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Chemical Engineering Science 57 (2002) 4697–4713

Chemical Engineering Science

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A mathematical model and decision-support framework for material recovery, recycling and cascaded use

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Abstract

To achieve more than incremental reductions in resource consumption and waste, it will be necessary to develop new approaches to the systematic use and re-use of materials in the kind of system termed an "industrial ecology". This paper presents a new methodology—CHAin Management of Materials and Products (CHAMP)—developed for modelling the flow of materials through a succession of uses with different performance requirements. Although developed specifically for polymers, the CHAMP approach is also applicable to other materials and products. Materials are characterised by a set of technical performance parameters, termed utilities. Geographical location is also treated as a utility to enable logistics—both distribution of products and collection of used products or waste—to be incorporated within the same modelling framework. Processing, transport and use are treated as activities through which a material can pass. The costs and environmental impacts of activities are included in the modelling framework, and are assessed on a life cycle basis by considering the complete supply chain of materials and energy used by each activity. The methodology includes acceptance criteria which determine whether a material is suitable for specific uses or activities. These criteria are applied within the model to guide selection of materials for specific applications and of successive uses for specific materials. A simple example of the CHAMP approach is given, to illustrate the kinds of problem to which it has been applied.

Keywords: Materials processing; Mathematical modelling; Integrated waste management; Environment; Life cycle assessment; Polymers

1. Introduction

1.1. Industrial ecology

Since the industrial revolution, use of material and energy resources and associated generation of wastes and dispersed emissions from human activities have been increasing (see e.g. Jackson, 1996). Recognition that this approach to material use is not sustainable is leading, inter alia, to the concept of Extended Producer Responsibility, which implies that manufacturers retain some responsibility for post-use management of the materials making up their products (see e.g. Clift, 2001). Extended Producer Responsibility is being driven, particularly in Europe, by "take-back legislation" which requires manufacturers and suppliers to accept materials and products back after use. While the overt motivation for take-back is to reduce the quantity of material entering the waste stream, greater environmental benefits often lie in the re-use of materials and components, thereby displacing waste generation earlier in the supply chain (see e.g. Clift & Wright, 2000). Extended Producer Responsibility is seen as a driver towards the development of industrial ecology illustrated by Fig. 1. This concept goes beyond re-use and recycling, to include use and re-use of materials in a series of different applications. Frequently these successive applications will have progressively lower performance specifications. Thus, in the sequence shown in Fig. 1, Use 1 has higher performance requirements than Use 2, so that material from Use 1 can pass to Use 2 but flow in the opposite direction requires reprocessing and may therefore be uneconomic. A sequence of applications like that in Fig. 1 is sometimes termed a *cascade of uses*.

While the ideal of moving towards a closed material economy may be desirable, it is already clear that implementation of Extended Producer Responsibility may sometimes lead to worse environmental performance overall (see e.g. Mayers & France, 1999). This is particularly the case where

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PII: S0009-2509(02)00282-8

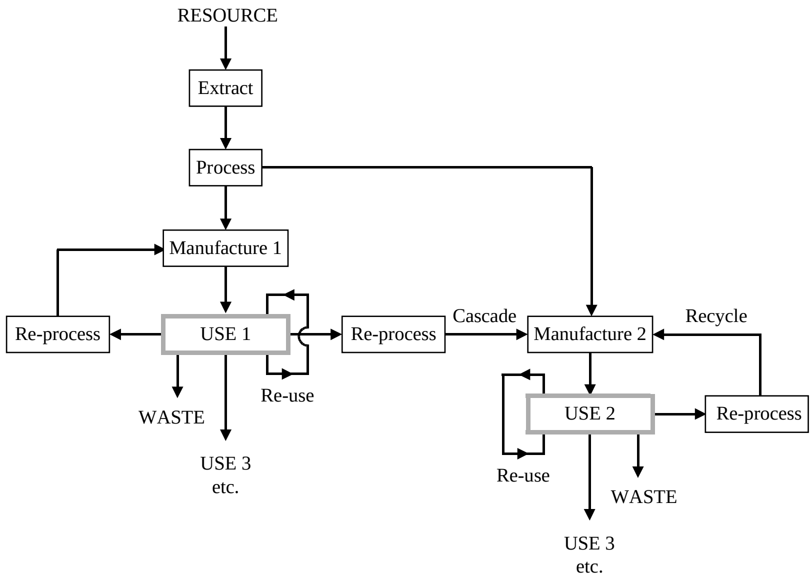

Fig. 1. Industrial ecology: cascaded use of materials.

transport contributes a significant part of the costs and environmental impact, which is frequently the case for collection of dispersed products and materials after use (Clift & Wright, 2000). Collection costs and impacts can be reduced for relatively large products, such as office machinery, which are leased rather than sold (Clift, 2001). However, even in these cases, selecting materials and designing products for recovery and re-use requires complex decisions to be made in which economic and environmental objectives may have to be traded off against each other. The methodology set out in this paper has been developed to support these decisions and thus aid the development of industrial ecologies. The modelling approach has been developed for the chain management of polymers but it is also applicable to chain management of products more generally. Therefore it could also provide the basis for decision-support in industrial ecologies of other materials.

Polymers have been selected as the focus for the CHAMP methodology because of the continuing growth of the polymer industry and the quantities of plastics in the waste stream. In 1999, more than 18 million tonnes of plastics were disposed of across Europe (APME, 1999) and this has been projected to increase to 25 million tonnes per year by 2006 (APME, 1998). Similar trends are predicted for North America (Bisio & Xanthos, 1995; Hadjilambrinos, 1996). Almost 80% of this waste is disposed of by landfilling or incineration without energy recovery (APME, 1999). Although the proportion of waste plastic recycled is progressively increasing, it is clear that new approaches to post-consumer waste management will be needed if plastic waste is to be reduced very substantially (Corto & Basar, 1998; Edgecombe, 1998; Nunan, 1999; Subramanian, 2000).

The general structure of a possible fully developed industrial ecology for polymers is shown in Fig. 2. It is characterised by nested possible loops (Clift, 1997). The principal material inputs are hydrocarbons, which must be extracted and processed to produce the monomer feedstock for polymerisation. The polymer must then be blended, usually with a range of additives, and formed into a plastic artefact. Following use, the artefact may simply be collected for *re-use* in the same application. If this is not possible—for example if the artefact is damaged—then the material may be recovered for *mechanical recycling* by physical treatment, for example by granulation and reforming. The new artefact may be returned to the previous use, or it may pass to a second application (see Fig. 1). If materials become contaminated or mixed, then mechanical recycling may not be an option. For some polymers, notably acrylics (Wright, 1997) and some polyurethanes (Markovic & Hicks, 1997), *depolymerisation* to monomers or feedstock is possible. *Chemical recycling*, usually by pyrolysis, recovers a mixture of lower molecular weight compounds for reprocessing, for example as cracker feedstock. Failing any of these options for material recycling, waste polymer can be used as a *fuel*, thereby displacing use of other fuels. Where none of these options is followed, the material must be subject to disposal to landfill or incineration without energy recovery.

In the kind of ecology shown in Fig. 2, the service lives of the polymer products considered so far are short, so that simple steady-state system modelling can be used. Alternative uses of metals can have very different service lives, some of them very long; some form of dynamic model is then needed (McLaren, Wright, Parkinson, & Jackson, 1999).

1.2. Environmental system analysis and life cycle assessment

The CHAMP approach to modelling multiple uses of materials is an example of environmental system analysis: the

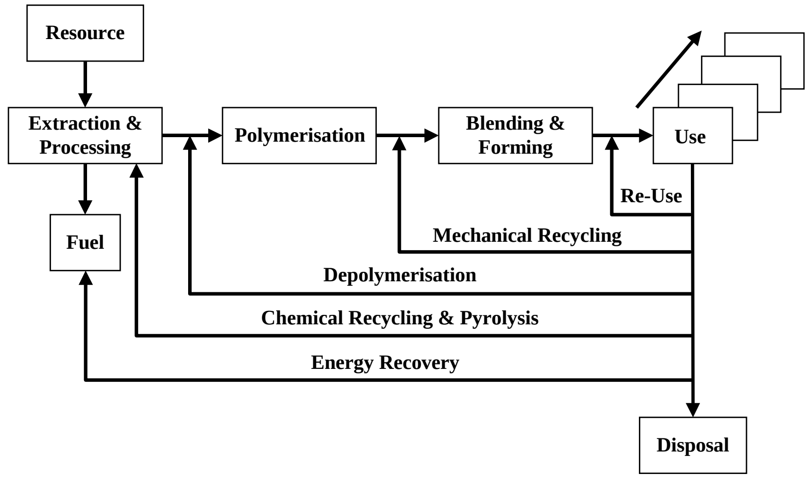

Fig. 2. An industrial ecology for polymers.

relationship between specific human activities and the environment is quantified, along with the significance of the burdens (or interventions) which pass between the economic system and the environment (Azapagic, 2002; Clift, 2001). The approach adopted draws on the established methodology of life cycle assessment (SETAC, 1993; Lindfors et al., 1995; ISO 14040, 1997; ISO 14041, 1998; ISO 14042, 1999; ISO 14043, 2000) by including the entire "cradle to grave" supply chains of energy and materials and by estimating environmental impacts of emissions and resource use. In particular, it incorporates the methodology developed to apply life cycle assessment (LCA) to waste management (Finnveden et al., 1995; White, Franke, & Hindle, 1995; Nichols & Aumônier, 1997; Finnveden & Ekvall, 1998; Clift, Doig, & Finnveden, 2000; Ekvall & Finnveden, 2000).

The first stages in LCA include defining the boundaries of the system to be studied, defining the functional unit [1] as the basis on which systems are to be analysed and compared, and identifying and quantifying the inputs to the system in the form of primary resources and emissions to the environment (SETAC, 1993; Lindfors et al., 1995; ISO 14040, 1997; ISO 14041, 1998). This set of inputs and emissions is termed the *environmental burdens* (or sometimes the environmental interventions), and the set of burdens is known as the Inventory Table. Fig. 3 shows schematically how the extended system approach (Tillman, Ekvall, Baumann, & Rydberg, 1994; Clift, Frischknecht, Huppes, Tillman, & Weidema, 1999; Clift et al., 2000) is used in this work to ensure that the analysis is carried out on a full life cycle basis. An activity—usually a processing operation or transportation—through which a material passes is treated as a Foreground Activity, and is ideally described by

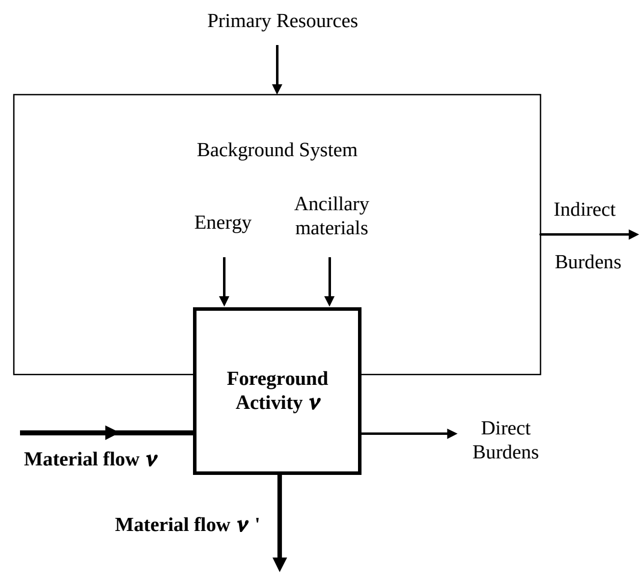

Fig. 3. Distinction between foreground activity and background system for life cycle assessment.

process-specific data. Environmental emissions from the Foreground Activity are termed *direct burdens*. However, the analysis must also include the environmental burdens associated with supplying both energy and ancillary materials; i.e. materials, such as fuels and lubricants, which are consumed in the Foreground Activity but do not become part of the material flow. The primary resource inputs and emissions from the Background System comprising these supply chains are termed *indirect burdens*. The indirect burdens can be described by generic industry data, obtainable from commercial or public life cycle inventory databases. This basic approach is also used to assess recovery of energy or materials by Foreground waste management activities (Clift et al., 2000).

Once compiled, the Inventory Table is expressed in terms of the contributions to a set of recognised Environmental

[1] Functional unit is a quantitative measure of the function, i.e. output of products or services, that a system delivers. For example, the function of beverage packaging is to contain a certain amount of liquid so that the functional unit can be defined as "the amount of packaging material used to contain a specified volume of beverage in units of specified size".

Impact Categories (Heijungs, 1992; SETAC, 1993; Lindfors et al., 1995; ISO 14042, 1999). Further details of this step, termed Impact Assessment, are given in Appendix A. In terms of the system model, Impact Assessment amounts to simple linear operations on the environmental burdens to aggregate them to a smaller number of impacts. This is done in terms of the potency factors representing their potential contributions to global impacts because, whereas the location of the direct emissions from the Foreground Activities may be known, the Background Activities generating the indirect burdens are not normally specified so that site-specific impact assessment is not possible.

Although the CHAMP methodology derives from life cycle assessment, it represents a new development in considering multiple uses of materials as shown in Figs. 1 and 2, whereas LCA conventionally considers single products, processes or services (Azapagic, 2002). Another development and application of LCA is *life cycle product design* (LCPD; sometimes known as Design for the Environment) which aims to optimise the environmental performance of a manufactured product over its entire life cycle (e.g. Wenzel, Hauschild, & Alting, 1997; Alting, Hauschild, & Wenzel, 1998; Azapagic, 1998). Whereas LCPD usually achieves only an incremental improvement in environmental performance (Udo de Haes, Wrisberg, Clift, Eder, & Triebswetter, 2002) the CHAMP approach can promote more substantial improvements by enabling product designers to consider the implications of recovering and re-using or recycling components and materials after use. CHAMP is complementary to and builds on the approach of whole system modelling combined with multi-objective optimisation developed by Azapagic (1998) and Azapagic and Clift (1995, 1998, 1999a).

2. Model structure

The approach taken in the CHAMP model is to track each material as it passes through a sequence of activities. These may be processing operations, use or transport, including both conventional logistics (i.e. distribution) and "reverse logistics" (i.e. collection of dispersed used product or waste material). The model is constructed so that all these types of activities can be accommodated within the same framework. Changes in material properties are modelled, along with economic costs and environmental burdens and/or impacts.

2.1. Material classification and functional unit

No distinction is made in formulating the model between *materials* (usually single polymers with additives), *components* (which may be formed from more than one material) and *products* (which are assemblies of different materials and components). This enables the CHAMP framework to describe all types of flow, in as much or as little detail as required, so that it can be applied to both products and materials.

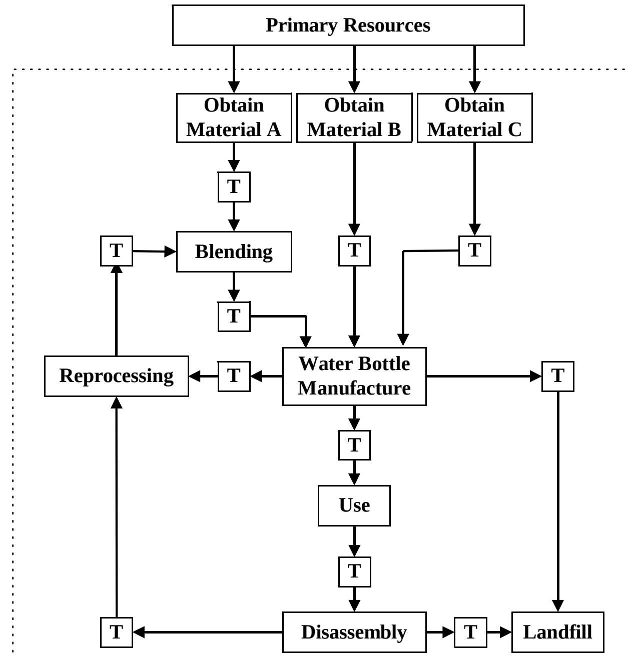

Fig. 4. An example of a sequence of activities forming part of a system to be modelled: a simple recycling scenario, with disposal of process scrap and off-specification product as well as used product. Note that T denotes some form of transport activity.

The flow of any type of material k $(k=1,2,\ldots,K)$ leaving an activity, whether it is a material, component or a product, is denoted by m_k (mass per unit time). The total material flow emerging from an activity is then defined as

$$M = \{m_1, m_2, \ldots, m_K\}. \tag{1}$$

Some elements of M may be assembled into a product, so that they then pass along a common path as shown in Fig. 4, before being disassembled to follow different routes again for recycling or disposal. (Note that this particular example is developed in more detail in a later section.) Thus the set M must include sufficient elements to represent all the constituent materials so that their properties can be tracked as they move through the system, plus further elements to represent components or products. Where materials are combined or assembled to form a product, as in "water bottle" manufacture" in Fig. 4, it is convenient to denote the product flow leaving the assembly activity by one of the elements in the set M. A non-zero value of m_k for a material then represents material leaving the activity (e.g. scrap). Similarly, on passing through a disassembly operation, the elements of M representing assembled product became zero but the elements representing materials increase. Even when a material is fully incorporated into a product so that its flow becomes zero, the vector describing its properties (see Section 2.3) is retained, so that information about the constituent materials is not lost.

In the following explanation of the model structure, the term "material" is used to denote any material flow, covering materials, components and products.

As in conventional life cycle assessment, the model is quantified in terms of a functional unit defined at some critical point in the system. For the example system shown in Fig. 4, the functional unit would be specified as packaging a defined total quantity of water in units of specified size; e.g. 1 m^3 in total in 1000 bottles of 1 l. The total material flow M through the system would then be the material quantities required for this packaging duty, allowing for losses from the supply chain in the form of process scrap and off-specification bottles. For other examples where the artefact is used in this form several times, M depends on the average number of times it is used before being reprocessed.

2.2. Material flow network

For a system comprising G activities in total, the possible routes for each material k through the system can be represented conveniently by a binary matrix, $\mathbf{P}_k$. If material k can pass to activity v from activity μ ($\mu, v = 1, 2, \ldots, G$), then element (v, μ) in $\mathbf{P}_k$ is set at unity. If the path to v from μ is not available, then the element (v, μ) is set to zero. Thus $\mathbf{P}_k$ summarises the network of routes available to material k. The set of matrices $\mathbf{P}_k$ form a simple binary tensor of order 3 and dimensions $K \times G \times G$. This is essentially the approach derived from the theory of graphs (e.g. Berge, 1962). More compact ways of representing the network are available, along with algorithms for rapid calculation (e.g. Sargent & Westerberg, 1964). The industrial ecologies considered so far are not sufficiently complex to justify use of these approaches but it may be noted that the CHAMP methodology could be adapted to process simulation approaches for more complex systems.

The first activity in any branch of the network normally consists of bringing the material into the foreground system, as illustrated by Fig. 4. Following the extended system approach to LCA illustrated by Fig. 3, this introduces the "background" costs and environmental burdens associated with producing the material in a way which is explained in more detail below.

2.3. Material properties

Central to the CHAMP methodology is the concept of material *utility*. A material at any point in the system is characterised by a set of technical characteristics which determine whether it can be used for any particular process or application; these properties form the utility vector $\boldsymbol{u}_k$ characterising material k. The elements of utility include intrinsic and extrinsic material properties such as melting point, impact strength, density, melt flow index and hardness. They also include geographical location; it is this feature which

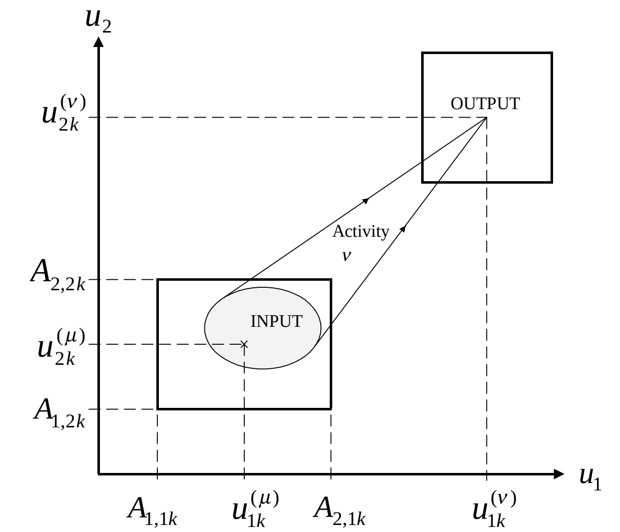

Fig. 5. Change of two utility parameters by a process or transport activity v.

enables logistics and reverse logistics to be included within the same model framework.

Each activity changes one or more of the components of a material's utility, as illustrated by Fig. 5. On leaving activity μ, for input to activity v, a material is characterised by a single set of utilities, represented in Fig. 5 by the two parameters $u_{1k}^{(\mu)}$ and $u_{2k}^{(\mu)}$. Alternatively, parts of the material may have different utilities, as shown by the shaded region in Fig. 5. These might be material properties, with the range dependent on how much service and therefore property degradation the material has experienced in use, or the utility parameters might describe location, so that the range corresponds to geographical dispersion. The activity changes the utility parameters and usually brings them to single values, by blending or processing the material to uniform quality or, in the case of reverse logistics, by bringing the dispersed material to a single location for processing or storage.

The CHAMP methodology models each activity by describing the changes in the utility parameters of materials passing through the activity, i.e. the change $\boldsymbol{u}_k^{(\mu)}$ to $\boldsymbol{u}_k^{(v)}$ ($k = 1, 2, \ldots, K$) brought about by activity v is represented by a function $\boldsymbol{X}_k^{(v,\mu)}$ such that

$$\boldsymbol{u}_k^{(v)} = \boldsymbol{X}_k^{(v,\mu)}(\boldsymbol{u}_k^{(\mu)}). \tag{2}$$

The functions describing utility changes may be non-linear in general, with the change in any individual utility parameter u_{hk} dependent on one or more of the other utilities. However, in many cases the changes represented by X_k are linear (or simple increments) so that Eq. (2) can be written as

$$\begin{aligned}\boldsymbol{u}_k^{(v)} &\equiv (u_{1k}^{(v)}, u_{2k}^{(v)}, \ldots, u_{Hk}^{(v)}) \\ &= (X_{1k}^{(v,\mu)}(u_{1k}^{(\mu)}), X_{2k}^{(v,\mu)}(u_{2k}^{(\mu)}), \ldots, X_{Hk}^{(v,\mu)}(u_{Hk}^{(\mu)})),\end{aligned} \tag{2'}$$

where $X_{hk}^{(v,\mu)}$ is the function within the operator set $\boldsymbol{X}_k^{(v,\mu)}$ representing the effect of activity v on utility h of material k.

2.4. Economic costs

The CHAMP model also calculates the costs associated with passing a material, component or product through the sequence of activities making up the industrial ecology system. Costs associated with each activity can be disaggregated by material j, and also between different components of cost such as energy, ancillary materials, capital costs, labour and transport. If there are L cost headings l, the cost of passing material k through activity v is expressed, per overall functional unit, as

$$\boldsymbol{c}_k^{(v)} = (c_{1k}^{(v)}, c_{2k}^{(v)}, \ldots, c_{Lk}^{(v)}). \tag{3}$$

If only total costs are of interest, then $L=1$ and $\boldsymbol{c}_k^{(v)}$ collapses to a single scalar value. It may be noted that, for a product or component, Eq. (3) in general requires the costs to be allocated between the different constituent materials; this is a common accounting problem, and is not explored further here. In general, the costs in Eq. (3) will depend on the utility change brought about by the activity, through the processing conditions or distance transported.

Eq. (3) refers to the costs associated with any individual activity. Costs are accumulated as a material passes through a sequence of activities; assuming that a material passes through a sequence of activities indexed in consecutive order (i.e. $1, 2, 3, \ldots$), then the total cost associated with material k leaving activity v is

$$\boldsymbol{C}_k^{(v)} = \sum_{\beta=1}^{v} \boldsymbol{c}_k^{(\beta)}, \tag{4}$$

where $\boldsymbol{c}_k^{(1)}$ is the initial cost of the material as it enters the system under analysis (see Section 2.2 above). In the form equivalent to Eq. (2), accumulated costs for material k leaving activity v can be expressed as

$$\boldsymbol{C}_k^{(v)} = \boldsymbol{C}_k^{(\mu)} + \boldsymbol{c}_k^{(v)}. \tag{5}$$

2.5. Environmental burdens and impacts

To complete the set of parameters characterising the flow of a material through the system, the environmental burdens associated with each activity are calculated and accumulated along the sequence of activities through which a material passes. The resource inputs and emissions associated with passing material k through activity v are expressed, per functional unit, as the corresponding set of environmental burdens:

$$\boldsymbol{b}_k^{(v)} = (b_{1k}^{(v)}, b_{2k}^{(v)}, \ldots, b_{Ik}^{(v)}). \tag{6}$$

The burdens in Eq. (6) include not only direct emissions from the processing or transport activity itself but also the burdens from the background system supplying energy and ancillary materials to the foreground activity (see Fig. 3). In LCA, the problem of allocating burdens $\boldsymbol{b}_k$ to the different materials has been the topic of a substantial body of literature (e.g. Huppes & Schneider, 1994; Azapagic & Clift, 1999b, c, 2000; Clift et al., 1999).

Similar to the economic costs in Eqs. (3) and (4), the environmental burdens are accumulated and in general related to the utility change effected by the activity. Assuming that a material passes through a sequence of activities indexed in consecutive order (i.e. $1, 2, 3, \ldots$), then the total burdens associated with material k leaving activity v are

$$\boldsymbol{B}_k^{(v)} = \sum_{\beta=1}^{v} \boldsymbol{b}_k^{(\beta)}, \tag{7}$$

where $\boldsymbol{b}_k^{(1)}$ are the burdens associated with the background activity of producing the material entering the system, in effect representing the environmental burdens "bought" with the product (cf. Section 2.2 and $c_k^{(1)}$ above). It is usually more convenient to convert the burdens to a smaller set of life cycle environmental impacts, as outlined in Appendix A:

$$\boldsymbol{e}_k^{(v)} = \mathbf{w} \cdot \boldsymbol{b}_k^{(v)}; \quad \boldsymbol{E}_k^{(v)} = \mathbf{w} \cdot \boldsymbol{B}_k^{(v)}, \tag{8}$$

where $\mathbf{w}$ is the matrix of potency factors for all the substances identified in the inventory. In the form equivalent to Eq. (2):

$$\boldsymbol{B}_k^{(v)} = \boldsymbol{B}_k^{(\mu)} + \boldsymbol{b}_k^{(v)}, \tag{9}$$

$$\boldsymbol{E}_k^{(v)} = \boldsymbol{E}_k^{(\mu)} + \boldsymbol{e}_k^{(v)}. \tag{10}$$

3. Mapping an industrial ecology

3.1. Sequences of activities

Once the activities making up the system have been modelled to describe their effects on the utilities, costs and environmental burdens and/or impacts, sequences of activities can be examined to investigate possible paths for the material through a series of possible uses. In the following explanation, α_k is used to denote any of the utility or system vectors for material k (i.e. $\alpha_k \in \{\boldsymbol{u}_k, \boldsymbol{C}_k, \boldsymbol{B}_k, \boldsymbol{E}_k\}$) and $\boldsymbol{X}_k^{(v,\mu)}$ denotes the component of the function changing $\alpha_k^{(v)}$ for the material passing through activity v (see Eqs. (2), (5), (9) and (10)). Fig. 6 uses network diagrams to illustrate the use of this approach for the example system given in Fig. 4, i.e. a simple cradle-to-grave recycling scenario with a nested loop.

It was mentioned in Section 2.2 that a material flow map can be described for each material k in the system by the binary square matrix $\mathbf{P}_k$, with order equal to the number of activities in the system, G. If the flow maps for individual materials are superimposed as

$$\mathbf{P} = \sum_{k=1}^{k=K} \mathbf{P}_k \tag{11}$$

then $\mathbf{P}$ represents the total network describing the system. The result for the system in Fig. 4 is shown in Fig. 6(a).

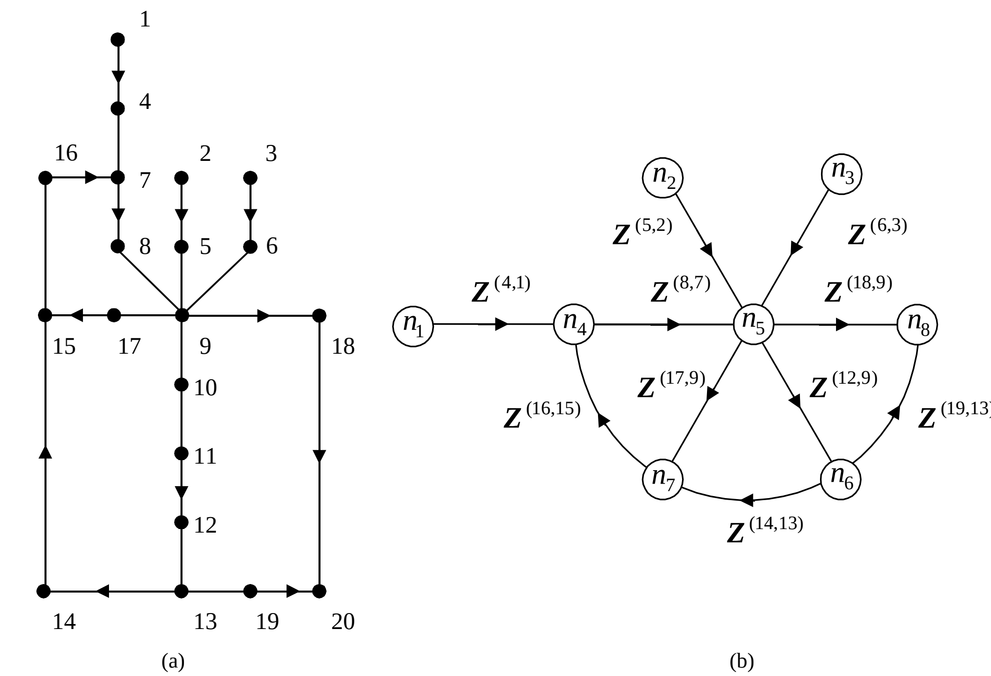

Fig. 6. Example of a system comprising sequences of activities, some of which may be repeated on different material paths: (a) Individual activities (see Fig. 4: 1, 2, 3—sourcing materials 1, 2, 3, respectively; 7—Blending; 9—Water Bottle Manufacture; 11—Use; 13—Disassembly; 15—Reprocessing; 20—Landfill; 10, 12, 18, 19—transport of all three materials; 4, 8, 14, 16—transport of material 1; 5—transport of material 2; 6—transport of material 3); (b) sequences aggregated by Eq. (15) to form an irreducible representation.

The 20 activities in this system are represented by the functions $\boldsymbol{X}_k^{(v,\mu)}$ with $\mu, v = 1, 2, \ldots, 20$ (see Fig. 6(a)). Passing material k for instance, from activity 3 through activities 6, 9 and 10 then through 11, would be written as

$$\boldsymbol{\alpha}_k^{(11)} = \boldsymbol{X}_k^{(11,10)}(\boldsymbol{X}_k^{(10,9)}(\boldsymbol{X}_k^{(9,6)}(\boldsymbol{X}_k^{(6,3)}(\boldsymbol{X}_k^{(3,0)}(\boldsymbol{\alpha}_k^{(0)}))))), \quad (12)$$

where the superscript 0 indicates the origin of a material stream (normally the primary resource for a full life cycle description; see Figs. 1, 2 and 4) and, as outlined above, the beginning of each material stream is the activity of obtaining the material.

Thus a sequence of activities such as that described in Eq. (12) can be represented by a single function $\boldsymbol{Z}_k^{(v,\mu)}$, where μ denotes the activity whose output enters the sequence, and v denotes the activity whose output leaves the sequence. The example given in Eq. (12) can thus be written as

$$\boldsymbol{\alpha}_k^{(11)} = \boldsymbol{Z}_k^{(11,0)}(\boldsymbol{\alpha}_k^{(0)}), \quad (13)$$

where, $\boldsymbol{Z}_k^{(11,0)}$ is expressed in function notation as

$$\boldsymbol{Z}_k^{(11,0)} = \boldsymbol{X}_k^{(11,10)} \circ \boldsymbol{X}_k^{(10,9)} \circ \boldsymbol{X}_k^{(9,6)} \circ \boldsymbol{X}_k^{(6,3)} \circ \boldsymbol{X}_k^{(3,0)}. \quad (14)$$

This formulation is used to represent in compact form the overall effect of any possible path which a material can take through the system. Some paths include one activity only. Others represent an ordered sequence of activities that can be followed by at least one of the materials present.

Using this approach, an irreducible representation of the system given in Fig. 6(a) can be formulated by aggregating activities into 10 sequences connecting eight nodes $(n_1, n_2, \ldots, n_8)$ as shown in Fig. 6(b). In function notation these sequences may be written as

$$\begin{aligned}
&\boldsymbol{Z}^{(4,1)} = \boldsymbol{X}^{(4,1)}; \quad \boldsymbol{Z}^{(5,2)} = \boldsymbol{X}^{(5,2)}; \quad \boldsymbol{Z}^{(6,3)} = \boldsymbol{X}^{(6,3)}; \\
&\boldsymbol{Z}^{(8,7)} = \boldsymbol{X}^{(8,7)}; \quad \boldsymbol{Z}^{(12,9)} = \boldsymbol{X}^{(12,11)} \circ \boldsymbol{X}^{(11,10)} \circ \boldsymbol{X}^{(10,9)}; \\
&\boldsymbol{Z}^{(14,13)} = \boldsymbol{X}^{(14,13)}; \\
&\boldsymbol{Z}^{(16,15)} = \boldsymbol{X}^{(16,15)}; \quad \boldsymbol{Z}^{(17,9)} = \boldsymbol{X}^{(17,9)}; \quad \boldsymbol{Z}^{(18,9)} = \boldsymbol{X}^{(18,9)}; \\
&\boldsymbol{Z}^{(19,13)} = \boldsymbol{X}^{(19,13)}. \qquad (15)
\end{aligned}$$

The nodes 1–8 in Fig. 6(b) correspond to the activities at which sequences branch or converge. For this system they are activities 1, 2, 3, 7, 9, 13, 15 and 20. Nodal activities are represented by the same function $\boldsymbol{X}$. The properties of material k are calculated at any node in the system by propagating the vector α_k along a particular route leading to the node. For instance, passing material $k = 1$ from cradle to grave along the route $\boldsymbol{Z}^{(4,1)} \to \boldsymbol{Z}^{(8,7)} \to \boldsymbol{Z}^{(12,9)} \to \boldsymbol{Z}^{(19,13)}$ which is from "obtain material 1" to "landfill" in Fig. 4, or equivalently from activity 1 to activity 20 in Fig. 6(a), would require the evaluation of the expression:

$$\alpha_1^{(20)} = \boldsymbol{X}_1^{(20,19)}(\boldsymbol{Z}_1^{(19,13)}(\boldsymbol{X}_1^{(13,12)}(\boldsymbol{Z}_1^{(12,9)}(\boldsymbol{X}_1^{(9,8)}(\boldsymbol{Z}_1^{(8,7)}(\boldsymbol{X}_1^{(7,4)}(\boldsymbol{Z}_1^{(4,1)}(\boldsymbol{X}_1^{(1,0)}(\alpha_1^{(0)}))))))))). \quad (16)$$

This expression quantifies the technical properties of material k entering the landfill site, the total environmental burdens and/or impacts leading up to landfilling, and the costs involved with processing the material up to its end of life.

Another route for material 1 through the system might include a single pass around the recycle loop $\boldsymbol{Z}^{(14,13)} \rightarrow \boldsymbol{Z}^{(16,15)}$ (see Fig. 6(b)) before landfill ($\boldsymbol{X}^{(20,19)}$), i.e.,

$$\alpha_1^{(20)} = \boldsymbol{Y}_1(\alpha_1^{(1)}), \tag{17}$$

where the symbol $\boldsymbol{Y}_1$ has been introduced to represent the sequence that material 1 has passed through, i.e.,

$$\begin{aligned}\boldsymbol{Y}_1 = {} & \boldsymbol{X}_1^{(20,19)} \circ \boldsymbol{Z}_1^{(19,13)} \circ \boldsymbol{X}_1^{(13,12)} \circ \boldsymbol{Z}_1^{(12,9)} \circ \boldsymbol{X}_1^{(9,8)} \\ & \circ \boldsymbol{Z}_1^{(8,7)} \circ \boldsymbol{X}_1^{(7,16)} \circ \boldsymbol{Z}_1^{(16,15)} \\ & \circ \boldsymbol{X}_1^{(15,14)} \circ \boldsymbol{Z}_1^{(14,13)} \circ \boldsymbol{X}_1^{(13,12)} \circ \boldsymbol{Z}_1^{(12,9)} \circ \boldsymbol{X}_1^{(9,8)} \circ \boldsymbol{Z}_1^{(8,7)} \\ & \circ \boldsymbol{X}_1^{(7,4)} \circ \boldsymbol{Z}_1^{(4,1)} \circ \boldsymbol{X}_1^{(1,0)}.\end{aligned} \tag{18}$$

Using the sequence relations exemplified by Eq. (14), another map may be produced for this process. It will be significantly more compact than the one defined by Eq. (11), with order equal to the number of nodes in the system N, but has properties and significance exactly parallel to $\mathbf{P}_k$. Its elements, $q_{\eta\lambda}$ (where $\eta, \lambda = 1, 2, \ldots, N$) are computed according to the rule:

$$q_{\eta\lambda} = \begin{cases} 0 & \text{if } n_\eta \text{ does not connect to } n_\lambda, \\ 1 & \text{if } n_\eta \text{ connects to } n_\lambda, \end{cases} \tag{19}$$

where "connect" implies the forward direction only. For the example shown in Fig. 6(b) this matrix would be

$$\mathbf{Q} = \begin{bmatrix} 0&0&0&1&0&0&0&0 \\ 0&0&0&0&1&0&0&0 \\ 0&0&0&0&1&0&0&0 \\ 0&0&0&0&1&0&0&0 \\ 0&0&0&0&0&1&1&1 \\ 0&0&0&0&0&0&1&1 \\ 0&0&0&1&0&0&0&0 \\ 0&0&0&0&0&0&0&0 \end{bmatrix}. \tag{20}$$

The 8×8 matrix $\mathbf{Q}$ represents an irreducible representation of the network describing the system shown in Figs. 4 and 6(a). At the other extreme, Eq. (11) describes the most expanded form of the system, i.e. a matrix of dimensions 20×20; this is exactly the representation in Fig. 6(a), where each transformation corresponds to one activity only. There are of course many other intermediate representations, so that sequences and nodes may be defined in any appropriate way. A representation with particular practical value has the "use" activities as nodes.

3.2. Material acceptance criteria

The CHAMP methodology includes a way of selecting materials which meet criteria defining acceptability for a use or for a process, and for routing a material to other activities if it does not meet the acceptance criteria. This feature is essential to enable the model to be used to explore possible industrial ecologies. The acceptance criteria are most commonly technical, as expressed by the set of utilities describing a material at any point in its life, but they may also apply to cost and environmental performance. All three types of acceptance criteria are included in the methodology.

Selection criteria can be applied at entrance to or exit from an activity, as shown schematically in Fig. 7. A material gains 'admission' to the activity provided its characteristics match the criteria applied by the entrance gate; this enables the material to be directed to the next most appropriate activity if the criteria are not met. An exit gate acts as a quality control function where this is required, and may also be used to direct the flow towards the next appropriate and compatible activity. In their simplest form, acceptance criteria are specified as a range of values within which the relevant material characteristics must lie, i.e. the material must meet criteria of the form:

$$A_{1,hk} \leqslant \alpha_{hk} \leqslant A_{2,hk}. \tag{21}$$

If property α_{hk} is not critical, the upper and lower acceptance bounds are set to arbitrarily high and low values.

Fig. 5 illustrates this kind of acceptance criterion. Only material whose properties or geographical location lies within the prescribed region is admitted to the activity. The properties of the material leaving activity v must lie within a different acceptable region; this may be expressed through an exit gate from activity v which fixes processing conditions or transport distance, or the region may represent entrance criteria for the next activity in the sequence. Acceptance criteria may be more complex than the form of Eq. (21), represented for example by the shaded region in Fig. 5.

Acceptance criteria can apply to all the materials making up a component or product, and to the total material flow M. Fig. 8 illustrates the operation of an acceptance gate for a set of materials. Different materials are represented by columns and their characteristics by rows. The first set of grids represents the characteristics of the material flow, and the second the acceptance criteria for the gate. The third set of grids represents the match of characteristics to criteria: a fully black grid indicates complete compatibility, with white elements indicating a mis-match between material characteristics and acceptance criteria. In the hypothetical case in Fig. 8, the set of materials is too expensive in two of the cost headings. It is then open to the user of the model to relax these criteria if appropriate, accepting the materials as meeting technical and environmental performance criteria notwithstanding the cost.

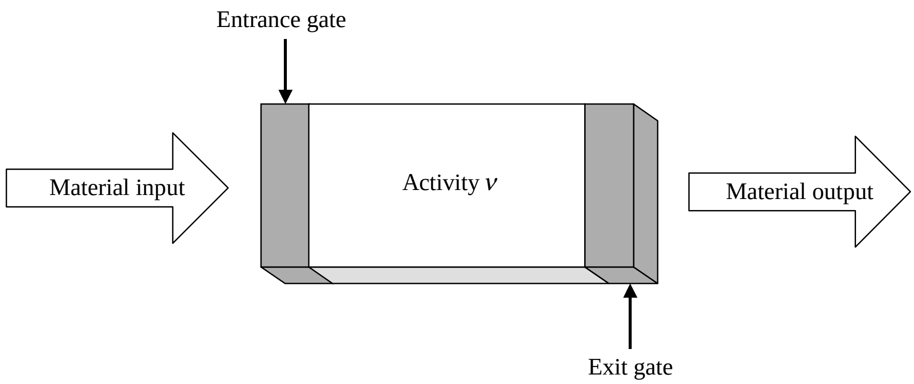

Fig. 7. Material flow through an activity where the acceptance criteria are met.

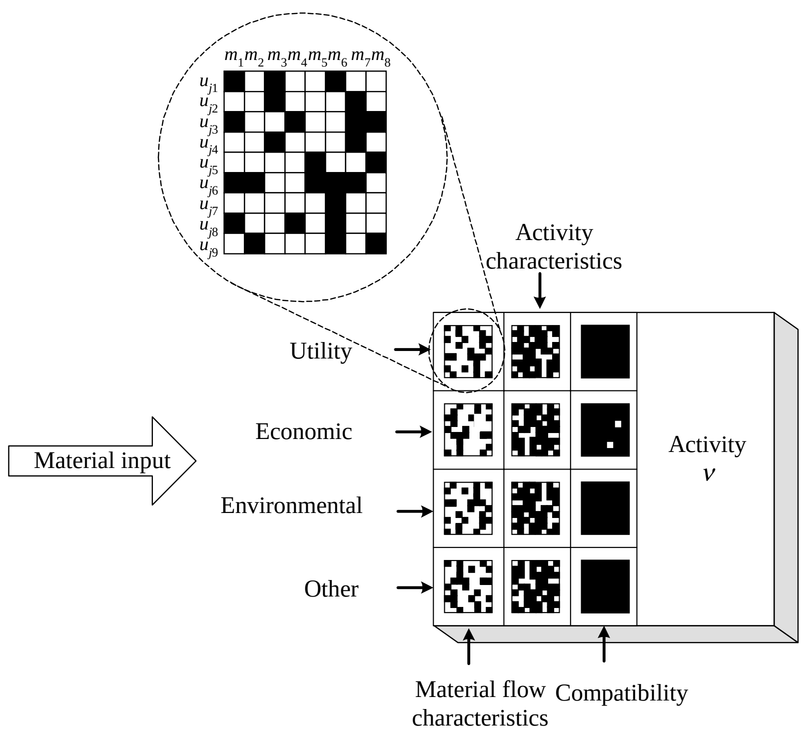

Fig. 8. Acceptance criteria applied to a group of different materials.

To simplify the treatment of "hard" criteria like Eq. (21), a Boolean matrix is formulated to summarise satisfactory (1) and unsatisfactory (0) matches. "Soft" interpretation, as in the example of Fig. 8, is facilitated by introducing parameters which express the relative deviation of a parameter from the strict acceptance criteria:

$$\delta_{1,hk} = (\alpha_{hk} - A_{1,hk})/A_{1,hk}, \tag{22}$$

$$\delta_{2,hk} = (A_{2,hk} - \alpha_{hk})/A_{2,hk}. \tag{23}$$

If both these parameters are positive, then the material meets the acceptance criteria and the Boolean parameter is set to 1. The total deviation from strict acceptance criteria for one activity is calculated as the sum over the different properties ($h = 1, 2, \ldots, H$) of the negative values of δ_{hk}. This sum can be accumulated amongst activities along the path of the material to show how far it departs from the ideal technical, economic and environmental performance criteria. Comparison or ranking of the accumulated relative deviations helps selection of the most appropriate materials for a given application, and of the most suitable successive applications for a given material.

3.3. *Application to decision-support*

The approach taken in the CHAMP model is to treat selection of materials, activities and applications as a multiple criteria decision problem, in the class of problems where the decision-maker selects between options on the basis of trading-off different performance objectives. Thus CHAMP is an example of a *generating method*: it presents a discrete or continuous set of options each of which is optimal in the Pareto sense; i.e. it is impossible to improve any one objective without worsening at least one other objective (Cohon, 1978; Stewart, 1992; Yoon & Ching, 1995). This approach is preferred over reducing the different criteria to a single metric, as for example in cost/benefit analysis, which may be appropriate for more limited decisions but which obscures information which may inform more strategic decisions of the kind for which CHAMP is relevant (RCEP, 1998; Clift, 1999). It represents a further application of a multi-objective approach which has been developed for process selection, design and optimisation (Azapagic, 1999; Azapagic & Clift, 1999d; Clift & Azapagic, 1999).

Fig. 9 shows schematically the way in which the different components of the CHAMP approach are combined to provide the information needed for multi-attribute decision support. Databases of material and process costs, life cycle environmental burdens and impacts and technical properties and performance (i.e. utilities) are needed to provide quantitative information. Processes and logistic operations are treated separately although, as explained above, there is a common modelling framework so that they can be combined within the CHAMP methodology. Separating processes and logistics in this way enables any activity to be optimised within itself, to select the route to be taken between the input and output utility parameters. This is particularly useful in the case of logistics (and especially reverse logistics) because it enables standard route-scheduling packages to be used in the logistics algorithm. The LCA algorithm combines a database for Background activities with appropriate models for the Foreground activities as outlined in Sections 1.2 and 2.4 above. As in the whole-system modelling approach to conventional LCA, standard multi-objective optimisation (e.g. Cohon, 1978; Azapagic, 1999; Azapagic & Clift, 1999d) generates the set of Pareto-optimal solutions on which the decision is based.

4. CHAMP application: an example

Application of the CHAMP methodology will now be illustrated for the relatively simple system introduced in Figs. 4 and 6: plastic bottles acting as water containers. This system is chosen to demonstrate how CHAMP uses economic, environmental and utility constraints to identify feasible routings and cascades of use for materials and products.

The functional unit was defined in Section 2.1 as packaging 1 m^3 of water in 1000 bottles of 1 l. Three materials are necessary to produce the 1000 water bottles: materials A, B and C whose quantities entering the "use" phase (activity 11) are 47, 2 and 1 kg, respectively. Each material is transported to the manufacturing site (activity 9) by three different transportation methods, denoted by T; these are activities 4, 5 and 6 in Fig. 6. The materials are combined to form bottles—for example, HDPE (A) bottles with PP (B) caps and paper (C) labels—which are transported to the use phase. After use, the empty bottles are collected and sent to a disassembly point (activity 13) where the labels and caps are separated from the bottles and sent to landfill. The bottles themselves are sent for reprocessing (activity 15); they are blended with virgin material before being used again for bottle production. Reprocessing of production waste is also possible. Both production waste and post-use waste can also be sent to landfill.

4.1. Materials and utilities

In the CHAMP methodology, the total flow through the system would be represented as in Eq. (1) by:

$$M = \{\text{HDPE}, \text{PP}, \text{Paper}, \text{Product}\}$$

or equivalently,

$$M = \{m_A, m_B, m_C, m_D\}. \tag{1'}$$

For any individual stream within the system, some elements of M may be zero. Thus $m_B = m_C = m_D = 0$ represents HDPE, while $m_A = m_B = m_C = 0$ for complete bottles with no single uncombined material; the quantities of elements of M change on passage through "Water Bottle Manufacture" (activity 9) and "Disassembly" (activity 13).

Each of the elements of M (including the zeros representing materials incorporated into a product) is characterised by a set of properties or characteristics which can be represented as a vector; four utility vectors are therefore necessary to describe the materials in the system. For each individual material to be suitable for use in the water bottle, its characteristics must meet the criteria for acceptance into the activity. These criteria define the critical utilities, and hence contribute to defining the utility vector and the material changes to be described by the model.

The utility constraints on the system in this example are taken as

- optical transparency of the HDPE bottle must be $\geqslant 75\%$;
- haze of the HDPE bottle must be $\leqslant 0.8\%$;
- quantity of material for recycling must be $\geqslant 5$ kg;
- tensile strength of the PP cap $\geqslant 25$ MPa;
- tear strength of the label $\geqslant 20$ N/mm.

For purposes of illustration, haze and optical transparency are taken to depend on contamination as shown in Fig. 10. Other utilities can be modelled in addition at the discretion of the operator. The utility vectors in this example include only the above parameters plus the level of contamination by 'foreign' material, and are thus formulated as

$$\boldsymbol{u}_A = (\text{haze}, \text{contamination level}, \text{optical transparency}, 0, 0, \text{mass}),$$

$$\boldsymbol{u}_B = (0, 0, 0, \text{tensile strength}, 0, \text{mass}),$$

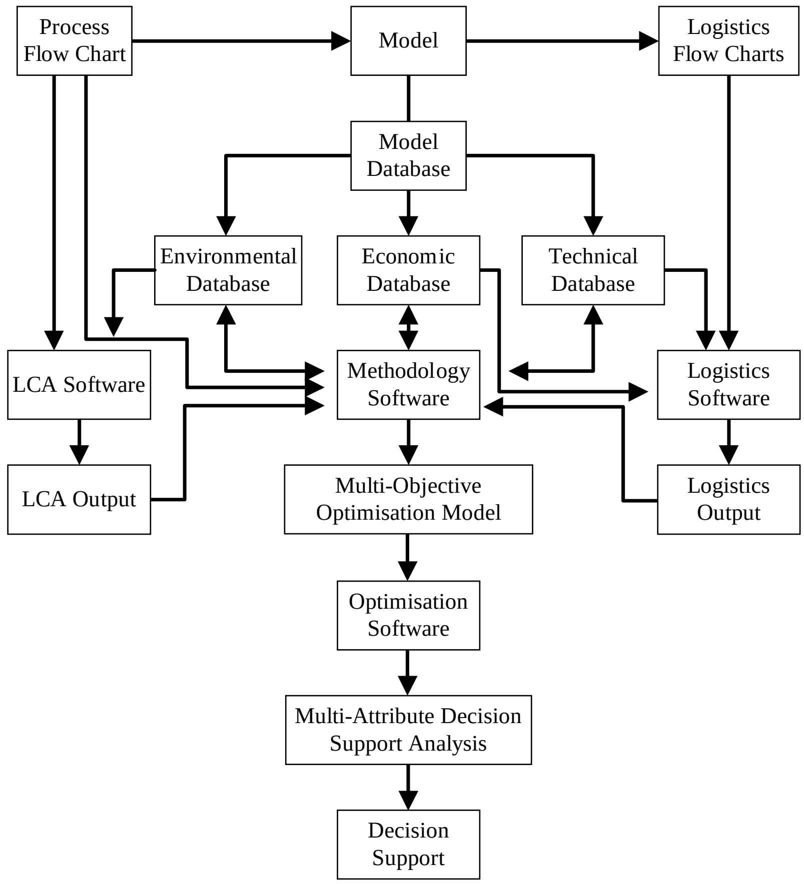

Fig. 9. CHAMP implementation—from model definition to decision support.

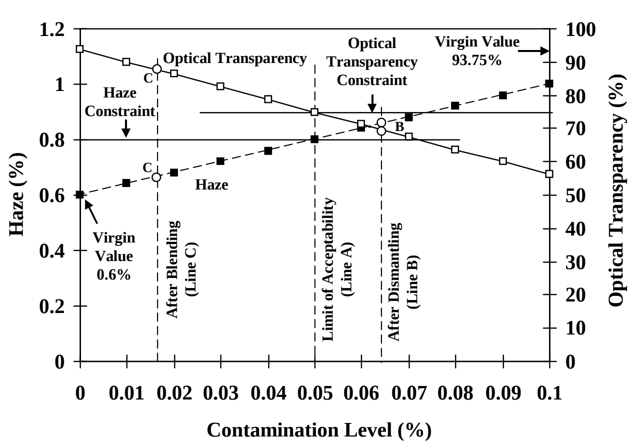

Fig. 10. Changes in Haze and Optical Transparency due to the Level of Contamination.

$$\boldsymbol{u}_C = (0, 0, 0, 0, \text{tear strength}, \text{mass}),$$

$$\boldsymbol{u}_D = (\text{haze}, \text{contamination level}, \text{optical transparency},$$
$$\text{tensile strength}, \text{tear strength}, \text{mass}).$$

To illustrate application of the gate-selection approach, it is also assumed to be uneconomic to recover and recycle less than 5 kg of any material per functional unit.

4.2. Economic costs

Economic costs are modelled as outlined in Section 2.4 above. The specific cost elements modelled can again be based on constraints of the system, or include other costs which the operator wants to model. In this example, the market price is taken as £300 per 1000 bottles. The economic constraint on the system in this example is:

- the market price of the water bottle must be greater than the total cost of production.

All costs incurred during the production of the water bottle must be included in the economic vector. For this illustration, only three of these costs have been considered: materials (1), energy (2) and transportation (3). For material A, HDPE (m_A), the economic vector associated with activity 1 (i.e. purchase of the material) would therefore be represented by

$$\boldsymbol{c}_A^1 = (\text{material cost}, \text{energy cost}, \text{transport cost})$$

or equivalently

$$\boldsymbol{c}_A^1 = (c_{1A}^1, c_{2A}^1, c_{3A}^1), \tag{3'}$$

where $\boldsymbol{c}_A^1$ is the cost of the raw polymer purchased into the system and $\boldsymbol{c}_{2A}^1 = \boldsymbol{c}_{3A}^1 = 0$. As the material passes through each successive activity, the economic vector is incremented by the components of cost associated with that activity, as in Eq. (4) or Eq. (5). Economic vectors for the polypropylene cap, paper label and the complete water bottle are developed in the same way, to give the total costs associated with the system.

4.3. Environmental burdens and impacts

In this example, one environmental constraint has been placed on the system: it has been assumed that total NO_x emissions for the blow moulding of 1000 water bottles must not exceed a compliance limit of 120 g. Consequently the quantity of NO_x emitted must be considered; it is represented as element 1 in the environmental vector. Other burdens can also be modelled; as an illustration SO_x emissions are also considered as burden 2 for material A, HDPE (m_A). The burdens are represented as environmental vectors as defined by Eq. (6). For activity 1 (raw material supply), they take the form:

$$\boldsymbol{b}_A^1 = (\mathrm{NO}_x, \mathrm{SO}_x)$$

or equivalently

$$\boldsymbol{b}_A^1 = (b_{1A}^1, b_{2A}^1) \tag{6'}$$

and represent the "background" burdens associated with polymer production (see Section 2.2). As with the economic costs, the environmental burdens are accumulated along the sequence of activities as in Eq. (7).

4.4. Analysis of the first life cycle

This example assumes that, in the first life cycle, the 1000 bottles are produced from virgin materials only, so that the ratio of virgin material to recyclate in activity 7 is 100:0. Fig. 6(b) shows that Material A passes through the sequence represented by $Z^{(4,1)}$ and $Z^{(8,7)}$, Material B passes through the sequence $Z^{(5,2)}$ and Material C passes through the sequence $Z^{(6,3)}$. At activity 9 (Fig. 6(a)) and equivalently at node n_5 (Fig. 6(b)) these three materials are aggregated together to form the water bottle product.

The properties of the three components at input to the system (i.e. as they leave activities 1, 2, and 3) are:

$$\boldsymbol{u}_A = (\text{haze } 0.6\%, \text{contamination level } 0\%,$$
$$\text{optical transparency } 93.75\%, 0, 0, \text{mass } 47 \text{ kg}),$$

$$\boldsymbol{u}_B = (0, 0, 0, \text{tensile strength } 30 \text{ MPa}, 0, \text{mass } 2 \text{ kg}),$$

$$\boldsymbol{u}_C = (0, 0, 0, 0, \text{tear strength } 22 \text{ N/mm}, \text{mass } 1 \text{ kg}).$$

To ensure the materials are suitable, the CHAMP method compares the material properties with the process requirements as outlined in Section 3.2 above. The properties of the three material inputs are within the utility constraints listed earlier, and they are consequently deemed fit for purpose. This step represents quality assurance of new material supply.

Table 1
Costs associated with the product as it passes from cradle to gate (per functional unit)

	Activity	Costs (£)	$\sum$ Costs (£)
1	HDPE production	79.90	79.90
4 and 8	Transport of HDPE	0.85	80.75
2	PP production	3.00	83.75
5	Transport of PP	0.36	84.11
3	Paper production	0.60	84.71
6	Transport of paper	0.20	84.91
9	Water bottle manufacture	4.31	89.22

Changes in polymer properties can occur as a result of many different processing and environmental effects. In this example, it is assumed that sufficient anti-oxidant has been added to the HDPE to prevent degradation during the moulding of the bottle and cap (activity 9). It is also assumed that because of the relatively short shelf-life of the products—several months—no significant UV degradation occurs. As a consequence, the utility vectors remain constant throughout use (activity 11). The utilities considered in this example also remain constant as the materials and product are transported around the system, because location has not been included as a utility in this simple example. However, costs and environmental impacts associated with transport are included.

Table 1 summarises the costs associated with the activities making up the system, up to water bottle manufacture (activity 9): costs for materials, transport and energy up to this point total £89.22. This easily satisfies the economic constraint that the total production cost must be less than the market price, taken as £300.

Table 2 illustrates how CHAMP tracks the burdens and impacts of materials as they flow through the system, enabling them to be readily determined at any point in the life cycle. Table 2 lists the NO_x formation from each activity and the associated acidification potential. Total NO_x emissions from the production of 1000 water bottles from virgin HDPE is therefore 652 g, equivalent to an acidification impact of 14.2 g eq. H+. It is clear from this assessment that the water bottle production activity which creates 115 g of NO_x is within the compliance limit of < 120 g of NO_x and consequently is suitable for use in this particular scenario. However NO_x emissions from the whole product system are much larger, mainly arising from HDPE production.

4.5. Cascaded use of materials

During disassembly (activity 13), the bottle is disaggregated into its components: label, cap, and bottle. If the materials are to be recovered, the constraints in force must continue to be met. Maximum efficiency for this activity would result in the mass utilities (i.e. quantity of each material) for the label, cap, and bottle being 1, 2 and 47 kg

Table 2
Cumulative NO_x formation from cradle to gate and resulting acidification potential

	Activity	NO_x (g)	Cumulative NO_x (g)	g eq. H+	Cumulative g eq. H+
1	HDPE production	517	517	11.24	11.24
4 and 8	Transport of HDPE	4.6	521.6	0.1	11.34
2	PP production	10.0	531.6	0.22	11.56
5	Transport of PP	0.2	531.8	0.004	11.56
3	Paper production	4.8	536.6	0.1	11.66
6	Transport of paper	0.1	536.7	0.002	11.67
9	Production of the water bottle	115.0	651.7	2.5	14.17

Table 3
Changes in the HDPE bottle component utility values after use

	HDPE leaving activity	Haze (%)	Contamination level (%)	Optical transparency (%)
11	Use	0.600	0	93.75
12	Transport to disassembly	0.600	0	93.75
13	Disassembly	0.856	0.064	69.75
14	Transport to reprocessing	0.856	0.064	69.75
15	Reprocessing	0.856	0.064	69.75
16	Transport to blending	0.856	0.064	69.75
7	Blending	0.664	0.016	87.75
8	Transport to bottle manufacture	0.664	0.016	87.75

respectively. The constraint which states that 5 kg of material is necessary for recycling to be economic means that the cap and paper are not suitable for recycling. Only the HDPE meets the recycling requirements and is allowed by the model to be transported to the reprocessing activity.

It is assumed that the efficiency of the disassembly activity is such that out of every 1000 bottles processed, 10 bottles pass through the activity unchanged. The associated PP and paper (materials B and C) represent contamination of the HDPE (material A) to the level of 0.064%. This and the other utilities for the recovered HDPE are listed in Table 3.

Reprocessing (activity 15) granulates the HDPE so that it is in a form which can easily be blended with virgin material. It is assumed here that the anti-oxidant used for original bottle processing is sufficient to stop any further material degradation and therefore the utility vector remains constant as it passes through this process.

Water bottle manufacture (activity 9) will only accept material whose utilities meet the criteria set out in Section 4.1. Contamination affects haze and optical transparency (see Fig. 10). It is assumed for illustration that a contamination level of 0.05% results in haze of 0.8% and optical transparency of 75%, at the limits of acceptability (Line A); to the right of this line the criteria do not satisfy the utility constraints. It is also assumed that an increase of 0.1% in the contamination level will result in a 5% increase in haze and a 5% reduction in optical transparency. The contamination level of 0.064% (Line B) therefore results in haze being increased to 0.856% and the optical transparency reduced to 69.75% (points B). The values of these utilities are beyond the limit of acceptability, meaning that in its current state the polymer does not meet the requirements for water bottle manufacture.

In order to improve the level of contamination and thus the haze and optical transparency of the polymer, blending of the recyclate with virgin polymer (activity 7) is carried out in the ratio of 75% virgin/25% recyclate. At this ratio (Line C) the haze and optical transparency values become 0.664% and 87.75%, respectively (points C) which are within the performance constraints. Consequently, with appropriate blending the polymer material can be sure to be suitable for re-use in the same application. In a practical application, different proportions in the blend would be explored.

Subsequent use cycles can also be modelled up to the final state in which all flows around the system are blended to steady composition. Given that this form of the model neglects "stocks" of material in the system, each use cycle is treated as being at steady state (see Section 1.1). For a simple recycle system like Fig. 4, which is representative of most industrial ecologies, the system converges monotonically towards the final state.

5. Real applications

The sample example in Section 4 provides an illustration of how the CHAMP methodology is applied. The methodology has already been applied to a number of real systems for material recovery, re-use and recycling. These applications include material selection, for polymer interlayers in laminated glass windscreens, the jackets of telecommunications cables and optical fibre cables; in the last case, the analysis led to the development of a new cable configuration. It has also been applied to selecting recycle and re-use options for the casings of office equipment. Applications deploying the ability of CHAMP to handle distribution and collection logistics include optimal scheduling of systems for delivery, collection and refilling of toner bottles, and the recovery of municipal and commercial waste from a defined geographical area.

In the applications to material selection and recovery and to product design, the driver for the users arose from impending legislation on Extended Producer Responsibility, particularly on measures flowing from European Commission Directives on the "take-back" of used products (see Section 1.1). By applying the CHAMP approach, the users were able to identify opportunities for cost reduction along with environmental improvements including waste minimisation and extended product lifetime. Thus CHAMP helps to achieve the increase in resource productivity and reductions in environmental impact which Extended Producer Responsibility is intended to promote.

The real applications have also illustrated the need to evaluate and compare the technical, economic and environmental performance of different materials, using some form of multi-attribute decision analysis. They have confirmed that system approaches like CHAMP, based on extended life cycle assessment, can present information in a way which supports this kind of decision.

Although CHAMP was developed specifically for polymeric materials, the general approach is applicable to other materials, products and processes. It is now being applied to two important metals: steel and aluminium. The industrial ecologies for these materials differ from the plastic artefacts considered in the present paper in having long service lives. This means that the "stocks" of materials in the economy are important, so that it is necessary to include time-dependency in the model (Davis, Geyer, Clift, Jackson, & Azapagic, 2002). The work on metals has emphasised the importance of the variation over time of supply and demand for recovered materials. This feature was already evident in some of the applications to plastics, highlighting the importance of developing recyclate "pools" to store recovered material and give quality assurance pending re-use of the material in the original or a different application.

6. Conclusions

A new methodology has been developed to model the flow of materials and products through a succession of uses with different performance requirements. The CHAMP model is based on a life cycle approach, but goes beyond conventional applications of Life Cycle Assessment in considering multiple use phases by describing material recovery, re-use and recycling. The model serves to generate the set of Pareto-optimal choices needed to support multi-attribute decisions in which technical, economic and environmental performance must all be considered. In this way, it can help the practical evolution of "take-back" and Extended Producer Responsibility. Although designed specifically for polymeric materials, the approach is applicable to other materials, processes and products, so that CHAMP provides a general tool for modelling of industrial ecology systems.

Notation

(Note: In these definitions, "material" is used in the general case of denoting a single material or a component or a product).

$A_{1,hk}$	lower acceptance bound on property h for material k
$A_{2,hk}$	upper acceptance bound on property h for material k
$b_{ik}^{(v)}$	environmental burden i per functional unit of putting material k through process or activity v
$\boldsymbol{b}$	set of environmental burdens
$\boldsymbol{b}_k^{(v)}$	set of environmental burdens per functional unit of putting material k through process or activity v
$B_{ik}^{(v)}$	accumulated environmental burden i associated with material k leaving process or activity v
$\boldsymbol{B}_k^{(v)}$	Set of accumulated environmental burdens associated with material k leaving process or activity v
$c_{lk}^{(v)}$	cost item l per functional unit of putting material k through process or activity v
$\boldsymbol{c}_k^{(v)}$	set of cost items per functional unit of putting material k through process or activity v
$C_{lk}^{(v)}$	accumulated costs in category l for material k leaving activity v
$\boldsymbol{C}_k^{(v)}$	set of accumulated costs for material k leaving activity v
e_j	contribution to environmental impact category j
$\boldsymbol{e}$	set of environmental impacts
$\boldsymbol{e}_k^{(v)}$	set of environmental impacts per functional unit of putting material k through process or activity v
$E_{jk}^{(v)}$	accumulated environmental impact j associated with material k leaving process or activity v
$\boldsymbol{E}_k^{(v)}$	set of accumulated environmental impacts associated with material k entering process or activity v
h	identifier of one utility parameter amongst the H considered
H	total number of utility parameters included in analysis
i	identifier of one element amongst the I in the Inventory Table
I	total number of environmental burdens comprising Inventory Table

j identifier of one impact category amongst the J included
J total number of environmental impact categories considered
k identifier of one material amongst the K present
K total number of materials passing through system
l identifier of one cost heading amongst the L distinguished
L total number of cost headings distinguished
m_k mass flow rate of material, component or product k through the system
M total flow of materials, individually or formed into components or products, emerging from an activity
N total number of nodes used in a network description of a system
$\mathbf{P}_k$ binary matrix summarising the network of routes available to material k
$\mathbf{P}$ matrix summarising the network of routes available to all materials M
$\mathbf{Q}$ binary matrix describing the total material flow network for the system of sequences and nodes
$\boldsymbol{u}_k^{(v)}$ utility vector describing material k leaving activity v
$u_{hk}^{(v)}$ utility number h in vector $\boldsymbol{u}_k^{(v)}$
w_{ij} potency factor for the contribution of burden b_i to environmental impact e_j
$\mathbf{w}$ sparse matrix of potency factors
$\boldsymbol{X}_k^{(v,\mu)}$ set of functions describing the effect of activity v on the utilities $\boldsymbol{u}_k$ of material k passed from activity μ
$X_{hk}^{(v,\mu)}$ function within $\boldsymbol{X}_k^{(v,\mu)}$ representing the effect of activity v on utility u_{hk} of material k passed from activity μ
$\boldsymbol{Y}_k$ function representing a group of sequences and/or activities associated with material k
$\boldsymbol{Z}_k^{(v,\mu)}$ set of functions describing the effect of a sequence of activities on utilities, costs and burdens and/or impacts associated with material k passing from the output of activity μ to output of activity v
$\boldsymbol{\alpha}_k^{(v)}$ set of properties of material k leaving activity v
$\delta_{1,hk}$ relative deviation of material k from lower bound on property h
$\delta_{2,hk}$ relative deviation of material k from upper bound on property h
η, λ identifier of one node amongst the N considered
μ, v number of activity (or process) on the path of a material through the system of G activities
$\circ$ operator denoting the composite of two functions, i.e. for the independent variable x, $f(g(x))$ can be written as $f \circ g$

Acknowledgements

We would like to thank the Engineering and Physical Sciences Research Council (EPSRC) and the Department of Trade and Industry (DTI) for supporting this work as a LINK project under the Waste Minimisation through Recovery, Re-use and Recycling (WMR3) Programme, and also the Energy Technology Support Unit (ETSU) and Environmental Technology Best Practice Programme (ETBPP) for their assistance in managing the project. We would also like to thank our partners in the LINK project for their constructive input: Biffa, Brand-Rex, Corning Cables, European Vinyls Corporation, Mann, Pilkington and Xerox.

Appendix A. Aggregation of resource consumptions and emissions into environmental impacts

In the Inventory phase of a Life Cycle Assessment, the entire supply chain supporting a product, process or service is analysed to identify and quantify the primary resource

Table 4
Environmental impact categories used in life cycle impact assessment (Heijungs, 1992; Guinée, Heijungs, Udo de Haes, & Huppes, 1993; Lindfors et al., 1995; Udo de Haes, 1996; Clift, 2001)

Impact category	description
Abiotic depletion potential	Extraction of non-renewable raw materials such as ores.
Energy depletion potential	Extraction of non-renewable energy carriers; can be included in abiotic depletion potential.
Global warming potential	Contribution to atmospheric absorption of infrared radiation leading to increase in global temperature.
Ozone depletion potential	Contribution to depletion of stratospheric ozone, leading to increase in ultraviolet radiation reaching earth's surface.
Human toxicity	Contribution to human health problems through exposure to toxic substances via air, water or soil (especially through the food chain).
Aquatic/terrestrial ecotoxicity	Contribution to health problems in flora and fauna caused by exposure to toxic substances.
Acidification	Contribution to acid deposition onto soil and into water.
Photochemical oxidant creation	Contribution to formation of tropospheric ozone.
Nutrification potential	Contribution to reduction of oxygen concentration in water (or soil) through providing nutrients which increase production of biomass.

inputs and environmental emissions per functional unit. These inputs and emissions constitute the environmental burdens, denoted here as b_i ($i = 1, \ldots, I$). To reduce this body of detailed numerical data to a comprehensible and manageable size, the burdens are aggregated in terms of their contributions to a set of recognised environmental impacts; the set most commonly used in Life Cycle Impact Assessment is summarised in Table 4.

The potential contribution of burden i to impact category j is expressed by its potency factor w_{ij} relative to same reference species. For example, for the specific category of global warming (see Table 4) the factors are expressed as the mass of carbon dioxide with the same greenhouse warming potential (GWP) integrated over some appropriate time period, for example 100 years. Thus the effects of all emissions which contribute to global warming are aggregated as an equivalent mass of carbon dioxide. The contribution of the set of burdens to impact category j is then given by

$$e_j = \sum_{i=1}^{i=I} w_{ij} b_i. \tag{A.1}$$

The vector of impacts is then

$$\boldsymbol{e} = \mathbf{w} \cdot \boldsymbol{b}, \tag{A.2}$$

where $\boldsymbol{e}$ is the vector of impacts, $\boldsymbol{b}$ the vector of burdens, and $\mathbf{w}$ is the (sparse) matrix of potency factors.

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