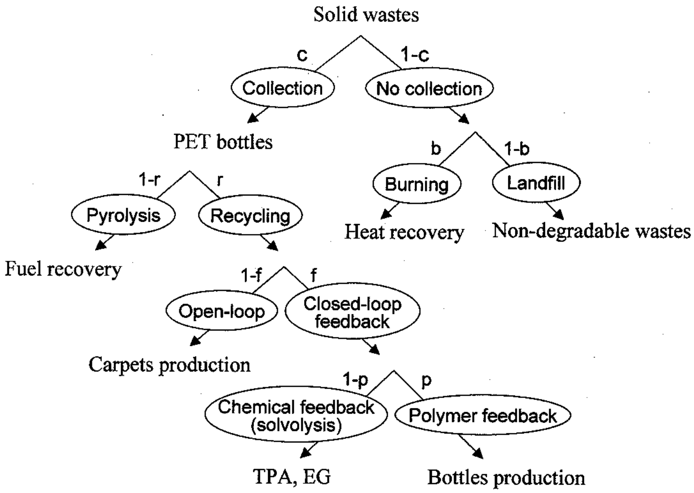


Fig. 2. Decision hierarchy diagram.

further clarifies this system of waste management scenarios. Table 1 illustrates some of the examples of this identification.

In order to derive the overall mathematical model for the total energy consumed and the total emissions released during the entire life-cycle by the functional units

Table 1
Various recycle pathways

Recycle pathways	Parameters					Environmental burdens F
	c	r	f	p	b	
L[a]	0	–	–	–	0	$F=A_0$
I	0	–	–	–	1	$F=A_0+A_5$
PL	$0<c<1$	0	–	–	0	$F=A_0+A_1c$
PI	$0<c<1$	0	–	–	1	$F=A_0+A_5+(A_1-A_5)c$
OL	$0<c<1$	1	0	–	0	$F=A_0+(A_1+A_2)c$
OI	$0<c<1$	1	0	–	1	$F=A_0+A_5+(A_1+A_2-A_5)c$
SL	$0<c<1$	1	1	0	0	$F=A_0+(A_1+A_2+A_3)c$
SI	$0<c<1$	1	1	0	1	$F=A_0+A_5+(A_1+A_2+A_3-A_5)c$
CL	$0<c<1$	1	1	1	0	$F=A_0+(A_1+A_2+A_3+A_4)c$
CI	$0<c<1$	1	1	1	1	$F=A_0+A_5+(A_1+A_2+A_3+A_4-A_5)c$
Example pathway	$0<c<1$	0.5	0.5	0.5	0.5	$F=A_0+0.5A_5+A_1c+0.5A_2c+0.25A_3c$ $+0.125A_4c-0.5A_5c$

[a] L, landfill; I, incineration; PL, pyrolysis + landfill; PI, pyrolysis + incineration; OL, open–loop recycle + landfill; OI, open-loop recycle + incineration; SL, solvolysis + landfill; SI, solvolysis + incineration; CL = (closed-loop) polymer feedback + landfill; CI, (closed-loop) polymer feedback + incineration; (–) not applicable.

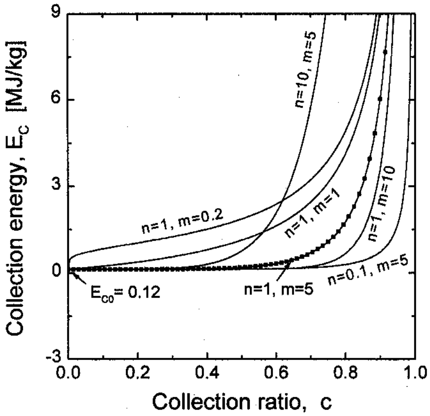


Fig. 3. Curves for the collection energy.

of the system, we need two things for each individual operation: (1) the input data of the process, and (2) the functional relationships in the process. Among many possible input data, we have chosen the energy and emissions data in this study since in most cases they are considered major input items. The available open literature was used to obtain the former information [12–15]. For the latter information, we need modeling for each operation. The modeling, however, turns out to be rather simple because there are linear relationships between the environmental burdens and the corresponding parameters for all the operations except for the collection operation of PET bottles as practised in Korea which has a nonlinear relationship. This is due to the fact that as explained earlier in this paper and also as Boustead pointed out [8], the energy required for the collection process becomes nonlinear as the collection ratio increases.

In this study, we choose the following simple nonlinear relationship for the collection operation:

$$E_C = E_{C0} + n\frac{c^m}{(1-c)} \tag{1}$$

where E_C denotes the collection energy required for unit kg of the bottles, and E_{C0} is the limiting value of E_C as the collection ratio, c, approaches zero (i.e. no collection), and n and m are the adjustable parameters making the model fit real field data.

This equation is based on the assumption that all PET bottles in this study are of similar specifications, which is not true in general. However, in order to deal with different kinds of PET bottles, we need of course many more relationships like Eq. (1) in the model. Leaving such more accurate modeling to future studies, we here adopt a simple relationship and assume it being capable of representing the collection process fairly well.

Fig. 3 shows several curves for Eq. (1) having the same E_{C0} plotted against c as the parameters of n and m take on different values. All the curves start from the same initial point at $c = 0$, increase with c and then go to infinity as c approaches unity. Depending upon the values of three parameters of E_{C0}, n, and m, the curves are considered flexible enough to portray the behavior of the collection process energy reasonably well.

Looking into the shape of the curves, we can say that the curves can be approximated by the combination of two parts, i.e. the linear part when c is small and the nonlinear part when c is large. Furthermore, if m has a large value, the linear part becomes almost a horizontal line. Hence we can say that when c is small and m is large, we have $E_C \approx E_{C0}$.

The parameters of the model of Eq. (1) can be determined if field collection data are available over the entire range of the collection ratio, i.e. $0 < c < 1$. Unfortunately this is not the case in Korea at the present time, i.e. the collection ratio is only around 10% [16]. So what we did in this study was determine the linear parameter E_{C0}, from the available data for a limited range of c and then estimated the other nonlinear parameters best as we can, exercising best judgements.

In the particular example of this study, we thus found $E_{C0} = 0.12$ from the field data [16], and estimated that $n = 1$, and $m = 5$. (m should take on a value not less than 1, because otherwise an inflection point appears in the curve, disagreeing with real field data. From Fig. 3 the curve with $n = 1$ and $m = 5$ is judged best for the collection energy curve.)

After choosing an appropriate functional relationship for the bottle collection process, we proceeded to derive, as illustrated in Fig. 1, the overall mathematical model for the system, taking into account the total energy consumed and the total emissions released by the functional units of the system (1000 units of PET bottles equal to 60 kg of PET) during the production and waste management stages of the life-cycle of the PET bottles. In Appendix A, explanation is given for the detailed procedure of this derivation for the case of total energy consumed over the above-mentioned parts of the life-cycle, counting all the steps involved shown in Figs. 1 and 2. The transport between the steps in Fig. 1 has not been considered in the study except for the collection process where transportation of the waste material represents an integral part of the process.

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

$$F = F(c, r, f, p, b) = A_0 + A_1c + A_2rc + A_3frc + A_4pfrc + A_5b(1 - c) \tag{2}$$

where the function F can represent any of five variables like 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, and the A_i's are the coefficients.

3. Comparison of various waste management scenarios

By setting appropriate values for the five parameters, we can make Eq. (2) represent any waste management routes or any combinations of them. Table 1 shows some examples of such cases. The environmental burdens for the various waste management scenarios are then evaluated calculating the values of the function F according to the equations given in Table 1. As an example, we here consider the case of energy (F denoting E in this case) for the different pathways in Table 1. Fig. 4 shows these energy results. Here we mean the process energy only, not including the embodied energy, which if incorporated, could lead to another set of interesting results.

We can now make the following observations from Fig. 4. Firstly, the curves show, in general, the decreasing trend of the energy with increasing collection ratio c and all go up to infinity as c approaches the limit of unity. These points show two things. One is that as the collection gets larger, the waste management scenarios get better in terms of a decrease in required energy, which confirms the utility of the scheme we consider here. The other is the obvious result of the functional form of Eq. (1) we have adopted in this study, which assumes the required energy to increase unbounded as the collection goes to the level of the theoretical possibility limit of 100%.

Secondly, there are two groups of curves depending upon which one of the two disposal alternatives is chosen for the uncollected bottles, i.e., landfill or incineration. Understandably the incineration routes which recover part of burning process energy shows less energy required than the landfill routes. If there is no bottle collection ($c = 0$), these incineration and landfill pathways are represented by two different starting points on the y-axis, respectively.

Thirdly, the best pathway as far as the required energy is concerned has turned out to be the CI pathway (closed-loop polymer feedback plus incineration) which has $r = f = p = b = 1$ with $0 < c < 1$ as shown in Table 1. In other words, as illustrated in Figs. 1 and 2, this pathway involves 100% of the collected bottles being recycled ($r = 1$) through the closed-loop feedback ($f = 1$) in the form of polymer input ($p = 1$) whereas 100% of the uncollected bottles are incinerated

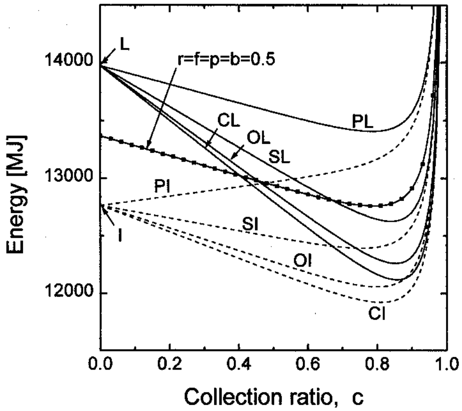


Fig. 4. Energy consumption for 60 kg PET bottles and 60 kg PET carpets for different pathways.

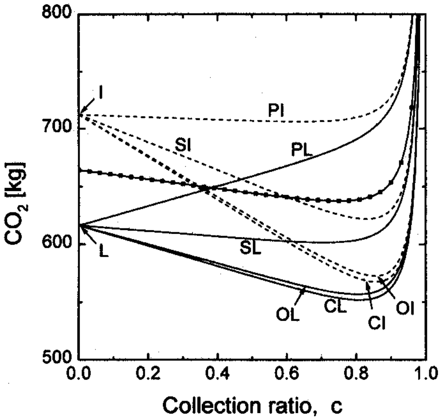


Fig. 5. CO_2 emissions for 60 kg PET bottles and 60kg PET carpets for different pathways.

($b = 1$). The second best pathway is the OI route which unlike the CI route employs open-loop recycle for the collected bottles while the uncollected bottles are disposed of by the same incineration method. Since the carpets and bottles need about the same amount of energy for their manufacture, these two routes CI and OI exhibit about the same behavior as in Fig. 4. The worst pathway is the PL route which is characterized by $r = b = 0$ as shown in Table 1, meaning 100% of the collected bottles are disposed of by pyrolysis and 100% of the uncollected by landfill as shown in Figs. 1 and 2. This is obvious because pyrolysis requires a lot of energy and landfill doesn't recover any energy.

Fourthly, waste management scenarios involving some combination of the individual routes of Table 1 can always be selected simply by assigning appropriate values to the corresponding parameters. As an example, we have tried the case of $r = f = p = b = 0.5$ with $0 < c < 1$ which is also shown in Fig. 4. Since all these parameters are linear ones, this particular curve depicts the middle points of the corresponding two limit cases. In other words, $r = 0.5$ means that out of the collected bottles 50% goes to pyrolysis while the other 50% is recycled, $f = 0.5$ means that out of the recycled 50% goes the closed-loop feedback route while the other 50% to the open-loop route, and so on.

Figs. 5–8 show the curves of the same waste management scenarios as considered in Fig. 4 for the other environmental burdens, i.e., CO_2, NO_X, SO_X, and solid wastes. From Fig. 5 we notice that unlike Fig. 4, the incineration curves display higher levels, i.e. higher CO_2 emission values, than the landfill curves due to the fact that incineration (burning) produces more CO_2 than landfill. So here the best pathway is the CL (close-loop polymer feedback plus landfill).

As seen in Figs. 6 and 7, as far as NO_X, and SO_X are concerned, the CI pathway is the best just as in the case of the energy in Fig. 4. Finally, as far as the solid wastes are concerned, the collection process itself is assumed to create no solid wastes, i.e. all curves become straight lines in Fig. 8. This is because the collection

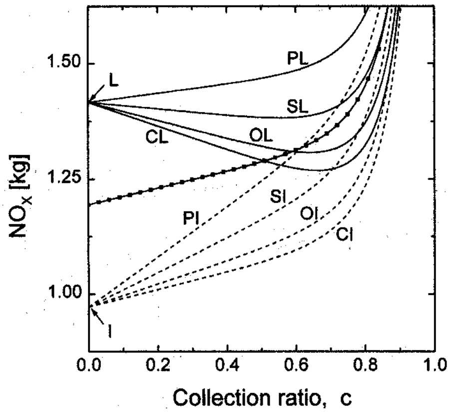


Fig. 6. NO_X emissions for 60 kg PET bottles and 60 kg PET carpets for different pathways.

process which is the only nonlinear stage in the waste management scenarios does not involve any solid waste production. Here the best pathway is found to be the PI route (pyrolysis plus incineration) which involves 100% of the collected bottles going to pyrolysis and 100% of the uncollected to incineration.

4. Parameter sensitivity analysis

In the block diagram of Fig. 1 explaining the production and waste management stages of the life-cycle of PET bottles, there are many junctions where multi-streams of materials are involved. One obvious utility of this kind of diagram is the fact that

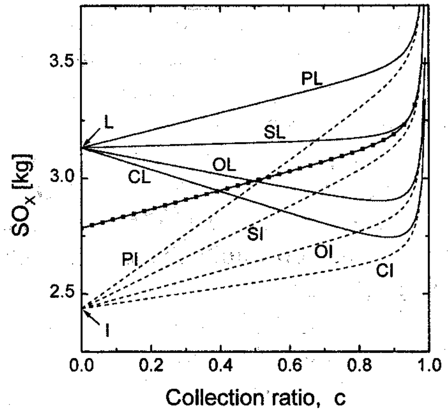


Fig. 7. SO_X emissions for 60 kg PET bottles and 60 kg PET carpets for different pathways.

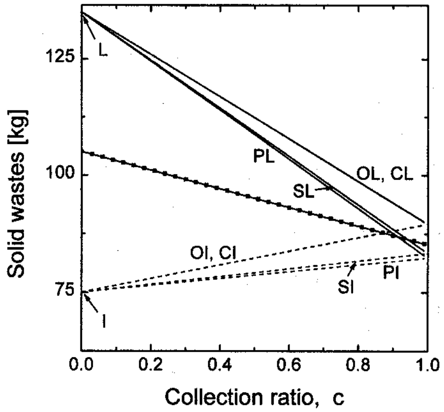


Fig. 8. Solid wastes generations for 60kg PET bottles and 60kg PET carpets for different pathways.

the effect of different waste management operations on the final environmental burdens can be easily determined. In other words, by computing the sensitivity of the environmental burdens, i.e. energy, CO_2, NO_X, SO_X, or solid wastes, to the different waste management operations, we can answer questions like whether we should increase or reduce that particular operation in a chosen pathway in order to improve the environmental burdens in question. This sensitivity is nothing more than the partial derivatives of the function F of Eq. (2) with respect to the five parameters, c, r, f, p, and b, i.e.:

$$\partial F/\partial c, \partial F/\partial r, \partial F/\partial f, \partial F/\partial p, \text{ and } \partial F/\partial b. \tag{3}$$

One remark we might add at this point is that in this sensitivity study the process efficiency concept is implicitly included although time is not directly involved. This is because every calculation of both required energy and released emissions by all the processes has the same quantitative basis and so the matter of efficiency as related to the time frame of the processes enters the picture indirectly. In other words, longer time, for example, invariably involves larger material quantities both in required energy and released emissions, which then mean lower efficiency.

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 pathway as to how beneficial the particular pathway is, against the environmental burdens in question:

$$M_J = \begin{bmatrix} \frac{\partial E}{\partial c} & \frac{\partial E}{\partial r} & \frac{\partial E}{\partial f} & \frac{\partial E}{\partial p} & \frac{\partial E}{\partial b} \\ \frac{\partial C}{\partial c} & \frac{\partial C}{\partial r} & \frac{\partial C}{\partial f} & \frac{\partial C}{\partial p} & \frac{\partial C}{\partial b} \\ \frac{\partial N}{\partial c} & \frac{\partial N}{\partial r} & \frac{\partial N}{\partial f} & \frac{\partial N}{\partial p} & \frac{\partial N}{\partial b} \\ \frac{\partial S}{\partial c} & \frac{\partial S}{\partial r} & \frac{\partial S}{\partial f} & \frac{\partial S}{\partial p} & \frac{\partial S}{\partial b} \\ \frac{\partial W}{\partial c} & \frac{\partial W}{\partial r} & \frac{\partial W}{\partial f} & \frac{\partial W}{\partial p} & \frac{\partial W}{\partial b} \end{bmatrix} \quad (4)$$

Let us consider, as an example, the same case we studied in the previous section, i.e. the recycle pathway of $r=f=p=b=0.5$ and $0<c<1$. Figs. 9–13 show the results. The important point in these figures is whether the partial derivatives take on negative values or not. Since we are dealing with the environmental burdens here, any positive values of the partial derivatives mean that the corresponding waste management operations worsen the particular environmental burdens.

The following observations from Figs. 9–13 are now in order. First, the effect of the parameters of f and p on the environmental burdens have turned out to be quite small, meaning that the question of closed-loop or open-loop (the parameter f effect), and the question of polymer feedback and chemical feedback (the parameter p effect) do not matter much in our chosen case of the waste management pathway. This can be explained by noting two things. One is that the differences between the closed-loop and open-loop and the differences between the polymer feedback and the chemical feedback are indeed relatively small in our system of the waste

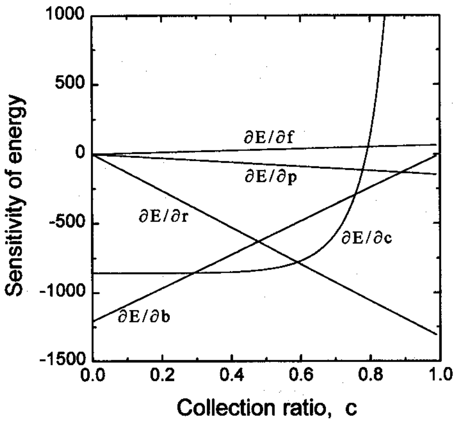


Fig. 9. Sensitivity of energy consumption for the recycle pathway of $r=f=p=b=0.5$.

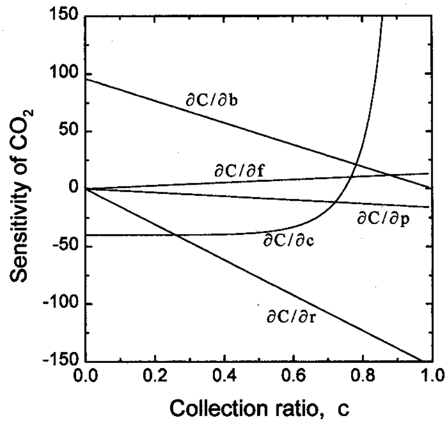


Fig. 10. Sensitivity of CO_2 emissions for the recycle pathway of $r=f=p=b=0.5$.

management scenarios because they involve basically similar process operations. The other point is that as shown in Fig. 2, both the parameters f and p affect the pathways in the later stages as compared to parameters like c and r which act in the earlier stages of the pathways. As is generally known [17], the effect of the later stages is smaller than that of the earlier stages in any hierarchic structures of operations like the one in Fig. 2.

Second, as seen in Fig. 13, all the sensitivities of the solid wastes are straight lines because as mentioned above, solid waste production is not involved in the bottle collection operation which is the only nonlinear step in the waste management scenarios considered here.

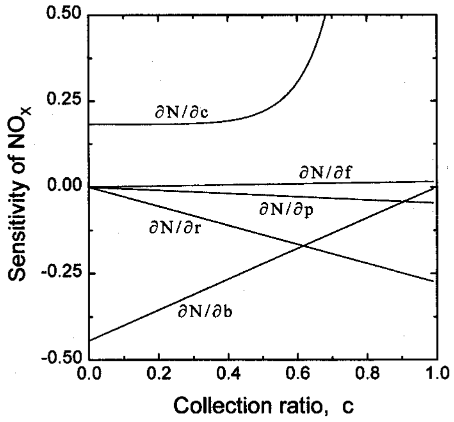


Fig. 11. Sensitivity of NO_X emissions for the recycle pathway of $r=f=p=b=0.5$.

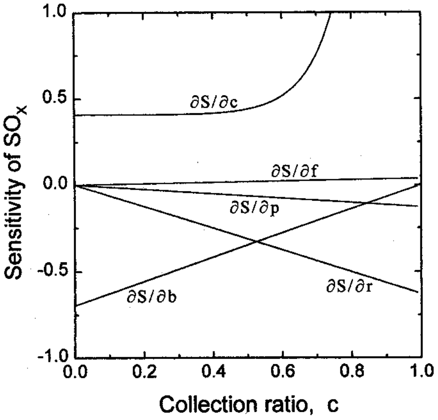


Fig. 12. Sensitivity of SO_X emissions for the recycle pathway of $r = f = p = b = 0.5$.

Third, the sensitivities with respect to the collection ratio (c) are all exhibiting nonlinear curves (except of course that of solid waste as explained above). Moreover, they are almost constant as far as the collection remains under the certain critical levels, and then rapidly increases as the collection gets larger than these critical levels. This suggests that in order to guarantee reasonable levels of environmental burdens for the PET bottles waste management scenarios, we have to maintain the bottle collection at moderate levels so as not to cause the unnecessarily high costs associated with too large values of the collection ratio.

In short, we can say that utilizing the results of the parameter analysis we can always determine the direction we have to go in choosing the best waste management scenario in order to reduce the particular environmental burdens in question.

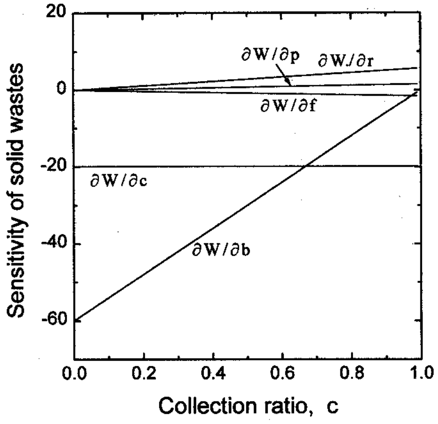


Fig. 13. Sensitivity of solid wastes generations for the recycle pathway of $r = f = p = b = 0.5$.

5. Conclusions

Using the case of PET bottles as an example, an LCA study on various possible waste management scenarios of plastic materials has been conducted. Mathematical models for the overall waste management system including a nonlinear relationship for the collection process of the PET bottles have been developed using the energy and material balances on each waste management operation involved. Based on this model, we have performed the comparison of various waste management scenarios, and the parameter sensitivity analysis through which we can determine both the environmental burdens of each processing operation and consequently the most favorable waste management route in terms of the environmental burdens in question. The simple algebraic manipulations of the model were performed for explaining the differences in various waste management scenarios, and the Jacobian matrix of partial derivatives representing the sensitivity of each environmental burden to the particular operation was used for the parameter sensitivity analysis. Finally, although the quantitative values in this study can vary depending on the choice of the particular collection model we employ, the conclusions and the methodology of this study can be easily applied to other wastes management problems. Some of the areas not covered in this study yet worth pursuing in future studies are different specifications for bottles, different collection systems, other input data than energy and emissions for individual processes, transport steps between the processes and other LCA areas like improvement analysis.

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Appendix A

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/shredding/cleaning)
+(reprocessing of flakes) +(depolymerization of waste bottles)
+(landfill of waste bottles) +(incineration of waste bottles)

$$
\begin{array}{ll}
+(\text{pyrolysis of bottles to fuels}) & +(\text{reprocessing of flakes}) \\
+(\text{EG production for carpets}) & +(\text{TPA production for carpets}) \\
+(\text{PET polymerization for carpets}) & +(\text{carpets production}) \\
+(\text{landfill of waste carpets}) &
\end{array}
\tag{A1}
$$

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:

$$
\begin{aligned}
&(\text{Energy required for EG production for PET bottles}) \\
&= \{\text{the EG mass term}\} \\
&\quad \times \{\text{required energy term for the production of unit mass of EG}\} \\
&= \{(\text{mass of EG for 1kg of PET bottle}) \times (60) \times [1 - pfrc]\} \\
&\quad \times \{(\text{energy equivalent for required crude oil}) \\
&\quad + (\text{energy equivalent for required natural gas}) \\
&\quad + (\text{process energy for EG production})\} \\
&= \{(\text{numerical value}) \times (60) \times [1 - pfrc]\} \\
&\quad \times \{(\text{numerical value}) + (\text{numerical value}) + (\text{numerical value})\} \\
&= (\text{constant}) + (\text{constant}) \times [pfrc]
\end{aligned}
\tag{A2}
$$

All the other items in Eq. (A1) can also be obtained in a similar fashion with the numerical values obtained from the literature like SAEFL, APME and PWMI technical report series, 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 Eq. (2):

$$
E = A_{E,0} + A_{E,1}c + A_{E,2}rc + A_{E,3}frc + A_{E,4}pfrc + A_{E,5}b(1-c) \tag{A3}
$$

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

$$
\begin{aligned}
A_{E,0} &= [(\text{oil for 1kg EG}) + (\text{gas for 1kg EG}) + (\text{energy for 1kg EG})] \\
&\quad (\text{EG mass for 1kg PET})(60) \\
&\quad + [(\text{oil for 1kg TPA}) + (\text{energy for 1kg TPA})] \\
&(\text{TPA mass for 1kg PET})(60) + (\text{energy for 1kg PET resin for bottles})(60) \\
&+ (\text{energy for 1kg PET bottles})(60) + (\text{energy for landfill of 1kg PET})(60) \\
&+ [(\text{oil for 1kg EG}) + (\text{gas for 1kg EG}) + (\text{energy for 1kg EG})] \\
&(\text{EG mass for 1kg PET})(60)
\end{aligned}
$$

$+$ [(oil for 1kg TPA) $+$ (energy for 1kg TPA)](TPA mass for 1kg PET)(60)

$+$ (energy for 1kg PET resin for carpets)(60) $+$ (energy for 1kg PET carpets)(60)

$+$ (energy for landfill of 1kg PET)(60)

$= (882.4) + (3353.3) + (1003.8) + (2759.4) + (0.0) + (882.4) + (3353.3) + (837.0)$

$+ (900.0) + (0.0) = 13971.7$

$A_{E,1} =$ (energy for collecting 1kg PET bottles)(60)

$-$ (energy for landfill of 1kg PET)(60)

$+$ (energy for pyrolysis of 1kg PET)(60)

$= [7.2 + 60c^5/(1-c)] - (0.0) + (-808.8) = -801.6 + 60c^5/(1-c)$

$\mathrm{A}_{\mathrm{E},2} =$ (energy for sorting, shredding and cleaning of 1kg PET bottles)(60)

$-$ (energy for pyrolysis of 1kg PET)(60)

$+$ (energy for reprocessing 1kg PET flakes)(60)

$-$ [(oil for 1kg EG) $+$ (gas for 1kg EG) $+$ (energy for 1kg EG)]

(EG mass for 1kg PET)(60)]

$-$ [(oil for 1kg TPA) $+$ (energy for 1kg TPA)]

(TPA mass for 1kg PET)(60)

$-$ (energy for 1kg PET resin for carpets)(60)

$= (228.0) + (808.8) + (2648.4) - (882.4) - (3353.3) - (837.0) = -1387.6$

$\mathrm{A}_{\mathrm{E},3} = -$ [(oil for 1kg TPA) $+$ (energy for 1kg TPA)]

(TPA mass for 1kg PET)(60)

$+$ (energy for solvolysis of 1kg PET)(60)

$-$ (energy for reprocessing 1kg PET flakes)(60)

$+$ [(oil for 1kg EG) $+$ (gas for 1kg EG) $+$ (energy for 1kg EG)]

(EG mass for 1kg PET)(60)

$+$ [(oil for 1kg TPA) $+$ (energy for 1kg TPA)]

(TPA mass for 1kg PET)(60)

$+$ (energy for 1kg PET resin for carpets)(60)

$= -(3353.3) + (1357.8) - (2648.4) + (882.4) + (3353.3) + (837.0) = 428.8$

$\mathrm{A}_{\mathrm{E},4} = -$ [(oil for 1kg EG) $+$ (gas for 1kg EG) $+$ (energy for 1kg EG)]

(EG mass for 1kg PET)(60)

$$\begin{aligned}
&- (\text{energy for 1kg PET resin for bottles})(60) \\
&+ (\text{energy for reprocessing 1kg PET flakes})(60) \\
&- (\text{energy for solvolysis of 1kg PET})(60) \\
&= -(882.4) - (1003.8) + (2648.4) - (1357.8) = -595.6 \\
A_{E,5} &= -(\text{energy for landfill of 1kg PET})(60) \\
&+ (\text{energy for incineration of 1kg PET})(60) = -(0.0) + (-1209.6) \\
&= -1209.6 \qquad \text{(A4)}
\end{aligned}$$

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), (A2), (A3) and (A4).

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