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A Prototype System for Evaluating Life Cycle Engineering of Chemical Products

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Associated with sustainable technology, in this paper, we have developed a prototype system for evaluating life cycle engineering of chemical products. For this purpose, giving a whole framework on the G2 software known as a graphical development environment of intelligent system, we have built a product life cycle model as one of its element technologies. Practically it is described as an object-oriented model having a hierarchical structure like IDEF0 model. Furthermore, due to the interdisciplinary nature of the problem-solving, highlighting an importance to facilitate a continuous improvement and to employ distributed information technologies, we also engage in developing a few related element technologies. Through a case study associated with the farm sheets, we have revealed that the developed system can analyze easily various kinds of life cycle scenarios just by giving certain values via a graphical user interface, and support strategic decision making on the life cycle engineering of chemical products.

Introduction

To reflect the environmental consciousness in process development is becoming a common and important concept in the coming industries. Accordingly, many interests have been paid to develop effective methods for evaluating environment management, and establish the sustainable technology. Among them, the life cycle assessment (LCA; Heijungs, 1992) is popularly known as a promising tool, but it concerns only with the analysis from the particular environmental aspects. Also recent studies in the process systems engineering formulate the problem as the synthesis problem, and derive the solution from its optimization (For example, see the special issue of Comp. & chem. Engng., 1999). However, after time-consuming solution procedures, we can obtain only a problem-specific result that seems far from comprehensive discussion about frameworks associated with the sustainable technology. It is highly desired, therefore, to provide a general decision-aid for the life cycle engineering (LCE) in quick and understandable manners.

With this point of view, in this paper, we have developed a prototype system through an object-oriented approach that provides us good procedures for continuous improvement. The object-oriented approach also enables us to use intelligent applications coupled with distributed information technologies. After explaining a life cycle model built on the G2 software and the related methods, we will present a case study regarding the evaluation of product life cycle scenarios of certain chemical products.

1. Scope of the Prototype System

1.1 General consideration

Due to the interdisciplinary nature of the concerned problem-solving, our approach will emphasize especially on establishing a framework easy for continuous improvement, i.e., model expansion and/or revision, application execution, and data collection/management and so on. For this purpose, we adopt the G2 software (Gensym Corp., 1995) as a development environment for intelligent applications. We also note a hierarchical modeling method known as IDEF0 (Marca and McGowan, 1988) and the outcomes of the distributed information technology.

By combining these element technologies, we aim at making a decision-aid whose whole scheme is shown in **Fig. 1**. There we focus mainly, in the present study, on a life cycle model that will work with the appropriate simulation engine and interfaces of G2 like G2 file interface (GFI), G2 standard interface (GSI) and G2 web-link. Based on it, we can carry out various numerical analyses whose results are processed visually, and then presented end users through a graphical user interface (GUI) for their decision supports. The GUI is also useful to set up some parameters and conditions characterizing the product life cycle scenarios to

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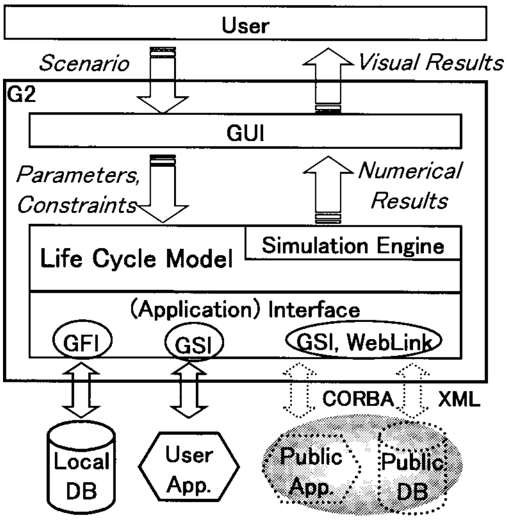


GFI: G2 File Interface
GSI: G2 Standard Interface
CORBA: Common Object Request Broker Architecture
XML: eXtended Makeup Language
(Broken-lined objects: Left for future studies)

Fig. 1 Whole scheme of the prototype system

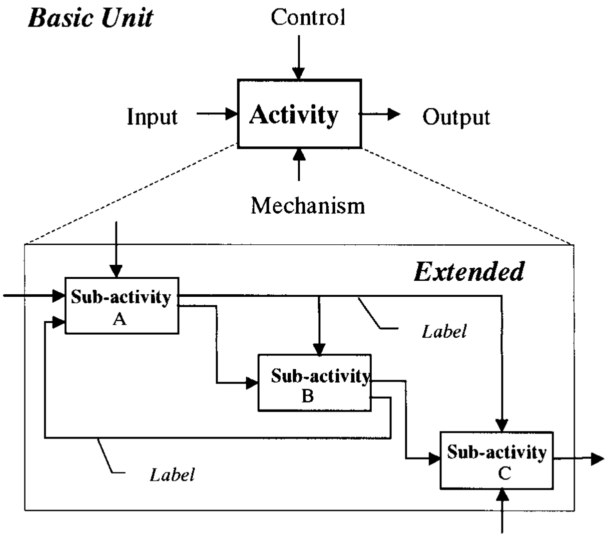
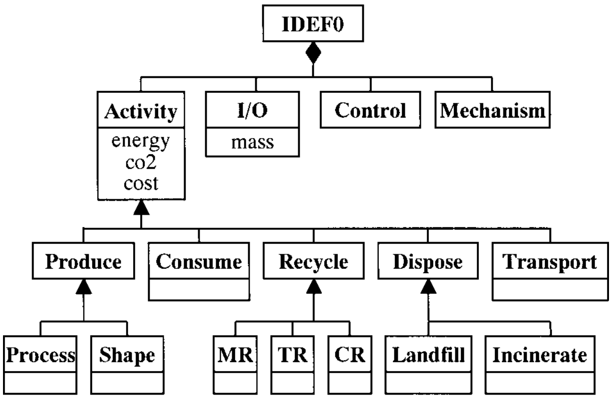


Fig. 2 Basic structure of IDEF0 model and its extension

be analyzed. Furthermore, through distributed information technologies, we are planning to build an environment suck that: we can use various data base (DB) and applications (APP) regardless where they are located locally or remotely; users at any sites only need specify parameters and conditions in the scenario, not worrying about the detail of the model and the configuration of their computers.

1.2 Activity-based approach for life cycle modeling

To build the life cycle model, we use a hierarchical activity-based modeling method like IDEF0 in our system. Being viewed as an effective tool for business process reengineering, IDEF0 is becoming an international standard for functional modeling method. Its basic structure is simple but definite enough as shown in the upper part of **Fig. 2**.



MR: Material recycle
TR: Thermal recycle
CR: Chemical recycle

Fig. 3 Class hierarchy of the life cycle model

It is composed of one box and four kinds of arrows named input, output, control, and mechanism respectively. There the box represents certain activity like “produce A” or “consume B”, the control instruction and/or regulation, and the mechanism resource and/or facility. In other words, relation between input and output represents what is done through the activity while the control describes why it is done, and the mechanism how it is done. By decomposing the activity into its sub-activities that inherit the properties from the upper level, we can deal with actual complicated systems without adding any extra modeling rules. (See the lower part of Fig. 2.)

Applying this hierarchical modeling method that matches quite well with the object-oriented approach, we can obtain simultaneously the following properties suitable for our approach.

(1) Careful assessment of the needs that complicated systems are to fulfill;

(2) To facilitate a modular design for modification and/or correction of the original model according to the particular concerns;

(3) To support collaborative works in model building and scenario setting.

2. Structure of the Prototype System

2.1 Modeling

Noticing that the life cycle activities are common to every industry as a whole, we construct the top level model composed of the activities such as “produce”, “consume”, “recycle” and “dispose”. Besides these, “transport” is added as a special activity of this level because the inputs are always equal to the outputs, and some special data such as load factors, transportation

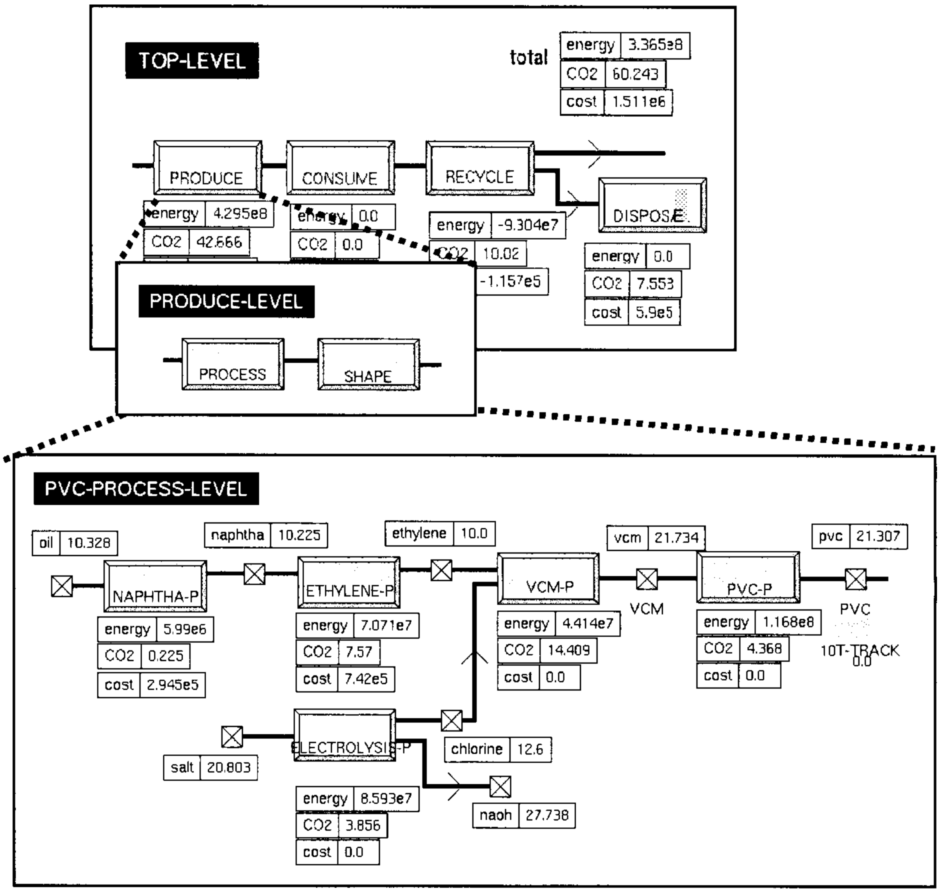


Fig. 4 A part of the life cycle model extended over three levels regarding the activity "produce"

distance and so on are necessary on the case by case basis. Next the lower level models that inherit the properties of their respective upper level are to be derived consecutively according to required fidelity of the analysis. In this aspect, the hierarchical model has an advantage since we need to modify only the lower level models according to the specific properties of the concerned problem. We also require the life cycle model to be general and flexible so that we can evaluate not only the target product but also its competing ones.

Having these aspects in mind, such modeling is carried out based on the object-oriented approach. It makes us achieve easily the above points only by augmenting certain instances into each class. We followed the IDEF0 description by viewing every activity and arrow as objects whose class hierarchy is shown in **Fig. 3**. Moreover, we prepare control class and mechanism class whose class definitions involve appropriate rules and/or procedures. By that, we can awaken end users by showing relevant messages when some activities in the life cycle model do not satisfy certain restrictions on regulations, and capacities.

Thus developed model a part of which is shown in **Fig. 4** ranges from supply of the raw material in the upstream to recycle and disposal in the downstream, i.e., over a life cycle of the chemical products. So we choose the amount of crude oil as the system input, and the recycle products and the waste discharged into the environment as the system outputs.

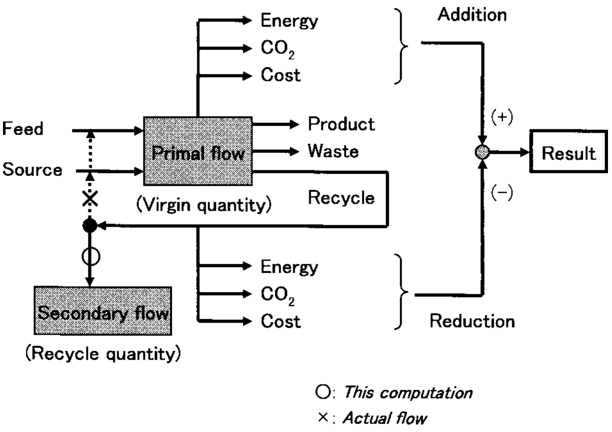
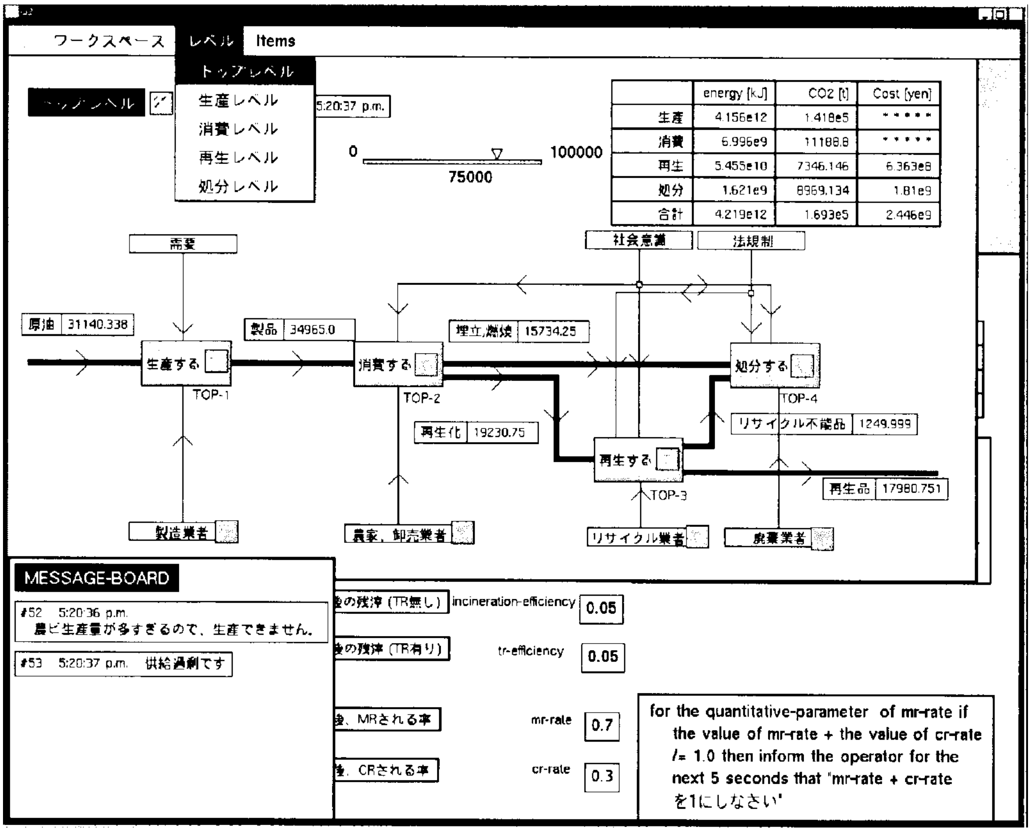


Fig. 5 Idea of equivalence reduction to account the effect of recycle flow

Calculations of balances regarding energy consumption, amount of CO_2 discharge, cost, and much more if necessary are to be described as the methods



	energy [kJ]	CO2 [t]	Cost [yen]
生産	4.156e12	1.418e5	* * * * *
消費	6.996e9	11188.8	* * * * *
再生	5.455e10	7346.146	6.363e8
処分	1.621e9	8969.134	1.81e9
合計	4.219e12	1.693e5	2.446e9

#52 5:20:36 p.m.
農ビ生産量が多すぎるので、生産できません。

#53 5:20:37 p.m. 供給過剰です

後の残滓 (TR無し) incineration-efficiency 0.05

後の残滓 (TR有り) tr-efficiency 0.05

後、MRされる率 mr-rate 0.7

後、CRされる率 cr-rate 0.3

for the quantitative-parameter of mr-rate if
the value of mr-rate + the value of cr-rate
/= 1.0 then inform the operator for the
next 5 seconds that "mr-rate + cr-rate
を1にしなさい"

Fig. 6 Multiple windows of prototype system attached Japanese user interfaces: ワークスペース, work space; レベル, level; トップ, top; 生産, production; 消費, consumption; 再生, recycle; 処分, disposal; 原油, crude oil; 製品, product; 再生品, recycle product

in the class method. Though they are presently on the unit consumption basis, or of linear relation, there is no problem to use nonlinear relation or an appropriate simulator outside the model referred as simulation engine in Fig. 1. As a nature of the object-oriented model, in addition, we can compute any values anywhere and in any directions by assuming no recycle flows. (For example, we can analyze such a scenario that prescribes not only the inputs but also the outputs.) To remove the recycled flows substantially, we use the concept of equivalence reduction whose idea is described in **Fig. 5**. That is, we will take the balance over the life cycle as follow: separate the recycle product flow as a secondary flow; then to involve the recycle effect in the evaluation; reduce the equivalent amounts necessary to generate them from those of the primal flow.

2.2 Interface

For the convenience sake of model builders and end users, we prepare a few interfaces respectively by merging the G2 user interface library into the G2 menu system. The former presents a development environment for designing a graphical user interface of the KB while the latter that for providing a customized menu bar in the KB. In **Fig. 6**, we show an example of the multiple windows attached various user interfaces such like the pull-down menu to move to any sub-level, and sliding bar to prescribe the amount of product on the top level. Moreover, a message board is appeared against improper prescriptions in the scenario setup menu showing at the bottom of the figure. (They are designed for the case study shown in the latter.)

In addition to the G2 file interface (GFI) for communication between the local databases, we plan to utilize the G2 standard interface (GSI) and the G2 weblink for various local and remote communications. In such environment, we can maintain the life cycle model ever in the latest manner by updating the employed applications and data sets.

2.3 Databases

For the simulation of the life cycle model, data is provided as a set of parameters that are extracted, in turn, from the linked local DB. For this purpose, we provide the DB after collecting various data into the EXCEL spreadsheets from the literatures (Takeshita, 1999; NIRE-LCA, 1997; NEDO Reports, 1995; JPWMI Report, 1992; JPRPC Report, 1995; Suzuki, 1996).

We can also prepare a certain KB for showing certain messages related to the control and the mechanism classes. In the present system, however, only a few rules are provided just to demonstrate the possibility already shown as the message board in Fig. 6.

Table 3 Evaluation of scenarios at downstream

Scenario	Product	Energy [10^8 kJ/km^2]	CO$_2$ [10^3 kg/km^2]	Cost [¥10^6/km^2]
No recycle	PVC	0.21	68.2	7.52
(landfill 50%, incineration 50%)	PE	0.16	154.0	5.87
Recycle	PVC	−10.58	33.2	6.60
(TR 50%, MR 40%, CR 10%)	PE	−7.17	158.1	4.59

Table 1 Statistics of farm sheet in 1997

		PVC	PE	Glass
Installed area = 5,200,000 m^2		77%	19%	4%
Released amount = 177,000,000 kg		60%	40%	
Details	Recycle	45%	4%	
	Landfill	26%	21%	
	Incineration	15%	64%	
	Others	13%	11%	

Table 2 Evaluation at production stage

Product (sheet)	Energy [10^8 kJ/km^2]	CO$_2$ [10^3 kg/km^2]	Weight [10^3 kg/km^2]
PVC	32.7	246.1	123
PE	16.8	199.0	96

(e.g., Rule A: if the demand exceeds the capacity of the facility, then the system suggests the user to reduce its amount; Rule B: if the total sum of details of the recycle option exceeds one, then the user is alerted, etc.) By using the GFI mentioned above for the linkage media between the local DB/KB and the G2, we can give the relevant values to the parameters involved in each object of the life cycle model. We should notice such a design is suitable for the data management of the system.

3. A Case Study

In Japan, chemical sheets have been popularly used in farm green houses (farm sheets). While the share of poly-vinyl chloride (PVC) sheet has been overwhelming the others (e.g., poly-ethylene (PE) and glass) in terms of economy and quality as well, disposal of the spent sheet is calling hot attention associated with what is known as the dioxin problem recently. In **Table 1**, we summarized some statistics of the farm sheets at Japan in 1997. As presented there, about 45% of the spent PVC sheet is recycled, and used as a raw material such as floor material and vinyl-sandals (material recycle; MR). On the other hand, thermal recycle (TR) is carried out demonstratively by mixing with other plastics, but it has a restriction associated with the dioxin problem and the corrosion of furnaces due to the hydrogen chloride (HCl). Furthermore, chemical recycle (CR) is still at R&D phases, and reuse is said to be hard on the badly polluted basis of the spent sheet.

As estimated from these facts, in the following case study, we cover the MR, TR, and CR as the recycle options, and the PE sheets as a competing product in the coming age. By adding disposal options like landfill and incineration (without TR) to them, there exist a variety of scenarios to be considered for the life cycle management of the farm sheet. For example, they are characterized by changing the amount of production, total recycle rates, its breakdown (MR, CR, TR), each processing efficiency and so on. It is significant, therefore, to show how helpful our system is for the decision making on the LCE through evaluating various scenarios characterized by the above parameters. Below we will explain some numerical results assessed using the data we could gather by now. (We provide a miscellaneous note regarding the numerical experiments in Appendix.)

As far as the production stage is concerned, we can assert that the PE sheets are superior to the PVC sheets from the aspects both of energy consumption and CO$_2$ emission from **Table 2**. However, turning our concern to the downstream management (**Table 3**), we need to reconsider the above conclusion depending on the scenario. If we don't carry out the recycling, and dispose the spent sheet through landfill and incineration at the equivalent rate (upper rows in the table), there occurs a tradeoff among the two environmental issues and cost. That is, the PVC sheet needs more amounts of energy and cost while less emission of CO$_2$ compared with the PE sheets. On the other hand, under the recycle scenario with the detail of the recycle rate like TR:MR:CR = 5:4:1 (lower rows), we know that the recycle of the PVC sheets cause more favorable effect on the environmental issues than the PE sheets. (This analysis is done under the condition that most spent sheets (90%) are recycled; the negative values in the energy column in the table mean that the reduced amount will exceed the necessary amount for the recycling.) The results also show that in both cases, recycling is quite acceptable from the environmental aspect and cost as well by virtue of the conservation of

Table 4 Evaluation of scenarios over life cycle

Scenario	Product	Energy [10^8 kJ/km^2]	CO$_2$ [10^3 kg/km^2]
No recycle	PVC	33.2	319.4
(landfill 50%, incineration 50%)	PE	17.2	381.2
Recycle	PVC	25.3	306.8
(TR 50%, MR 40%, CR 10%)	PE	9.74	387.2

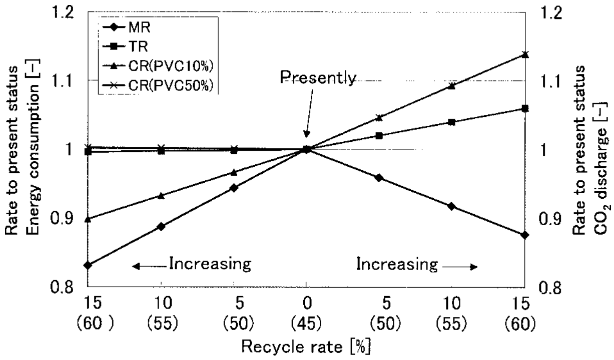


Fig. 7 Effect of recycle options on the energy consumption and CO$_2$ discharge (PVC sheet)

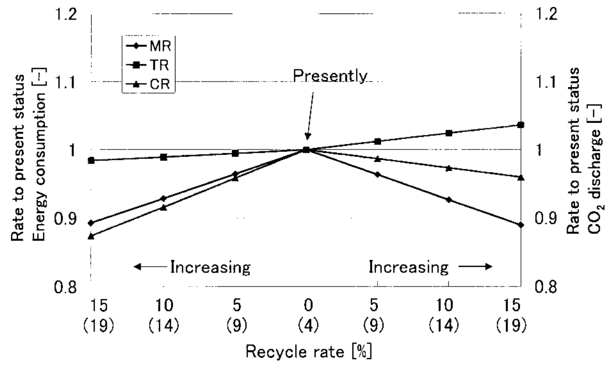


Fig. 8 Effect of recycle options on the energy consumption and CO$_2$ discharge (PE sheet)

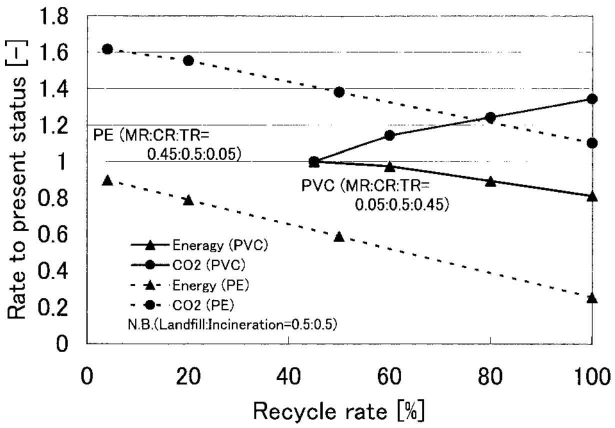


Fig. 9 Consideration on the possibility of the shift from PVC to PE under a certain scenario

Table 5 Detail of the supposed scenario

Product	MR	CR	TR
PVC	5%	50%	45%
PE	45%	50%	5%

virgin resin and crude oil. (Only the downstream cost is accounted in the present study.)

In the LCE, we emphasize the importance to evaluate the system totally, and to derive a final decision based not on each stage but on over the whole stages. In **Table 4**, we present a result evaluated over the life cycle of the products. Since most of the energy consumption and CO$_2$ emission occur at the production stage, we can know the MR (or reuse if possible) is very effective regarding the PVC sheets. Also, if we would shift to the PE sheets, we could considerably reduce the energy consumption at the expense of a little increase in CO$_2$ emission regardless of recycling. Below we will present a few results analyzed from some different aspects.

In **Fig. 7**, we show the change in the amounts of energy consumption and CO$_2$ discharge of the PVC sheets depending on the difference of the recycle options. (Drawn as the rate to the present status.) It describes a situation where each recycle option is to be used alone to deal with the increase in recycle rate from the present status (i.e., recycle rate in Table 1). The scale of abscissa increases in both sides from the half of the axis by letting the present state locate at zero (actual value is shown in the parenthesis). Two cases are shown regarding the CR, i.e., the rate of the PVC in the feed mixture is 10%, and 50% respectively. Then the MR is shown preferable as the recycle option under an assumption that the demands for the recycle products are sufficient. This is because both the energy consumption and CO$_2$ emission decrease most rapidly as the increase in recycle rate. To promote the MR further, developing new recycle products, and expanding their markets are known essential. On the other hand, both the TR and the CR are not so attractive under the present level of the recycling technologies.

On the other hand, the CR for PE is a more promising option comparable to the MR as shown in **Fig. 8** (both scales are drawn just like Fig. 7). This is derived

Table A-1 Conversion rate

Activity	Input	Input rate	Output	Output rate
Production (naphtha)	crude oil	1.01	naphtha	1
Production (ethylene)	naphtha	0.363	ethylene	0.355
Electrosis	salt	0.984	chlorine sodium hydroxide	0.569 1.312
Production (VCM)	ethylene chlorine	0.473 0.596	VCM	1.028
Production (PVC)	VCM	1.02	PVC	1.0
Sheet processing (PVC)	PVC plasticizer	0.74 0.26	PVC film	1.0
Production (PE)	ethylene	1.04	PE	1.0
Sheet processing (PE)	PE	1.0	PE film	1.0

from the fact that nevertheless the reduction rates of energy and CO_2 of the MR are rather small compared with the foregoing PVC case, the efficiency of the CR becomes higher for the PE case.

From taking these analyses into account, we depicted **Fig. 9** to examine further the possibility of the shift from the PVC to the PE. First, we supposed the MR of the PVC is hard to expand due to the small market for the recycle products, and the CR for the PE will become more popular. Under these assumptions, we set up the respective details of the rates of recycle options as shown in **Table 5**. Then, the results show the PE sheets become preferable more and more along with the increase in recycle rate, and there might arise a possibility of the shift over the recycle rate around 80% regardless of the tradeoff problem between the CO_2 discharge and energy consumption. Thus using the developed system, we can carry out easily a variety of analyses as examples shown here.

Conclusion

In this paper, we have developed a prototype system available for evaluating the LCE. Actually, we have built an object-oriented life cycle model on the G2 software in terms of the IDEF0 modeling method. Running the system, we can calculate the energy consumption, CO_2 emission and cost (in part) over the life cycle under a variety of life cycle scenarios. The case studies have shown how we can carry out the assessment for the strategic decision making for the LCE using the system.

Usefulness of the approach is verified by the following facts: our system can make it clear that optimizing the recycle system, and improving the technology levels have a real effect besides increasing social consciousness about the environment; it can point out the bottleneck technologies; it makes us consider the sustainable technology faithfully.

However, to deal with more general concerns, and to derive more reliable conclusions*, reliable sets of data seem to play a key role. Besides the standardization of data specification, therefore, it is quite important to collect and refine various data for the LCE through collaborative efforts as at SPOLD (Society for the Promotion of LCA Development).

Acknowledgment

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Appendix

Miscellaneous for the data and usage

(1) Conversion rate

We carried out the following computation using the rates in **Table A-1**.

(output quantity) × (output rate) = (input quantity) × (input rate)

(2) Employed parameters

Unable to get every data from the single source, we gathered them from various sources as mentioned already, and estimated the missing data under certain assumptions. After all, we summarized the outcomes in **Table A-2**.

Moreover, in the computation, contribution due to the transportation, the consumption of products and the collection of spent sheets are also included under certain assumptions, but those are treated to be not so large compared with the other activities listed above.

(3) Abbreviation

CORBA = Common Object Request Broker Architecture
CR = Chemical Recycle
DB = Data Base
GFI = G2 File Interface
GSI = G2 Standard Interface
GUI = Graphic User Interface
IDEF = Integrated function modeling DEFinition
I/O = Input and Output
KB = Knowledge Base

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* To improve our system in advance, we are willing to have any correspondences.

Table A-2 Employed data

Activity		Energy [J/kg]	CO_2 [kg/kg]	Cost [¥/kg]
Crude oil supply		3.90×10^5	0.029	N/A
Production of industrial salt		3.39×10^6	0.246	N/A
Production of chlorine[a)]		7.57×10^6	0.306	N/A
Production of naphtha		5.86×10^5	0.022	28.8
Production of ethylene		7.07×10^6	0.757	74.2
Production of VCM		2.03×10^6	0.663	N/A
Production	(PVC)	5.48×10^6	0.205	N/A
	(PE)	4.31×10^6	0.871	N/A
Processing to sheet	(PVC)	6.23×10^6	0.425	N/A
	(PE)	3.96×10^6	0.299	N/A
MR	(PVC)	4.06×10^6	0.487	10.0
	(PE)	4.06×10^6	0.487	–5.6
CR[b)]	(PVC)	-6.44×10^6	1.733	16.0
	(PE)	-3.81×10^7	1.733	16.0
TR[c)]	(PVC)	-6.06×10^5	1.042	14.0
	(PE)	-2.07×10^5	3.143	14.0
Incination	(PVC)	0.0	1.042	20.0
	(PE)	0.0	3.143	20.0
Landfill	(PVC, PE)	0.0	0.0	35.0

[a)] The value is divided at the equivalent rate between Cl_2 and Na

[b),c)] Assumed to be recovered as oil and electricity respectively, and given the values appeared in the pilot scale data

LCA = Life Cycle Assessment
LCE = Life Cycle Engineering
MR = Material Recycle
TR = Thermal Recycle
XML = eXtented Makeup Language

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