A Petri Net Approach for Green Supply Chain Network Modeling and Performance Analysis

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Abstract. Green supply chain has become a promising and challenging field during the last decade driven by rising environmental conscious business and governmental legislation. In this paper, we develop a Petri-net based model to describe the green supply chain and to evaluate the essential performance. Generalized stochastic Petri nets (GSPN) are introduced to model the network of a general green supply chain with time characteristics. Performance analysis is carried out using the embedded Markov chain. Furthermore, we perform a comparison between green and normal supply chain to assert the superiority of the green supply chain in terms of profits.

Keywords: Green supply chain network · Generalized stochastic Petri net · PIPE2 · Modeling · Performance measures

1 Introduction

Under the global trend of circular economy and sustainable development, there is an increasing need for integrating energy-saving and environmental protection consciousness in business practice. As a consequence, green supply chain [7] becomes an attentive focus among researchers and industrial practitioners. According to the comprehensive reviews [16, 19], legions of relevant exiting studies are empirical and conceptual, while green supply chain modeling and network design is still a challenging and complicated issue in this area. Green supply chain network (GrSCN), known as closed-loop supply chain network, is the integration of the traditional forward supply chain process and reverse part. Forward chain has already been fully studied; reverse flow, namely recovery process, has been highly concerned and widely researched in recent years. Thierry et al. [12] distinguished three classes of activities for the returned products: direct reuse/resale without reprocessing; product recovery activities including repair, refurbishing, cannibalization, remanufacturing and recycling; and disposal. Fleischmann et al. [5] analyzed the general characteristics of recovery networks based on nine cases studies in different industries. Dowlatshahi [6] considered and analyzed the relevant literature in reverse logistics and generate a cost-benefit analysis regarding reverse logistics. Kumar et al. [17] explored a simple model for companies to understand and improve supply chain sustainability practices, and the model applied in two case studies proved that a green supply chain is a requirement for profitability. Even though the current achievement in GrSCN research is

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encouraging, it seldom conducted in global business strategy. More research is necessitated in determining how green supply chain makes sense in different products. Besides, in terms of the methodology and approach adopted, Petri nets are seldom used.

Such a promising field is required for trying out new methodologies and using traditional techniques for overall design. In this respect, Petri net seems a novel method in GrSCN design. Moore et al. [11, 12] investigated a Petri net approach in making disassembly process plans automatically in product recycling or remanufacturing. Hanafi et al. [5] utilized a fuzzy colored Petri net in predicting the return of the end-of-life products in different locations for designing the collection strategies. However, these researches did not focus on integrity. Therefore, our work intends to study on the Petri net approach regarding the whole green supply chain network. It is also an encouraging area of trying out new applications of Petri nets.

In this paper, we view the green supply chain as a discrete event dynamic system and put forward a stochastic Petri net approach. Now that Petri net is such a perfect tool in system modeling and analysis, and less utilized in green supply chain area, our work is rewarding and innovated. More precisely, we aim at modeling the general GrSCN with Petri net, and then, analyzing the essential performance of the model.

The introduction of Petri net approach is presented in Sect. 2. Section 3 models the green supply chain network in a generalized stochastic Petri net. Performance analyses are discussed in Sect. 4 and 5. Section 6 draws conclusions.

2 An Overview of Petri Net Approach

Petri nets are used for modeling discrete event systems, first put forward by Carl Adam Petri [13] in 1962. As to its component, a Petri net consists of places, transitions, arcs and tokens. Places and transitions are model conditions and model activities respectively. They are connected by arcs. Tokens are in places, while a token transform from one place to another after firing the related transition.

Generalized Stochastic Petri nets (GSPNs), an extension of ordinary Petri nets with the additional behavior of timing, were originally proposed by G. Balbo and G. Conte [1] in order to better model, analysis and evaluate the real-life system with complexity and time-related features.

A GSPN [9] is a 6-tuple, $GSPN = \{P, T; F, W, M_0, \lambda\}$, where $P = \{P_0, P_1,\ldots,P_m\}$ is a finite set of places; $T = \{T_0, T_1,\ldots,T_n\}$ is a finite set of transitions, which can be divided into two types: timed transitions $T_i = \{T_0, T_1,\ldots,T_k\}$, firing in exponentially distributed random times, which represent actions required some time to be completed, and immediate ones $T_i = \{T_{k+1},\ldots,T_n\}$, firing in zero time, which represent logistical events; $F \subseteq (P \times T) \cup (T \times P)$ is a set of arcs associated with the firing relationship; Inhibitor arcs are additional in GSPN, which define that the appearance of tokens in the input places of inhibitor arcs will disenable the firing of the output transitions; W is the weight function, defining the weight of arcs, with $w_{ij}(T_i, \mathrm{P}_j)$ is the weight of the arc from the transition T_i to its output place P_j and $w_{ij}(P_j, T_i)$ is the weight of the arc to the transition T_i from its input place P_j; M_0 is the initial marking of the Petri net; $\lambda = \{\lambda_0, \lambda_1\ldots,\lambda_k\}$ is the array of firing rate of the corresponding timed transitions; $P \cap T = \emptyset$, $P \cup T \neq \emptyset$. Graphically, places are represented by circles, while transitions by rectangle boxes with immediate ones in black and timed ones in white. An inhibitor arc is drawn as a line with a small circle in end.

The behavior of the system can be described as the marking process. A marking in GSPN changed by the firing of the transitions according to the following firing rules:

1. *A transition T_i is enabled only when each input place P_j directing to T_i contains at least $w_{ij}(P_j, T_i)$ tokens. It fires by moving $w_{ij}(P_j, T_i)$ tokens from each input place node and depositing $w_{ij}(T_i, P_j)$ tokens in each output place node.*
2. *Immediate transitions have priority over timed transitions.*
3. *If more than one immediate transition is enabled at a marking M, which one can fired is based on the priorities and weights. The firing probability $P\{T_k\}$ can be illustrated in expression:*

$$P\{T_k\} = \frac{W(P_i, T_k)}{\sum_{j:T_j \in E(M)} W(P_i, T_j)} \quad (1)$$

where $E(M)$ is the set of enabled immediate transitions with the highest priority in marking M; $W\{P_i, T_j\}$ is the firing weight of transition T_j.

3 Modelling of the Green Supply Chain Network

Referring to the related literature, the general GrSCN is shown in Fig. 1. The raw materials gathered by the supplier are sent to the manufacturer for production, and then the finished products are delivered to the distributor and allocated to the retailer for selling. Used products from the customer are collected by the recycling collection center and detected for recovery process.

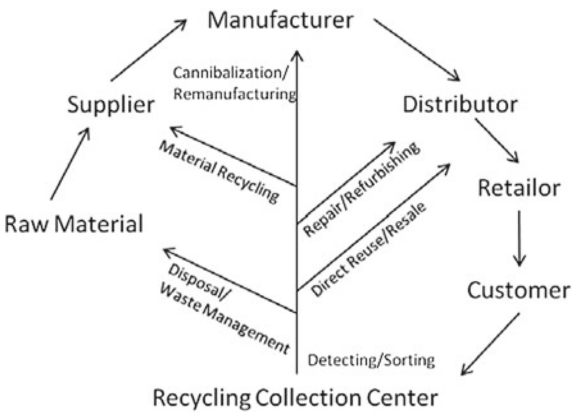

Fig. 1. A general green supply chain

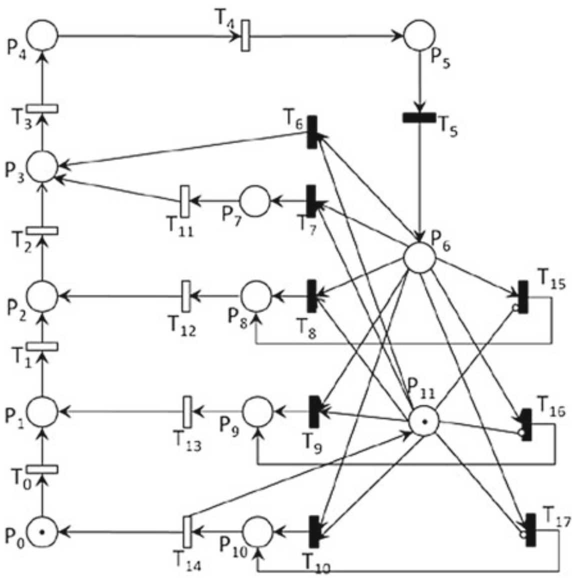

Fig. 2. GSPN model of green supply chain network

In this study, we model the GrSCN with the framework of GSPN (hereinafter referred to as GSPN-GrSCN). Figure 2 illustrates the GSPN model of the green supply chain network given in Fig. 1. Tables 1 and 2 give the description of each place and transition in the GSPN model respectively.

The token in place P_0 represents the initial state of the product, namely in raw material. And the flow of the token reveals the flow of the product in the GrSCN. The raw material is delivered to the supplier (P_1), and the manufacturer (P_2) obtains the material for production. The finishing product stored in distributor (P_3) is assigned to the retailer for selling (P_4). When the product is used out, it is collected (T_5) by the

Table 1. Interpretation of places in the Petri net

Places	Description
P_0	The raw material
P_1	Material stored in supplier
P_2	Manufacturer engages production
P_3	The product stored in distributor
P_4	Retailer sells the product
P_5	Customer uses the product
P_6	The recovery product inspected in collection center
P_7	Repair/Refurbish of the product
P_8	Cannibalization for remanufacturing of the product
P_9	Material recycling of the product
P_{10}	Disposal of the product
P_{11}	Assigning recovery mode

Table 2. Interpretation of transitions in the Petri net

Transitions	Description
T_0	Transportation of the raw material to supplier
T_1	Transportation of the material from supplier to manufacturer
T_2	Delivery of the product from manufacturer to distributor
T_3	Distributor provides the product to retailer
T_4	Customer buys the product from retailer
T_5	The used product delivered to collection center
T_6	The product is classified for direct reuse
T_7	The product is classified for repair/refurbish
T_8	The product is classified for cannibalization
T_9	The product is classified for material recycling
T_{10}	The product is classified for disposal
T_{11}	The repaired/refurbished product send to distributor
T_{12}	Delivery of the disassembled parts for remanufacturing
T_{13}	Delivery of the recycling material
T_{14}	Finishing disposal of the useless product
T_{15}	The once reused product is classified for cannibalization
T_{16}	The once reused product is classified for material recycling
T_{17}	The once reused product is classified for disposal

recycling collection center for detecting (P_5). Due to the fact that the customer using time of a product is much longer than other time consumption during the whole logistic flow, such as transporting time, manufacturing time, etc. We define T_5 as an immediate transition, not considered in performance evaluation. After the inspection, the collection center makes the decision of the recovery mode, including reuse (T_6), repair/refurbishing (T_7), cannibalization for remanufacturing (T_8), material recycling (T_9) and disposal (T_{10}). The function of the place P_{10} is to assign the recovery mode, that is the product only can be recovery through cannibalization (T_{15}) or material recycling (T_{16}) or disposal (T_{17}) if it has once be reused. We use an inhibitor arc to realize this. The token returns to place P_0 for another new recycling after material reclamation (T_{14}). Firing weight of immediate transitions T_6, T_7, T_8, T_9, T_{10}, T_{15}, T_{16}, T_{17} and firing rate of timed transitions T_0, T_1, T_2, T_3, T_4, T_{11}, T_{12}, T_{13}, T_{14} should be assigned according to the actual situations.

4 Stochastic Analysis

In this section, we show how the proposed model can be performed in performance analysis of green supply chain network. Note that the GSPN model is isomorphic with a semi-Markov process with a discrete state space, thus, performance analysis can be obtained by solving the underlying Markov chain problem. After generating the reachability tree, including tangible sates (the state only timed transitions are enable) and vanishing ones (the state at least one immediate transition is enable), the embedded Markov chain can be established, so does the calculation of stationary probabilities $P[M_i]$, equal to the steady state distribution of tangible states.

Various performance measures can be derived from the known stationary probability distribution as follow.

- The efficiency of each process e_i:
  This corresponds to the average number of tokens $\bar{u}_i$ in place P_i.

$$e_i = \bar{u}_i = \sum_j j \times P[M(P_i) = j] \quad (2)$$

  where $M(P_i)$ is the number of tokens in place when the marking is M, j is the probable number of tokens in P_{i}.
- The efficiency of the sub-procedure $E^{(l,k)}$:
  This corresponds to the sum of the average number of tokens $\bar{u}_i$ in the places of sub-system from place P_l to P_k.

$$E^{(l,k)} = \sum_{i:s_i \in S} \bar{u}_i = \sum_{i:s_j \in S} \sum_j j \times P[M(P_i) = j] \quad (3)$$

  where S is the sub-set starts from place P_l to P_k.
- Sojourn time for steady sate$\bar{\tau}[M_i]$:

$$\bar{\tau}[M_i] = \left(\sum\nolimits_{T_j \in H} \lambda_j\right)^{-1} \quad (4)$$

  where H is the set of enabled transitions in M_{i}.
- The utilization of each workflow et_{i}:
  This corresponds to the transition utilization $U[T_i]$:

$$et_i = U(T_i) = \sum_{M_j \in E} P[M_j] \quad (5)$$

  where E is the set of markings where T_{i} is enabled.
- The throughput of each workflow r_i:
  This corresponds to the transition throughput $R(T_{\mathrm{i}})$:

$$r_i = R(T_i) = \sum_{P_j \in O} W(T_i, P_j) \times U(T_i) \times \lambda_i \quad (6)$$

  where O is the set of output places of T_{i}.
- Time consumption of sub-procedure $T^{(l,k)}$:

$$T^{(l,k)} = \overline{N}/\lambda = E^{(l,k)}/R(T_i) \quad (7)$$

  The Little's Law [18] is used above, where $\overline{N}$ is the average number of tokens of the certain sub-system of the Petri net.

- Total time consumption T:

$$T = 1/R(T_{14}) \quad (8)$$

It reflects the efficiency of the whole system, and change in structure can promote the time performance.

- Manufacturing throughput *MT*(P_2):

$$MT(P_2) = \bar{u}_2/\bar{u}_0 \tag{9}$$

This can be used for comparison. We define the average number of tokens in P_0 as the basic value, and thereby gaining the throughput as in (9). Variational parameters or different structures result in different manufacturing throughput.

With the above measures, we can also obtain the economic performance of the reclamation, which is discussed in the next section by considering the cost of each recovery process and the additional profit brought by reclamation.

5 Numerical Analysis

We use Platform Independent Petri net Editor 2 (PIPE 2) [8], a Java based editing and analysis software for Petri nets, as a tool for both model description and performance analysis. It is user-friendly and fully functional for this paper. It generates the reachability tree as seen in Fig. 3, where white ovals represent tangible (steady) sates and blue, vanishing (unstable) ones. Apparently, there are 13 stationary states and 4 vanishing ones in the GSPN-GrSCN model. Then, we have the embedded Markov chain (shown in Appendix A1).

To conduct a more visualized study, we first define the transition parameters. We assume the firing rate of timed transitions as $\lambda_{0,1,2,3,4,11,12,13,14} =$ [6, 3, 1.5, 6, 2, 6, 3, 2, 3] and firing weight of immediate ones as $W_{(P_6 \to T_6,T_7,T_8,T_9,T_{10},T_{15},T_{16},T_{17})} = [1, 5, 7, 5, 2, 2, 3, 15]$. The Petri net state analysis shows it a bounded, safe and deadlock-free net.

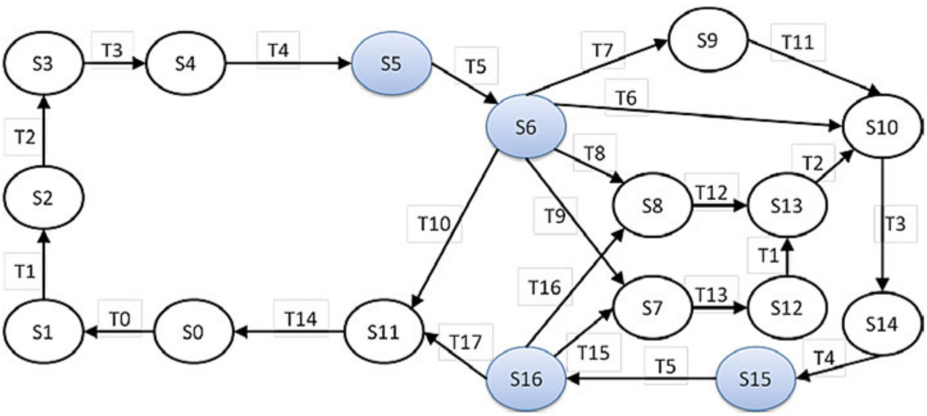

Fig. 3. The reachability graph of the GSPN model of GrSCN

The steady state probability of each state is illustrated in Table 3. Then we can compute the basic performance measures, including sojourn time, average tokens of places, transition utilization and transition throughput, of the GrSCN-GSPN model as indicated in Appendix A2, while Appendix A3 presents the results of the model when removing all the recovery parts (only remaining P_0, P_1, P_2, P_3, P_4, P_5, P_6, P_{10} and T_0, T_1, T_2, T_3, T_4, T_5, T_{10}, T_{14}).

Table 3. The steady probability of each state

State	Probability	State	Probability	State	Probability	State	Probability
M_0	0.04042	M_4	0.12126	M_8	0.038	M_{11}	0.14551
M_1	0.08084	M_5	0.08084	M_9	0.05214	M_{12}	0.03476
M_2	0.16168	M_6	0.0485	M_{10}	0.14551		
M_3	0.04042	M_7	0.01011				

The efficiency of each process can be attained in the light of (3) and (4). Specifically, Supplying efficiency contains material gathering and supplying process is 15.6 %; manufacturing efficiency is 30.7 %; product distribution efficiency is 8.9 %; retailer selling efficiency is 26.7 %; repair/refurbish efficiency is 1 %; disassembling efficiency is 3.8 %; material recycling efficiency is 5.2 % and disposal efficiency is 8.1 %. Supply managers can make wise decisions based on the above data, while arranging more staffs and more attentions to high-efficiency processes and reducing workers in low-efficiency processes for the maximization of the resource allocation. The utilization results show that the transportation of the product from manufacturer to distributor needs to be improved firstly. Besides, sales and material transportation are also two bottlenecks in the whole system, requiring attentions.

Manufacturing throughput of the GSPN-GrSCN model and the none-recovery one is 7.6 and 4, respectively. Obviously, recovery process nearly doubles the manufacturing performance, and enhances the manufacturing efficiency and utilization ratio.

Now we investigate the economic performance of green supply chain compared with traditional supply chain without recovery. Referring to [3], the values of the cost parameters for each process are given in Table 4.

Table 4. Value of the cost parameter for each process

Cost Parameter	*Value* (%)
Virgin unit price p_1	100
Second good's price p_2	80
Holding, Shortage and non-utilized capacity cost per unit per period c_1	10
Material cost per unit c_2	10
Manufacturing cost per unit c_3	10
Repairing cost c_4	5
Disassembly cost per unit c_5	3
Recycling cost per unit c_6	5
Disposal cost c_7	1

The economic benefit of none-recovery SCN per unit can be:

$$P_{n-re\text{covery}} = p_1 - c_1 \times \sum_{i=0}^{4} \tau[M_i] - c_2 - c_3 - c_7 = 60.67\,\%$$

and the additional profit brought by reclamation ΔP has:

$$\Delta P = p_2 - c_1 \times \sum_{i=5}^{11} \overline{\tau}[M_i] - c_4 \times \frac{U(T_{11})}{\sum_{k=11}^{14} U(T_k)} - (c_3 + c_5) \times \frac{U(T_{12})}{\sum_{k=11}^{14} U(T_k)} - (c_3 + c_5 + c_6) \times \frac{U(T_{13})}{\sum_{k=11}^{14} U(T_k)} - c_7 \times \frac{U(T_{14})}{\sum_{k=11}^{14} U(T_k)} = 44.7\,\%$$

Then, the economic benefit of GrSCN per unit has:

$$P_{GrSCN} = P_{n-re\text{covery}} + \Delta P = 105.37\,\%$$

Clearly, reclamation increases the total profit more than half, bringing in great economic benefit to the company. This is also definitely a powerful proof of the necessity of green supply chain except its environmental factors.

6 Conclusions

This paper presents a Petri net approach for modeling and analyzing the green supply chain network, a promising research field both in academic and industrial area. The proposed model indicates the general green supply chain network pictorially and logically, consequently can be used in diverse industries in describing green supply chain. Base on the performance measures calculated by PIPE2, we put forward the approach to analyze the time performance, efficiency, manufacturing throughput and economic performance of the GSPN-GrSCN model. Results show that compared with traditional none-recovery supply chain, green supply chain improves the manufacturing throughput, drastically increasing the economic profit.

Green supply chain is not only a “hot” area under the global tendency of environmental business, but a promising field for trying out new application of Petri nets. This paper is just the first step towards a comprehensive research of green supply chain analysis, further work should extend to the following aspects: (1) discussing and analyzing more complex and realistic GrSCN; (2) applying Petri net approach in other fields of green supply chain, such as life-cycle analysis (LCA) of the product; (3) integrating Petri net with other tools to improve and optimize the proposed model.

Appendix

A1. Set of Steady States

State		P_0	P_1	P_2	P_3	P_4	P_5	P_6	P_7	P_8	P_9	P_{10}	P_{11}
S0	M_0	1	0	0	0	0	0	0	0	0	0	0	1
S1	M_1	0	1	0	0	0	0	0	0	0	0	0	1
S2	M_2	0	0	1	0	0	0	0	0	0	0	0	1
S3	M_3	0	0	0	1	0	0	0	0	0	0	0	1
S4	M_4	0	0	0	0	1	0	0	0	0	0	0	1
S11	M_5	0	0	0	0	0	0	0	0	0	0	1	0
S10	M_6	0	0	0	1	0	0	0	0	0	0	0	0
S9	M_7	0	0	0	0	0	0	0	1	0	0	0	0
S8	M_8	0	0	0	0	0	0	0	0	1	0	0	0
S7	M_9	0	0	0	0	0	0	0	0	0	1	0	0
S14	M_{10}	0	0	0	0	1	0	0	0	0	0	0	0
S13	M_{11}	0	0	1	0	0	0	0	0	0	0	0	0
S12	M_{12}	1	0	0	0	0	0	0	0	0	0	0	0

A2. Performance Measures of GSPN-GrSCN

Steady state M_i	Sojourn Time $\bar{\tau}[M_i]$	Place P_i	Average tokens $\bar{u}_i$	Transition T_i	Transition utilization $U(T_i)$	Transition T_i	Transition throughput $R(T_i)$
M_0	0.16667	P_0	0.04042	T_0	0.04042	T_0	0.24252
M_1	0.33333	P_1	0.1156	T_1	0.1156	T_1	0.34681
M_2	0.66667	P_2	0.30719	T_2	0.30719	T_2	0.46079
M_3	0.16667	P_3	0.08892	T_3	0.08893	T_3	0.53355
M_4	0.5	P_4	0.26677	T_4	0.26678	T_4	0.53355
M_5	0.33333	P_5	0	T_{11}	0.0101	T_{11}	0.06063
M_6	0.16667	P_6	0	T_{12}	0.038	T_{12}	0.11399
M_7	0.16667	P_7	0.01011	T_{13}	0.05214	T_{13}	0.10428
M_8	0.33333	P_8	0.038	T_{14}	0.08084	T_{14}	0.24252
M_9	0.5	P_9	0.05214				
M_{10}	0.5	P_{10}	0.08084				
M_{11}	0.66667	P_{11}	0.44462				
M_{12}	0.33333						

A3. Performance Measures of GSPN-SCN without Recovery

Place P_i	Average tokens $\bar{u}_i'$	Transition T_i'	Transition utilization $U(T_i)$	Transition T_i'	Transition throughput $R'(T_i)$
P_0	0.07692	T_0	0.07692	T_0	0.46153
P_1	0.15385	T_1	0.15384	T_1	0.46153
P_2	0.30769	T_2	0.30769	T_2	0.46153
P_3	0.07692	T_3	0.07692	T_3	0.46153
P_4	0.23077	T_4	0.23077	T_4	0.46153
P_5	0	T_{14}	0.15384	T_{14}	0.46153
P_6	0				
P_{10}	0.15385				

References

1. Ajmone Marsan, M., Balbo, G., Chiola, G., Conte, G.: Generalized stochastic petri nets revisited: random switches and prioritiesn. In: Proceedings of the International Workshop on Petri Nets and Performance Models, Madison (1987)
2. Dowlatshahi, S.: A cost-benefit analysis for the design and implementation of reverse logistics systems: case studies approach. Int. J. Prod. Res. **48**, 1361–1380 (2010)
3. El-Sayed, M., Afia, N., El-Kharbotly, A.: A stochastic model for forward-reverse logistics network design under risk. Comput. Ind. Eng. **58**, 423–431 (2010)
4. Fleischmann, M., Krikke, H.R., Dekker, R., Flapper, S.D.P.: A characterization of logistics networks for product recovery. Omega **28**, 653–666 (2000)
5. Hanafi, J., Kara, S., Kaebernick, H.: Generating fuzzy coloured petri net forecasting model to predict the return of products. In: IEEE International Symposium on Electronics and The Environment, vol. 245–250, pp. 7–10 (2007)
6. Hanafi, J., Kara, S., Kaebernick, H.: Reverse logistics strategies for end-of-life products. Int. J. Logistics Manag. **19**, 367–388 (2008)
7. Handfield, R.B.: Green supply chain: best practices from furniture industry. In: Proc 3th Annual Conference Decision Sciences Institute, New York, pp. 1295–1297 (1996)
8. http://pipe2.sourceforge.net/
9. Huang, Z.Q., Yi, R.H., Da, Q.L.: Study on the efficiency of the closed-loop supply chains with remanufacture based on third-party collecting. Chin. J. Manage. Sci. **3**, 73–77 (2008)
10. Lin, C.: Stochastic Petir Nets and System Performance Evaluation II. Tsinghua University Press, Beijing (2004)
11. Moore, K.E., Gungor, A.K., Gupta, S.M.: A petri net approach to disassembly process planning. Comput. Ind. Eng. **35**, 165–168 (1998)
12. Moore, K.E., Gungor, A.K., Gupta, S.M.: Petri net approach to disassembly process planning for products with complex AND/OR precedence relationships. Eur. J. Oper. Res. **135**, 428–449 (2001)
13. Petri, C.A.: Kommunikation mit Automaten. Thesis(PhD), Universität Bonn (1962)
14. Salema, M.I., Póvoa, A.P.B., Novais, A.Q.: Dynamic network design model with reverse flows. In: Sixteenth Annual Conference of POMS, Chicago, pp. 003–0036 (2005)

15. Kumar, S., Teichman, S., Timpernagel, T.: A green supply chain is a requirement for profitability. Int. J. Prod. Res. **50**, 1278–1296 (2012)
16. Samir, K.: Srivastava: green supply-chain management: a state-of- the-art literature review. Int. J. Manag. Rev. **9**, 53–80 (2007)
17. Thierry, M., van Wassenhove, L.N., van Nunen, J.A.E.E., Salomon, M.: Strategic issues in product recovery management. Calif. Manag. Rev. **37**, 114–135 (1995)
18. Travedi, K.S.: Probability and Statistics with Reliability, Queuing, and Computer Science Applications II. Wiley, New York (2001)
19. Zhang, X., Qiang, L., Teresa, W.: Petri-net based applications for supply chain management: an overview. Int. J. Prod. Res. **49**, 3939–3961 (2011)