Working Paper

LIFE-CYCLE ANALYSIS

IDEA
AN INTERNATIONAL DATABASE
FOR ECOPROFILE ANALYSIS

A Tool for Decision Makers

*Barbara Lübkert, Yrjö Virtanen, Manfred Mühlberger,
Jyrki Ingman, Bruno Vallance and Sebastian Alber*

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⊞IIASA

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Preface

Environmental impacts of products and production processes are receiving increasing social attention. In searching for solutions with less impacts, there is a need for comparing competing products with regard to their life-cycle demands for raw-materials and energy as well as their emissions to the environment. It is however necessary to consider the entire systems, because decreased emissions in one part can easily increase the emissions in another part of the system.

IIASA has developed a methodology and database for life-cycle analysis of products and production processes. Data for more than 1000 so-called unit processes of the industrial sectors pulp and paper, steel, aluminum, petrochemicals, plastics, inorganic chemicals, glass, energy conversion, transportation and waste management is currently stored in the database.

The model and database is intended to support analysis of the impacts of products and production processes. Examples of possible applications are:

- comparison of the environmental impacts of different stages of the production cycle, eg. basic materials, processing, fabrication, packaging and shipping;
- comparison of two competing products with respect to their direct and indirect environmental impacts;
- comparison of alternative production processes for the same product.

The assessment can be performed at any level of aggregation, from a single factory to regional or national averages. The results can be used for targeting improvements of the production processes, for assessing the impact of new regulation or to support international negotiations on environmental protection.

Results from calculations indicate the importance of considering the whole life-cycle of a product. At the same time it is necessary to build "transparency" both into the models and the data used. Possible disagreements in results have to be traceable back to the specific assumptions made.

A deliberate effort was made to make the model and the database "user friendly", to make it possible for a person with a background in production to understand the assumptions without excessive effort. The model and database have been built in the dBASE IV database program to make it easily transportable and expandable.

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Summary

This report documents IIASA's work in the field of life-cycle analysis (LCA) between February 1990 and May 1991. During this time, the LCA Project developed a database and materials and energy flow model which can be used to quantify the cumulative energy-, material- and environmental impacts of consumer products. Since beverage packaging systems constitute a good example of consumer goods for comprehensive life-cycle analysis and since they are discussed frequently by policy makers, the project chose beverage containers of different materials and sizes as examples for which to create the relevant database. It should be noted though, that the purpose of the study was not to furnish results of the life-cycle impacts of beverage containers, which are already amply available in the literature, but to supply a transparent database to those who want to carry out their own LCA studies. As a result, a tool was created - IDEA, consisting of the database, the flow model and a scenario creation option, intended to help policy makers compare alternative products for their environmental friendliness or harmfulness.

The present document describes IDEA in detail. The report is divided into two parts:
(1) Theory,
(2) Technical Annex.
The first part starts with a short discussion of life-cycle analysis, its uses, advantages and limitations. It then describes the structure, content and use of the database; the following section discusses the theoretical background and potential uses of the materials and energy model, and the last section outlines the various options of generating scenarios. The second part describes all data presently contained in the database; it gives, in particular, the sources of the raw data and details their derivation for use in IDEA. This part is divided into 11 sections, each dealing with one of the following economic sectors:

(1)   fuel and minerals mining,
(2)   energy conversion,
(3)   goods transportation,
(4)   inorganic chemicals production,
(5)   organic chemicals production,
(6)   glass production,
(7)   pulp and paper production,
(8)   aluminum production,
(9)   iron & steel production,
(10) beverage container manufacture,
(11) waste management & recycling.

Due to the large amount of data gathered for the evaluation of beverage containers, the IDEA database constitutes a good basis for life-cycle analyses of other products. In some cases, the present database may already be adequate, in others, some new processes and/or economic sectors may have to be added.

The present report does not include an evaluation of results from any life-cycle study made with IDEA; it is rather intended as the technical background document for the various studies. IDEA has so far been used to compute the cumulative impacts of several beverage container systems, different grades of paper, as well as raw aluminum and steel. The model was applied in the joint study between IIASA and the Austrian Association for Agrigultural Research on "World Trade and Environment"; The forthcoming publication from this study includes a description of results as well as the IDEA system (Schmidt-Bleek and Wohlmeyer, forthcoming). Other results are given in Virtanen and Lübkert (forthcoming).

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Technical Annex

Life-Cycle Analysis -- Its Use, Advantages and Limitations

The principle of life-cycle analysis implies that products, activities, or even entire economic sectors are analyzed from an end-use perspective. Contrary to the more traditional assessment of environmental impacts from industrial installations or sectors, the life-cycle approach allows the quantification of the cumulative impacts that a product generates from the point onwards where materials and energies for this product are extracted from the earth, up to either a certain point in the product's life-cycle, or in the most complete case, the final disposal of the remaining wastes back into the earth.

Life-cycle analysis is therefore based on comprehensive inventorying of the various cumulative environmental impacts, which has its roots as far back as the early 1960's. At the World Energy Conference in 1963, Harold Smith published a report on the cumulative energy requirements for the production of chemical intermediates. In the late 1960's and early 1970's, several researchers undertook global modeling studies in which they attempted to predict how changes in population would affect the world's total mineral and energy resources (e.g., Meadows et al., 1972; Mesarovic and Pestel, 1974). Around the period of the major world oil crises in the mid- and late 1970's, the United States commissioned about a dozen major "fuel cycle" studies to estimate costs and benefits of alternative energy systems. Later similar studies were commissioned by both the US and British governments on a wide range of industrial systems. In 1985, the Commission of the European Communities introduced a "Liquid Food Container Directive" (CEC, 1985) which charged countries with monitoring the raw material and energy consumption as well as the amounts of solid waste generated. As concern increased about global air and water pollution problems, these emissions were then also routinely added to energy, raw material and solid waste considerations.

Among the initial and/or more well-known studies on comprehensive life-cycle analyses of products are those by Ayres et al. (1974), Barber et al. (1977a & b), Franklin Associates Ltd. (1985), Sellers and Jere (1989), and the US EPA (1972) in the United States, and by Bojkow (1989), Boustead (1989), Boustead and Hancock (1979), Franke (1984), Kindler and Nikles (1979 & 1980), Lundholm and Sundström (1985 & 1986), Thalmann and Humbel (1985a & b), and UBA (1988) in Europe. Most recently, two workshops were held to review the European and North American activities in this field, one in Smugglers Notch, Vermont, the other one in Leuven, Belgium. The proceedings from these workshops give probably the best and most up-to-date overview of research on life-cycle analysis (Society of Environmental Toxicology and Chemistry and SETAC Foundation for Environmental Education, Inc., 1991; IMSA and IPRE, 1990).

In order to carry out a life-cycle analysis, the product to be evaluated needs to be analyzed for all production-, use- or consumption-, transportation and final disposal steps that it undergoes. Backwards from the desired output, all material and energy inputs into, and outputs from, each of these steps have to be quantified. With the help of an accounting system, one can then calculate the cumulative amounts of all materials, energies and pollutants.

In the first place, *life-cycle analysis is an inventorying method of all material and energy flows*, and generates as results a long list of substances that are
- *produced* by the production system studied, either as *useful products* or as *wastes* discharged to the various environmental media;
- *consumed* by the production system studied, either in *material* or *energy* form.

In order to use these results for policy decisions, these long lists of substances need to be interpreted, and generally reduced to a few numbers. Some researchers consider this step still part of the life-cycle analysis itself, whereas others call this step *ecoprofile analysis*. This can be done by either
- using one or several of the individual substances as *indicator(s)* of the overall impacts;
- *aggregating* these lists *into a few numbers* such as, for example,
  - (a)   total material requirements;
  - (b)   total air emissions;
  - (c)   total water emissions;
  - (d)   total solid waste discharges.

Both methods involve, however, some *value judgement*. In the first case, representative indicators have to be selected; these probably always depend on the goals set out by the person(s) studying the respective production system. If the main objective is, for example, to reduce the amounts of solid waste generated, the representative indicator(s) will be different than if the goal is to limit the release of toxic substances into the environment.

In the second case, different substances have to be added together into one or several still meaningful number(s). This requires value judgement on the comparability of these various substances and on their relative harmfulness to the environment. This is often done by using existing legal limits in order to translate, for example, all air pollutants into a so-called *critical volume of air*, which is the amount of clean air required to assimilate the total quantity of air pollution released into the atmosphere. Note that this is, however, only possible if legal limits exist for *all* pollutants released and if these are *not equal to zero*. Even if these two conditions are fulfilled, the aggregation will probably still be a mixture of legal limits for human health, natural environment and welfare protection.

When talking about life-cycle analysis, it is therefore very important to separate between the two steps of
- (1)   *physical inventorying and quantification of the impacts;*
- (2)   *interpretation of results in order to answer policy questions.*

When referring to life-cycle analysis in the remainder of this report, we mean only the physical inventorying of impacts, whereas by ecoprofile analysis, we mean the interpretation of these results.

1. Use of Life-Cycle Analysis

Life-cycle analyses are used to quantify and compare relative stresses on the environment caused by alternative products or by different production systems and technologies to make the same products. In the same way, the method can be used to compare impacts of entire industries, economic sectors, and even total national economies. The information can then be used in ecoprofile analysis to help answer a number of technical and policy-oriented questions in several areas:

(1)   *Comprehensive environmental impact assessments:*
   •   What are the life-cycle impacts generated by a certain product and how do different products compare?

(2)   *Environmental labels:*
   •   Furnish a quantitative basis for awarding labels for environmentally benign products (eco-labels).

(3)   *Assessment of industrial process efficiencies for a given output:*
      Calculate energy and material usage efficiencies within a given economic sector or activity and identify possible areas of improving the efficiencies.

(4)   *Evaluation of policy alternatives to minimize environmental impacts:*
   •   Assess the impacts of possible alternative environmental regulations through the analysis of different scenarios in order to find the best regulation.

(5)   *Comparison of environmental performance:*
   •   How do different countries compare in their environmental performance in certain economic sectors?

(6)   *International negotiations on environmental policies:*
   •   Assess and compare industrial efficiencies for different geographic regions, or countries, in order to detect margins for savings.

(7)   *Optimization of policies for the eco-restructuring of the economies:*
   •   Supply an important tool that allows to evaluate alternative ways as to how to best restructure a national economy in an environmentally sound way.
   •   Supply an important tool for finding least-cost strategies for optimizing environmental benefits during economic restructuring of, for example, the post-communist countries.

2. Advantages of Life-Cycle Analysis

In the traditional approach of environmental impact analysis, the industries or industrial sectors themselves are usually studied and their impacts are implicitly taken as representative of the products made by these industries. Although in most cases the traditional approach gives a rough indication of the product's impacts, it does not identify all sources of pollution associated with this product and, in many cases, may not even identify the largest or major sources. For this reason, the traditional approach is not comprehensive enough to identify all possible strategies for reducing a product's environmental impacts.

The following example illustrates the above points: When **comparing basic oxygen and electric arc furnaces** *in the traditional way,* one would only look to the difference in pollution that is generated per tonne of steel at the production facilities themselves. In this case, the pollution generated in the steps preceding these production facilities is not included. In comparison, *in a life-cycle approach,* one computes the cumulative pollutant emissions that are generated by a tonne of steel, including the steps leading up to the final production of a tonne of steel. Those preceding steps include transport of the input materials, electricity generation for the consumed electric power, pig iron production, and other processes.

Assessing, for example, carbon monoxide (CO) from basic oxygen furnaces versus electric arc furnaces in the traditional way, one obtains a difference in emissions of a factor of about 7 if both plants are either uncontrolled or controlled to the same degree (in the uncontrolled case, 69.5 kg CO/t of steel vs. 10 kg/t). In a life-cycle comparison, however, a tonne of steel made in a basic oxygen furnace generates about 8.5 times more CO than a tonne of steel from an electric arc furnace (115 kg/t vs. 14 kg/t). This approach further provides a more comprehensive assessment of the total pollution impact of a tonne of steel from either of the two processes. In the case of basic oxygen furnaces, 65 % more CO per tonne of steel is computed using the life-cycle approach as compared to the traditional approach. The additional CO emissions are mainly due to the steps of coking and pig iron production in blast furnaces which precede the steel production in basic oxygen furnaces. The corresponding steps for electric arc furnaces produce lower CO emissions.

3. Limitations to Life-Cycle Analysis

Although life-cycle analyses identify the amounts of known pollutants from the products or production systems studied, *they cannot, and should not, without further interpretation* be used to compare these products or production systems *for their environmental toxicity*. One can readily compare different products or production systems for their amounts of *identical* pollutants, but one cannot deduce from life-cycle analyses whether or not one specific pollutant, or a group of pollutants, is more harmful to the environment than another one.

Take, for example, **the production of bleached versus unbleached, coated paper.** The quality of both papers is about the same; the bleached paper is made white by using chlorine as a bleaching agent whereas the unbleached, coated paper is made white by using titanium oxide (TiO_2) as a pigment in the coating. Between 60 and 180 kg of chlorine per tonne of paper are released into the waste water from the bleaching process. About 2 kg of TiO_2 per tonne of paper are released into the waste water from the coating process. The chlorine is ecotoxic to fish and, once reacted with organic matter, the chlorinated organic compounds bio-accumulate. The TiO_2 is contaminated with heavy metals, such as vanadium pentoxide and chromium oxide, and with phosphor pentoxide, all from the ilmenite and rutile ores of which it is made; these are as well ecotoxic and bio-accumulate. Further, the production of 1 tonne of TiO_2 generates 1.55 tonnes of concentrated sulfuric acid, of which only 0.55 tonnes are further used, and 4.5 tonnes of ferro-sulfate. Both are discharged into the ocean where they are harmful to the aquatic environment.

In the quantitative inventorying of life-cycle analysis, these amounts are all calculated per desired amount of paper, but it requires knowledge on the toxicity and comparative risk analysis, and finally some value judgement, in order to determine which type of paper is ultimately better for the environment.

Another potential weakness of life-cycle studies is the tremendous amount of data involved. It is extremely difficult to document clearly and understandably all data and assumptions that go into the final results from any life-cycle analysis. If different studies for the same product(s), however, come up with different final results, one should be able to trace these discrepancies back to the different assumptions made. This is only possible if all base data are accessable and well documented as regards their sources.

Now even if this is the case, data may still be disputable unless they have some official character. It would therefore be desirable if some nationally, and preferably internationally, accepted database could be established, at least, for the major products, intermediates and/or economic sectors, and those products and sectors that reccur in every life-cycle analysis, e.g., goods transportation and energy mining and conversion.

This could be done in a stepwise approach where, first, base data for the most important, i.e. most often-used and recurring, products and sectors would be put into an (inter)national database; once these are verified and agreed upon, the cumulative results for the production of the main products and intermediates could as well be stored for direct further use. As other data become available for less common products and processes, the database could then gradually be extended and completed.

Description of the IDEA Model

IDEA -- the International Database for Ecoprofile Analysis -- is a user-friendly, interactive tool for decision makers to assess quantitatively the cumulative materials and energy requirements as well as the environmental discharges to air, water and land from one, or several, product(s). With IDEA, these cumulative impacts of a product can be computed from the point onwards where materials and energies for this product are extracted from the earth, up to either a certain point in the product's life-cycle, or in the most complete case, the final disposal of the remaining wastes back into the earth.

The IDEA system currently comprises three main features:

(1)   a *database;*
(2)   a *materials and energy flow model;*
(3)   a *scenario creation* option.

The database is constructed around so-called *unit processes;* these can be combined in the materials and energy flow model so that any production and consumption system can be modeled for which all relevant processes are included in the database. Since the database can easily be expanded through the addition of new unit processes, the complexity and application of the IDEA system can vary widely from highly aggregated production and consumption systems that represent, for example, national economies, to very detailed studies of comparisons of individual unit processes, for example, for the evaluation of alternative production technologies for the same product. Products evaluated can be of material or utility type, and several products and/or utilities can be evaluated simultaneously.

The software environment within which IDEA has been developed is Dbase IV, whose advantage is wide-spread availability and relatively easy use; this makes IDEA accessible to many users. IDEA has been designed as a user-friendly, interactive tool that allows *flexibility and transparency:*

- **Flexibility** is important for IDEA to be applied to various economic activities of different degrees of complexity and to allow the creation of freely selected, alternative policy scenarios.
- **Transparency** is essential in order to allow the user of IDEA to be able to understand, and to make understood to others, all assumptions made in the system modeled.

Due to the hierarchical structure of the database, IDEA allows easy separation between base data and any further assumptions or aggregations made at any stage in the analysis. This means that the user is free to change any of these assumptions or aggregations so that

- the assumptions match his/her understanding of what the system modeled should look like;
- the user can create various policy scenarios that he/she wants to evaluate and compare.

In the following sections, we describe the current features of the IDEA system. In the future, however, IDEA may easily be expanded by either

- expanding the present database to include new processes and/or entire economic sectors;
- writing additional dBase programs for new applications.

1. Database

The IDEA database is built around so-called *unit processes* and *products*. In this context, "unit processes" are defined in the following way: any transformation that a product undergoes in order to make a new product, for which additional material and/or energy products are needed as inputs. "Products", in turn, are defined as material and energy inputs into, or outputs from, these unit processes.

In the following sections, we describe
- the type of data needed for life-cycle analysis with the IDEA system;
- the IDEA database structure, including the description of the various files and their interrelationships;
- the mass balancing of inputs into, and outputs from, the unit processes before the data are used in the IDEA system to actually compute cumulative environmental impacts.

1.1. Description of the Data

Unit processes make up the basic elements, and thus reference points, of the IDEA database. Since these unit processes can be defined flexibly, examples in the current database range from aggregated processes such as "oil refining", which is actually comprised of a multitude of individual process steps, to "pickling", which is one process step in the production of cold rolled steel. Each unit process belongs to a unique sector which reflects either an economic sector or a logically-linked group of processes.

In general, there are many ways to describe an economic activity, or a national or regional economy on a more aggregated level, in terms of these so-called unit processes. The level of detail should be determined so that the unit processes defined:
- match the available input/output data of materials and energy flows;
- match as far as possible the available emission factors to air and water;
- distinguish between different technologies that could be used to generate the same main output.

Due to this flexible definition of unit processes, the complexity of the system analyzed can vary widely from highly aggregated systems that represent national economies where unit processes are defined as entire economic sectors, to very detailed studies of comparisons of alternative production technologies for the same product where unit processes are defined as these individual alternative production technologies.

Currently, the IDEA database contains approximately 1000 unit processes and also about 1000 products. The unit processes describe either entirely or in part the following eleven economic sectors:

(1) fuel and minerals and mining,
(2) energy conversion,
(3) goods transportation,
(4) inorganic chemicals production,
(5) organic chemicals production,
(6) glass production,
(7) pulp and paper production,
(8) aluminum production,
(9) iron & steel production,
(10) beverage container manufacture,
(11) waste management & recycling.

All data are stored with reference to a unit process and organized according to inputs into, and outputs from, each process. These *inputs and outputs* constitute flows which are uniquely identified through three attributes:

• unit process name;
• product name;
• calculation type.

The *calculation type* defines the role of a product in a process, i.e. whether it is a
• reference output,
• non-reference output,
• reference input,
• non-reference input.

In the database, reference flows are identified as such through a "main output" or "main input" flag. Each process can only have one reference flow, i.e. depending on whether it is a production or consumption process, the reference flow is either an input or output. All other flows are expressed per rate of the reference flow, that is, they are linearly related to the reference flow. The rates of the flows of each unit process must be unit-consistent; this means that, if the reference output is given in "tonnes", all non-reference flows must be given "per tonne" of main output.

In the IDEA database, the flows into each unit process include all material and utility consumptions, those out of each unit process should include all co-products (i.e. intermediate and final products that are indeed further used and thus have an economic value), as well as all waste streams resulting either from the material or utility inputs. Waste streams include both types: the total waste streams as well as individual components of these waste streams. Total waste streams are included in IDEA to make input and output balancing easier because, as a rule, this is done via the total waste streams and not via the individual waste components.

1.2 Database Structure

The database has been conceived as *a set of dependent tables related to unit processes*. These unit processes are the main reference points in the database and are contained in the reference file. The tables, which are each stored as an individual file, are constructed as a relational database (see Figure 1.):

The first set of tables is *process-dependent:*
- substitution tables
- allocation tables

The next set of files is *product-dependent*:
- property tables
- mixture tables
- distribution tables

The final set of tables is *product- and process, i.e. flow-dependent*:
- input and output tables
- transportation tables

1.2.1 Relational Structure of Files

The relational structure of the nine tables, or files, is created and maintained by an interface program that uses process- and product names as keys. Therefore, all data related to a specific process contain a field for the "process name" in their file structure; those related to a specific product, a field for the "product name". Data related to a flow, i.e. a specific process and product, include fields for both names in their file structure. In order to define the relationships uniquely, it is thus essential that all process- and product names are unique. This uniqueness of names is of particular importance in a network, i.e. multi-user, environment because the "write" access for editing the data is controlled by it.

There are two types of relationships in the database:
- one-to-one;
- one-to-many.

A *one-to-one relationship* exists between
- *products* and *property tables*,
        mixture tables,
        distribution tables,
- *flows* and *transportation tables*.

This means that one product or flow may only have one of each of the above tables linked to it. In turn, mixture- and distribution tables may each contain a maximum of ten processes, transportation tables up to 15 different modes.

A *one-to-many* relationship exist between
- *processes* and *input tables,*
    - *output tables,*
    - *allocation tables,*
    - *substitution tables.*

This means that one process may have an unrestricted number of the above products or tables linked to it.

1.2.2 File Description

Input and output tables

Input flows into, and output flows out of, a unit process are defined by
- *a unique product name;*
- *actual units* in which inputs or outputs are given;
- *the average rate,* i.e. the best estimate of a representative product flow;
- *the minimum rate* - to indicate the lower bound of uncertainty or the best technologies available;
- *the maximum rate* - to indicate the upper bound of uncertainty or the worst technologies still in use.

A *"type" attribute* allows the classification of each product flow as one of the following:
- (1) *useful products* (type 1) (these leave the system modeled):
    - final main product;
    - co-product;
- (2) *intermediate products* (type 2) (these are further used within the system analyzed);
- (3) *energy utilities* (type 3):
    - electric power;
    - steam;
    - heat;
- (4) *non-energy utilities* (type 4):
    - process water;
    - cooling water;
    - process air;
- (5) *raw materials:*
    - depletable raw materials (type 5);
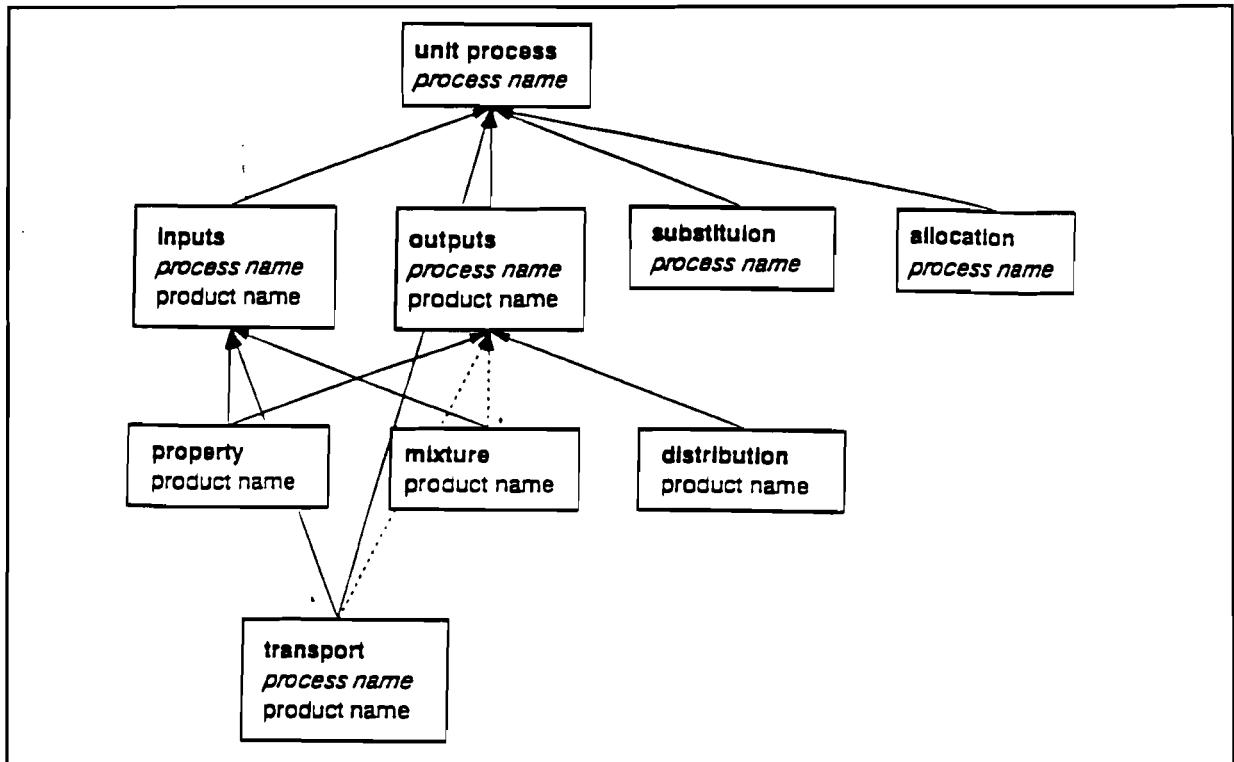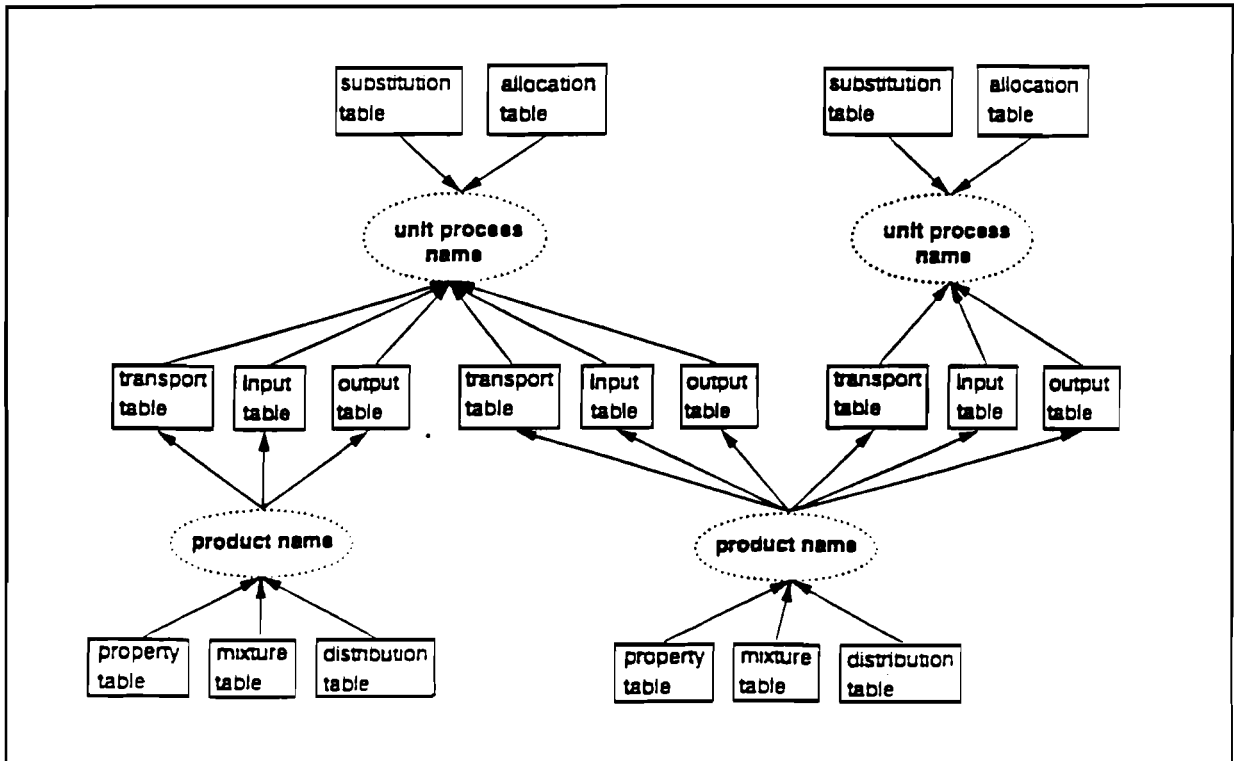   - common raw materials (type 6);

FIGURE 1.1: Database Structure

FIGURE 1.2: File Interrelationships

(6) *waste components:*
  • air pollutants (e.g., SO_2) (type 11);
  • water pollutants (e.g., BOD_5) (type 12);
  • particular municipal solid wastes (e.g., waste glass) (type 13);
  • particular special solid wastes (e.g., spent sulfuric acid) (type 14);
  • particular industrial solid wastes (e.g., mine tailings) (type 15);
(7) *total waste streams:*
  • total waste air (type 21);
  • total waste water (type 22);
  • total municipal solid waste (type 23);
  • total special solid waste (type 24);
  • total industrial solid waste (type 25).

Substitution tables

On the input side, substitutions denominate alternative products (different product names) equally well suited as inputs into one process. Substitutions on the output side represent recycled versus discarded wastes. Substitutions are given as fixed relative shares between the alternative inputs or outputs. The information is only *process-specific*. The actual production rates of all but one of the alternative products are generally set to zero and the total amount is reflected only in the production rate of one of the products. A substitution table with the product names of the alternative inputs or outputs contains their *fixed relative shares*. These shares may reflect
  • the actual percentages of the alternative inputs used;
  • the actual percentages recycled versus discarded;
  • the number of return trips translated into return and waste rates.

Example of an input-related substitution: in secondary aluminum production from scrap, the salt used in "rotary furnaces" can be either sodium or potassium chloride; the relative amounts of either salt as currently used in Western Europe in this process are contained in a substitution table linked to the input data into "rotary furnace".

Example of an output-related substitution: in the transport of filled beverage containers from the bottler to the retail store, wooden pallets are used which usually make 20 trips before being discarded to the municipal waste collection. The unit process "retail" thus has, among others, two outputs "pallet" (with the total output rate) and "solid waste/municipal" (with an output rate of zero); these two names are contained in a substitution table with a 95% share for "pallet" and a 5% share for "solid waste/municipal".

Allocation tables

Allocations identify the relative fixed shares of all different intermediate product inputs into, or useful product outputs from, the same process. This information is only process-specific. It is used to allocate input flows into, or output flows from, one aggregated process for which these data are available, to the various respective outputs or inputs.

Example of output-related allocation: light fuel oils, middle distillates and heavy fuel oils are outputs from a refinery (unit process for which input and output data are available); an allocation table contains the output product names together with their relative shares under current Western European conditions.

Example of input-related allocation: waste paper and board, -plastics, -glass, -metals, etc., are all categories of input into municipal solid waste handling (unit process for which input and output data are available); an allocation table contains the product names of these inputs and their relative shares under current conditions in Western Europe.

Property tables

Properties include the following data linked to each input and output product:
- *global calculation unit* to be used uniformly throughout the system for the input or output product;
- *specific weight* of the input or output product;
- *specific volume* of the input or output product;
- *specific energy* content of the input or output product;
- *product group identifier* to link the specific input or output product to a product group for which transportation profiles are available (see Section 2.2).

This information is only product-specific, so if it has been given once for a specific product name, it is automatically linked to all inputs or outputs with the same product name, irrespective of the unit process.

Mixture tables

Mixtures describe the relative fixed shares between identical products (same product name) into, or from, alternative processes. The information is only product-specific, i.e. it applies to all products with the same name irrespective of the process by which they are consumed or generated.

Example of an input-related mixture: raw steel can be made either in basic oxygen or electric arc furnaces (each a unit process); a mixture table is linked to the product-specific input data into "steel casting" and contains the unit process names of the two alternative production processes as well as their fixed relative shares for the current situation in Western Europe.

Mixtures on the output side are possible in the database logic, but only make sense for the final product of the process chain if this can be manufactured by different processes. If, for example, the process chain of soda ash (Na_2CO_3) production is to be modeled, this chain ends with two unit processes, i.e. the Solvay and Trona process, both making Na_2CO_3. In this case, a mixture table linked to the final product output is necessary which specifies the two process names and the relative shares of soda ash produced by each of them.

Distribution tables

Distributions describe the relative fixed shares of one output product into different processes. This information is only output product-specific; this means that if the information has been given once for a specific product name, it is automatically linked to all outputs with the same product name, irrespective of the unit process by which they are generated.

Example of output-dependent distribution: waste glass comes out of several consumption processes; in Western Europe, 29% are recycled, of the remainder, 73% are landfilled and 27% are incinerated. A distribution table thus contains "cullet recycling" 29%, "waste glass landfilling" 52%, and "waste glass incineration" 19%.

Transportation tables

Transportation information describes for each product input or output the modes of transport, their fixed relative shares in the total transport of this product, and the gross transport distance, i.e. including empty return trips, for each mode. This information is flow-, i.e. process- and product-specific.

As a rule, data are given as *input flow-dependent* in the production stream of a product, but if necessary, they may also be given as output flow-dependent. Priority is given to input-related transportation tables. That is, the model first looks for the input flow into a process and searches for the related transportation table; only if it does not find any table linked to this input flow, it proceeds to look for the matching output flow and then takes the transportation data from the transportation table linked to this output flow.

Output-related transportation information may be necessary in cases of recycling because different transportation modes or distances may be associated with the primary and recycled input. Since the names of the input flows (defined as process-product pairs) of the primary and recycled materials are, however, identical, only one transportation table could be given on the input side. On the output side, however, the flows still have different names because they come from different processes so that two transportation tables can be given.

Currently 14 different **transport modes** are possible:
- *rail, diesel*   • *light duty gasoline trucks (< 3.5 t own weight) - urban*
- *rail, electric*   • *light duty gasoline trucks (< 3.5 t own weight) - rural*
- *ship, seagoing* • *light duty gasoline trucks (< 3.5 t own weight) - highway*
- *ship, inland*   • *diesel trucks (3.5-16 t own weight) - urban*
- *pipeline*   • *diesel trucks (3.5-16 t own weight) - rural*
- • *diesel trucks (3.5-16 t own weight) - highway*
- • *heavy duty diesel trucks (> 16 t own weight) - urban*
- • *heavy duty diesel trucks (> 16 t own weight) - rural*
- • *heavy duty diesel trucks (> 16 t own weight) - highway*

Each of these 14 modes are contained in the database as a unit process with a main output of 1 tonne-km and their specific inputs and outputs on energy requirements and air pollution emissions.

If for any material input or output no transportation table is given, the input should, and can, be assigned into one of the following eleven **product groups:**
(1) foods, incl. grains
(2) sand, clay
(3) stones, minerals, salt
(4) ore, metal wastes
(5) solid fossil fuels
(6) oils, petroleum products
(7) fertilizers .
(8) mineral/construction products, glass
(9) iron and steel, incl. intermediates
(10) machinery
(11) other goods, incl. chemical products
For these eleven product groups, transportation tables are available in the database, based on German data extrapolated to the Western European situation.

1.3 Mass Balancing

Before actually computing the cumulative material and energy flows through the system, each unit process can be checked for mass consistency, i.e. the amounts of materials going into, and coming out of, each unit operation should balance to zero. In order to do so, all flows to be accounted for in the materials balance are converted to mass equivalent units. The flows included are:

(1) on the *input side,* i.e. entering a unit process, all
 - materials,
 - non-energy utilities;
(2) on the *output side,* i.e. leaving a unit process, the
 - main product,
 - co-products,
 - amount of total waste air,
 - amount of total waste water,
 - re-usable non-energy utilities (same name as inputs),
 - amount of industrial solid waste,
 - amount of municipal solid waste,
 - amount of special solid waste.

In general, therefore, mass balancing is done over the total exhaust gas, waste water and waste streams and not over the individual pollutants contained in these streams. That is also the reason that the masses of the individual pollutants are not converted to mass equivalent units as long as the total amounts of waste streams are given. However, if these total waste streams are not given, the individual pollutants are, indeed, converted to mass equivalents and included in the mass balance calculation.

After conversion, the program sums up all mass equivalents on the input and output sides and then subtracts them from each other. The resulting balance should be zero, or as close to zero as possible.

Take, for example, the unit process of "steam generation from hard coal"; on the input side, we add up:

```
+   34.14 kg hard coal
+ 285.72 kg process water
+ 984.04 kg process air
-----------------------------------------
+ 1303.90 kg total
```

From this, we subtract the following outputs:

  - 285.71 kg steam/hard coal
  -1013.30 kg waste air
  -    4.88 kg solid waste/other industrial

  -1303.90 kg total

Note, that the individual pollutants do not enter the mass balance since the total waste air stream is available in the database. On the other hand, take "salt mining and preparation", a process for which no total waste water and waste air quantities are given. Here we have on the input side only one material input:

  + 1131.30 kg salt rock

  + 1131.30 kg total

and, on the output side, we subtract from this:

  -1000.00 kg NaCl
  - 130.90 kg solid waste/other industrial
  -   0.30 kg TSP (i.e. total suspended particulate, or dust, to air)
  -   0.08 kg acids (to water)
  -   0.02 kg heavy metals (to water)

  -1131.30 kg total

2. Materials and Energy Flow Model

Calculations to determine the composite environmental impacts of one or several product(s) are made with a general purpose *materials and energy flow model*, also written in Dbase IV, which simulates process chains of any given economic activity. The model can thus handle any number of simultaneously produced products, alternative production processes, and substitutions through, for example, recycling.

As *input*, the model takes the materials, energy and environmental data directly from the database for those processes that are involved in the production and consumption of the desired output(s). The model assumes *linear production functions*, and calculations are carried out in three consecutive steps:
(1)   The direct impacts of *production and consumption* are computed, including the final energy (i.e. heat, electric power, etc.) and fuel (i.e. light fuel oil, natural gas, hard coal, etc.) demands.
(2)   The impacts of all *transportation*, including fuel transport, are computed.
(3)   The final energies and fuels from the first two steps are added together and the impacts of *energy conversion* and *fuel mining* are computed.

The last two steps both require *iterations*. In the case of energy conversion and fuel mining, additional energy is necessary for running these process steps, and in the case of transportation, the energy conversion and mining as well as the fuel transport itself generate new transport requirements. The first iteration is done within the energy conversion and mining sectors, and the result from this is then fed back into the transportation sector calculations in order to proceed with the second iteration (see Section 2.3.2).

As *output*, the model generates tables with the inputs and outputs of each process as calculated for the desired final demand. These listings show the processes in the order of model calculation and, below each process, first all inputs and then all outputs.

Model output can also be grouped by input and output products. In those listings, first all inputs are listed alphabetically and below each input, all processes that consume it are shown. Then all outputs are listed alphabetically and, below each, all processes that generate the respective output are indicated.

All material and energy needs and pollution discharges are computed at the unit process level, but may be aggregated to
• one sector;
• several sectors;
• the entire system.
At each level, model output includes overall materials and energy balances.

Through an interface program, model output is further linked to two options of *graphical representation* in Lotus Freelance Plus. For each input or output product, *pie charts* of relative shares can be drawn up from the model results; these can represent:

- the *relative shares* of the product coming *from*
  (a) the *production and/or consumption* itself;
  (b) *energy conversion* for the energy needed in the production and/or consumption;
  (c) *transportation* requirements of both the production and/or consumption, and the energy conversion steps.
- the *relative shares* of the product coming *from the various process steps that consume or generate it.*

2.1 Direct Production and Consumption Impacts

The first calculation step in the IDEA model involves
- the creation of the production and consumption system for which the cumulative material and energy requirements and environmental impacts are to be calculated;
- the computation of the direct impacts from production and consumption.

Both parts are detailed in the following sections. The description includes the general flow solution as well as the handling of recycling, alternative production processes and products, etc. Although described here, these general principles apply not only to the calculation of direct impacts from production and consumption, but also to the computation of impacts from transportation and energy conversion and mining.

2.1.1 Generation of the Production and Consumption Chains

In the IDEA database, all processes must have one *reference flow* which is to be identified as such through a *"main output"* or *"main input"* flag. On the production side, these are always main outputs whereas, on the consumption side, such as waste management and recycling, they are always main inputs. Note that the outputs from recycling processes, in which the outputs carry the same product names as from the primary production processes, are not flagged as main outputs; these processes must, however, have a main input flow. This is so that the recycled material always takes priority over the primary material in the solution algorithm of the general flow model (see Section 2.5). Examples of flow definitions as presently contained in IDEA are given in Table 1.

TABLE 1. Examples of Flow Definitions in the IDEA Database.

PROCESS	PRODUCT	CALCULATION TYPE
glass melting & fining	molten glass	reference (main) output
cullet melting & fining	molten glass	non-reference output
municipal waste incineration	municipal waste	reference (main) input

The input(s) into a process usually lead(s) to the main output(s) from (an)other unit process(es), so that the systematic definition of these *process-product pairs*, or flows, determines the relationships between all unit processes of the process chains modeled.

These flows are then used to construct the production and consumption trees of the entire system. Generally there are several trees of both types in one system. The model therefore builds them stepwise:

(1)   In the first round, the model creates a *primary production tree* going *upwards* from the final products via the intermediate products to the virgin raw materials by systematically *scanning for "main" outputs*. For example, if the desired output is 1 tonne of cold rolled steel, the model first identifies all inputs into the unit process "cold steel rolling mill", it then searches for those processes that produce these inputs as main output, in this case, only one unit process "pickling". The model proceeds in the same way from "pickling" and finds here three inputs, i.e. hot rolled steel, limestone and sulfuric acid (H_2SO_4) (**Figure 2**). It now identifies the next set of unit processes that produce these three materials as main outputs. This procedure is repeated until all inputs found are either virgin raw materials or external inputs for which no further production processes are given in the database.

(2)   Once all virgin raw materials and external inputs have been found, the model identifies *all non-reference outputs* of the primary production tree in order to build the first level of *consumption trees downwards*. In this step, the model traces all material output and waste streams towards their ultimate disposal through the *scanning of the "main" inputs*. Taking most consumer goods as the desired final output, the model finds, for example, as an output stream from the primary production tree "waste paper". It searches for the process into which waste paper is the main input, and finds "paper recycling", "municipal landfill" and "municipal waste incineration" (**Figure 4**). It now identifies all outputs from each of these unit processes, again looks into which processes these outputs become main inputs, and repeats the above steps until all materials have been found that are either disposed of in the ground or leave the system as co-products, i.e. those for which no further consumption processes are given in the database.

(3)   In the third round, the model identifies *all non-reference inputs* into the consumption trees in order to build the *second level production trees upwards*. Here, the model traces all inputs into the tree until it again reaches all virgin raw materials via the *scanning of the "main" outputs*. Take again "paper recycling" as an example of one of the processes in a consumption tree; this process again requires new inputs other than waste paper, namely electric power, process water and some additives (**see Figure 3**). The model again identifies the next set of unit processes that produce these three inputs as main outputs. As in the primary production tree, this procedure is repeated until all inputs found are either virgin raw materials or external inputs.

(4)   The model proceeds in the same way until it creates the *final level of consumption or production trees* which require no more upstream or downstream processes.

FIGURE 2. Construction of the Production Tree(s) in the IDEA Materials and Energy Flow Model -- Example of the Production of Cold Rolled Steel.
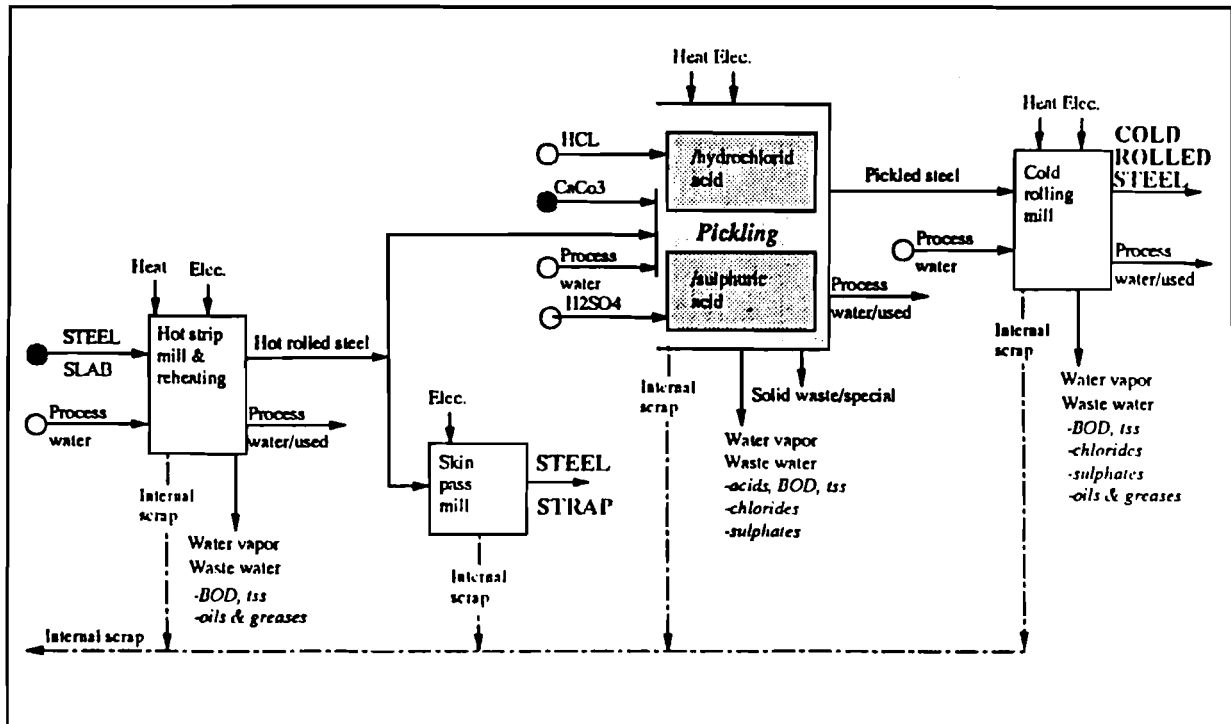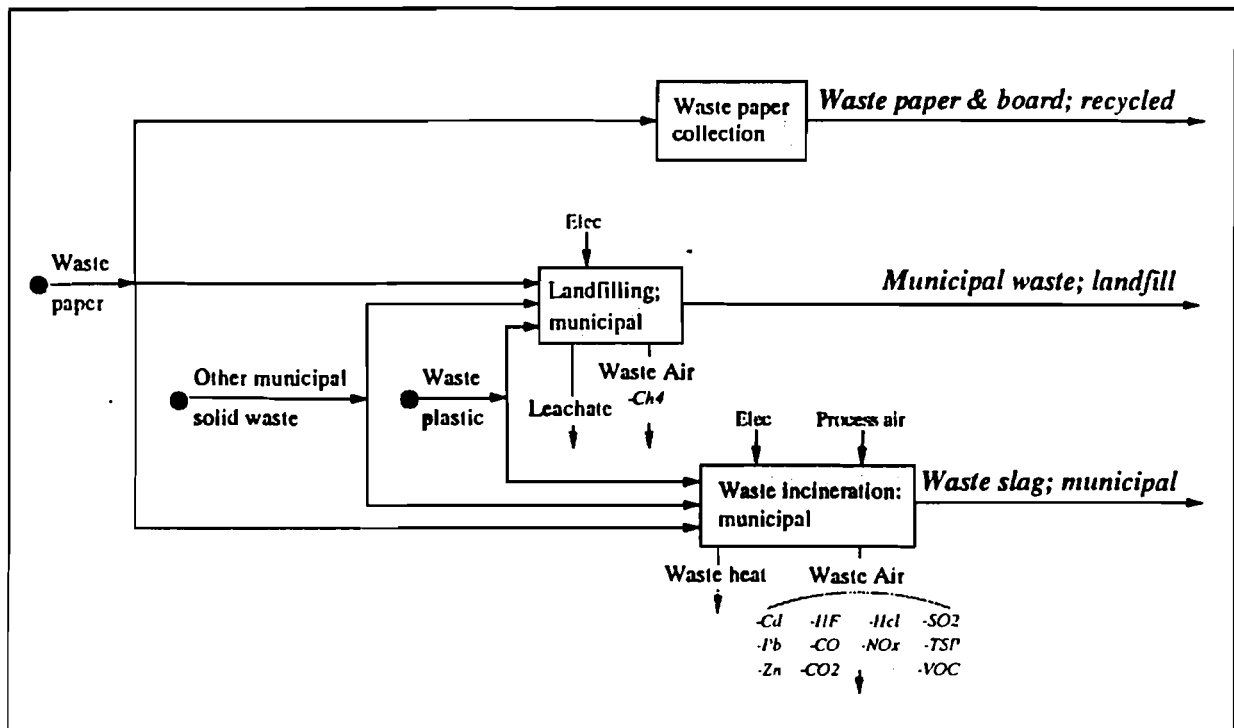

FIGURE 3. Construction of the Consumption Tree(s) in the IDEA Materials and Energy Flow Model -- Example of the Waste Paper Handling.

During the generation of this tree structure, the model creates so-called subject and object files. The *subject file* contains the actual flows through definition of:

- process name;
- product name;
- calculation type specification;
- actual rate of demand in global calculation units given in the IDEA database;
- actual rate of demand in mass equivalents given in the IDEA database.
- actual rate of supply in global calculation units given in the IDEA database;
- actual rate of supply in mass equivalents given in the IDEA database;
- a logical field that indicates the status of supply vis-à-vis demand; this field is set to "incomplete" as long as an imbalance exists between the demand and supply, and it is set to "complete" when the imbalance has been adjusted. In most cases this means that the supply equals the demand.

While the tree structure is being built, only the first three fields are filled in. The next four fields for the actual flows of supply and demand are only filled in during the calculation step. The last field of each record is initially set to "complete" as both supplies and demands are zero (see **Table 2**).

The object file contains the relationships between the input and output flows. These flow pairs represent relationships between:

- flows into and out of one process;
- flows between two processes.

These flow pairs are defined through:

- process name;
- product name;
- calculation type specification;
- calculated rate of change in the object (i.e. target, or related flow) for a unit rate change in the subject flow.

These rates of change, or relative weights, are obtained in two ways, depending on the type of relationship:

- *Within one process*, i.e. if the flow pair identifies a relationship between input and output flows of the same process, the weights are calculated as ratios of flows to the reference flow. For example, run-of-mine brown coal as a main output from "surface brown coal mining" is related inside the same process to TSP (total suspended particulate, or dust) emissions from "surface brown coal mining". The weight is calculated from the rate of TSP per tonne of run-of-mine brown coal.

- *Between different processes,* i.e. if the flow pair identifies a relationship between flows into one and out of another process, the weights are,
  - (a) for a single object, equal to one;
  - (b) for several objects with the same product name, identical to the relative shares from the mixture tables on the input side, and from the distribution tables on the output side. Note that a mixture or distribution table should be given in the database if there are several objects with the same product name because, otherwise, a default of equal shares is used in the calculation.
    For example, waste paper comes out of "paper consumption" and is related to the input flows of three processes. The weight is calculated from the distribution table of waste paper into "waste incineration", "landfill" and "paper recycling".

All fields in the object file are filled in while the tree structure is being built; this file will not be modified during the calculation step, it will only be used to identify the relationships between flows (see **Table 3**).

The final step, once the production and consumption trees have been built, is the identification of relationships, or flow pairs, that define recycling possibilities. This is done by name-matching of reference and non-reference inputs and outputs:

(1) All non-reference outputs from the completed tree are scanned for product names identical to reference, or main, outputs.

(2) Whenever such a matched name pair is found, this relationship is recorded into the object file; i.e. a record is appended for this flow pair. If more than one reference-output is found, several records are created and the relative shares of the mixture table are used to compute the weights.

(3) Steps (1) and (2) are repeated for non-reference and reference inputs.

(4) Lastly, the non-reference outputs are scanned for product names identical to non-reference inputs.

(5) These relationships are recorded into the object file in order to allow so-called by-product allocation (see Section 2.1.2).

With the creation of the complete subject and object files, the solution area for the process chains to be modeled has been constructed and can be saved. This is so that several runs can be made without regenerating the production and consumption trees each time. Such additional runs may be scenarios related to changes in the data and/or structure of the transportation and/or energy conversion and mining sectors, since the solution for these sectors is done separately, and none of the weights calculated in the object file of the production chains are changed.

For all other scenarios, as well as corrections in the original data, some of the weights, or relationships between flows, change. In principle, it is therefore necessary to regenerate the solution area, including the object file. In simple cases, however, where only a few changes in mixture-, distribution-, and/or transportation profiles, or in recycling schemes, are involved, this can be done directly in the object file through an interface program. For all other scenarios in which the production data are changed, or new processes are added or existing ones taken out, the production and consumption tree structure has to be regenerated.

2.1.2 Flow Solution Principles

The previous section described how
* the production and consumption trees are created stepwise;
* the flows are defined in parallel, and stored in the subject files;
* the relationships between flows are computed as relative weights of flow pairs, and stored in the object files.

The *principle of the solution algorithm* is based on the stepwise *balancing of demands and supplies of each flow* in the respective fields of the subject file; that is, to make the difference between the demand and supply of each flow equal to zero, if possible. In order to better understand this solution of actual flows, we shall use the following definitions of "subjects" and "objects":
* *subject:* the flow to be balanced;
* *object:* the target flow that is adjusted in order to balance the present subject.

Basically, the algorithm proceeds in the same order as the generation of the tree structure:

(1) Initially, all demands and supplies in the subject file are equal to zero.

(2) When starting the calculation, the demand for the final subject(s) is set in the subject file equal to the desired final external demand(s). These final subjects make the first set of the subjects to be balanced, and are recorded to the respective table. The calculation proceeds from here on by scanning the table of the subjects to be balanced and balancing the difference between demand and supply for each subject.

(3) The object file is scanned to identify flows related to the subject(s) currently being balanced.

(4) The supply or demand of these objects is computed as:

supply = supply + weight * subject_difference
for non-reference output objects and reference input objects in case the subject is not the start of a recycling chain;

supply = supply - weight * subject_difference
for reference input objects in case subject is the start of a recycling chain;

demand = demand + weight * subject_difference
for non-reference input objects and reference output objects in case subject is not the end of a recycling chain;

demand = demand - weight * subject_difference
for reference output objects in case subject is the end of a recycling chain.

In the recycling case, the weights are adjusted to the maximum adjustment potential; for output objects this is the present demand and, for input objects, the present supply. Negative demand or supply values are not possible.

(5) These new supplies or demands calculated for the objects are recorded in the subject file into the respective records. They cause an imbalance in these records, i.e. the logical field for complete/incomplete is set to "incomplete"; thereby, these records are marked and recorded into the table of next subjects to be balanced.

(6) The rates for the open supply or demand fields of the present set of subjects are calculated as:

supply = supply + Σ (weight * subject_difference)
for non-reference input subjects;

supply = supply + subject_difference
for reference output subjects;

demand = demand + Σ (weight * subject_difference)
for non-reference output subjects;

demand = demand + subject_difference
for reference input subjects.

(7)   These rates are recorded into the subject file, and when the supply equals the demand of a given flow, the logical field for complete/incomplete is set to "complete". Note that balancing of inputs and outputs is dependent on the availability of objects; i.e. if no further flow pair is found in order to balance the supply or demand, the imbalanced flow remains as the amount of external input required or output generated. In this case, the logical field is also set to "complete".

Adjusting a reference flow means to set its production or consumption level to meet the demand/supply directed to it. Therefore, reference flows can always be balanced and their objects adjusted accordingly. For non-reference flows, such as raw materials or emissions, the difference remains and constitutes the amount of external demand, or by-product or waste supply.

(8)   Once all subjects of the present set have been balanced, that is, all logical fields have been set to "complete", the model proceeds to the next set of subjects to be balanced. This is done by replacing the table of current subjects to be balanced with the one of next subjects to be balanced, and clearing the new table of next subjects.

(9)   Steps (1) through (8) are repeated until no subjects remain to be balanced.

After balancing all flows as far as possible, the final step of the flow solution takes place, i.e. *by-product allocation*. This allocation of by-products is done by name matching of non-reference inputs and outputs:
(1)   The object file is scanned for relationships between non-reference flows with identical product names.
(2)   The supply surpluses of non-reference outputs are added to the imbalanced supplies of the matching non-reference inputs.
This allocation is done in the order of the production and consumption tree structure; this means that processes closest to the final demand are first adjusted.

2.1.3 Model Treatment of Alternative Production Processes

Alternative production processes are those that generate the same desired, i.e. main, output product, but may require different material and energy inputs and produce varying co-products and waste streams. In our calculations, we attempt to model as closely as possible a Western European reality and, therefore, specify in the product-dependent *mixture tables* of the database the relative, output-weighted shares of the different processes in place in Western Europe. The model computes the total impact from a process step for which alternative processes exist by multiplying the data for each alternative production process with its actual share and then adding them up. Once a product-specific mixture table has been given, this is always used by the model to allocate its production shares.

If, however, the user wishes to use different and/or flexible mixtures for the same product at different stages in the product system, additional unit processes are introduced into the chain which contain the relative shares either as rates or alternatively, in a process-specific substitution table. In the case of final electricity production, for example, an additional process is given in the database for "electric power production/Western Europe" which takes as inputs electric power products from fuel-specific production processes, like "electric power/hard coal", electric power/brown coal", etc., in shares representative of Western Europe. Alternatively, a substitution table could be given. The output produced from "electric power production/Western Europe" is "electric power". All of these product names represent the same product, i.e. electric power. Although they all represent this one product, they can be called by their different names and can be combined flexibly.

Take the following example: 700 Wh of electric power is required in pulping for each kg of dry pulp. Of this total, 280 Wh comes from the general Western European electricity production (i.e. 40%) and 420 Wh comes from electricity made from heavy fuel oil. In the database, therefore, both "electric power" and "electric power/heavy fuel oil" need to be given as inputs. Then, there are two ways to specify the rates:

(1) The actual rates of 280 Wh and 420 Wh are given under the respective input names.

(2) One of the input rates is set to zero, the other one to 700 Wh, and a substitution table gives the percentages, 40 and 60%, respectively.

If the additional process "electric power production/Western Europe" were not given in the data base, there would be no way to distinguish between these inputs into pulping because the same information from one input-related mixture table would be taken for *all* electric power inputs.

2.1.4 Model Treatment of Alternative Material and Energy Inputs

Alternative material or energy inputs into a unit process are those
• that, in equal quantities, are equally well suited as inputs for this process;
• that require the same amounts of energies and generate the same amounts of material and pollution flows from this process.

As we attempt to model as closely as possible the Western European reality, we therefore specify in the process-dependent *substitution tables* of the database the relative amounts of those alternatives as currently used in Western Europe. The model computes the total impacts from the previous process steps according to these relative shares.

Take the process "glass forehearth" as an example. Associated to this process is a substitution table between "molten brown glass" and "molten external cullet" with a 52 % to 48 % ratio. Therefore, when calculating the demand for molten virgin brown glass, the model finds in the object file a weight of 0.52 relating the flow "molten brown glass into glass forehearth" to "molten brown glass out of virgin glass melting and fining". All demands into virgin glass melting and fining are therefore computed according to this weight.

2.1.5 Model Treatment of Recycling

Materials and products as well as energy can be recycled. In such cases, the system should be credited for the savings in materials, energy, and/or emissions that the recycling incurs. Before we decide, however, what the actual credit that we give to the system modeled is, we have to consider what can happen in reality. First, materials and energy can be recycled within the system that we model; in this case, the recycled, or secondary, product is used in order to reduce the primary inputs into its own production process and we have a so-called *closed recycling loop*.

Alternatively, materials and energy can be recycled so that they either leave the system or are introduced into the system from the outside; we then speak of *open recycling loops*. In the case of materials, this usually means that the recycled product is not of high enough quality to use it again in its own manufacture; we call this *cascade recycling* where a material can actually pass through the cycle several times, but each time at a lower level. A prominent example of cascade recycling are polycarbonate bottles. After being discarded they are ground up and the granulate is made into transparent display parts; once these are discarded, they can consecutively be re-manufactured into household appliances, automotive parts, and pallets; these can then either be made into building materials for the construction industry or they can be burnt for energy recuperation (Mekel and Huppes, 1990).

Open recycling loops, in general, cannot be handled without involving some value judgement as to how much credit should be given to the system modeled for those material or energy flows that are recycled outside the system. One has several alternatives; for example, one can simply treat anything that leaves the system as a by-product and not give the system modeled any additional credit for it. Alternatively, one may choose to credit the present system by a certain fraction of the material or energy that leaves this system to be recycled to another system. DeRohe et al. (1990) suggest to credit the system modeled according to the economic values of the co-products that leave the system. This, however, means to include cost information in the database.

If the recycled stream is used to produce something very similar in quality (e.g., colored glass compared to white glass), or if it were practically possible to reuse the recycled material for the same product (e.g., aluminum cans could be used to make new cans, but this is currently not done), one may decide to simplify the system and treat the open recycling loop as a closed one, i.e. give full credit to the system modeled. IDEA can model both cases as two possible scenarios where, in one case, we treat the outputs from open recycling loops as by-products, and in the other case, we simply close the recycling loops.

The IDEA model handles *closed recycling loops* as a substitution between primary and recycled, i.e. secondary, products. In general, the model allows

- *"fixed" substitution* where a mixture or substitution table is given: in this case, only a fixed portion of the total input into a process may be a recycled material and the substitution is done *on the input side*;
- *"open" substitution* of outputs where no "main output" flags are given to the recycled material: in this case, substitution depends only on the amount of recycled product available and is done *on the output side*.

Dependent on the type of substitution, there are two basic possibilities in the model to solve for closed recycling loops:

- *On the input side:*
  If the secondary material is used in a fixed ratio with the primary input, the outputs from all processes making the same material are marked with a "main output" flag and a *mixture or substitution table*, depending on whether or not identical product names are used for the primary and secondary inputs, identifies the fixed relative shares of inputs coming from the different processes, including those for recycling. In this case, however, the input(s) into the recycling process(es) do(es) not get marked with a "main input" flag.

- *On the output side:*
  If the secondary material is always preferred over the primary product, the recycling process(es) that produce the desired secondary output are not marked with a "main output" flag. In this case, the model recognizes these outputs as always preferable over those that have a "main output" flag, and automatically reduces the outputs from the primary production processes by the amounts from the secondary processes as long as the output product names are identical. In the secondary production process it is then, however, necessary to flag the main input as such in order for the model to be able to proceed.

In the latter case, actual calculation of the recycling loops is done in the following way:
(1) Whenever a certain subject, say a non-reference output flow, is to be balanced, the object file is scanned for all related flows.
(2) If an object is found with an identical reference output name, the supply surplus available for this subject (i.e., the amount of supply from this non-reference output not yet balanced) is used to adjust the object, or reference-output, flow rate.

(3) This means that the remaining demand to be covered by primary materials is automatically reduced.

(4) In a similar way, recycling of materials that are to replace main inputs, is done as part of the general algorithm of the flow solution.

Take "internal cullet" as an example. This is produced at several stages in the glass bottle manufacture and is fully recycled into the glass making processes. So, at the point where the non-reference output "molten glass" of the process "cullet melting and fining" is to be balanced, a related process "glass melting and fining" which produces a reference output "molten glass", is found through the object file. Now, the amount of molten glass from "cullet melting" is used to adjust the "molten glass from virgin glass melting", or object flow. This automatically lowers the demand left open and passed over as supply of "molten glass" from virgin "glass melting and fining."

The supply of "molten glass from cullet melting", in turn, was computed via the relationships between the reference input "internal cullet" into "cullet melting and fining" and non-reference outputs of "internal cullet" from glass forming, glass annealing, and glass finishing.

Within the open substitution, we have to yet consider another particular case. If no primary production processes exist in the database which produce as a main output the specific product that is required as an input into some process, this means that
- open substitution occurs between virgin raw materials and recycled products;
- the supply has to be satisfied from products recycled within the system and, possibly, external inputs;
- the supply has to be satisfied entirely from external inputs if the specific product is not produced as an output anywhere within the system.

In the latter case, the external input is treated as a virgin raw material and no substitution is necessary; in the first two cases, substitutions are solved by so-called *by-product allocation*. This by-production allocation allows us to model complicated recycling schemes which might otherwise result in infinite iteration loops. Two examples of by-product allocation within recycling are:

(1) The pulp digester in pulp and paper production requires as inputs, among others, wood chips and white liquor and produces as outputs pulp and black liquor. Black liquor is the only source to satisfy through a number of process steps the demand for white liquor, i.e. there is no primary production process that makes white liquor. When the model now calculates the demand for white liquor and the resulting supply of white liquor, the two numbers will not be identical because no one-to-one linear relationship exists between the black liquor output and the white liquor input. Since the model does not find any other processes making white liquor, it would, in the general solution of open recycling, replace the input demand with the amount actually produced, and repeat the calculation until the two numbers converge. The model would, however, keep repeating this iteration, and thus not be able to proceed with its solution, since an imbalance would remain between the demand and supply sides.

Through by-product substitution, the model accepts this imbalance, reserves calculation of final input demand to the very end, and then calculates the difference between supply and demand. The model, however, cannot distinguish whether this constitutes
- a real external demand or supply;
- only a theoretical calculation imbalance.

This will be up to the model user to decide.

(2) Steel production from scrap takes as an input iron scrap. There is no unit process in the system that produces iron scrap as a main output but many processes that produce it as a by-product. In by-product substitution, all amounts of iron scrap by-products are added up, subtracted from the total input demand, and the remaining difference is taken as an external input requirement, in the same way as any virgin raw material.

2.1.6 Computation of Environmental Loads

Environmental discharges and wastes are identified as such in the database by their appropriate type number. Pollutant emissions to air and water as well as solid waste components are explicitly calculated with the help of emission factors which are part of the output coefficient list. In this case, the relationship between the reference input or output flow and the pollutant is described by this emission factor, and the weight in the object file is calculated accordingly. Total waste streams are calculated in the same way as useful co- or by-products; however, in order to distinguish them from these, they have different type numbers so that they can be summed up separately in the mass and energy balances. Terminal wastes, both total waste streams and individual pollutants can be considered the equivalents on the output side to virgin raw materials on the input side.

2.2 Transportation Impacts

In IDEA, the requirements and environmental impacts from transportation are computed for
- the goods transport in the production and consumption sectors;
- the fuel transport for the transportation sector itself;
- the goods transport in the energy conversion and mining-related sectors.

For the last two impact calculations, *iterations* are necessary. The transport of fuels used in transportation itself generates energy requirements. These energy requirements together with those from production and consumption of the goods cause additional transport needs, first for the materials needed within energy conversion and mining, and second for fuels used for this additional transport.

After having computed all direct impacts, including the actual rates of all product flows, from production and consumption, the IDEA model proceeds to compute the transportation impacts from the related goods transport. This determines the fuel requirements for this goods transport, and thus allows the model to compute, in the following step, the impacts from the fuel transport for all transportation so-far calculated. Before the final impacts from *all* fuel transport within the system modeled can be calculated, energy conversion and mining impacts need to be computed. After that step (see Section 2.3), the resulting transportation needs are fed back into the transportation calculation step and the iteration loop of the system (see Section 2.3.2) is started (see **Figure 4.**).

2.3.1 Allocation of Transportation Profiles to Product Flows

The data currently available in IDEA to compute energy requirements and environmental impacts from transportation consist of
- 14 different *unit transportation processes* with their related inputs and outputs;
- *product flow-specific transportation profiles* contained in the transportation table and linked to the specific input or output product flow;
- *group-specific transportation profiles* contained in the transportation table and linked to the product group name, together with *group identifiers* specified in the property table and linked to all those products which belong to the respective groups.   .

Unit transportation processes are stored in the IDEA database in the same way as all other unit processes which contain, for example, production data. They include fuel or energy inputs, as well as combustion air inputs where necessary, and total waste air and air pollution emission outputs per 1 tonne-km of reference output. The derivation of the data for the current 14 transportation processes is described in Part 2 of this report.

FIGURE 4. Iteration Between the Energy and Transportation Calculation Modules of the IDEA Materials and Energy Flow Model.
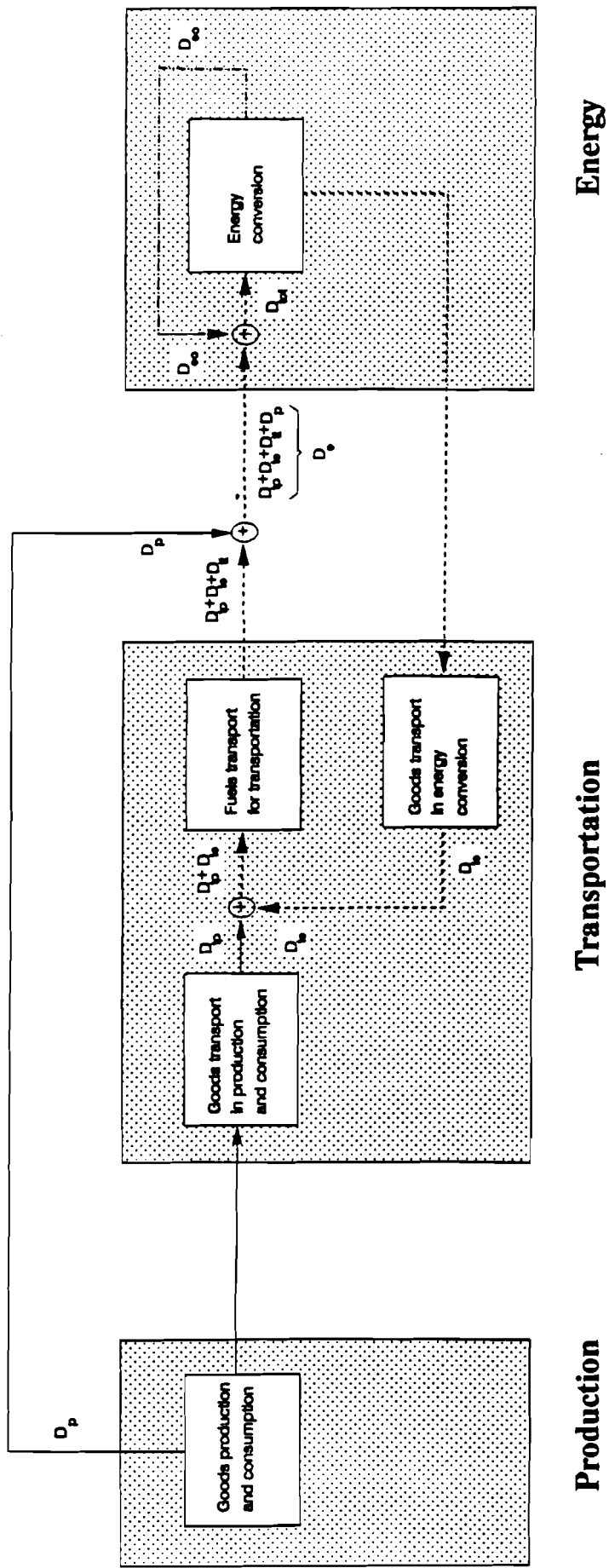
Product flow-specific as well as group-specific transportation profiles contain average distances, including all empty return, or other, trips, and mass shares of those unit transportation processes that are involved in carrying the specific product to which the transportation profile is linked, or all products of a group to which the profile is related. The mass shares reflect the modal split between different means of transportation. In the transportation profiles, unit processes can be connected in series and in parallel. Take, for example, paperboard from board manufacturing; this is first transported with seagoing ships and then with rail. Thus, the product-specific transportation profile for "paperboard from board manufacturing" should contain for both "ship/seagoing" and "rail" the same total mass share of 100%, since the total amount of paperboard is transported consecutively by both means. On the other hand, of all rail transport, 75% is by electric and 25% by diesel trains, which means that 25% of all goods are transported on diesel and 75% on electric trains. "Rail/diesel" and "rail/electric" are therefore parallel transport modes. The actual transportation profile for "paperboard from board manufacturing" thus contains:

- ship/seagoing   100%
- rail/diesel   25%
- rail/electric   75%
- etc.

Group identifiers are group numbers that refer to general product group names for which transportation profiles are available in the transportation table of the IDEA database. All input and output products which fall within one of the general product groups, and for which, in general, no product flow-specific transportation profile is given, can be linked to the group-specific transportation profiles by specifying the respective group identifier in the property table linked to the product names.

The basic idea in determining the cumulative transportation impacts of an entire production system is to relate each product flow between different production and/or consumption places to only *one* specific transportation profile. Although only one transportation profile is associated with a particular product flow, there may be various profiles available for the same product name. It is therefore necessary to establish a certain "search" hierarchy so that products are not transported once as an input flow and again as an output flow. The IDEA model searches in the following sequences:

(1) input product flow-specific profile;
(2) output product flow-specific profile;
(3) group-specific profile.

In the first computation step, all *input flows* are scanned to search for *product flow-specific profiles*. If such a profile is found, all output flows with matching product names are excluded from the next search steps, and transportation requirements are calculated for the input product flow.

In the following step, all *output flows* still included in the search list are scanned again for *product flow-specific profiles*. Once again, if such a profile is found, transportation requirements are calculated and, in turn, all input flows with matching product names are excluded from the last, group-specific profile search.

In the third and last search, all remaining *input flows* are scanned to seek for *group-specific profiles*. Here, the group identifier for the remaining input product names is read from the property table, and the related group-specific transportation profile is read and used to calculate the transport requirements.

2.3.2 Calculation of Transportation Impacts

The actual calculation of transportation impacts is done in the same way for the *production and consumption* and *energy conversion and mining-related sectors*; it is done slightly differently for the fuel transport used within the *transportation sector* itself in order to save computation time. The computation of the first two transport-related sets of impacts is carried out in two steps:

(1) Actual transportation demands in tonne-kilometers are calculated *for each transportation process* involved; they are, at the same time, the actual rates of reference outputs from the various unit transportation processes:

$$\text{demand}_i = \Sigma \, \text{demand}_{i, n}$$

where:

demand_i = total actual transportation requirement in tonne-km for i;

i = unit transportation process;

n = product flow for which a transportation profile is given which includes the unit transportation process i.

(2) Using these actual reference outputs calculated, and the reference output rates given in the IDEA database, all non-reference inputs, i.e. fuels or energy, and combustion air, and all non-reference outputs, i.e. total waste air and the specific air emissions, are calculated:

$$rate_{(i, j)} = demand_i/demand_{ref, i} * rate_{ref, (i, j)}$$

where:

$rate_{(i, j)}$ =	total rate of j for the total demand for i;
$demand_i$ =	actual transportation requirement in tonne-km for i;
$demand_{ref, i}$ =	reference transportation requirement, i.e. 1 tonne-km;
$rate_{ref, (i, j)}$ =	reference rate of j per 1 tonne-km;
i =	unit transportation process;
j =	non-reference input or output flow of the unit transportation process;

Results of these transportation calculations are recorded into two corresponding files, each containing the results from transportation impacts in the
- production and consumption sectors;
- energy conversion and mining-related sectors.

Their records have two key fields, one for the unit transportation process name, the other for an input or output product name of this unit transportation process. Altogether, these files thus contain records for the rates of the cumulative tonne-km, fuel and energy requirements and air emissions from each of the 14 transportation processes. For example, there are records for
- tonne-km (one of the outputs) from 16t truck/diesel/rural (one of the unit transportation processes);
- NO_x from rail/diesel;
- middle distillate (i.e. diesel fuel) into ship/inland;
- light fuel oil (i.e. gasoline) into light duty trucks/gasoline/urban;
- etc.

Once the final rates of all flows in these two files have been computed, we have also available the total amounts of fuels and energies needed by each unit transportation process, that is, the amounts of transportation fuels and energies per unit transportation process. For the transportation data included in the IDEA database, these are
- diesel (i.e. middle distillate);
- gasoline (i.e. light fuel oil);
- electric power.

Within each file, they are summed up to give together the *total transportation fuels and energies needed*.

Now the IDEA transportation impact module of the materials and energy flow model proceeds to compute the impact from the fuel transport used within the *transportation sector* itself. This sector only involves the transport of the fuels and energies needed in transportation fuel transport. Only diesel and gasoline constitute material flows and thus are the only ones for which transportation profiles have been given in the IDEA database. Therefore, each time the transportation calculation module of the IDEA materials and energy flow model is activated, the module computes, based on the given transportation profiles for diesel and gasoline, *the average input and output product flows per kg of transportation fuel,* which are no longer transportation process-specific but are averaged over the various transportation processes involved in fuel transport. These rates are recorded into a temporary file which is then used in all calculations of impacts from transportation fuel transport. Records in this file have only the product names as key field.

In the following step, the actual demands of transportation fuel in kg are read from the other two result files for transportation impact calculations described above. Now the model makes use of the temporary file containing the average input and output product flows per kg of transportation fuel, which have been averaged over the various transportation processes involved in fuel transport, and calculates the impacts from the fuel transport used within the transportation sector itself. These results are stored in the results file for the impacts from the fuel transport used within the transportation sector itself, which again only has one key field, i.e. the product names.

This last step of calculating the impacts of fuel transport used for transportation itself has to be repeated several times because the additional fuels needed will require additional fuel production and, as a result, also additional transportation needs, and so forth. Before this can be done, however, the impacts from energy conversion and mining need to be computed for all energies and fuels required in the production and consumption sectors as well as in the transportation sector so-far.

2.3 Energy and Fuel Conversion and Mining Impacts

The total cumulative impacts from energy and fuel conversion and mining also need to be calculated in several rounds because the conversion and mining processes themselves will generate additional fuel and energy needs and, as a result, also additional transportation needs. These needs are calculated in iterations
- within the energy conversion and mining sectors;
- between the energy and transportation calculation modules.

This section describes therefore
- the conventions used in IDEA for the various fuels and energies currently included in the database;
- the two iteration principles used in the IDEA materials and energy flow model.

Although described in this section, the iteration principle within the energy conversion and mining sectors is used as well in the production and consumption calculation step wherever needed. It is, however, explained here because the conversion and mining of fuels and energy always requires new energies and/or fuels as inputs. The iteration between the energy and transportation calculation modules is explained here as it is the last step in the overall impact calculations.

2.3.1 Conventions in the Energy and Fuel Impact Calculations

The third step in the IDEA model computes the requirements and environmental impacts from the conversion and mining of fuels and energies. This calculation can only be carried out for those final energy and fuel types for which unit processes are contained in the IDEA database which produce them. Table 4 lists those fuel types available in the present database as reference outputs from the energy conversion or mining sectors. In addition, the following three types of final energies are available as reference outputs from the energy conversion sector:
- electric power;
- heat;
- steam.

For these three final energies, there are currently unit processes in the database to generate them
- from different fuels (see Table 4[1]);
- for a Western European fuel mix.

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[1] For electricity generation, hydropower and nuclear power are also included with no emission discharges.

The model user can choose either the European mix by only specifying the energy without any further extension, e.g.,

- electric power;
- heat;
- etc.

or the model user can specify a fuel-specific production by giving the appropriate extension, e.g.,

- electric power/natural gas;
- heat/heavy fuel oil;
- etc.

You can also specify whether heat is generated in co-production plants, i.e. made simultaneously with electricity. In this case, heat is identified as "heat/co-generation" if the industrial fuel mix of Western Europe is assumed, or you may give a further extension if the heat is made from a specific fuel[2], e.g.,

- heat/co-generation/hard coal;
- heat/co-generation/light fuel oil;
- etc.

If any of the demands for heat or steam are from co-generation, the model subtracts automatically the co-generation output of "electric power" (produced at a ratio of 20% electricity and 80% heat or steam) from the system's total electricity demand.

Fuel and energy outputs from the energy conversion and mining sectors are identified as *type 1, i.e. final main output*. On the input side, that is in the input coefficient list of the various production, consumption and transportation processes, fuels are again identified as *type 1, i.e. inputs coming as a main final output from another sector*, and final energies as *type 4, i.e. energy utilities*.

In both the first computation step of the direct impacts of production and consumption, and the second step of impacts of transportation, the model adds together the energy demands by type of fuel, e.g. heavy fuel oil, middle distillate, light fuel oil, etc., and type of final energy, e.g., heat, steam, electric power, etc. In the computation of the production and consumption impacts, the model already calculates the *net* requirements of fuels and final energies through the last solution step of by-product allocation. This means that, if the production and consumption processes generate anywhere in the system one of the fuels or final energies as a by-product, these are allocated to reduce the final external demand still needed from the energy conversion and mining sectors. For example, rotary furnaces in the aluminum industry generate as one of the by-products "heat". The model thus reduces the external heat requirement of the total production and consumption system by the amount of heat that these furnaces, and possibly other processes of the entire system, generate. This reduction is done globally over the entire system, that is, the by-products are allocated to wherever there is a demand for them.

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[2]   For a *complete list of all fuel and energy names* as used in the IDEA system, see the Annex. It is important to follow the exact naming convention because **only these names** are recognized by the IDEA system.

TABLE 4. Fuel Types Contained in the IDEA Database as Reference Outputs from the Energy Conversion and Mining Sectors.

FUEL	HEAT CONTENT	
	[kcal/kg]	[MJ/kg]
hard coal	6995.80	29.29
brown coal	2694.18	11.28
derived coal[3]	6995.80	29.29
crude oil	10294.26	43.10
heavy fuel oil	9912.10	41.50
middle distillate[4]	10150.95	42.50
light fuel oil[5]	11392.95	47.70
natural gas	12000.00	50.24
refinery gas	12133.37	50.80
coke oven gas	9744.91	40.80
wood	3821.53	16.00

The solution of the energy impact calculations is done in the same way as the demands and supplies of the production and consumption system are computed, using the unit processes contained in the energy conversion and mining sectors. However, energy conversion as well as mining require additional energy inputs so that the system needs to be iterated.

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[3] includes *coke, briquette,* etc.
[4] includes *diesel,* etc.
[5] includes *gasoline,* etc.

2.3.2 Iteration Principles

There are two types of iteration necessary within the IDEA materials and energy flow model:

(1) the *internal iteration* within the energy conversion and mining sectors;
(2) the *iteration between* the energy and transportation *calculation modules* of the IDEA materials and energy flow model.

The *iteration within the energy conversion and mining sectors* is done as part of the general flow solution algorithm as described in Section 2.1.2, which itself is iterative. In the stepwise balancing of supplies and demands, the already balanced subjects are repeatedly imbalanced again whenever a process requires additional fuel or energy inputs. This causes the model then to perform several rounds of internal iterations until the maximum tolerance of 1% is no longer exceeded for any flow.

As a *result*, this iteration step gives us the *total demand vector* D_{tot} for all fuels and final energies from *all* sectors (including energy conversion and mining itself). This D_{tot} is part of the overall vector M_e which includes *all* input and output flows in the energy production-related sectors.

The *iteration between the energy and transportation calculation modules* is done according to the following general equation (**compare Figure 4.**):

$$D_e = D_p + D_{tp} + D_{te} (M_e (D'_e)) + D_{tt} (D_{tp} + D_{te} (M_e (D'_e))) \tag{1}$$

where:

D_e = total external demand vector (i.e. excluding own use for energy conversion and mining) calculated for all i's;

i = final main product, or reference output, from the energy conversion or mining sectors, i.e. fuels and final energies;

D_p = total demand vector for all i's from the production and consumption processes;

D_{tp} = total demand vector for all i's from the *transportation* of products and fuels between the various *production and consumption processes;*

D_{te} = total demand vector for all i's from the *transportation* of products and fuels between the various *energy production-related processes*, that is, in the energy conversion and mining sectors themselves, but also in sectors affected by the energy conversion, e.g., waste management, inorganic chemicals production;

M_e = solution vector of all (material[6]) input and output flows for the *energy production-related sectors;*

D'_e = total external demand vector previously calculated for all i's;

D_{tt} = total demand vector for all i's from the *transportation* of fuels needed for *transportation* itself.

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[6] The calculation algorithm checks all flows although only material flows incur transportation demands.

The initial condition for this equation is

$$\mathbf{D_c} = \mathbf{D_p} + \mathbf{D_{tp}} + \mathbf{D_{tt}} (\mathbf{D_{tp}})$$

because $\mathbf{D_{tc}}$, the demand vector for all fuels and energies from the transportation within energy conversion and mining, is ϕ since no impacts from energy conversion have yet been computed. In the next step, $\mathbf{M_c}$ is computed by iteration within energy conversion and mining so that, in the following iteration between energy and transportation calculations, a new $\mathbf{D_c}$, including a $\mathbf{D_{tc}} \neq \phi$ can be determined.

Also, initially $\mathbf{D_{tt}}$, the total demand vector for all i's from the transportation of fuels needed for transportation itself, is only dependent on $\mathbf{D_{tp}}$, again since no energy and fuel conversion impacts have yet been computed. In the following round, $\mathbf{D_{tt}}$ is then increased by the demands arising from energy conversion. Its *final* demand, however, also needs to be solved by recursion because the fuels used in transportation need to be transported themselves. This is done in the following way (see Figure 5.):

$$D_{tt} = D_{tt} + \Delta D_{tt}(\Delta D'_{tt})$$

where:

D_{tt} = total demand vector for all i's from the transportation of fuels needed for transportation itself;

$\Delta D'_{tt}$ = fuel load increment for transportation;

ΔD_{tt} = fuel need increment needed to carry $\Delta D'_{tt}$

This recursion is repeated until:

$$|\Delta D_{tt}(\Delta D'_{tt})| \leq \zeta$$

where:

ζ = maximum absolute tolerance, i.e. 0.01 kg.

FIGURE 5.   Iteration Principle of the IDEA Materials and Energy Flow Model for the Energy and Fuel Demands Arising from the Transportation of Fuels Needed for Transportation Itself.
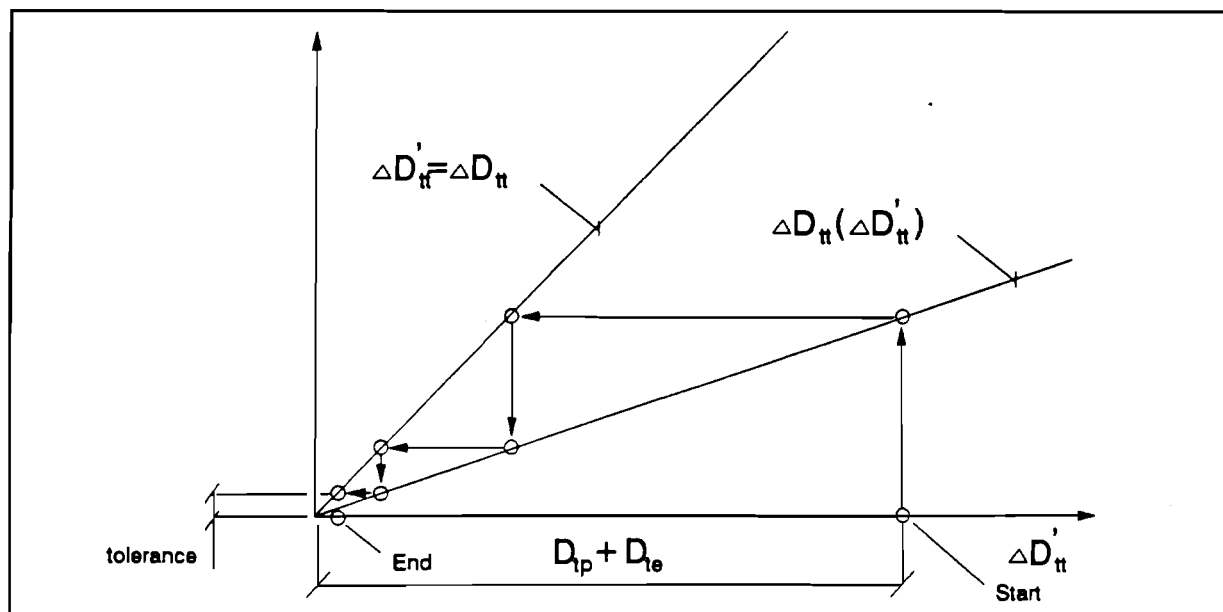
The recursion of iteration steps between transportation and energy calculations expressed by the general equation (1) is repeated for all external fuel and energy demands until the difference between consecutive steps meets the following condition (see **Figure 6.**):

$$\max \{ \, | (D_{e,i} - D'_{e,i}) / D_{e,i} | \, \} \leq \delta \qquad \text{for all i's;}$$

where:

$D_{e,i}$ =   total external energy and fuel demand from the production and consumption and transportation sectors calculated for i;

$D'_{e,i}$ =   previous energy and fuel demand from the production and consumption and transportation sectors calculated for i;

i =   final main product, or reference output, from the energy conversion or mining sectors, i.e. fuels and final energies;

δ =   maximum relative tolerance, i.e. 1%.

FIGURE 6. Iteration Principle of the IDEA Materials and Energy Flow Model for the Total External Energy and Fuel Demands.
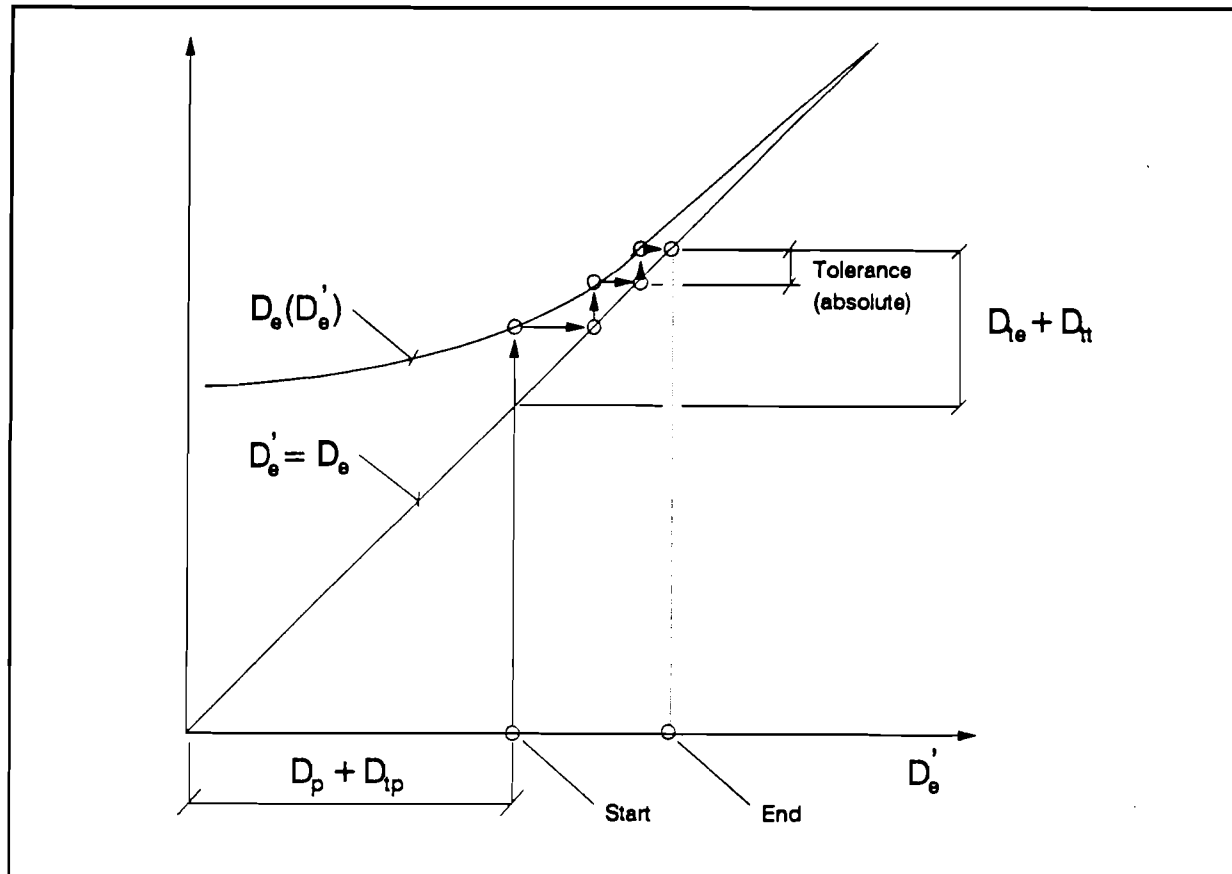
Now that we have explicitly calculated the total overall energy demand vector D_{tot} and the total external energy demand vector D_e, we can also compute the *final own use in the energy and fuel conversion and mining sectors:*

$$D_{eo} = D_{tot} - D_e$$

where:

D_{eo} =	energy and fuel demand vector for all i's within the energy conversion and mining;
D_{tot} =	total energy and fuel demand vector from all sectors (i.e. including energy conversion and mining) for all i's;
i =	final main product, or reference output, from the energy conversion or mining sectors, i.e. fuels and final energies.

This step then *concludes* the IDEA model run of *all cumulative impact calculations.*

3. Scenario Creation

Next to the database and the flow model, IDEA has a third feature of creating *alternative scenarios* in order to
- change assumptions made in the base case model runs;
- evaluate different policy options.

In general, the IDEA user can create scenarios that reflect
- *quantitative* changes under changing external demands;
- *structural* changes in the production, consumption and transportation profiles;
- *qualitative* changes in the unit processes themselves.

Scenarios of *quantitative changes* only due to changes in the output demands are created by simply inputing the new final demand(s). The IDEA model then recalculates the new impacts according to its linear production and consumption relationships.

Structural changes are introduced into scenarios by modifying the existing:
- mixture and distribution profiles between processes;
- substitution profiles into unit processes;
- transportation profiles for certain, or all, products;
- demand profile for the mix of final output demands.

In the scenario creation option of IDEA, these changes are made through an interface program directly in the object file so that the production and consumption tree structure does not have to be re-created before re-running the IDEA model part.

For scenarios of *qualitative changes* in process performance, such as increased energy efficiency or pollution control over time, or the replacement of a particular process by a new technology, no systematic or automized features are yet installed in the scenario creation option. The IDEA user can, however, create such scenarios by using the existing interface program for data editing; instead of using, however, the original database, a copy of these data should be used to make the desired modifications in the existing unit processes, or to add new unit processes.

The IDEA user can decide which database he/she wants to use as a starting point for creating any scenario. Generally, all scenarios should be created in working copies of the base data so that the original data are not modified. When the user wants to create his/her first scenario, obviously he/she has to start with the copy of the base data. Once he/she has already created a number of scenarios, however, the user can freely combine different scenarios from, for example, those already created in the energy and/or transportation sectors with others in the production and consumption sectors.

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Technical Annex

The Technical Annex describes the production processes covered in the IDEA database. It contains the data themselves for approximately 1000 so-called unit processes; the derivation of these data is described, the references to the appropriate literature are given, and the degree of aggregation as well as reliability are indicted as far as possible.

The IDEA database also contains about 1000 products which are described in this annex. Wherever relevant, the modes of transportation, their relative shares and the transport distances are described for these products.

The annex is organized according to the main economic sectors or, in some cases, logically-linked groups of processes covered in IDEA; these are:

(1) fuel and minerals and mining,
(2) energy conversion,
(3) goods transportation,
(4) inorganic chemicals production,
(5) organic chemicals production,
(6) glass production,
(7) pulp and paper production,
(8) aluminum production,
(9) iron & steel production,
(10) beverage container manufacture,
(11) waste management & recycling.

Most process and process chain descriptions are accompanied by flow charts that illustrate the linkages between the different processes and process steps. Each box on a flow chart represents a unit process for which data are contained in the IDEA database.

1. Minerals and Fuel Mining

1.1. Fuel Mining

This section describes the mining or extraction of following primary energy sources:
(1) hard and brown coal,
(2) oil,
(3) natural gas,
(4) wood.

1.1.1. Coal

Coal is not only an important primary energy source, but it is also used as a raw material in several processes, e.g., in coke production. Major coal producers are the United States, the Soviet Union and China. Most of the coal consumed in Western Europe comes from Germany, Great Britain and Yugoslavia. In 1988, coal ranked second in the production of useful energy and remained the dominant source of electricity generation from fossil fuel in Western Europe.

Mining

Coal is mined both from underground and surface mines. Run-of-mine coal from either of these mine types contains water, which was added during mining to suppress dust. Most important water emissions arise from the underground mining operation, because this operation consumes most water for dust suppression.

Air emissions from mining activities are highly dependent upon the mining technology used as well as on the control technology applied. The main atmospheric emissions are dust and those stemming from power generation. Water emissions are mainly in the form of acids, sulfates and suspended and dissolved solids. At the cleaning stage it is therefore important to distinguish between brown coal and hard coal as they have significantly different sulfur contents which translate into different emissions.

Acid mine drainage (AMD) is usually formed by the oxidation of sulfur bearing minerals in an aqueous environment, such as may exist in abandoned coal mines. The principal source of sulfur is iron pyrite, commonly found in coal seams and adjacent strata. The vast majority of the AMD pollution originates from abandoned coal mines. The principal adverse effects of AMD on surface and ground waters are excessive increases in dissolved solids, including calcium (Ca), manganese (Mg) and aluminum (Al), and a low Ph value. In the IDEA database we took account of AMD by including manganese and aluminum (Down and Stocks, 1977).

FIGURE 1.1: Coal mining and cleaning
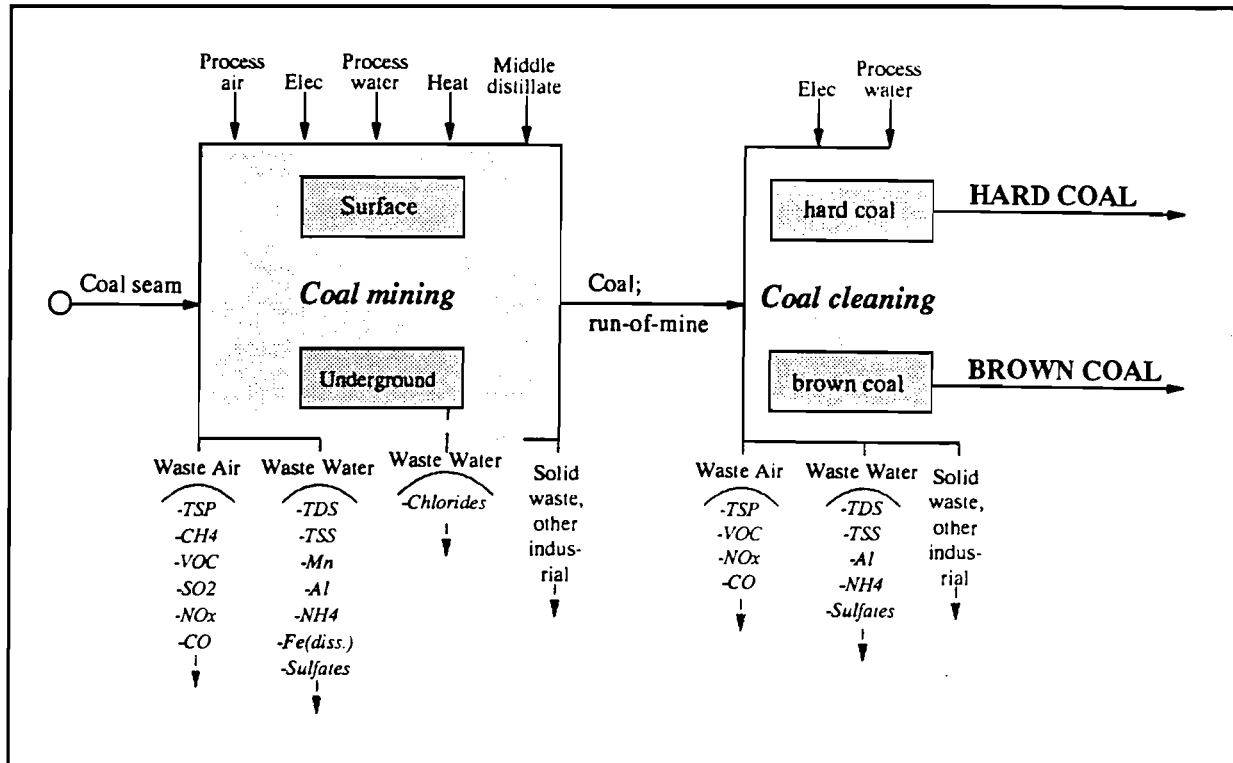
A. Surface Mining

In surface mining, coal seams that lie near the surface of the earth are exposed by excavators and shovels. In IDEA, we did not distinguish between the various mining types, but used data "typical" mining operations as employed by the major coal suppliers of Western Europe (Hittman Associates, 1974; Bechtel Corporation, 1975; OECD, 1989). Surface mining for European supply of brown coal is done mainly in Germany and Yugoslavia.

Water is required to suppress the large amounts of dust that are created by the excavation operations. Once discarded, this water may contain acid pollutants which contribute to acid mine drainage. Surface mining operations require relatively little electricity, and comparatively much middle distillate which powers the shovels, excavators, and other equipment.

Methane (CH_4) originates from the biochemical and geochemical conversion of organic substances. Mining processes can set free the methane produced during the formation of coal. The release of methane depends on the depth of the coal mined. As surface operations occur at low depths, emissions should be low and we used the OECD figure of 2.28 m^3/t (OECD, 1989).

B. Underground Mining

Underground mining for European supply is done mainly in Germany and Great Britain at medium depths. In underground coal mining, all equipment needs to be electrically powered, because otherwise air pollution emission would make the working conditions impossible. For this reason, we have different inputs and emission figures. We used energy data for underground mining mainly from Gelb and Pliskin (1979); Bechtel Corporation (1975) and CH_4 emission figures from OECD (1989).

Water consumption is very high in underground mining, since dust suppression is difficult in underground operations. Therefore the total suspended and dissolved solids load of the waste water is relatively high. Also, acid mine drainage may occur. As most equipment has to be electrically powered, electricity consumption figures are in underground mining significantly higher than for surface operations. Air pollutants from electrical equipment are not considered a problem and can thus be neglected.

Methane (CH_4) emissions increase with depth. Methane is adsorbed on the inner surface of the coal. It is significantly larger a problem in underground mining because surface, or close-to-surface mining activities only release a comparably small amount of CH_4. As underground mining for European supply is done at medium depths, we use in IDEA the OECD estimate of 14 m^3/t for an average depth of 14 m (OECD 1989).

Coal beneficiation

Coal beneficiation is a process for cleaning coal prior to its use for metallurgical or utility purposes. The purpose is to remove impurities (e.g. ash and/or sulfur). Coal beneficiation is done at, or close to, the mines so that we assume no transport for run-of-mine coal. In coal cleaning, raw coal is crushed by means of rotary screen breakers typically to a maximum size between 50 and 100 mm. After screening, the crushed coal is washed to reduce its sulfur content and to clean it from other impurities. Therefore, the solid waste generated is relatively high (i.e. 300 kg/t). On average, 1.42 t of run-of-mine coal are required per t of cleaned coal. This figure was calculated from data by Hittman Associates (1974), assuming a "typical" beneficiation operation.

We distinguish between hard coal cleaning and brown coal cleaning, as it is the different qualities, such as sulfur content, heating value and ash content of the coal types which translate into different emissions.

Emission data for brown coal cleaning are from Bechtel Corporation (1975). Brown coal has lower emission levels compared to hard coal, because of its lower sulfur and ash contents and calorific value. The data for hard coal cleaning are extrapolations of the figures given in the literature for brown coal and those from Loftness (1984). The figure for solid waste was taken from Hittman Associates (1974) and is based on averages calculated by the company. Table 1.1 shows different sulfur, ash and carbon contents as assumed in IDEA, of hard coal and brown coal.

TABLE 1.1: Different Fuel Qualities of Hard and Brown Coal.

%	Sulfur	Ash	Carbon
Hard Coal	2.5	10.0	78.0
Brown Coal	0.5	5.0	41.0

Before the cleaned coal is transported, it is usually dried to reduce its free moisture content and thus its likelihood to freeze. This is especially done in areas such as Northern Europe where coal has to be transported in sub-zero temperatures. Within Western Europe, coal is mainly transported by rail. Only little is also transported by inland ships and a few percent are brought to Europe by ocean going ships.The average distance (incl. empty return trips) over all brown coal consumed in Western Europe is 203 km by train. The average transport distance over all hard coal consumed in Western Europe is 1816 km by seagoing ships to Europe and 380 km by rail within Europe and abroad. Some coal is also transported by inland ships.

1.1.2 Oil and Natural Gas

Crude oil is drilled from deep wells, predominantly in the following three ways:

(1)   direct drilling, where the oil is directly extracted from the earth with pumps and the pressure comes from the natural hydrostatic pressure of the reservoir;

(2)   secondary drilling, where the oil is extracted with pumps, but the pressure is created by water injected into the reservoir;

(3)   tertiary drilling, where the oil is extracted in the same way as in secondary drilling, but chemicals are added to the water in order to seal the pores of the shaft and to increase the temperature in the reservoir so that the pressure increases.

Natural gas is obtained either from natural gas reservoirs (75 %) or as a by-product of so-called combined wells for oil and gas (25 %). At the drilling sites, the oil and gas are stored in floating roof tanks; from here they are transported to the refineries by pipeline or tanker. Oil and gas extraction generate both waterborne as well as airborne emissions. In the IDEA database, we include one unit process for "oil well" and one for "natural gas well and processing", and one process each for oil and gas distribution. These processes contain the losses from the products, but not the transportation emissions.

FIGURE 1.2: Oil Drilling

Natural Salt Light Heavy
gas water Elec fuel oil fuel oil   Natural gas

Crude oil/reservoir → Oil well → Extracted oil → Oil distribution → CRUDE OIL

Waste Air   Waste Water   Solid waste, other industrial
-CH4   -TDS
-VOC   -Oils
         -Salt
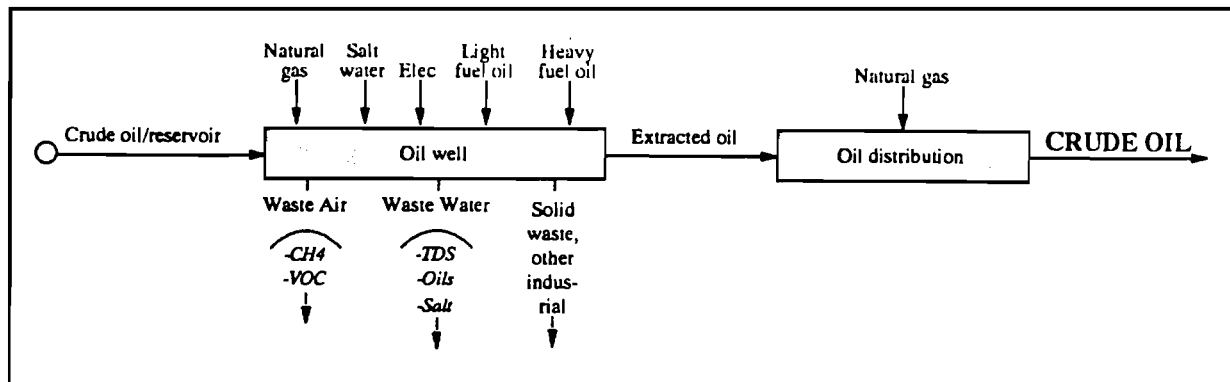
Oil Wells

Although there are significant differences between onshore and offshore drilling operations, insufficient data were available to allow us to distinguish between these two types. Data in IDEA are therefore an average over the various types of crude oil drilling. The open literature (Gelb and Pliskin, 1979; API, 1989) as well as personal communication with Oxley (1991) served as sources of our data. On average, the main input into oil drilling operations is salt, or brine, water. This water also comes out of the process again. According to the American Petroleum Institute (API), about 3350 million m3 of brine water were produced worldwide from crude oil production in 1985. This means that 5.4 m^3 of brine are generated per m^3 of oil and gas produced. Ninety % of this water is injected into wells specifically designed to accept production-related waters. Therefore, we only count the remaining 10 % of brine to determine the pollution emissions to water. This brine water carries a relatively high load of total dissolved solids (12.65 kg/t oil drilled) and oils (0.16 kg/t).

Atmospheric emissions are primarily in the form of volatile organic compounds (VOC) and methane (CH_4). These emissions come mainly from the gas contained in the oil well, as well as from losses and unflared venting operations during transport. These figures vary greatly between drilling sites and countries; in IDEA, we use the data provided by the OECD (1989) for CH_4 and by Bechtel (1975) for VOC.

FIGURE 1.3: Natural Gas Extraction
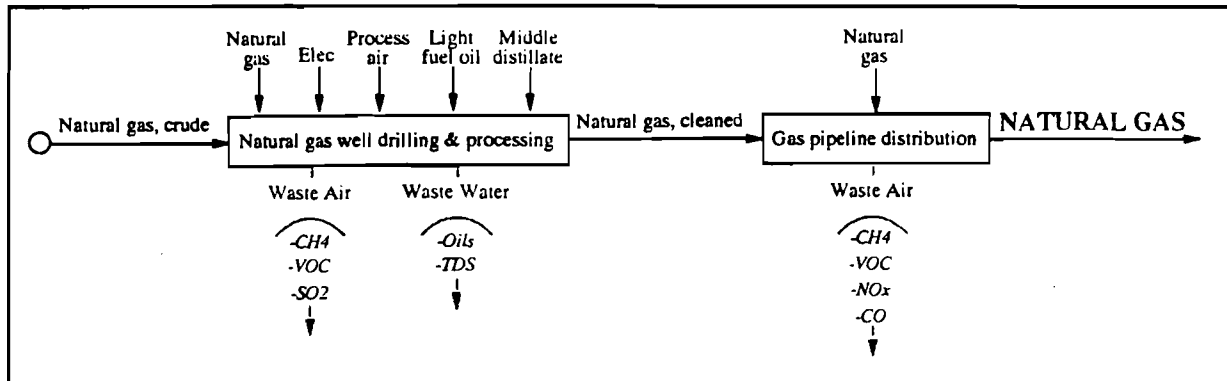
Natural Gas Well and Processing

Natural gas is a comparably clean fuel, although it may have a relatively high sulfur when coming out of the reservoir; this is removed by processing at the well. This operation is included in the IDEA unit process on gas wells. Data for drilling and processing are to be representative of typical operations. They were taken from Sellers and Sellers (1989). The major pollutants from gas drilling and processing include CH_4, VOC and SO_x to air, and oils and total suspended solids to water. The CH_4 and VOC from natural gas wells are significantly higher than from oil wells due to the higher volatility of the gas. The sulfur emissions originate from the gas processing an the sulfur originally contained in the gas. Emissions to water stem both from drilling and processing, and are oily in composition.

FIGURE 1.4: Wood harvesting
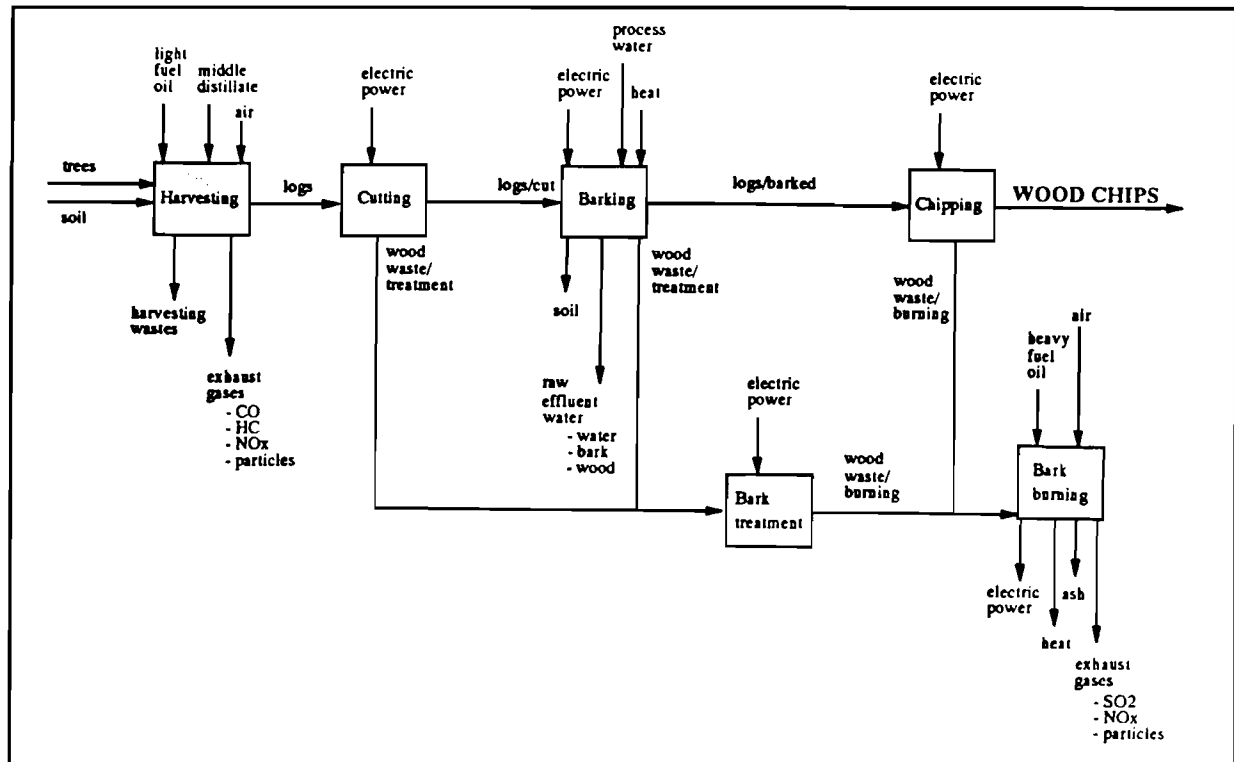
1.1.3. Wood Harvesting

Of all trees harvested, about 65% of the total biomass is recovered as logs. These are used by pulp mills, the wood products industry, and utility and industrial boilers.

There are several methods of logging, for example, using different types of saws, etc., as well as combinations of technologies. Only one unit process for wood harvesting is contained in IDEA. Data have been derived from Finnish forest statistics and constitute an average over the five main methods and technology combinations (Figure 1.3).

The only process inputs are fuels, mainly light fuel oil for chain saws, etc., as well as some middle distillate for other equipment. The outputs are 65% of the input trees as logs and the remaining 35% as waste trees that remain in the forest. The only emissions are those to air from combustion processes (i.e. CO_2, CO, SO_2, NO_x, VOC and TSP).

1.2. Minerals Extraction and Mining

The IDEA database contains the mining operations for several minerals which are basic primary material inputs into many production processes; these include:
- quartzsand,
- limestone,
- dolomite,
- feldspar,
- iron ore,
- iron-manganese (Fe-Mn) ore,
- bauxite,
- salt.

Quartzsand extraction is typical of all types of sand extraction and is thus described as a generic process; also, limestone, dolomite and feldspar are mined alike and are therefore described by the same data for stone quarrying.

FIGURE 1.5: Rock mining and rock and quartzsand preparation
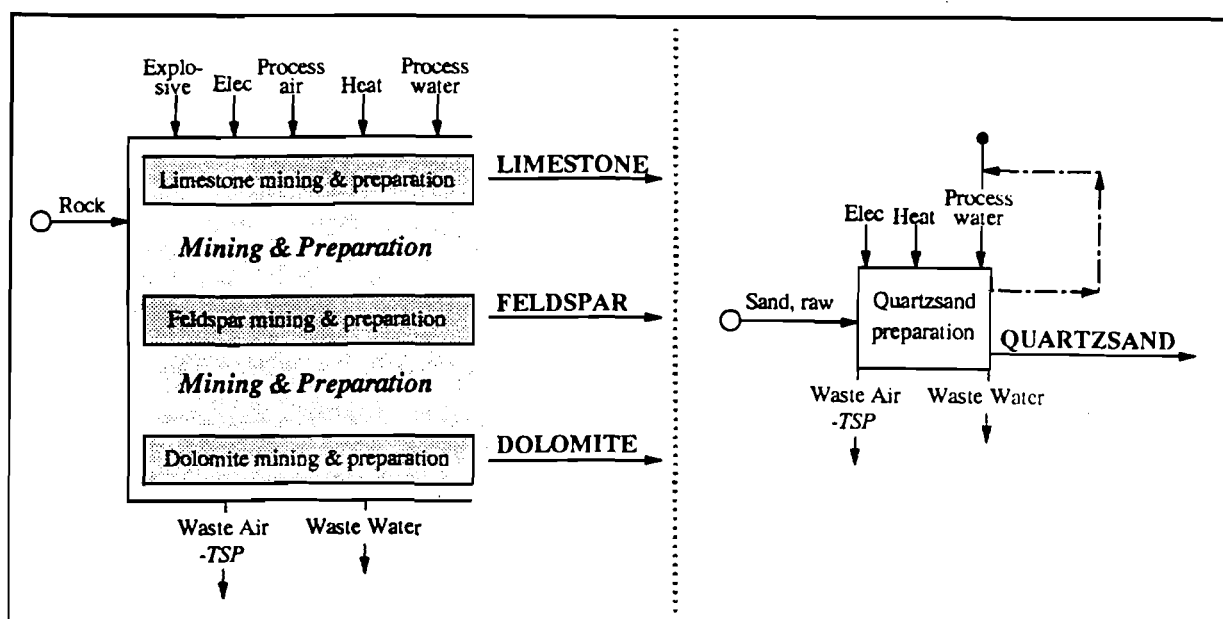
Sand Extraction

The process of (quartz)sand preparation is shown in Figure 1.4. The process basically involves repeated washing, drying and sieving. Inputs are thus energy and water; outputs include dust emissions to air (TSP) and waste water.

Stone Quarrying

Rock mining is shown in Figure 1.4. There are three unit processes included in IDEA, producing limestone, dolomite and feldspar. Process steps include excavation, crushing, grinding, sieving, washing and drying. Input and output quantities are identical for all three. In addition to energy and water, explosives are generally required. Environmental discharges include TSP to air and waste water.

Bauxite Mining

Aluminum is among the most widespread metals in the earth's crust. Naturally, it occurs as aluminum oxide, i.e. alumina (Al_2O_3), in corundum and as hydrated alumina in bauxite. In Europe, most bauxites are monohydrate aluminum oxides. Commercially, aluminum is made from alumina which, in turn, is produced from bauxite. The composition of bauxite varies according to where it is found; it contains 45 to 60 % alumina next to iron oxides and silica (SiO_2). It takes about 2 t of bauxite for each tonne of alumina, and again 2 t of alumina for 1 t of aluminum.

Iron ore mining

Iron (Fe) is found in various ores of which hematite (Fe_2O_2) is the most common one. Ore preparation includes
(1) mining,
(2) preliminary ore preparation, and
(3) ore concentration.
Iron ore is extracted both from deep mines and open-cast mines. Ore preparation basically involves repeated crushing, sifting, grinding and washing; emissions are mostly dust to the air and waste water containing suspended solids.

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2. Energy Conversion

The extraction of primary energies (i.e., crude oil, natural gas, brown and hard coal) from the earth is described in Section 1 "Fuel and Minerals Mining." This section describes their transformation into final energies or energy feedstocks.

2.1. Crude Oil Refining

Crude oil is made into fuels and chemical feedstocks at *refineries* that comprise several different plants. Since these plants make use of the various co-products produced in other production units on-site, refineries can generally be seen as a system of several nearly-closed production cycles.

Crude oils consist of hydrocarbons of varying composition with different boiling points. Imported oil, and crude from European oil fields, are first fractionated under atmospheric pressure in a *crude oil distillation plant* to yield the so-called naphtha-cut which includes gasoline, gas-oil and residual fuel oil. This naphtha stream goes to the *ethylene plant*, i.e. the *steam cracker*. Top-gas forms at the top of the distillation column and comes from the gas originally dissolved in the crude oil; it is further used to produce ethane, propane, butane and the C_4-fraction.

The portion of the crude oil that cannot be fractionated under atmospheric pressure is led to a *vacuum distillation plant*. The resulting vacuum distillates are then broken down in a *catalytic cracker* into gasoline, gas oil and various fuels for heating. The residue from the vacuum distillation plant goes to the *bitumen oxidation plant* where it is processed for further use by the road construction industry.

In the IDEA database, we treat *"crude oil refining" as one unit process*. This was decided after consultation with various oil refineries (Richter, pers. comm., ÖMV; etc.) and CONCAWE (Lyons, 1991) for the following reasons:

(1) In Western Europe, there are refineries of different degrees of complexity, and it would be extremely difficult to identify one, or even several, "typical" one(s).
(2) Different refineries include different processes, process steps and combinations of processes, and none of them require "typical" inputs or produce "typical emissions."
(3) Through CONCAWE, on the other hand, the environmental impacts of refineries in Western Europe have been studied extensively.
(4) As a result, CONCAWE (Lyons, 1991) has had available data for input requirements as well as emissions and effluents aggregated for Western Europe.
(5) The total amount of crude oil input to Western European refineries as well as the total output of marketable products is available from oil statistics (International Petroleum Institute; Lyons, 1991).

Refinery data in the IDEA database have therefore been determined from these aggregated data, that is, total emissions, energy inputs, etc., have been related to total crude oil input. Since, for production processes, however, IDEA requires output-related flows, we had to decide how to distribute energies and emissions to the various refinery output products. Again, this was done in concordance with CONCAWE (Lyons, 1991). According to Lyons (pers. comm., 1991), it is not possible to allocate emissions, etc., to specific refinery outputs in specific ratios. We therefore agreed to use emissions factors, energy requirements, etc., for *all* refinery outputs, although we are aware that certain outputs require more process-steps, or more energy intensive ones, than others. Since different emission data were available for the distribution of fuels and chemical feedstocks, we distinguish between these two categories in the distribution step which constitutes a separate unit process. Table 2.1 lists the refinery output products as supplied by CONCAWE (Lyons, 1991) and used in IDEA. Within the scope of our study it was, however, not possible to make any more-detailed investigations.

IDEA thus includes unit processes for *"fuel refining"* and *"chemical feedstock refining"* which contain identical data, and unit processes for *"fuel distribution"* of each of the fuels produced, again with identical data, as well as unit processes for *"chemical feedstock distribution"* of each of the feedstocks from the above list (see figure 2.1).

FIGURE 2.1: Oil refining and petroleum product distribution
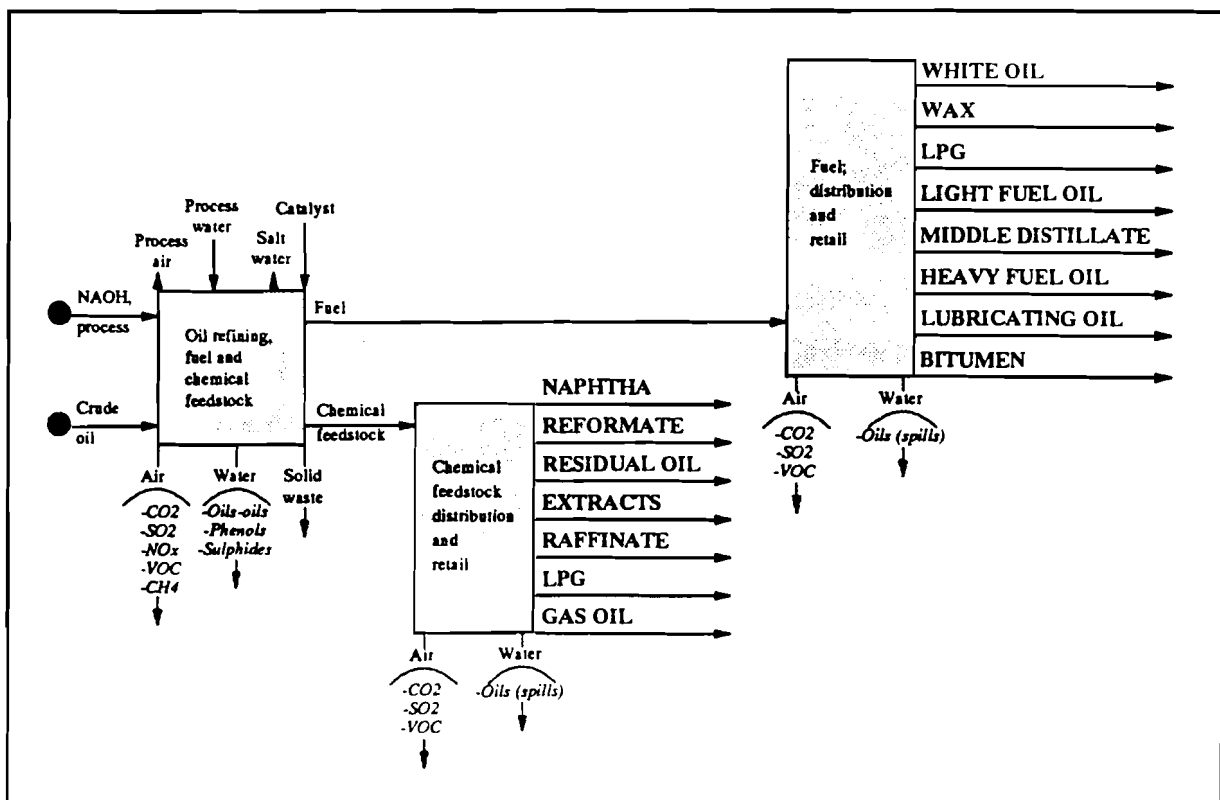
2.2. Coking

In the production processes presently covered in the IDEA database, coke, or derived (i.e., carbonized) coal is mainly needed in the iron production and in industrial fuel combustion, such as boilers, but it is also used in some other processes. Coke ovens are generally part of the iron and steel plants. The coal is first crushed, screened and blended, and then charged into the *coke oven*. In coking, which is a batch process, the coal is carbonized and coke oven gases are formed. When the batch is finished, the hot coke is pushed from the oven and quenched with water. It is dried on the coke wharf, screened and used on-site or shipped for further use elsewhere. Approximately 1.3 t coal is needed to produce 1 ton coke.

The coke oven gases are vented to a by-product plant where they are cleaned and salable products such as ammonia, tar, liquor, light oils, etc., are recovered. The cleaned gas, which mainly consist of methane (CH_4) and carbon monoxide (CO), is recycled for further use within the steel plant. In addition to the by-products from coke oven gas, coke breeze is also recovered from coke screening and used in industrial processes such as sintering.

2.3. Electricity Production in Western Europe

The electricity consumed by an industry, or by electric trains, has to be converted into primary energy requirements, and the correct share of air and water pollutant emissions resulting from the production of this electricity has to be allocated to its use. In order to be able to do so we have to know the conversion efficiency of electricity production, and the relative shares of primary fuels that produce this electricity.

From the Economic Commission for Europe (UN ECE, 1986) and the International Energy Agency (OECD IEA, 1987), we know the total consumption of fuels for electricity production in power stations in Western Europe. This information was extracted from IIASA's RAINS database (Alcamo et al., 1990) and used in IDEA.

In 1985, the 17 Western European countries (Austria, Belgium, Denmark, Finland, France, the Federal Republic of Germany, Greece, Ireland, Italy, Luxembourg, the Netherlands, Norway, Portugal, Spain, Sweden, Switzerland, and the United Kingdom) consumed a total of 18,463 Petajoule (PJ) of fuel to generate 7,464 PJ of electricity; 9,219 PJ were from fossil fuels whereas the remainder was from nuclear- and hydro-power. From the OECD energy balances (OECD IEA, 1986), we know that the distribution and pump losses and own consumption of the electricity generating plants make up about 13 % so that the final electricity consumed amounts to 6494 PJ. From these figures we can calculate an overall conversion efficiency for net electricity consumption of 35.2 %. Table 2.2 gives the absolute amounts, as well as the relative shares, of the individual fuels used in 1985 in West European electricity production.

In this table, nuclear and hydro-power are given in primary fossil fuel energy equivalents needed to produce a given output of electricity; a theoretical efficiency of 38.5 % has been used (OECD IEA, 1986).

This profile and the 35.2 % efficiency serve as the basis in IDEA to convert demands for "electric power" which has no further fuel-specific extension into primary fuel requirements. If further fuel-specific extensions, e.g., electric power from hard coal" are given, the fuel-specific production data are used.

TABLE 2.1: Refinery Output Products (Lyons, 1991)

Petroleum product	Product name in IDEA
Fuels:	
LPGs	LPG
gasolines	light fuel oil
kerosines	
diesel fuels	middle distillate
heating/gas oils	
residual fuels oils	heavy fuel oils
lubricating oils	lubricating oils
bitumens	bitumen
white oils	white oil
waxes	wax
Chemical Feedstocks:	
LPGs	LPGs
naphthas	naphtha
reformats	reformat
gas oils	middle distillate/chemical feedstock
residuals	heavy fuel oil/chemical feedstock
extracts	extract
raffinates	raffinate

Air pollution emission factors from electricity production in power plants

In order to calculate the composite air emission factors for European electricity production, we used the relative contribution of the different fossil fuels to the production of one unit of electricity, as well as the specific emission factors for each fossil fuel type from power plants. Fuel-specific emission factors were either taken directly from the literature or derived from total European emissions from power plants. In the latter case, we made use of the IIASA RAINS model (Alcamo et al., 1990). RAINS gives total sulfur dioxide (SO_2) and nitrogen oxide (NO_x) (as NO_2) emissions per country, fuel and major emission sector, one of which is power plants; the model further contains the energy inputs by the individual fuel types (see Table 2.2). We added, for each fuel type, the total emissions of SO_2 and NO_x from power plants in the 17 West European countries, and then divided these by the total fuel input into electricity generation; in this way we obtain a specific emission factor per Petajoule of fuel input, representative of Western European conditions (see Tables 2.3 and 2.4). From these emission factors and the relative shares of fuel in West European electricity production (see Table 2.2), we compute a composite emission factor of 533 t/PJ fuel input for SO_2 and of 132 t/PJ fuel input for NO_x (as NO_2). To relate these emission factors to 1 PJ of electricity consumption, we have to take the 35.2 % conversion efficiency into account so that the resulting emission factors are as follows: 1514 t/PJ of electricity consumption for SO_2 and 375 t/PJ of electricity consumption for NO_x (as NO_2).

In addition to SO_2 and NO_x, electricity production also emits carbon monoxide (CO), carbon dioxide (CO_2) and volatile organic compounds (VOC). For CO and CO_2, we use emission factors characteristic of Western Europe which have been elaborated by the Energy and Environment Group of OECD for a project on climate change (OECD, 1989). From these emission factors we have calculated fuel-specific total emissions of CO and CO_2 and weighted composite emission factors per 1 PJ fuel input as well as per 1 PJ electricity consumption; these are presented in Table 2.5 for CO and in Table 2.6 for CO_2.

For VOC, the weighted composite emission factors were determined in a similar way, using the RAINS energy data (Alcamo et al., 1990) and fuel-specific VOC emission factors from the Swiss Environment Agency (BfU, 1987). This results in xx t/PJ of fuel input and xx t/PJ of electricity consumed.

Table 2.7 summarizes all emission factors based on 1 PJ of electricity consumed.

TABLE 2.2: Fuel Consumption for Electricity Generation in Western Europe in 1985 (Alcamo et al., 1990)

FUEL	CONSUMPTION		
	PJ	**% OF TOTAL FUEL**	**% OF FOSSIL FUEL**
Brown coal	1429.0	7.7	15.5
Hard coal	4900.0	26.5	53.2
Derived coal	0.0	0.0	0.0
Light fuel oil	0.0	0.0	0.0
Middle destillate	42.0	0.2	0.5
Heavy fuel oil	1654.0	9.0	17.9
Gas	1025.0	5.6	11.1
Other solids	169.0	0.9	1.8
TOTAL FOSSIL FUEL CONSUMPTION	9219.0		100.0
Nuclear-power	5468.0	29.6	
Hydro-power	3776.0	20.5	
TOTAL PRIMARY FUEL CONSUMPTION	18463.0	100.0	
ELECTRICITY PRODUCTION	7464.0		
Distribution and other losses (13 %)	970.0		
NET ELECTRICITY CONSUMPTION	6494.0		
NET EFFICIENCY [%]	35.2		

TABLE 2.3: SO₂ Emissions per Fuel Type from Power Plants in Western Europe (Alcamo et al., 1990)

FUEL	SO2 EMISSIONS [kt]	ENERGY CONSUMPTION [PJ]	SO2 EMISSION FACTOR [t/PJ]
Brown coal	2732.1	1429.0	1911.9
Hard coal	4409.2	4900.0	899.8
Middle destillate	9.5	42.0	226.2
Heavy fuel oil	2679.9	1654.0	1620.3
TOTAL (per primary fuel consumption)	9831.0	18463.0	532.5
TOTAL (per net electricity consumption)	9831.0	6494.0	1513.9

TABLE 2.4: NO$_x$ Emissions per Fuel Type from Power Plants in Western Europe (Alcamo et al., 1990)

FUEL	Nox EMISSIONS [kt]	ENERGY CONSUMPTION [PJ]	Nox EMISSION FACTOR [t/PJ]
Brown coal	385.9	1429.0	270.0
Hard coal	1561.4	4900.0	318.7
Heavy fuel oil	330.8	1654.0	200.0
Gas	154.0	1025.0	150.2
TOTAL (per primary fuel consumption)	2432.0	18463.0	131.7
TOTAL (per net electricity consumption)	2432.0	6494.0	374.5

TABLE 2.5: CO Emissions per Fuel Type from Power Plants (OECD, 1989b)

FUEL	ENERGY CONSUMPTION [PJ]	CO EMISSION FACTOR [t/PJ]	CO EMISSIONS [kt]
Brown coal	1429.0	28.0	40.0
Hard coal	4900.0	13.0	63.7
Middle destillate	42.0	14.0	0.6
Heavy fuel oil	1654.0	14.0	23.2
Gas	1025.0	17.0	17.4
TOTAL (per primary fuel consumption)	18463.0	7.8	144.9
TOTAL (per net electricity consumption)	6494.0	22.3	144.9

TABLE 2.6: CO_2 Emissions per Fuel Type from Power Plants (OECD, 1989b)

FUEL	ENERGY CONSUMPTION [PJ]	CO2 EMISSION FACTOR [kt/PJ]	CO2 EMISSIONS [Mt]
Brown coal	1429.0	109.6	156.6
Hard coal	4900.0	99.7	488.5
Middle destillate	42.0	73.0	3.1
Heavy fuel oil	1654.0	73.0	120.7
Gas	1025.0	50.6	51.9
TOTAL (per primary fuel consumption)	18463.0	44.5	820.9
TOTAL (per net electricity consumption)	6494.0	126.4.0	820.9

Table 2.7: Weighted Composite Emission Factors for Air Pollutants Emitted by Fossil-Fueled Power Plants in Western Europe

EMISSION FACTORS [per PJ electricity consumed]				
CO2 [kt/PJ]	CO [t/PJ]	SO2 [t/PJ]	Nox [t/PJ]	VOC [t/PJ]
126.4	22	1514	375	8

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3. Transportation

Transportation of materials is an important component when calculating total air pollution impacts and energy requirements of production systems. Raw materials have to be transported to the place of production, intermediate products have to be shipped to their place of final assembly, the finished products have to reach the retail stores, and finally, the discarded products have to be taken to their ultimate disposal sites.

Our data base contains 15 different unit processes for road, rail, ship and pipeline transportation, as well as transportation mode and distance profiles for each input product; these profiles are generally linked to the input and sometimes to the output flows (see report "Theory", Section 1.2.2.)

Description of the different transportation modes

The majority of goods is transported by rail, ship and truck. Total energy requirements as well as air emissions depend predominantly on the transport distances, mode of transportation and fuels used. This section describes the derivation of the unit energy requirements and unit air pollutant emission factors as they are used for all transport calculations in IDEA. Unit energy requirements as well as emission factors are given on a per tonne-kilometer basis so that the only material-specific transportation information needed is the average transport distance in Western Europe and the transportation mode.

In cases where no product- and process-specific transportation information is available, a group specific average transportation profile is applied; 11 different groups of goods are included. These data were selected from German transportation statistics for which distances and model splits are available (Bundesminister für Verkehr, 1985). From OECD statistics, we had available the modal split of all freight transport in Western Europe (OECD, 1991). The average transportation distance for all goods transport was a weighted average net haul distance per tonne of goods transported for each transportation mode, based on European transportation statistics from the UN ECE (1986). These distances were obtained by dividing the net freight kilometers by the total freight volume in Western Europe.

In order to make these Western European averages goods-specific, German data were adjusted to match the weighted average data for OECD Europe for distance as well as for modal split. The resulting modal split for Western Europe is given in Table 3.1; the average goods-specific transportation distances are given in Table 3.2.

TABLE 3.1: Average European freight transportation profile [%] (OECD, 1991).

FREIGHT TRANSPORT year = 1988	OECD-EUROPE [%]	COMMENTS
road/truck	65.0	
urban	24.7	38.0 % of truck
rural	28.3	43.5 % of truck
highway	12.0	18.5 % of truck
rail	18.0	
electric	13.5	75.0 % of rail
diesel	4.5	25.0 % of rail
inland ship	8.0	
pipeline	9.0	
sum	100.0	

2.1. Rail

Freight trains in Europe use either diesel or electricity as fuel, which determines their energy requirements as well as their unit emission factors.

Energy requirements

From the European transportation statistics (UN ECE, 1986), we know that in Western Europe in 1984, the total gross freight transport by train was 534,311 million t-km, and that 75 % of this transport was by electric trains and 25 % by diesel engines. From the OECD IEA 1984 energy statistics (1986), we know that rail transport consumed a total of 142 PJ of electricity and 121 PJ of diesel fuel.

In order to compute the energy requirements per gross tonne-kilometer transport, we would need, in addition, either the total gross passenger tonne-kilometers, or the fuel consumption by freight trains alone, neither of which is given in the statistics. Thus, we have to make a few assumptions that allow us to compute these.

TABLE 3.2: Goods-specific transportation profile for OECD-Europe [%]

GOODS TYPE	RAIL electric	RAIL diesel	SHIP inland	TRUCK highway	TRUCK rural	TRUCK urban	PIPELINE	SUM
year = 1988	goods transported [%]	goods transported [%]	goods transported [%]	goods transported [%]	goods transported [%]	goods transported [%]	goods transported [%]	goods transported [%]
foods	.5.2	1.7	3.2	19.6	46.2	24.1	0.0	100.0
incl.: grains	0.0	0.0	100.0	0.0	0.0	0.0	0.0	100.0
sand, clay	3.7	1.2	17.0	3.3	7.9	66.8	0.0	100.0
stones, minerals, salt	5.9	2.0	8.6	5.9	13.8	63.8	0.0	100.0
ore, metal wastes	41.6	13.9	26.9	3.6	8.5	5.4	0.0	100.0
solid fossil fuels	45.7	15.2	23.9	2.3	5.4	7.6	0.0	100.0
oils, petroleum products	6.3	2.1	10.3	2.2	5.2	17.6	56.3	100.0
fertilizers	42.8	14.3	20.4	4.9	11.6	6.0	0.0	100.0
mineral/construction products, glass	4.3	1.4	1.2	15.3	36.1	41.7	0.0	100.0
iron & steel, incl. intermediates	30.6	10.2	8.5	11.8	27.9	11.0	0.0	100.0
machinery	6.9	2.3	0.6	23.1	54.4	12.7	0.0	100.0
other goods	16.4	5.5	4.6	16.8	39.5	17.2	0.0	100.0
incl.: chem.products	0.0	0.0	0.0	29.8	70.2	0.0	0.0	100.0
OECD average over all goods	13.5	4.5	8.0	12.0	28.3	24.7	9.0	100.0

TABLE 33: Goods-specific average transportation distances in OECD-Europe

GOODS TYPE	RAIL	INLAND SHIP	TRUCK HIGHWAY/RURAL	TRUCK URBAN	PIPELINE
year = 1984	avg. distance [km]	avg. distance [km]	avg. distance [km]	avg. distance [km]	avg. distance [km]
foods	311	208	134	17	0
incl.: grains	0	212	0	0	0
sand, clay	172	112	81	10	0
stones, minerals, salt	118	136	106	4	0
ore, metal wastes	123	81	115	11	0
solid fossil fuels	102	176	119	8	0
oils, petroleum products	156	148	82	17	144
fertilizers	243	197	119	14	0
mineral/construction products, glass	175	155	106	16	0
iron & steel, incl. intermediates	145	154	147	19	0
machinery	386	187	164	14	0
other goods	312	165	144	11	0
incl.: chem.products	0	0	158	0	0
OECD European average	215	147	138	12	144

Note: German goods-specific distances adjusted to the overall average European distances.

From the difference between gross and net freight transport, we have calculated an average weight per freight train of 410 t. We assume that a passenger train only weighs about 25 % of a freight train, and that it carries a load of 4 t, i.e. 500 persons at 80 kg/person. By multiplying the resulting gross passenger train weight of 106 t with the total passenger train kilometers (1955 million km), we obtain the gross passenger tonne-kilometers (208,169 million t-km). Using an equal ratio between electricity (75 %) and diesel (25 %) for passenger trains as for freight trains, we can compute that, of total rail transport, 559,273 million t-km were by electric trains and 183,206 million t-km by diesel trains. When dividing the total electricity and diesel consumptions by the respective freight volumes, we obtain an average energy requirement of 0.25 MJ per gross t-km for electric trains, and 0.68 MJ/t-km for diesel trains.

Since average transport distances are given in net km/t, we have to still divide these figures by the freight train load efficiency, i.e. net tonne-kilometers over gross tonne-kilometers, or 43.2 %. This then gives us an average energy requirement of 0.59 MJ of electricity per net t-km for electric trains, and an average fuel requirement of 1.57 MJ per net t-km for diesel trains. Note that, in this context, "net" means only per tonne of good transported *excluding* the weight of the trains themselves, but *including* all empty trips.

Air pollution emission factors

Emissions from railroads are those typical of combustion; they are listed in Table 3.4 on a per PJ energy consumption basis. By taking the above energy consumption figures, we can convert these emission factors to a mg/t-km basis (see Table 3.5). For electric trains, emission factors correspond to those of energy production in power plants. Although these are included in Table 3.5 for comparative purposes, they are not included in the unit process "electric train transport"; in the IDEA database, electric trains only require as input the final amount of electricity per t-km; the emissions are only calculated when this electric power demand is converted to primary energies in the energy conversion sector.

TABLE 3.4: Rail Emission Factors [per unit energy consumption]

TRANSPORT MODE	FUEL	EMISSION FACTORS					
		CO_2 [kt/PJ]	Nox [t/PJ]	VOC [t/PJ]	CO [t/PJ]	TSP [t/PJ]	SO_2 [t/PJ]
RAIL	diesel	69.7	1200	100	570	60	235
RAIL	electric	126.4	375	8	22	0	1514

TABLE 3.5: Rail Emission Factors [per net t-km]

TRANSPORT MODE	FUEL	EMISSION FACTORS					
		CO_2 [g]	Nox [mg]	VOC [mg]	CO [mg]	TSP [mg]	SO_2 [mg]
RAIL	diesel	109.3	1884.0	157.0	894.9	94.2	369.0
RAIL	electric	74.6	221.3	4.7	13.0	0	893.3

2.2. Ship

In shipping, we have to differentiate between inland and ocean-going vessels. Both types of vessels are mostly diesel-fueled, although ocean-going ships often use lower grades of fuel, and sometimes even heavy fuel oil. As a result, the emission factors for ocean-going ships are higher.

Energy requirements

The energy requirements for inland ships have been derived from 1984 data for three countries: France, the Federal Republic of Germany and the Netherlands. These countries were chosen because (1) the European transportation statistics (UN ECE, 1986) and the OECD IEA 1984 energy statistics (1986) had sufficient data available, and (2) these countries have extensive goods transport by inland ships. By dividing their total diesel consumption used in 1984 in inland shipping (50 PJ) by the total net freight tonne-kilometers (94,469 t-km), we obtain an average energy requirement of 0.53 MJ/t-km.

Based on available data in the European transportation statistics (UN ECE, 1986), energy requirements for seagoing vessels have been computed for Western Europe (with the exception of the Federal Republic of Germany, Ireland and Italy) per tonne of goods loaded, by dividing the fuel consumption for seagoing ships in 1984 by their total freight loaded in the ports during the same year. This gives an average value of 1592 MJ/t loaded. By knowing the average transport distance, one may arrive at a fuel requirement per tonne-kilometer. However, no general statistics are available on such distancès. On the other hand, Sauer (1974) gives an average energy consumption for tankers of 0.46 MJ/t-km. Dividing the 1592 MJ/t by this value gives an average transport distance of 3460 km, which appears reasonable.

Emission factors

Again, emissions from boats are those typical of combustion and, for the two types of ships, the different emission factors are listed in Table 3.6, In Table 3.7, these emission factors have been converted to mg/t-km. Conversions are based on the average fuel requirements of 0.53 MJ/t-km for inland and 0.46 MJ/t-km for transatlantic shipping.

TABLE 3.6: Ship Emission Factors [per unit energy consumption]

TRANSPORT MODE	FUEL	EMISSION FACTORS					
		CO_2 [kt/PJ]	Nox [t/PJ]	VOC [t/PJ]	CO [t/PJ]	TSP [t/PJ]	SO_2 [t/PJ]
SHIP, seagoing	diesel	72.6	1200	300	320		235
SHIP, inland	diesel	70.4	1100	140	320		235

TABLE 3.7: Ship Emission Factors [per net t-km]

TRANSPORT MODE	FUEL	EMISSION FACTORS					
		CO_2 [g]	Nox [mg]	VOC [mg]	CO [mg]	TSP [mg]	SO_2 [mg]
SHIP, seagoing	diesel	33.4	552.0	138.0	147.2		108.1
SHIP, inland	diesel	37.3	583.9	74.3	169.9		124.8

2.3. Road Transport

In most European countries, the predominant mode, to-date, of transporting goods between different locations are probably trucks. Especially relatively small, finished consumer products reach the end-user by truck. Also, all household wastes are collected by trucks. Since trucks are so often used, this transportation mode should receive particular attention. We have to distinguish between trucks in urban and long distance transport, and more specifically, between rural and highway driving, and between gasoline- and diesel-fueled trucks. Due to their different driving conditions, these trucks have very different energy requirements as well as emissions.

Energy requirements and emission factors used in our calculations are predominantly based on the work of an EC working group on emissions from vehicles (Eggleston et al., 1989; Samaras and Zierock, 1989). In this section, we explain the assumptions behind these Western European average values.

Energy requirements

Average European fuel consumption figures for the three vehicle classes

(1) light duty gasoline-fueled vehicles,
(2) diesel-fueled trucks between 3.5 and 16 t,
(3) diesel-fueled trucks larger than 16 t,

and the three driving modes

(1) urban,
(2) rural,
(3) highway,

are based on Eggleston et al. (1989) and are given in Table 3.8. By using the average energy content values of 47.7 MJ/kg for gasoline and 44.7 MJ/kg for diesel, we have computed the average energy consumption figures per kilometer travelled, which are also listed in Table X15, and which are used in the IDEA database. These fuel consumption data represent composite average values weighted over the fleets in the different EC countries. Implicit in these consumption figures are the fleet composition and average load of the vehicles. They are further based on the average speeds, which, in the EC countries, are 25 km/h for urban, 70 km/h for rural and 95 km/h for highway travel. In cases where no data are available on the fractions of travel on the different road types, the working group gives average shares of 38 % for urban, 43 % for rural and 18 % for highway driving.

In order to convert the energy requirements to a per tonne-kilometer basis, we need information on the average load of the vehicles in each class. From (R. Rijkeboer, pers. oral comm. 1990) we know that the average load for all trucks is approximately 50%; this is derived from Dutch figures indicating that 70% of the full load capacity is utilized on loaded trips, and that 30% of all trips are empty trips. Resulting energy requirements per t-km are presented in Table 3.9 and are based on average vehicle weights of 3.5t, 12t and 16t for the three classes, respectively.

TABLE 3.8: Fuel Consumption for the Different Driving Modes at Average EC Speeds and Average Vehicle Loads

TRANSPORT MODE	FUEL CONSUMPTION [kg/100 km]			ENERGY CONSUMPTION [MJ/km]		
	URBAN	RURAL	HIGH WAY	URBAN	RURAL	HIGH WAY
Light duty, gasoline, > 3.5 t	22.5	10.0	16.5	10.7	4.8	7.9
Heavy duty, diesel, 3.5-16 t	21.5	20.6	20.6	9.6	9.2	9.2
Heavy duty, diesel, > 16 t	36.3	37.1	30.5	16.2	16.6	13.6

Emission factors

Emission factors for the various pollutants from transportation are taken from Eggleston et al. (1989) for CO, VOC, NO_x and TSP, from OECD (1989) for CO_2, and from Veldt and Bakkum (1988) for SO_2; they are given on a per kilometer basis and represent composite average values weighted over the fleets in the different EC countries. Implicit in these factors are the different climate conditions in Europe and thus, hot/cold start ratios, etc., the fleet composition and average age of vehicles, average vehicle load, average fuel consumptions as given above, and average speeds as given. They represent the best available Western European averages.

Within each driving mode, we distinguish between emission factors for light duty gasoline-fueled vehicles and the two sizes of diesel-fueled trucks, those between 3.5 and 16 t, and those larger than 16 t. For urban, rural and highway driving, these are listed in **Tables 3.9, 3.10 and 3.11**, respectively.

In **Tables 3.12-3.13**, these emissions have been converted to a per tonne-kilometer basis.

TABLE 3.9: Truck Emission Factors for Urban Driving [per km travelled]

TRANSPORT MODE	FUEL	EMISSION FACTORS					
TRUCK: urban		CO_2 [g/km]	NO_x [g/km]	VOC [g/km]	CO [g/km]	TSP [g/km]	SO_2 [g/km]
Light duty, > 3.5 t	gas	590.7	4.5	7.0	70.0	0.0	0.0
Heavy duty, 3.5-16 t	diesel	669.8	11.8	2.6	6.0	0.9	2.3
Heavy duty, > 16 t	diesel	1130.2	18.2	5.8	7.3	1.6	3.8

TABLE 3.10: Truck Emission Factors for Rural Driving [per km travelled]

TRANSPORT MODE	FUEL	EMISSION FACTORS					
TRUCK: rural		CO_2 [g/km]	Nox [g/km]	VOC [g/km]	CO [g/km]	TSP [g/km]	SO_2 [g/km]
Light duty, > 3.5 t	gas	265.0	7.5	5.5	55.0	0.0	0.0
Heavy duty, 3.5-16 t	diesel	641.8	14.4	0.8	2.9	0.9	2.2
Heavy duty, > 16 t	diesel	1158.1	24.1	3.0	3.7	1.6	3.9

TABLE 3.11: Truck Emission Factors for Highway Driving [per km travelled]

TRANSPORT MODE	FUEL	EMISSION FACTORS					
TRUCK: highway		CO_2 [g/km]	NO_x [g/km]	VOC [g/km]	CO [g/km]	TSP [g/km]	SO_2 [g/km]
Light duty, > 3.5 t	gas	436.1	7.5	3.5	50.0	0.0	0.0
Heavy duty, 3.5-16 t	diesel	641.8	14.4	0.8	2.9	0.9	2.2
Heavy duty, > 16 t	diesel	948.8	19.8	2.4	3.1	1.3	3.2

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4. Inorganic Chemicals

A number of inorganic chemicals are important inputs into many production processes covered by the IDEA database. In a complete life-cycle analysis, the production of these chemicals should thus be described. Since the inorganic chemicals industry is, however, not one of main industrial sectors covered in this study, the presentation processes of each chemical are generally depicted as one unit process although, in reality, they consist of several steps.

Wherever possible, we took data for the most commonly-used production process in Western Europe. Since chemical companies rarely allow access to their production data, we had to rely predominantly on published literature. The current data set should thus be regarded as a starting point for further investigation in the field of inorganic chemicals production.

Table 4.1 gives an overview of all chemicals for which production data are contained in the IDEA database.

The following section describes briefly their production processes. For transporting these chemicals from the manufacturer to the consumer, an average transportation profile for OCED Europe was taken: Chemicals are transported by truck over 158 kilometers, 30% on highways, 70% on rural roads.

4.1. Nitrogen and Oxygen Production

Both are gases naturally contained in air and are produced by liquefaction of air. Based on the Linde process, air is compressed and then flows through a expansion valve, which reduces the temperature of the air. This cool, expanded air is then directed back and is cooling down the compressed air in a countercurrent stream via a heat-exchanger. The air is continuously cooled down to liquefaction temperature. Afterwards, nitrogen and oxygen are separated in a rectification tower. The liquid air flows down over several rectification baffles in a countercurrent stream with the uprising gaseous air. The liquid takes up the oxygen and releases the nitrogen, so that the liquid becomes continuously more oxygen-enriched whereas the gas becomes nitrogen-enriched. Nitrogen and oxygen are then transported and stored either in insulated tank vessels in liquid form or in gaseous form compressed to 200 bar in pressure vessels (Veranneman, 1987; Rubner, pers. comm., 1990).

IDEA contains data for the production, liquefaction and compression of oxygen and nitrogen. As they are produced simultaneously by the same process, the respective unit processes contain production data normalized to 1 kg oxygen and 1 kg nitrogen produced.

TABLE 4.1 (a): Inorganic chemicals production - an overview

Chemical	Symbol	Source	Production process	Product name in IDEA
Nitrogen	N_2	Brown et al. (1985) Linde AG, Germany	Air liquefaction	n2/process n2/liquid n2/compressed
Oxygen	O_2	Brown et al. (1985) Linde AG, Germany	Air liquefaction	o2/process o2/liquid o2/compressed
Hydrogen	H_2	Brown et al. (1985)	Steam reforming of natural gas Byproduct chlorine/alkali process	h2/process
Carbon monoxide	CO	PEP Yearbook, 1989	from synthesis gas by cryogenic separation	co/process
Carbon dioxide	CO_2	CO_2 Lambach, Austria	by-product from chemical processes	co2/process co2/purified
Chlorine	Cl_2	PEP Yearbook, 1989	Diaphragm process	cl2/process
Caustic soda	NaOH	PEP Yearbook, 1989	Diaphragm process	naoh/process
Calcium chloride	$CaCl_2$		(unwanted byproduct of propylene glycol)	
Sodium Hypochlorite	NaOCl	PEP Yearbook, 1989	from caustic soda by chlorination	naocl/process
Sulfuric acid	H_2SO_4	PEP Yearbook, 1989	from sulfur	h2so4/process

TABLE 4.1 (b): Inorganic chemicals production - an overview

Chemical	Symbol	Source	Production process	Product name in IDEA
Sodium sulfate	Na_2SO_4		by-product from ClO_2 production	na2so4/process
Nitric acid	HNO_3	PEP Yearbook, 1989	HNO_3 (60%) from ammonia by catalytic oxidation	hno3/process
Ammonia	NH_3	Brown et al. (1985)	Steam reforming of natural gas	nh3/process
Soda ash	Na_2CO_3	PEP Yearbook, 1989	Solvay process	na2co3/process
Phosgene	$COCl_2$	PEP Yearbook, 1989	from chlorine and carbon monoxide	cocl2/process
Lime	CaO		lime manufacture	cao/process

4.2. Hydrogen Production

Hydrogen (H_2) is produced:
(1) from petrochemicals: 77%
(2) from coal: 18%
(3) through electrolysis of aqueous solutions: 44%
(4) from other sources: 1%

The hydrogen production from petrochemicals is thus the predominant route, here catalytic reforming is the most important process with natural gas as the major feedstock (Ullman, 1985). Therefore IDEA contain data on steam reforming of natural gas for the production of hydrogen (Brown et al., 1985).

Desulfurized natural gas is mixed with steam and reformed under high pressure and temperature into a mixture of hydrogen (H_2), carbon dioxide (CO_2), methane (CH_4) and steam, then cooled to 340°C and passed through a series of high and low temperature catalysts to reduce the carbon monoxide content to approximately 0.5%. The CO_2 is removed by scrubbing with an amine solution. Finally, the residual carbon oxides in the hydrogen-rich gas are converted to methane. Air emissions originate from the CO_2 and methane removal. Hydrogen is then transported and stored either in isolated tank vessels in liquid form or in gaseous form compressed to 200 bar in pressure vessels.

4.3. Carbon Monoxide Production

Carbon monoxide (CO) is produced from synthesis gas by cryogenic separation. Synthesis gas is predominantly a mixture of H_2 and CO with a ratio of 3 to 1. In a molecular sieve adsorber CO_2 and water are removed. The sieved gas is cooled down in the cold box to minus 130°C before countercurrently scrubbed with liquid methane to absorb the CO. The unabsorbed gas stream is a hydrogen product of 98.5 volume % purity. The CO-containing liquid stream is reduced in pressure and subjected to a second liquid methane wash. In a third column CO is separated from methane (PEP Yearbook, 1989). Carbon dioxide is removed from the synthesis gas and emitted to the atmosphere. Methane is collected and recycled to the liquid methane loop.

4.4. Carbon dioxide Production

To date carbon dioxide (CO_2) in Western Europe is extracted in three ways:
(1) from chemical processes > 70%
(2) from natural sources < 30%
(3) from alcoholic fermentation < 1%
Since CO_2 is an unwanted byproduct generated in significant quantities of a variety of chemical processes, this route is the most important and most economical one of marketable CO_2. In the ammonia synthesis, for example, CO_2 is an unavoidable product of the synthesis gas generation and must be removed before further processing.

As ammonia production is included in IDEA, its production data have been converted to 1 kg CO_2 main output. This, however, is only necessary if the CO_2 demand of the system model exceeds the amount of CO_2 produced as a by-product from all other chemical production processes involved in the system.

The extracted CO_2 is then cooled, dried and liquified in several steps in order to clean the gas to its wanted purity. Raw CO_2 has a purity of > 99,5%, sold qualities are more than 99,99% pure. Separate unit processes for compression and liquefaction of CO_2 are included in IDEA. Emissions to air include hydrogen (H_2), nitrogen (N_2), oxygen (O_2), argon (Ar), methane (CH_4), and carbon monoxide (CO_2). The majority, however, comes from the H_2 and N_2, but is still below 1%; these therefore are the only ones included in the IDEA database. (Bauer, pers. comm., 1991).

Carbon dioxide is transported and stored either in isolated tank vessels in liquid form or in gaseous form compressed to 200 bar in pressure vessels.

4.5. Chlorine and Caustic Soda Production

Chlorine (Cl_2) and caustic soda, or sodium hydroxide (NaOH), are produced in nearly equal amounts by electrolysis of brine in the:
(1) diaphragm cell,
(2) the mercury cell
(3) the membrane cell.
Currently, only data for the diaphragm process is included in the database (Brown et al., 1985; PEP Yearbook, 1989). Data have been computed for 1 kg of chlorine as main output as well as 1 kg of caustic soda as main output and is stored in two unit processes.

In the diaphragm cell, the electrodes are separated by a porous diaphragm made of asbestos and a polymer to prevent contact of the chlorine produced at the anode with either the alkali hydroxide formed or the hydrogen liberated at the cathode (see figure 4.1).

FIGURE 4.1: Caustic soda and Chlorine via Diaphragm Process
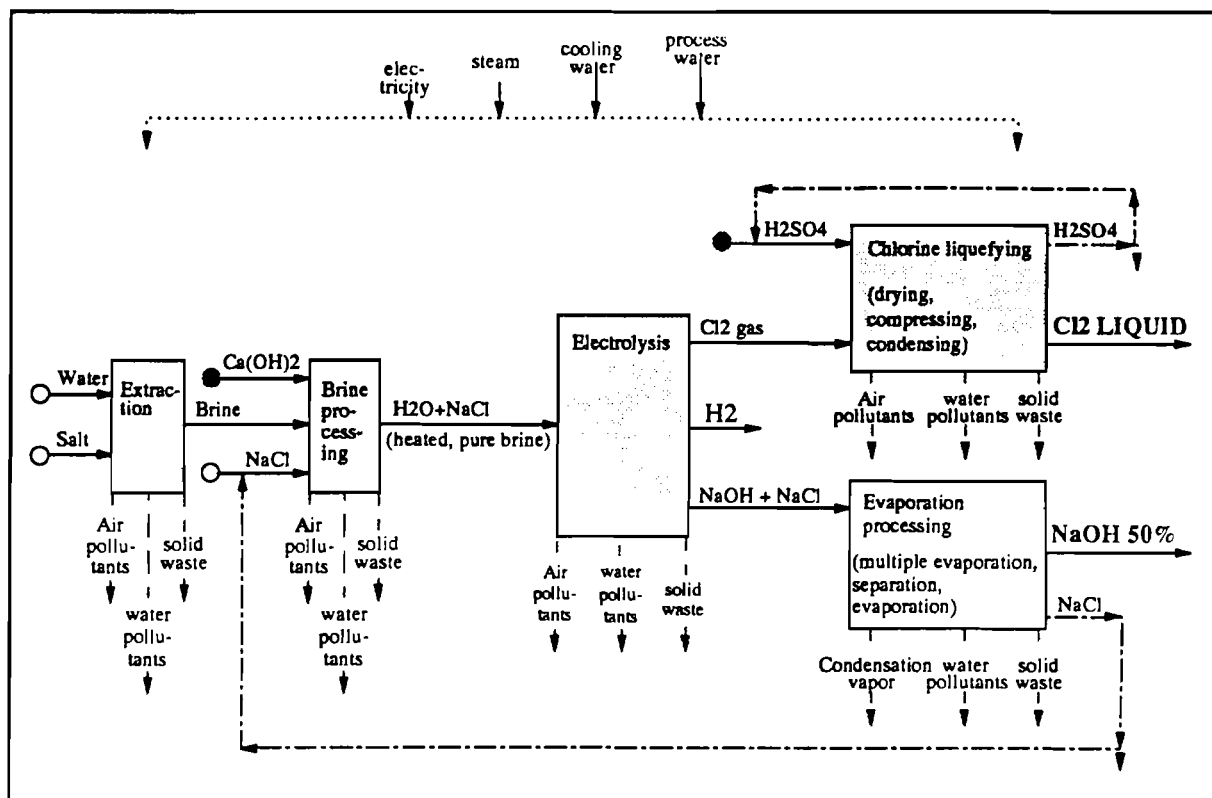
The dry chlorine gas is then compressed for in-plant use, or is cooled further to liquefy the chlorine. Caustic soda leaves the cells as a dilute solution along with unreacted brine. The solution is evaporated to increase the concentration to a range of 50 to 73 %; this evaporation also precipitates most of the residual salt which is then removed by filtration.

Air emissions from the diaphragm cells are mainly chlorine and hydrogen. Emissions to water include salt, hydrochloric acid, sulfate, and some caustic soda. Also some asbestos is emitted to the water (Reinders, 1984).

4.6. Chlorine Dioxide and Sodium Sulfate Production

Chlorine dioxide (ClO_2) used in pulp mills, is produced from sodium chlorate ($NaClO_3$) in the presence of sulfuric acid (H_2SO_4) and salt (NaCl). The acidified sodium chlorate is reduced by salt to produce chlorine dioxide (ClO_2), chlorine (Cl_2)and sodium sulfate (Na_2SO_4) (PEP Yearbook, 1989). The IDEA database contain these production data, but no emission figures. There is a separate unit process in the IDEA database for chlorine dioxide as main output and for sodium sulfate as main output.

4.7. Sodium Hypochlorite Production

Sodium hypochlorite (NaOCl) is obtained from a 15 weight % caustic soda (NaOH) solution which is chlorinated to produce a sodium hypochlorite solution. The solution is then withdrawn from the chlorinator and is sent to a settling tank where the impurities from the caustic soda are settled out. The resulting solution is stabilized by adjusting the alkalinity (PEP Yearbook, 1989). The IDEA database presently only contains these production data, and no emission data yet.

4.8. Sulfuric Acid

All sulfuric acid (H_2SO_4) is made by either
(1) the lead chamber process,
(2) the contact process.
The latter has a market share of 97% in the United States; its data, therefore, are stored in the IDEA database.

The contact process uses elemental sulfur as the major feedstock and consists of three basic steps:

(1) Manufacture of SO_2: SO_2 is usually produced by burning liquid sulfur, but can also be produced by roasting ores such as pyrites, zinc and copper.

(2) Catalytic oxidation of SO_2 to SO_3: in modern sulfuric acid plants with so-called double absorption systems, a conversion efficiency of 99.7% can be achieved.

(3) Reaction of SO_3 in a strong aqueous solution of sulfuric acid (98.5%) with water to form sulfuric acid of a concentration of about 93%.

Atmospheric SO_2 emissions originate mainly from the incomplete conversion of SO_2 to SO_3. Therefore emission factors vary considerably between different plants. For the emission data contained in the IDEA database we assumed a conversion efficiency of 99.5% which can be achieved in new sulfuric acid plants.

Further contributions to air pollutants are unabsorbed SO and unabsorbed H_2SO_4 droplets as a mist. Emissions to coater consists of H_2SO_4 and Na_2SO_4 (Reinders, 1984 USEDAS, 1985).

4.9. Nitric acid Production

Most of the nitric acid (HNO_3) is produced by catalytic oxidation of ammonia; production data included in IDEA are thus based on process. It typically consists of three steps:

(1) A 1:9 ammonia:air mixture is oxidized at high temperature (750-800°C) as it passes through a platinum/rhodium catalyst.

(2) After cooling down the process stream, the nitric oxide (NO) reacts with residual oxygen (O_2) to form nitrogen dioxide (NO_2).

(3) Finally, the gases are introduced into a bubble cap plate absorption column for contact with a counter-current stream of water.

The final product is a 57% HNO_3 solution. For the production of further concentrated nitric acid dehydrating agents are required.

Atmospheric emissions from nitric oxide production consists primarily of NO, NO_2 and trace amounts of nitric acid mist. Since ammonia is used as raw material, there are some ammonia emissions. The major source of the Nox emissions is the tail gas from the absorption tower. These emissions can be effectively controlled by almost two orders of magnitude through the catalytic reduction or extended absorption (Reinders, 1984; USEPA, 1985).

4.10. Ammonia Production

Ammonia (NH_3) is manufactured by catalytic reaction between nitrogen (N_2) and hydrogen (H_2) in the Haber-Bosch process (market share in Western Europe > 90%). The hydrogen feedstock is predominately produced from:

(1) natural gas: 73 %

(2) naptha: 13 %

(3) heavy fuel oil

Eighty-five percent of the world-wide ammonia output is made by steam reforming (ref.). Therefore steam reforming of natural gas is by far the most important production process and described in IDEA.

Its major steps are

(1) synthesis gas preparation:
   - reforming of natural gas with steam and air;
   - conversion of CO with water to CO_2 and H_2;
   - removal of CO_2;
   - methanation;

(2) compression to 80-450 bar;

(3) ammonia synthesis: hydrogen and nitrogen react over a catalyst in a converter to NH_3;

(4) recovery of hydrogen from the purge gas.

Although all ammonia plants use this basic process, data on pressure, temperature, catalysts and quantities of feedstock vary from plant to plant. Typical values can be found in literature (Brown et al, 1985; PEP Yearbook, 1989); these are the ones included in the IDEA database.

The final ammonia product is then stored either in pressure vessels or at low temperatures; it is transported with truck, rail, barge, sea-going vessels or pipelines.

The CO_2 is removed from the synthesis gas with mono-ethanolamine or potassium carbonate solutions. The regeneration of this scrubbing liquid with steam produces mainly CO_2 emissions which are however, often used for on-site production of urea or sold to producers of liquid/solid CO_2. The scrubbing liquid must be periodically renewed which is done by draining off part of the solution. This causes ammonia and mono-ethanolamine or potassium carbonate emissions of water. Other air emissions include NO_x, NH_3, CO and H_2, which come from the condensate steam strippers, used to remove NH_3 and methanol from water. The emission factors vary within one or more orders of magnitude depending on the type of pollution control equipment in place (Reinders, 1984; UNESPA 1985). The IDEA database includes emission factors for relatively well-controlled processes as currently in place in Western Europe.

4.11. Lime Production

Lime (CaO), or burnt lime, is made by calcination of limestone (CaCO3), also called lime burning: $CaCO_3$ + heat --> CO_2 + CaO. This is done in various types of different kilns. There are two kinds of lime,
   (1) high-calcium lime (CaO)
   (2) dolomitic lime (CaO·MgO). About 10 % of all CaO is further converted to hydrated (slaked) lime $(Ca(OH)_2)$. The basic production steps(ref.) are:
   (1) preparing the limestone for the kilns by crushing and sizing;
   (2) calcining the limestone;
   (3) hydrating the quicklime;
   (4) transfer, storage and handling.

IDEA contains separate unit processes for the burning of limestone to produce CaO and for the hydration to form $Ca(OH)_2$ (see figure 4.2). Crushing, sizing and handling is included in the mining of limestone (see Section 1.1 "Minerals Extraction and Mining"). Large amounts of CO_2 are formed in the kilns and vented to the atmosphere; particulate matter (TSP) is also emitted from several operations, as well as some gaseous emissions like SO_2, NO_x and CO. The major emission source is the kiln. Hydrator emissions are 1 because the exhaust gases are usually filtered to prevent product losses (USEPA, 1985).

**FIGURE 4.2:** Slaked Lime Production
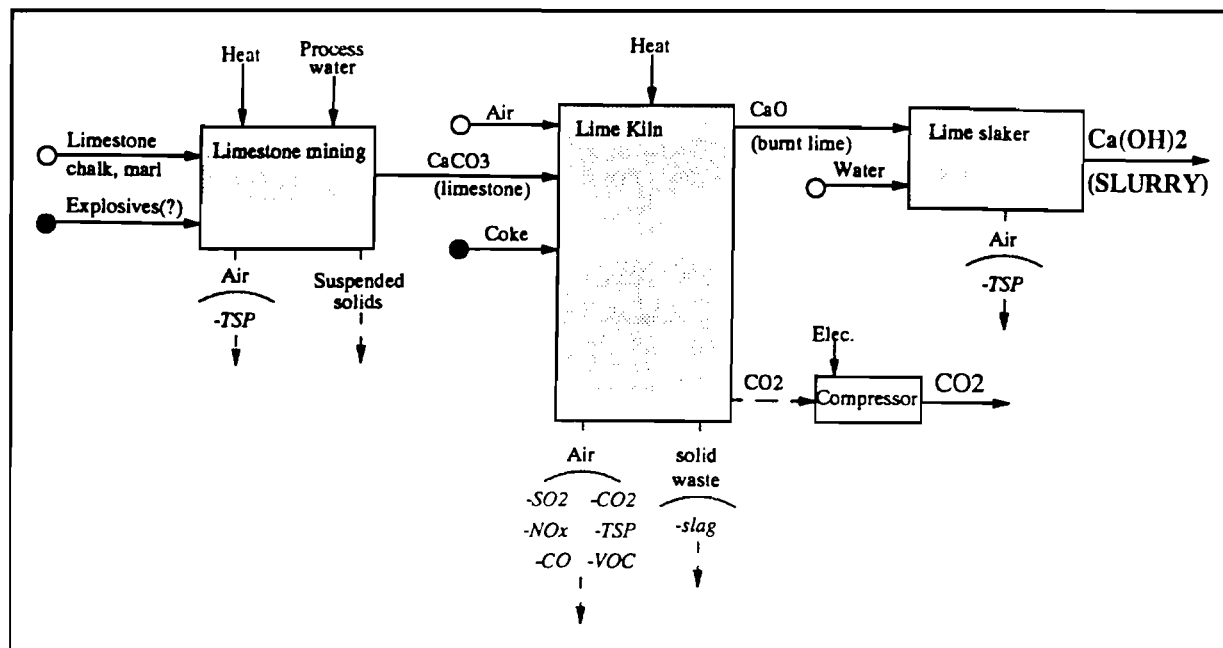
4.12. Soda Ash Production

In Western Europe most of the soda ash, or sodium carbonate (Na_2CO_3), is made by the so-called Solvay process, where ammonia, calcium carbonate (limestone) and sodium chloride (brine) are the basic raw materials. The limestone is burnt and further mixed with water to produced slaked lime ($Ca(OH)_2$). The brine is purified and goes then through an ammonia absorber where ammonium hydroxide (NH_4OH) is formed. Through the addition of carbon monoxide (CO), sodium hydrogen carbonate ($NaHCO_3$) is formed which goes to the calciner where the final sodium carbonate is produced. There are ammonia losses in the absorbing system, and particulate emissions from lime manufacture and from the calciner.

Data in IDEA for the Solway process include all requirements and emissions of limeburning and slaking so that these steps are not calculated separately with the separate unit process data also available in the database.

4.13. Phosgene Production

Carbonyl chloride (COCl$_2$) or phosgene is produced by direct reaction of carbon monoxide (CO) and chlorine (Cl2) in the presence of an activated carbon catalyst. The crude phosgene is distilled to remove so-called heavy ends and then dechlorinated by passing it through an activated carbon adsorption bed. Residual phosgene in the exhaust gases and excess CO must be removed and can be recycled to the main process reactor. Due to its toxicity, phosgene is produced only at the sites where it is used. It must thus be totally removed from the exhaust gases; this is done either by hydrolyzing it to Hcl and CO$_2$ or through reaction with NaOH, the excess CO formed by both methods can be burnt as afterburners (see figure 4.3).

FIGURE 4.3: Phosgene Production
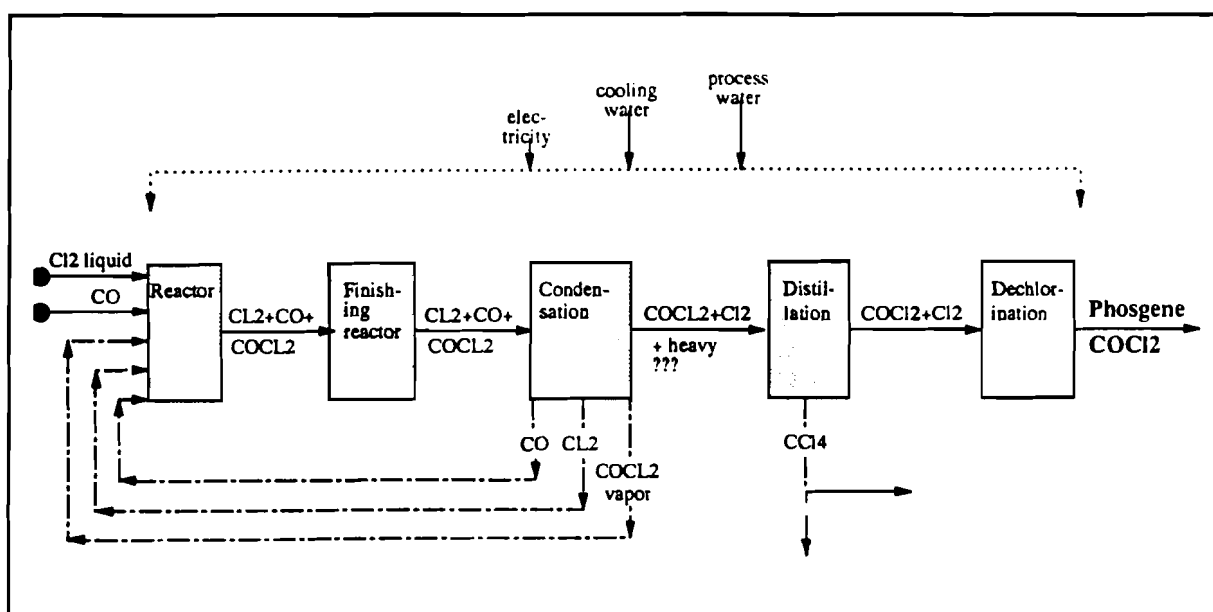
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5. Organic Chemicals Production

This section describes the production of basic organic chemicals used in the manufacture of plastics, as well as the production of certain plastics, or polymers themselves.

5.1. Basic Organic Chemicals

This section describes the production of three basic organic chemicals used in the manufacture of plastics:

(1) Olefins,
(2) aromatics,
(3) ethylene.

Olefin production

Olefins are the principal chemicals needed for the manufacture of plastics such as ethylene, propylene, butylene and butadiene. Annual production of olefins for the plastics manufacturing in Europe is well over 25 million tonnes of which approximately half is ethylene. The basic process is thermal cracking of a hydro-carbon feedstock at high temperatures in the presence of steam. The major feedstock in Europe, at present, is naphtha (around 80%) (see refinery outputs: chemical feedstock Table 2.1, Section 2.1 "Crude Oil Refining") a major change expected in the future is a shift from naphtha to ethane, propane and butane, i.e. natural gas liquids from the North Sea, or top-gas liquids.(CEC,1988), (Conser et al, 1990)

FIGURE 5.1: Production of olefins
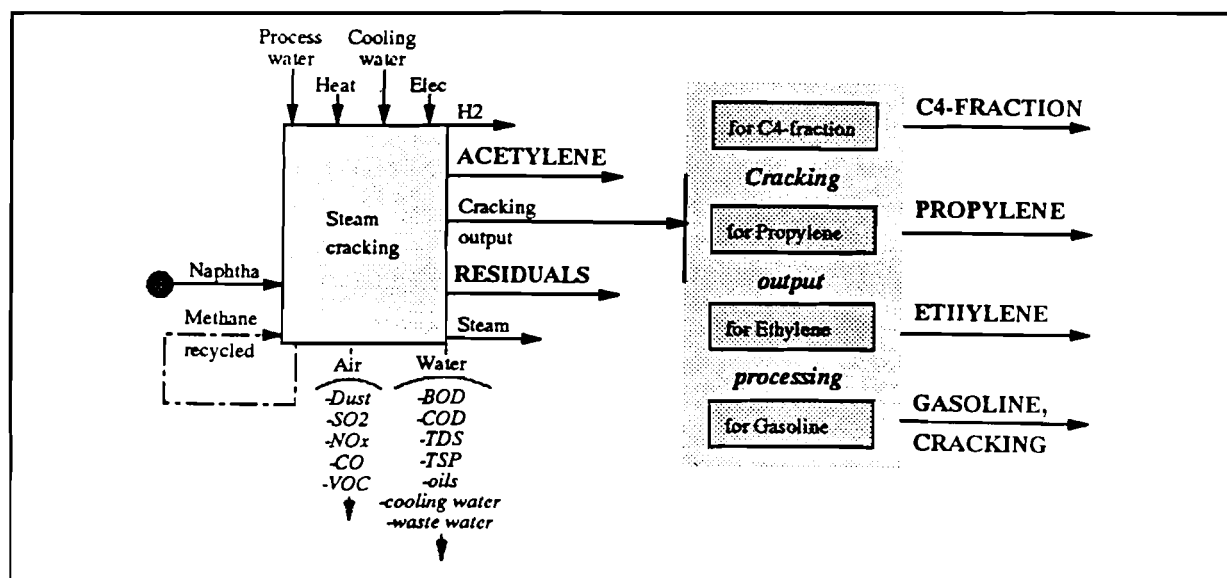
Thermal cracking of the hydrocarbon feedstock yields a mixture of olefin gases (ethylene, propylene, acetylene) and liquids which are separated by distillation. The gas is normally used as fuel on-site. The liquids (hydrocarbons from C_4/C_5 upwards) generally have a high aromatic content; they are either (Richter, 1991; Lyons, 1991)

(1) further processed to extract these aromatics in a catalytic reformer,
(2) used as gasoline blending components in close-by refineries, or
(3) burnt as fuel on-site.

The yield pattern from an olefin plant depends on the hydrocarbon feedstock used and the cracking conditions. A typical yield pattern of efficient cracking is shown in Table 5.1. In contrast to old plants, modern ones have a high energy efficiency since they extensively recycle materials and recover waste heat.

TABLE 5.1: Typical Yield from Cracking Hydrocarbon Feedstocks [% by weight](Aere, 1984)

Product	Hydrocarbon Feed Stock				
	Ethane	Propane	Butane	Naphtha	Gas oil
Ethylene	80-81	44-46	35-38	31-33	24-26
Propylene	1-3	15-17	16-18	14-16	14-16
Butadiene	1	1-2	1-2	4-5	4-5
Butylenes	0	0	0	4-5	4-6
Fuel gas	14-16	28-30	30-32	15-18	10-11
C_5 +	1-2	7-9	12-14	24-27	36-39

Aromatics (benzene, toluene and xylene) production

The common source of aromatics is the "C_6-C_8 cut" from a catalytic cracker in the refinery or the naphtha/gasoline-cut as steamcracking-output. This heart cut containing benzene, toluene and xylene is routed to the extraction tower in order to dissolve the aromatics. Here, solvents, such as sulfolane or dimethylsulfoxide, are dispersed and the rich solvent is stripped. From this rich solvent, the individual aromatics are fractionated and the solvent is recycled to the extraction tower. Benzene and toluene are removed overhead, whereas the xylene leaves the bottom of the fractionator as a by-product. Finally, benzene and toluene are separated in a benzene tower (see Figure 5.2).

FIGURE 5.2: Aromatics production
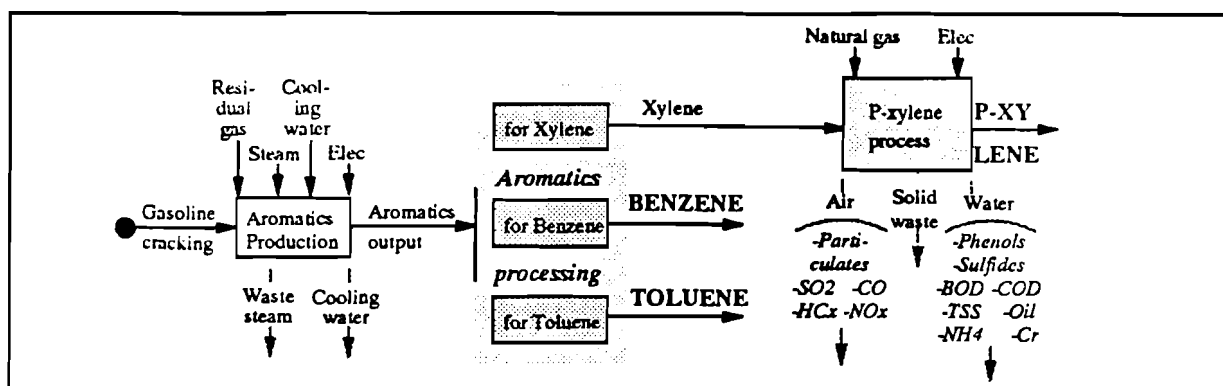
The xylenes-fraction (ethylbenzene, o-xylene,p-xylene, m-xylene) can be separated by crystallization, adsorption (Toray-process, Parex-process), or distillation (only o-xylene). (UOP, 1990)

Energy requirements vary widely, being relatively low for the extraction and purification processes and considerably higher for the reforming process. Data representing a Western European average are contained in IDEA; these data are duplicated for each major output as reference output from a separate unit process.

Ethylene production

Ethylene is produced in the ethylene plant of the refinery by pyrolytic steam cracking from naphtha, liquid gas and washed waste gases, such as top-gas, etc. In our further calculations, we assume a ratio of 250 : 64 : 13 for these three inputs. (Mosthaf/Nikles, 1989, 1990)

The pyrolytic steam cracking is done at temperatures around 850 °C, mostly in directly heated reactors. Heating is done mostly with fuel or gas produced as by-products in the various plants of the refinery so that the only external energy needed is electricity.

The important steps in the pyrolytic steam cracker are:
(1) splitting of the naphtha into shorter C chains with as high as possible a fraction of ethylene;
(2) several separation and cleaning steps.

When splitting the naphtha, ethylene gas, still mixed with other gas fractions, forms at the top of the cracker and pyrolytic gasoline and gas-oil are withdrawn from the bottom to be recycled as fuels for the cracker. The gases are quenched, cooled and then purified to separate hydrogen sulfide (H_2S) and carbon dioxide (CO_2) which are released to the atmosphere.

The remaining liquid stream is fractionated through condensation into an azeotrope mixture of acetylene or ethylene, and propylene. The acetylene and ethylene mixture is separated by a selective catalyst or extractive distillation with acetone.

Water is added to the cracker to produce steam which, in turn, improves the heat transfer to the feedstock and prevents corrosion of the reactor's coat by sulphur compounds. The steam is, at the same time, considered a co-product because it can be further used as an energy source. (Mosthaf/Nikles, 1989, 1990)

A typical steamcracker produces from 1 t of feed:
- 313 kg   ethylene;
- 165 kg   propylene (crude);
- 95 kg   "C$_4$" fraction;
- 20 kg   hydrogen (H$_2$);
- 170 kg   methane (CH$_4$) (for own consumption);
- 5 kg   acetylene;
- 205 kg   gasoline;
- 25 kg   residual fuel oil and
- 2 kg   hydrocarbons that are either burnt or lost to the atmosphere as VOC.

Only ethylene, propylene, the "C$_4$" fraction, gasoline are regarded as valuable co-products which together amount to 778 kg. In order to represent data for all four output products, the same set of data has been recalculated per t of each of these products as the main, or reference, output.

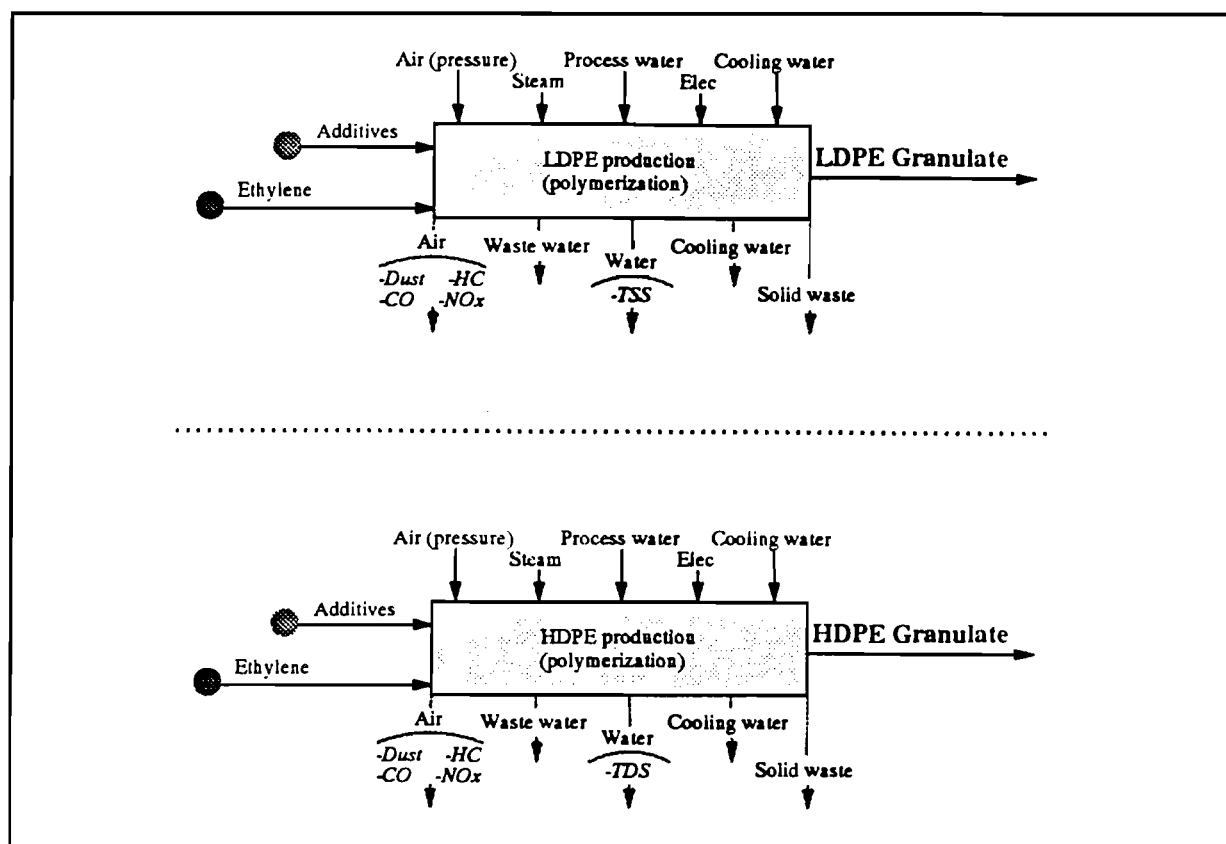## 5.2. Production of Polymers and Intermediates

This section describes the production of the following plastics, or polymers:

- polyethylene and polypropylene,
- polyethylene terephthalate (PET),
- polycarbonate.

Also included is the description of the intermediate organic chemical needed in the final production of these plastics.

Whereas the description of the manufacture of ethylene and propylene from naphtha have been described in Section 5.1. on "Olefin production", the following paragraphs describe the polymerization process to make high or low density polyethylene and polypropylene.

FIGURE 5.3: Granulate production from ethylene

Air (pressure)   Process water   Cooling water
Steam   Elec

Additives

Ethylene

LDPE production
(polymerization)

LDPE Granulate

Air   Waste water   Water   Cooling water
-Dust -HC   -TSS   Solid waste
-CO -NOx

Air (pressure)   Process water   Cooling water
Steam   Elec

Additives

Ethylene

HDPE production
(polymerization)

HDPE Granulate

Air   Waste water   Water   Cooling water
-Dust -HC   -TDS   Solid waste
-CO -NOx

5.2.1. Polymerization of polyethylene and polypropylene

Polymerization means the addition of the relatively short chains of monomers to produce longer chained polymers which have significantly higher stability; they can then be used to manufacture textured products of various desired qualities. There are three commercially important systems for polyethylene and polypropylene production:

(1) **High pressure polymerization** by free-radical initiation, using oxygen, peroxides, or other strong oxidizers as initiators: this produces low density polyethylene (LDPE) with a density of 0.910-0.940 g/ml. Pressures of 60-350 Mpa at up to 350 °C are applied. Low density polyethylene is, for example, further used as lining of the beverage cartons, bottle caps and for shrink film as secondary packaging material. (BUWAL, 1990), (BASF, 1990)

(2) **Low pressure polymerization** by heterogenous catalysis using as initiators:
    (a) transition metal oxides, such as molybdenum oxide or chromium oxide, supported by inorganic carriers;

(b) Ziegler catalysts, such as aluminum alkyls or titanium halides, also supported by inorganic carriers.

Polymerization temperatures range from 50 to 300°C and pressures from 0.1 to 20 Mpa. This process produces high density polyethylene (HDPE) with a density of 0.941-0.970 g/ml used, for example, for blow-molded products.(BASF, 1990)

(3) **The UNIPOL process:** this gas-phase polymerization in a fluidized-bed reactor takes place at a pressure of 2 Mpa and a temperature of 100 °C. Close process control is possible through the fluidized bed so that polyethylene with a very wide spectrum of densities (0.88 - 0.98) and molecular weights (0.1 - 1000) can be produced; it also allows close control over the distribution of molecular weights within the polyethylene. In contrast to the other processes, the UNIPOL process can manufacture all different grades of polyethylene products in one reactor. To date, approximately 25 % of all polyethylene is produced by this process world-wide. Due to better materials- and energy efficiencies, its share is constantly increasing. (Union Carbide, 1990)

In our calculations with IDEA, all HDPE is made with process (2) and all LDPE with process (1) (see Figure 5.3). The gas phase polymerization process is used for the production of polypropylene.

The main emissions to air and water are from the solvents, used in the first two processes to dissolve the co-monomers, and from the combustion processes necessary to heat the inputs. They are mainly organic compounds in water and typical combustion gases (CO, CO_2, NO_x, VOC, SO_2) to air.

FIGURE 5.4: PET bottle production
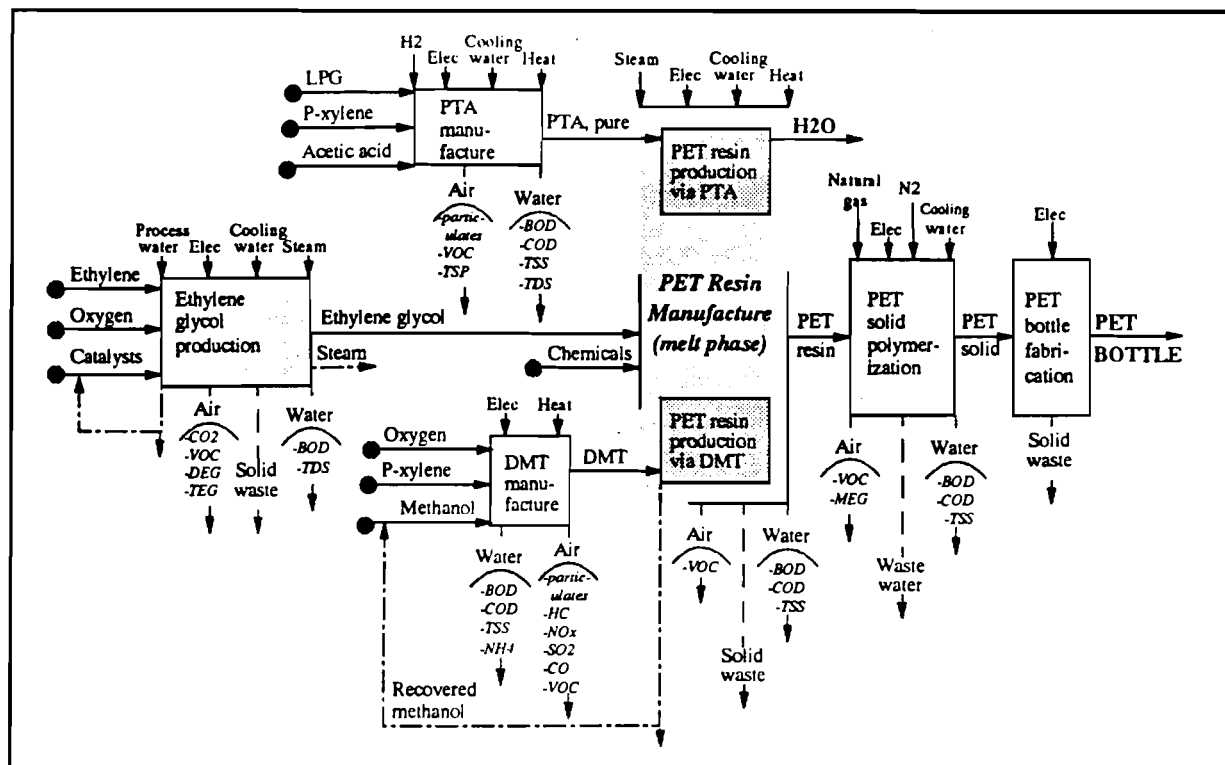
5.2.2. Production of polyethylene terephthalate (PET)

The polyethylene terephthalate (PET) resin is currently made by two major methods:

(1) esterification of pure terephthalic acid with ethylene glycol, or

(2) trans-esterification of dimethyl-terephthalate with ethylene glycol.

Ethylene glycol is therefore needed in both methods, and dimethyl-terephthalate and terephthalic acid, in turn, are produced through catalytic reaction of para-xylene and acetic acid. Whereas the production of xylene and other aromatics can be found in Section 5.1, the following sections detail the manufacture of acetic acid, ethylene glycol, crude and purified TPA, DMT and PET polymer (see figure 5.4).

A. Acetic acid production

Acetic acid can be produced in several ways. The most common method of production, and the one included in the IDEA database, is by liquid phase oxidation of butane or liquefied petroleum gas (LPG). It can also be made by oxidation of acetaldehyde or reaction of carbon monoxide with methanol. (Sellers, 1989), (PEP, 1989)

B. Ethylene glycol production

Ethylene glycol is manufactured in two steps: (1) ethylene feedstock is reacted with oxygen in the presence of a silver-based catalyst to yield ethylene oxide; (2) ethylene oxide is hydrated (i.e. reacted with water) to make ethylene glycol. The first oxidation step is highly exothermic and produces medium pressure steam as a by-product, which is used on-site as a heat source. The main reactor effluent from this oxidation step is mixed with water to dissolve unreacted gases. This water-rich stream of ethylene oxide is fed to a stripper where pure ethylene oxide is recovered and the water discarded to the sewer.(Sellers, 1989), (PEP, 1989).

The IDEA database contains one unit process describing the ethylene glycol production.

D. Crude TPA production

Crude terephthalic acid (TPA) is manufactured primarily by oxidation of para-xylene in the liquid phase. Liquid para-xylene, acetic acid, and a catalyst, such as manganese- or cobalt-bromides, are combined as the liquid feed to the oxidizers. The reaction effluent is continuously removed and routed to a series of crystallizers, where they are cooled by flashing with water. (Sellers, 1989), (Thalmann ,1991)

The partially oxidized impurities are more soluble in acetic acid and tend to remain in solution, while crude TPA crystallizes from the liquor. The slurry from the crystallizers is sent to solid/liquid separators, where crude TPA is recovered in the solid state. The liquid portion is distilled and acetic acid, methylacetate (an intermediate product) and water are recovered overhead and are recycled. Some water is discarded as waste water.

E. PTA production

There are two main methods of pure PTA production:
(1) direct production of fiber grade, pure therephthalic acid (PTA);
(2) conversion of crude TPA to dimethyl-terephthalate (DMT).

The IDEA database contains a unit processes for both production methods, and a mixture table indicates the relative shares as typical of Western European conditions of X% for the direct production and X% for production via DMT.

Pure PTA production. In order to produce fiber grade PTA from crude TPA, the crude acid is dissolved under pressure in water at 225 to 275 °C. This solution is hydrogenated in the presence of a catalyst to convert some intermediate products that might otherwise interfere in some of the following steps of PET production. The solution is then cooled, causing pure TPA to crystallize out.
By the Amoco-process p-xylene is oxidized together with aldehydes. Acetic acid is used as solvent, in which terephalic acid is suspended. (Enimont, 1990)

DMT production. Crude TPA is purified by reaction with methanol at moderate temperature and pressure to yield DMT. In this case, any intermediate products that were still present in the crude TPA do not react with the methanol and can therefore be easily separated from the DMT. The methanol is recovered to over 90 % from the PET resin manufacture in the melt phase. The DMT is then brought to fiber grade by crystallization and distillation. (Buwal, 1990), (Winnacker/Küchler,1985)

F. Polyethylene theraphthalte (PET) production

The first step in the manufacture of polyethylene terephthalate (PET) resin is the melt phase polymerization, of which there are currently two main methods, as already mentioned above: (Enimont, 1990), (Buwal, 1990), (Thalmann, 1991)

(1) esterification of pure terephthalic acid with ethylene glycol and loss of water;
(2) trans-esterification of dimethyl-terephthalate with ethylene glycol and loss of methanol which is recycled to the DMT production.

The IDEA database contains two unit processes for these two methods and a mixture table with the relative shares of each process as currently being employed in Western Europe, i.e., X% for esterification of pure TPA, and X% for trans-esterification of DMT.

Reactions occur at 100 to 150 °C in the presence of a catalyst and produces an intermediate, bis-(2-hydroxyethyl)-terephthalate. This intermediate then undergoes polycondensation at 10 to 20° C above the melting point of PET (246 °C) under vacuum. Ethylene glycol is distilled and recycled, and the resulting PET resin with an intrinsic viscosity of 0.60 to 0.65 is cooled and pelletized.

The final step in PET resin manufacture is a solid state polymerization process. This step raises the temperature of the pellets to below the melting point in the presence of a catalyst, in order to continue polymerization and, thereby, increase the final molecular weight and intrinsic viscosity to 0.72 to 0.80. This step further ensures a polymer with a very low acetaldehyde content.

5.2.3. Production of polycarbonate

The two main chemicals necessary to make polycarbonate are phosgene and bisphenol A; phosgene, in turn, is made from chlorine (Cl_2) and carbon monoxide (CO), and bisphenol A from phenol and acetone. The production processes for phosgene, bisphenol A and polycarbonate are described in the following sections; for the manufacture of carbon monoxide, chlorine and phosgene see Section 4 "Inorganic Chemicals". (Heidenreich, 1983), (GE Plastics, 1990)

**FIGURE 5.5:** Phenol/Acetone production via Cumene Process
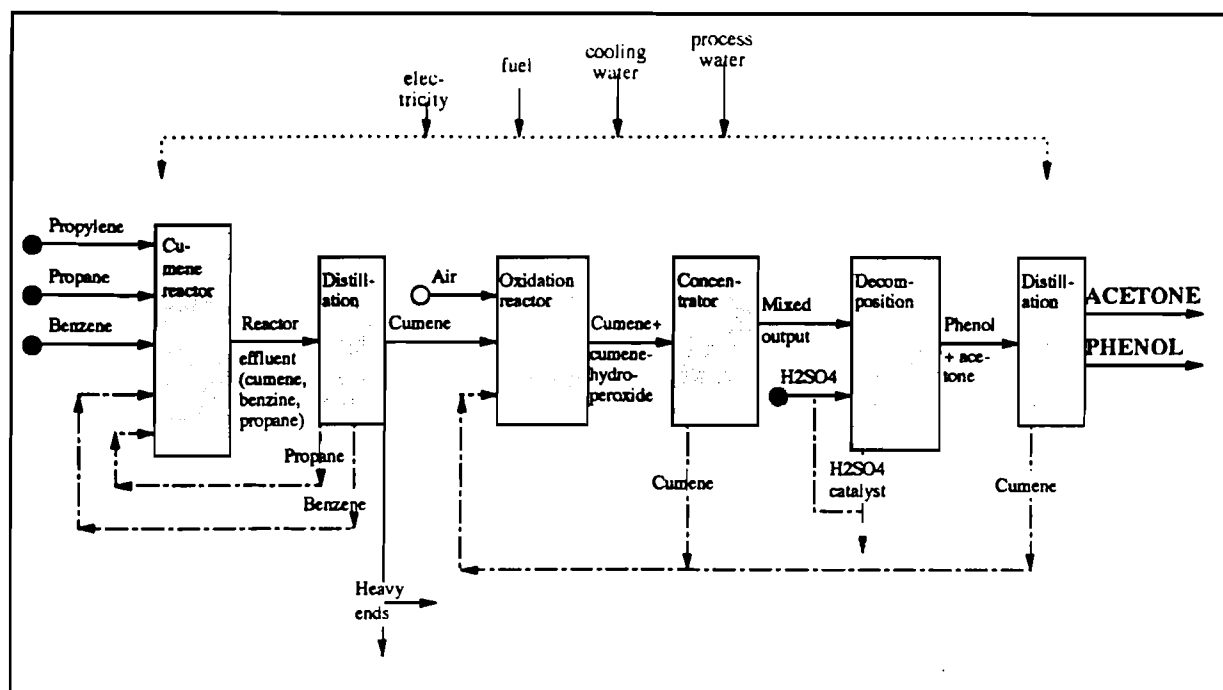
A. Phenol and acetone production

Phenol and acetone are produced in the same process in two steps. First, propylene diluted with propane, and a large excess of benzene are reacted over a phosphoric catalyst on kieselguhr to produce cumene. This practically completes the propylene conversion, whereas the propane and benzene are recovered by distillation, and are recycled. In the second step, the so-called Hock-process, cumene is oxidized with air to convert about 20 % to hydroperoxide. Most of the unreacted cumene is recycled; the hydroperoxide solution is concentrated to 85 % and is then decomposed to phenol and acetone by using a sulfuric acid catalyst. Phenol, acetone, and residual unreacted cumene are separated by distillation. Again, the cumene is recycled. The process steps are illustrated in Figure 5.5. (PEP, 1989)

This technique has the advantages that it is inexpensive, and that it produces both reagents needed for bisphenol A without any by-products.

FIGURE 5.6: Bisphenol A production via Ion Exchange Catalyst
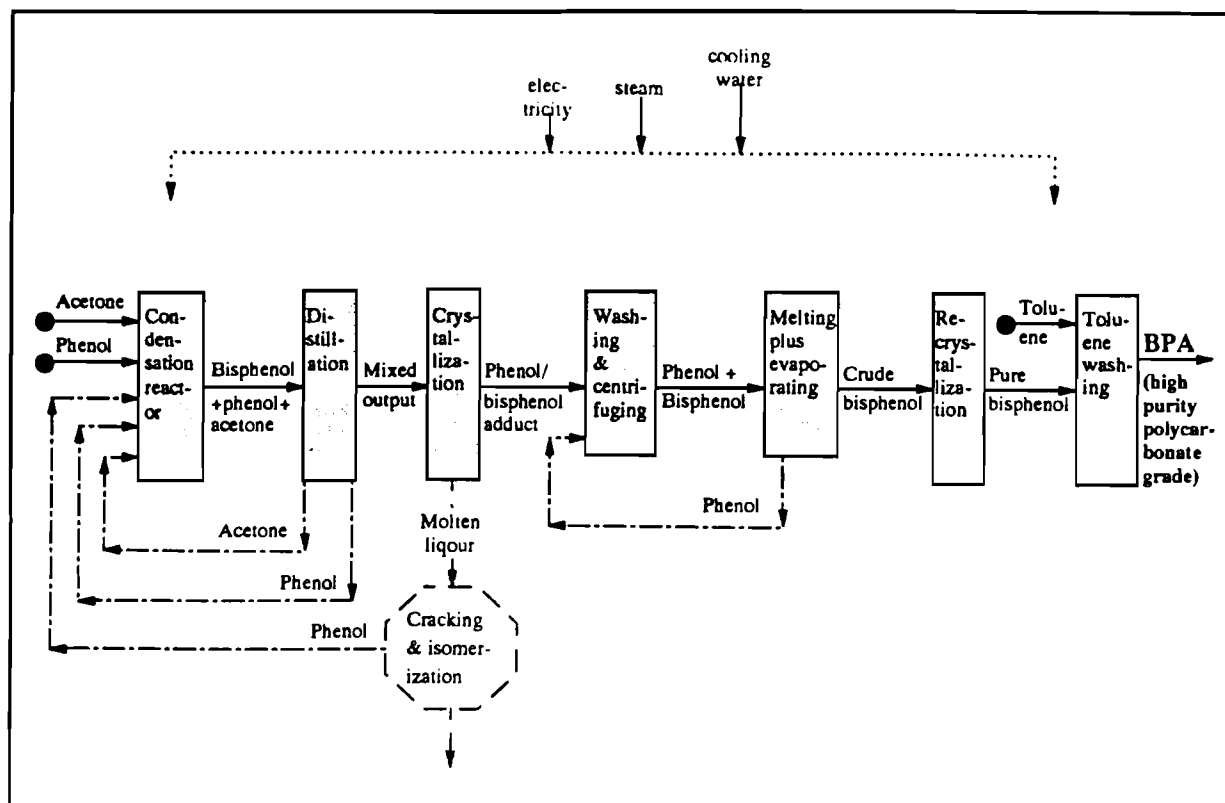
B. Bisphenol A production

Bisphenol A is made by an ion-exchange catalyzed process from phenol and acetone. Acetone and excess phenol are reacted in the presence of a cation exchange resin catalyst in a condensation reactor to form crude bisphenol A. Unreacted acetone and part of the phenol are separated from the reaction mixture by distillation and are recycled to the condensation reactor. The crude product (i.e. bisphenol A still containing some phenol) is crystallized to a phenol/bisphenol adduct; this is then centrifuged, washed with additional phenol, melted and evaporated in order to strip the phenol. The product is washed with toluene and re-crystallized to yield the final high purity (polycarbonate-grade) bisphenol A (see Figure 5.6). Product yield on phenol is 91 %. The mother liquor from the first crystallization, after cracking and isomerization, is recycled to the condensation zone. (PEP, 1989)

C. Polycarbonate production

Todate, the "polycarbonate batch interfacial process with polymer recovery from aqueous phase" is the most common process to manufacture polycarbonate. The polymer is formed in two stages by (1) batch phosgenation, and (2) polycondensation. Both stages contain a caustic aqueous and an organic (methylene chloride) phase.

First, bisphenol A is phosgenated in the presence of p-tert-butylphenol to form a prepolymer. The prepolymer mixture is polycondensated (promoted by tri-ethylamine) in a second reactor. After this reaction, the aqueous phase is separated from the organic phase and sent to neutralization. The polycarbonate solution (in methylene chloride), i.e. the organic phase, is purified and washed with dilute caustic soda (NaOH), hydrochloric acid (Hcl) and water. (PEP, 1989)

The purified polymer solution is mixed with antisolvents and water, and the polymer precipitates into the aqueous phase. This, in turn, is centrifuged to separate the polymer precipitate from the aqueous solution which is discarded as waste water (polycarbonate separation). The wet polymer is dried, compounded with additives and pelletized. Common additives are glass fiber, flame retardant, UV-stabilizer, colorant, etc. Both the methylene chloride and the antisolvent from the organic phase are recovered, purified and recycled. Product yields on bisphenol A and phosgene are 99.5 and 81.9 %, respectively.

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6. Glass Production

This section describes the various process steps involved in the manufacture of container glass. In simple terms, glass making starts with mixing a batch of dry ingredients (raw material mixing), heating this batch until molten and uniform in composition (melting and fining), adjusting the batch's temperature (forehearth), forming the molten glass into the desired shape (drawing and forming), reducing the temperature of the product in a controlled way in order to minimize residual stresses that might otherwise be retained (annealing), and ends with several finishing steps (finishing, inspection, palletizing, and packaging). Figure 6.1 depicts these various process steps.

Ninety % of all glass produced, and 100 % of mass-produced glass, is soda-lime glass. Its typical chemical composition is around 73 % silicon oxide (SiO_2), 14 % sodium oxide (Na_2O), 10 % calcium oxide (CaO), about 1 % each of aluminum oxide (Al_2O_3) and magnesium oxide (MgO), and 1 % additives (e.g. Suess et al., 1985; Lubisch; Krock; Chiogioji, 1979). These latter can include iron oxide (Fe_2O_3), titanium oxide (TiO_2), potassium oxide (K_2O), and others, which aid in giving special properties or color to the glass.

The raw materials involved in the manufacture of glass are sand (SiO_2), limestone ($CaCO_3$), dolomite, feldspar, soda ash (Na_2CO_3), phonolite, and some metal ores, such as chromium and cobalt, to impart color. In addition, the charge to the furnace contains 10 to 50 % cullet, i.e. recycled glass. This cullet can be from internal and external sources; typically, the amount ranges around 20 and 30 %, but it depends on the color of the glass to be produced and on the availability of cullet of suitable composition. The amount of external cullet used is continuously increasing as more glass is being recycled by the consumer. As we try to represent state-of-the-art technologies in Western Europe, we use in the IDEA database a rate of around 50 % external cullet depending on the color of the glass (Schweingruber, person. comm., 1991).

Mass produced glass is melted in large continuous, regenerative furnaces. These are equipped with automated machinery for mixing and delivering the raw materials, including the cullet, to the melting tank, and for drawing, forming, annealing and handling the glass product taken from it. Melting itself takes place at temperatures between 1450 and 1600 °C. The first stage of the melting process is the formation of silicates; this is then followed by dissolution of the remaining sand and lime to form the glass. Any gas occlusions and heterogeneities in the glass melt are subsequently removed in the so-called fining step. Afterwards the glass is adjusted in temperature until it attains a viscosity suitable for forming. After the product has been formed and cooled, it has to still be finished, inspected, palletized and shrink film packaged. Those bottles or other glass containers that break during forming, annealing and finishing, or do not pass the inspection stage, are sent back as internal cullet and are directly mixed back into the batch.

The process continues steadily for a few years until the condition of the furnace indicates that the refractory lining is no longer serviceable, and the "campaign" is terminated (Burwell, 1982).

Waste gases and particulate matter are generated during glass melting from the combustion of fuels to fire the furnace and from the glass making process itself. Air pollutants emitted from the glass furnace include those typical of any combustion process, i.e. CO_2, CO, SO_2, NO_x and dust (i.e. TSP) and those from the evaporation of the toxic materials that are either contained as contaminants in the raw materials, or added in small quantities to the glass. These include primarily alkalies, borates, fluorides, lead compounds, and some other heavy metals.

Fuel oil and natural gas are the most frequently employed fuels, although coke oven gas is used in some regions (Suess et al., 1985). Additional electrical heating (electric boosting) is frequently employed to increase the production rate; in this case, 5 to 10 % of the total input energy is in form of electrical energy directly into the batch through electrodes (Suess et al., 1985). In EC Europe in 1985, of the total energy input for making container glass, 48 % was fuel oil, 42 % gas, and 10 % electricity. In the IDEA database, we include only natural gas melting with electrical boosting since this is the fuel combination most commonly used in the more modern glass furnaces.

FIGURE 6.1: Glass production
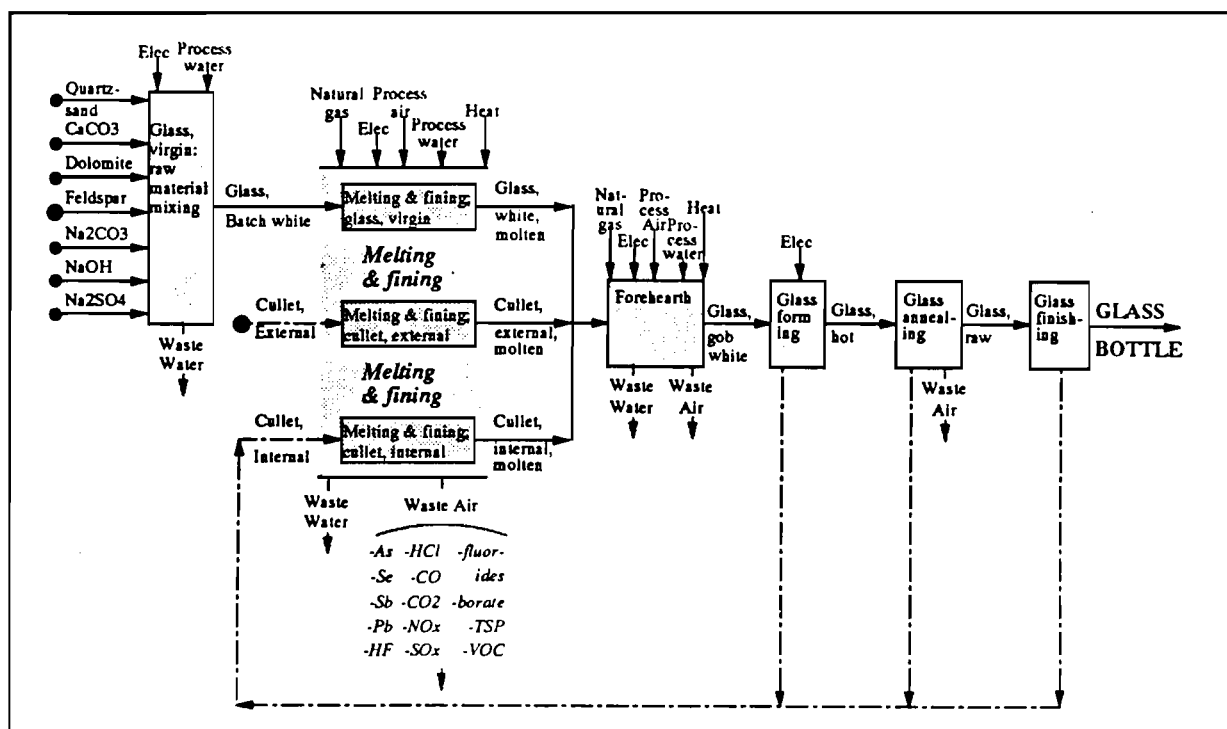
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7. Pulp and Paper

The production of pulp and paper can be broken down into three main steps:

(1) wood harvesting and transporting,
(2) wood pulp production,
(3) paper or board production.

The major part of paper board is produced in so-called integrated mills, that is, pulping and paper or board production take place at the same mills so that no transport of intermediate products is involved. The rest is produced in separate board mills using market (bale) pulp. The difference in energy use between the two ways of production is significant. In the current IDEA database, we only include data for integrated mills.

7.1. Wood Pulp Production

This section describes the chemical wood pulp production sulphate technology. Both short fiber (birch) and long fiber (pine) wood are used as basic raw materials in this process. Todate, in Europe, it is estimated that the percentages of short to long fibers are about 50/50 % for bleached pulp, and 25/75 % for unbleached pulp.

Sixty % of the logs for pulping are transported to the pulp mill by truck; the rest is transported either by boat or by train. When the logs arrive at the pulp mill, they are prepared for digesting. First, on their way to barking, part of the logs are cut, and the bark is removed in barking drums. The barked logs are then led to chippers, and the wood chips, after being screened, go to the digester. Bark residue is treated and used as fuel in the bark boilers.

In the digester, lignin is separated from the fibers by cooking the wood in an highly alkaline liquor (white liquor) under high temperature and pressure. The active alkali are sodium hydroxide (NaOH) and sodium sulfide (Na_2S). Both batch and flow digestion are used. In modern mills, extended cooking ensures high lignin removal rates which, in turn, reduces the amount of bleaching needed.

After digestion, the cooking liquor (black liquor) is separated from the fiber stock by washing. The washed pulp is then led to the knot separator and screening. Screen rejects become part of the waste water stream, whereas knots are sometimes returned to the digester. The screened pulp is thickened and stored in pulp chests. The unbleached pulp is then pumped either to (1) the stock preparation of the board-making machine, (2) the drying section from where it is prepared for sale, or (3) the bleaching section (Figure 7.1). In wood pulping, the white liquor is chemically recovered, recycled and re-used in the digester in the following way.

FIGURE 7.1: Pulp production
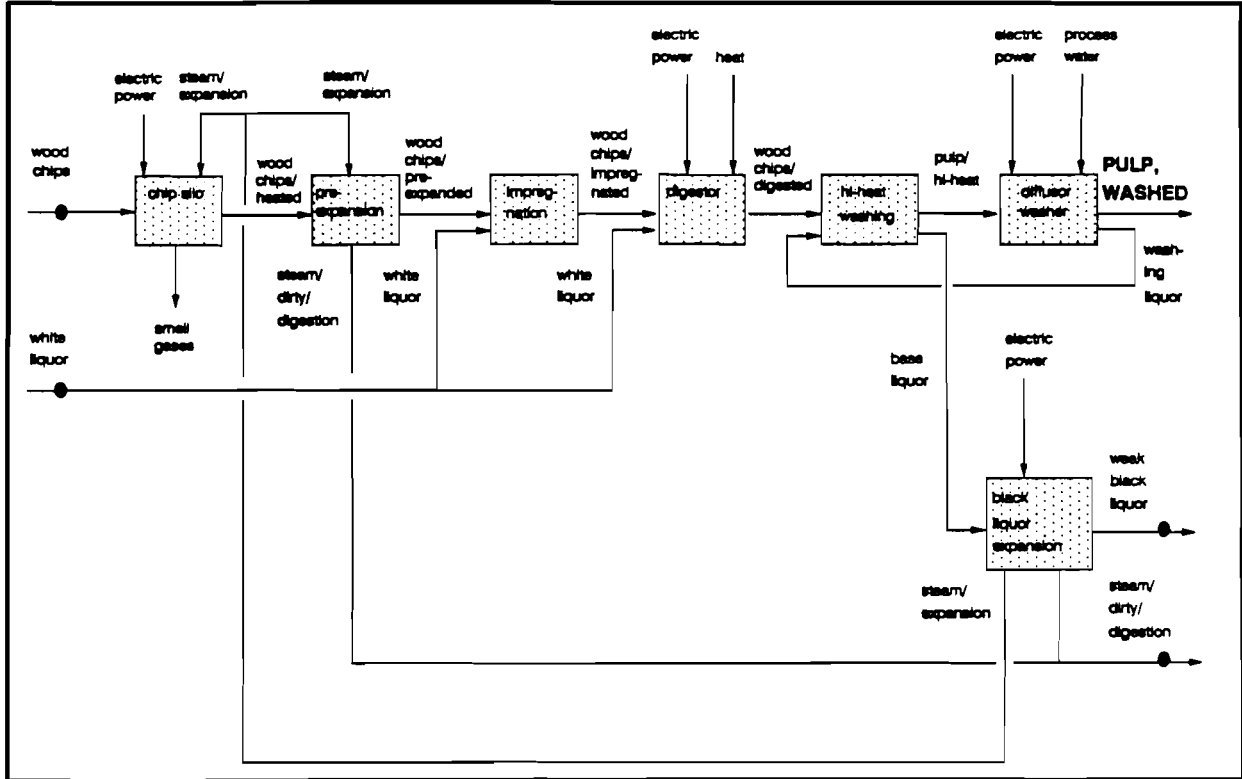
The mixture of base and washing liquors (weak black liquor) from washing is sent to multistage evaporators, where their dry content is raised to a level that sustains combustion. From the evaporators, the concentrated liquor (strong black liquor) is led to a recovery boiler for burning. Before burning, sodium sulfate (Na_2SO_4) is added to make up for chemical losses that occur in the liquor circulation. In the recovery boiler, the liquor is burned and molten sodium carbonate (Na_2CO_3) and sodium sulfide (Na_2S) are generated. These molten chemicals are then dissolved in weak white liquor (secondary condensates and supply water), and the solution (green liquor) is led through a clarifier into a caustisizer (slaker). In the caustisizer, Na_2CO_3 reacts with calcium hydroxide ($Ca(OH)_2$) forming sodium hydroxide (NaOH) and calcium carbonate ($CaCO_3$), i.e. lime sludge. The $Ca(OH)_2$ comes from the reaction between water and calcium oxide (CaO) that also takes place at the front end of the caustisizer; the CaO is fed in from the lime sludge burner. The $CaCO_3$ sludge is extracted from the remaining white liquor to which, before pumping it back to the digester, NaOH is added in order to adjust the sulfide/sodium balance. The $CaCO_3$ is burned in the lime sludge burner to regenerate CaO.

Bleaching is generally done in two main stages. There are four bleaching processes that are employed in sequence in these two stages:

(1)   O = oxygen delignification,
(2)   C = chlorine gas oxidizing,
(3)   D = chlorine dioxide oxidizing, and
(4)   E = alkaline extraction.

In the first stage, most of the residual lignin is removed by the following handling sequence: O-(D+C)-E. In the second stage, delignification is completed and colored compounds are dispersed to meet the final brightness demand of the pulp. A commonly used handling sequence in this stage is D-E-D, and this one is thus included in the IDEA database. Whereas the washing filtrate from the oxygen stage is re-used as part of the washing liquor in the digester, filtrates from the other stages are discarded in the sewage stream.

In the current IDEA database, there are production data included for bleached pulp from both pine and birch trees. For unbleached pulp, data for pine wood pulp only is included. In detail the following characteristics are assumed for different pulping processes.

Bleached pine pulp: a conventional batch cooking followed by an oxygen delignification to kappa number of 18. For bleaching both chlorine and chlorine-dioxide are used with alkaline extraction.

Bleached birch pulp: an extended flow cooking followed by the oxygen bleaching to kappa number of 13. Only chlorine dioxide is used for bleaching with alkaline extraction.

Unbleached pine pulp: a conventional batch cooking to kappa number of 80.

Chlorine and chlorine-dioxide are produced on site by ERCO R5 and ERCO R8 methods.

7.2 Paper and board production

Paper board production takes place in three main steps:

(1) stock preparation,
(2) board making (board machine),
(3) coating and finishing.

In the stock preparation for paper board production pulp is mixed, cleaned and refined to the degree needed for the final product. In so-called liquid paperboard, i.e., paperboard used for the manufacture of beverage containers, several layers of different quality are combined to make the final board product. There is a separate industrial line for each layer.

In the mixing step, a multistage process, different types of pulp are combined to form the final mixture for the particular layer; in this process, the consistency of the stock is also adjusted. Additives are used in small amounts as retention agents, slime preventers, fillers, pigments, etc. For liquid paper board, virgin, long- and short-fiber wood pulp is used. Only the broke (rejects) from the board machine and finishing section, and most of the cleaning rejects of the top layer, are re-used for the base layer stock. Generally, no other recycled pulp is used because of the high quality demands which would lead to high purifying costs. All other rejects are discarded as sewage.

The stock entering the head box of the board machine is diluted to 0.7-1.5 % solids. This mixture then goes through a cleaner. The rejects from this cleaner are passed through several reject sorters and a clarifier, from where the slurry is led back to broke handling and then to the base layer stock. In the board machine itself, the different pulp layers are formed, laminated and dried. The combined pulp layers enter the drying section with a solids content of about 40 to 45 %; here the water is evaporated so that the dry content increases to about 94 %. The water extracted during forming and pressing is recovered and recycled to dilute the incoming pulp in the head box of the board machine.

After drying, the board is optionally coated, wound and packaged for shipping. The coating and winding sections are generally part of the board machine. The coating stock is typically a mixture of latex, kaoline, starch, pigments (carbonates, TiO_2), carboxy-methyl cellulose (CMC), additives and water. Additives are used in small amounts for hardening, optical brightening, etc. The coating stock is pressed onto the board which is then dried by heated cylinders and infrared heaters. Coating and coating stock preparation produce pigment-containing effluent waters; these are typically treated with aluminum compounds and polyelectrolytes. The pigment-containing sludge is then separated for disposal and the remaining effluent water is discarded as sewage. (Figure 7.2).

FIGURE 7.2: Paper board production, duplex type
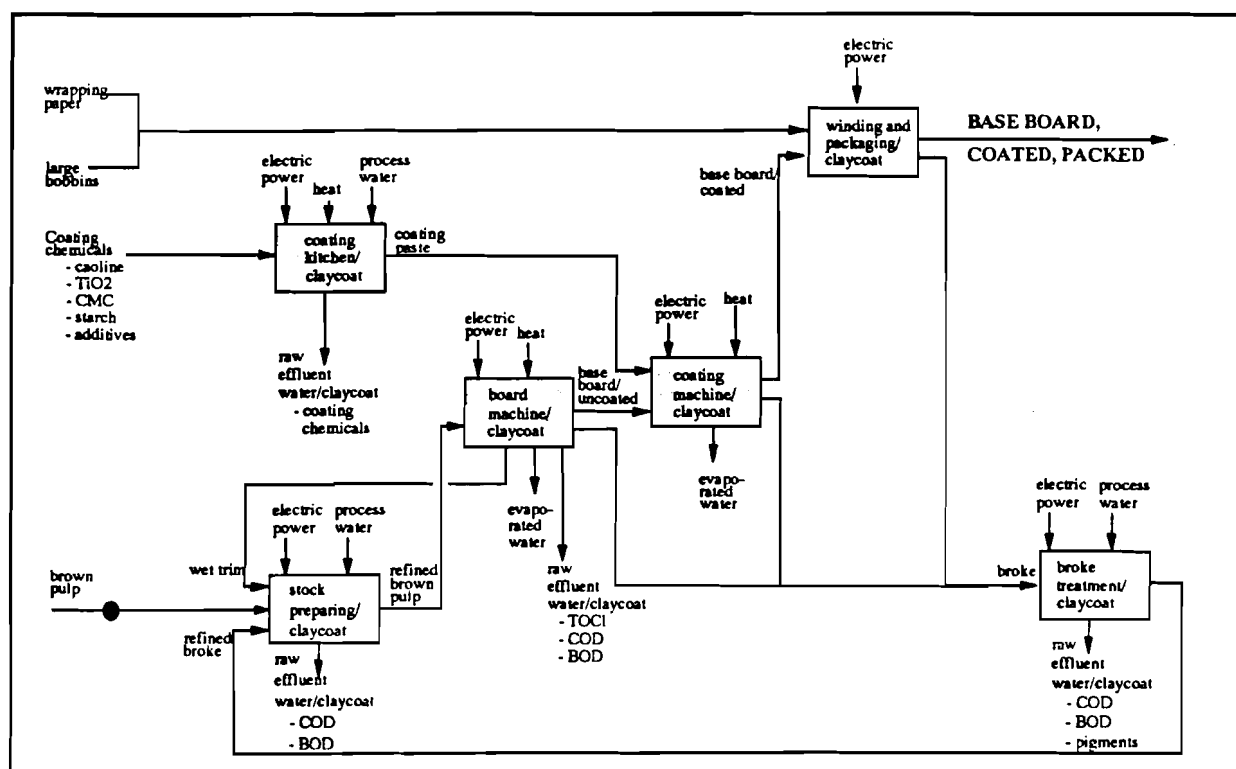
In the current IDEA database, there are data for three types of liquid packaging boards, which are

Duplex, uncoated : total weight 245 g/m2, bleached top layer 70 g/m2. In top layer 70% of bleached birch pulp and 30% of bleached pine pulp. Back layer all unbleached pine pulp.

Duplex, coated : total weight 260 g/m2, bleached top layer 70 g/m2. In top layer 70% of bleached birch pulp and 30% of bleached pine pulp. Back layer 170 g/m2, all unbleached pine pulp. Coating 20 g/m2

Gable Top, uncoated : total weight 295 g/m2, one layer, all bleached pulp. 50% of bleached birch pulp and 50% of bleached pine pulp.

There are also data for **boxboard of recycled fibre** (c-95) with the following characteristics:

Total weight 300 g/m2, coated. Coating 20 g/m2. 95% recycled fibre, 5% unbleached pulp.

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8. Aluminum Production

8.1 Alumina Production

The Bayer process is uses to obtain alumina from bauxite; it is an extractive hydro-metallurgical process in which concentrated caustic soda (NaOH) is used to extract in a digester alumina from bauxite at elevated temperature and pressure. First, the bauxite crushed and ground, then it is digested. In the digester, the aluminum hydrate from the bauxite is dissolved in the NaOH solution to form sodium aluminate solution. This produces a slurry which consists of a super-saturated sodium aluminate solution and a solid phase, commonly called red mud, or bauxite residue. This red mud consists of iron oxide, titania, silica, calcium oxide, alumina, phosphorus pentoxide, and several trace elements, and is separated from the saturated aluminate solution.

The sodium aluminate solution is cooled and precipitated to yield insoluble aluminum hydroxide and a NaOH solution. Aluminum hydroxide is then washed and filtered, and the large particles of aluminum hydroxide, the so-called seeds, are returned
to the solution of sodium aluminate in order to:

- Obtain a large grained crystallized precipitate.
- Accelerate precipitation.

This seeding results in a much finer product and eliminates a classification step. The spent liquor,containing NaOH, from filtering the precipitate is passed through a heat exchanger and a purification and evaporation step, and is then recycled to the digester. From the purification of the spent liquor, vanadium (V) and gallium (Ga) are recovered. Here again, the evaporated water is recycled as washing water.

The red mud, which forms the largest and most environmentally problematic effluent from alumina plants, is usually washed and filtered, and the solid residues are disposed of as waste The filter effluent is evaporated to remove the excess water from washing; the residual liquor is used to dilute the aluminate solution before precipitation, and the evaporated water is recycled as washing water.

The fine precipitated aluminum hydroxide crystals from precipitation are washed to remove impurities and go to the calciner, which can be a rotary kiln or a fluidized bed calciner, to remove at high temperatures (1300°C) free hydration water and obtain non-hygroscopic alumina (Al_2O_3) which is a white powdery material which is cooled, stored and finally transported to aluminum smelters.

The various steps of the Bayer process are shown in *Figure 8.1*.

**FIGURE 8.1:** Bayer Process for Alumina production
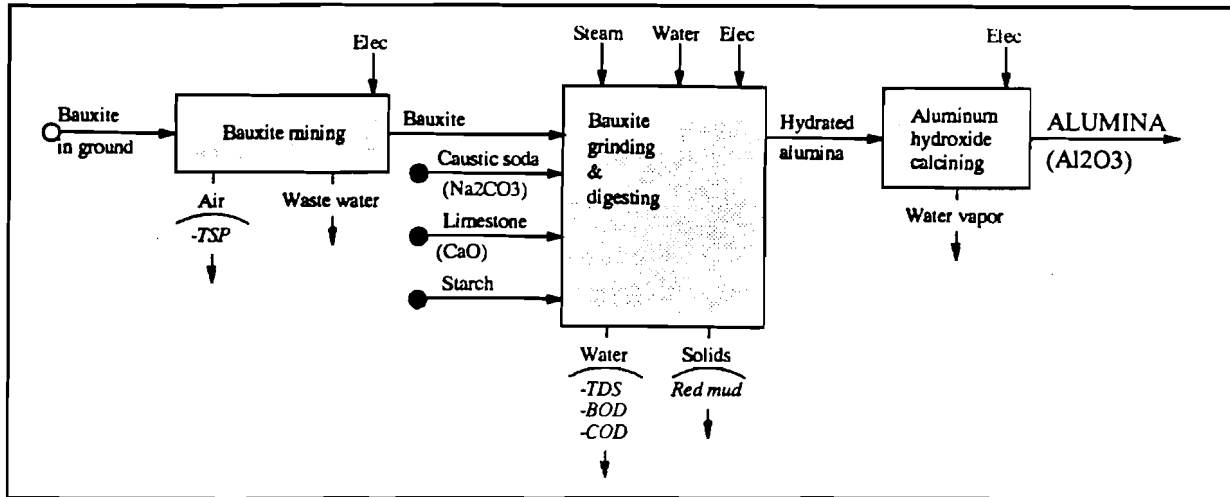
8.2. Primary aluminum smelting and semi-manufacturing

The only process being used on an industrial scale for smelting of primary aluminum is the Hall-Heroult process (*Figure 8.2*). The essence of this process is the electrolytic reduction of crystallized alumina (Al_2O_3) in a cryolite (Na_3AlF_6) melt at 960 °C in 50 to 280 kA cells with a consumable carbon anode and an aluminum pole cathode. The electrolysis yields aluminum (Al) at the cathode and oxygen (O_2) at the anode. The O_2 reacts with the carbon of the anode to create carbon oxides (CO and CO_2) which become part of the exhaust gas stream.

During the electrolysis, the so-called anode effect occurs periodically, where the aluminum fluoride (AlF_3), and not the Al_2O_3, is reduced, and fluorine compounds are formed. These are generated in large quantities, they are vented from the smelter and washed repeatedly to recover fluor in the form of cryolite. The water of each washing step is recirculated and losses are made up by fresh water.

The reduction cell, or electrolysis pot, is the main unit of an aluminum smelter and is made from sheet steel, lined internally with insulating blocks and provided at the base with a layer of carbon which acts as the cathode. Basically two anode types are available: prebaked anodes are baked in a special furnace before being used in the electrolysis while, in Söderberg systems, the paste is continuously baked at the cell by the heat of the electrolysis and the so-called Joule effect. The baking is done in furnaces with open or closed chambers at a temperature around 1100°C. These furnaces are usually heated by fuel oil or natural gas. The baking of anode materials is the principal source of polycyclic aromatic hydrocarbons. Prebaked anode are changed after having been consumed up to about 85%, the rest is reused for producing new anodes.

FIGURE 8.2: Hall-Heroult process for the production of primary aluminum
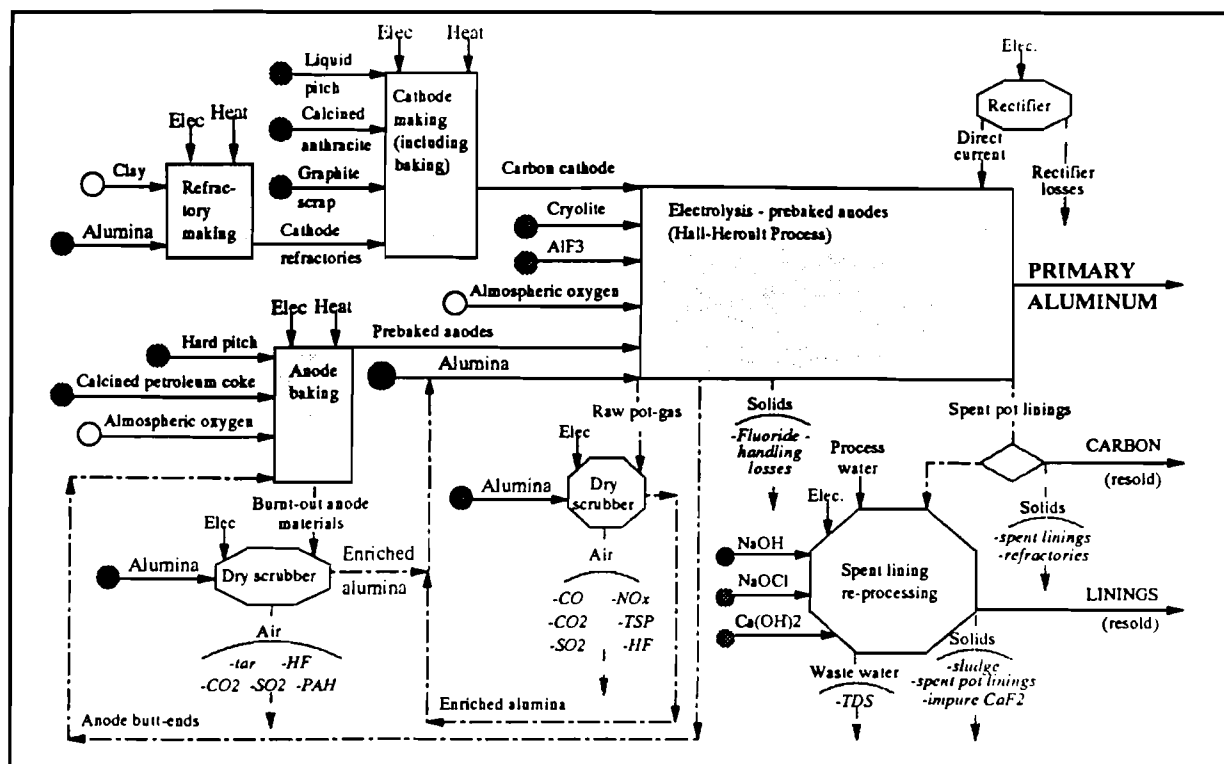
The density of the electrolyte, i.e., the cryolite, at 960°C is lower than that of the molten aluminum which enables the latter to form a layer at the base of a cell from which is drawn off by tapping or by suction. Alumina is introduced regularly into the electrolyte through the crust which forms on the surface, and cryolite losses are made up as required.

The liquid metal withdrawn from the reduction cells is transported to the casting plants. Here it is mixed with alloying constituents such as manganese (Mn), silicon (Si), iron (Fe), copper (Cu), magnesium (Mg), chromium and zinc (Zn) according to final product requirements. The liquid metal has to also be degassed to eliminate the hydrogen which is the only gas that has a measurable solubility in molten aluminum and calcium; this is done by fluxing with a mix of chlorine gas and argon or nitrogen. Afterwards the aluminum can be cast into billets (for producing profiles), slabs (for producing flat products) or ingots (usually not alloyed and dedicated for remelt to foundry or wrought alloys).

In 1985, there were 33 aluminum reduction plants in EC Europe; the total annual output was 2.3 million t of aluminum.

Air Emissions

In the early years of the aluminum industry, most of the effort was directed toward controlling fluoride emission from the cells. The technology for fluoride control is now well established throughout the industry. Other significant air emission sources exist in the anode production process; these involves polycyclic aromatic hydrocarbons, tars and fluorides from the reuse of unconsumed anode materials, called anode butt-ends. Atmospheric emissions produced by an aluminum cell consist of particulate and gaseous fluoride (predominantly HF), alumina, carbon dust, sulfur dioxide, carbon dioxide, and carbon monoxide. Typical values (before cleaning) for total fluorides generated by the cell range from 20 to 30 kg/tonne product. Approximately the same amounts of alumina and carbon dusts are also produced. Sulfur dioxide varies according to the sulfur content (around 3%) of the coke used to prepare the anodes. Because of the inherent disadvantages in wet systems, not the least of which is potential water pollution, new smelters employ dry scrubbers for controlling cell emission. A dry scrubber uses either a fluidized bed or direct injection of metal grade alumina into the gas stream to remove the hydrogen fluoride gas by adsorption. The alumina usually is recovered from the gas stream by a fabric filter, which also removes the other entrained particulate species. Dry scrubber efficiencies are generally greater than 98% for both the gaseous fluoride and the particulate matter, while the SO_2 adsorption efficiency remains below 33%. Dry scrubbers are considered to be the state-of-the-art control technology. The aluminum fluoride that is recycled to the cells represents a significant material recovery value.

Emission data contained in the IDEA database represent the application of state-of-the-art pollution control technology.

Wastewater Discharges

Wastewater effluent is usually not a major problem, except in those plants where wet processes are still used to scrub the air emissions from the cells and the anode baking furnaces. As we, however, do not include data for those plants in IDEA, there are no significant waste water effluents.

Solid Waste

Cathode linings in aluminum cells are removed when lining failure occurs and large amount of this material, called spent pot linings, must be discarded. The USEPA initially classified spent pot lining as hazardous waste because of its cyanide content, in the meantime: these, however, have been removed from the hazardous waste list pending further studies. Present disposal practices are "temporary" storage in curbed, roofed, protected areas to minimize leachate generation, or burial in landfills lined with impervious materials to prevent contamination of the surrounding environment. These procedures are costly because of the large volumes involved.

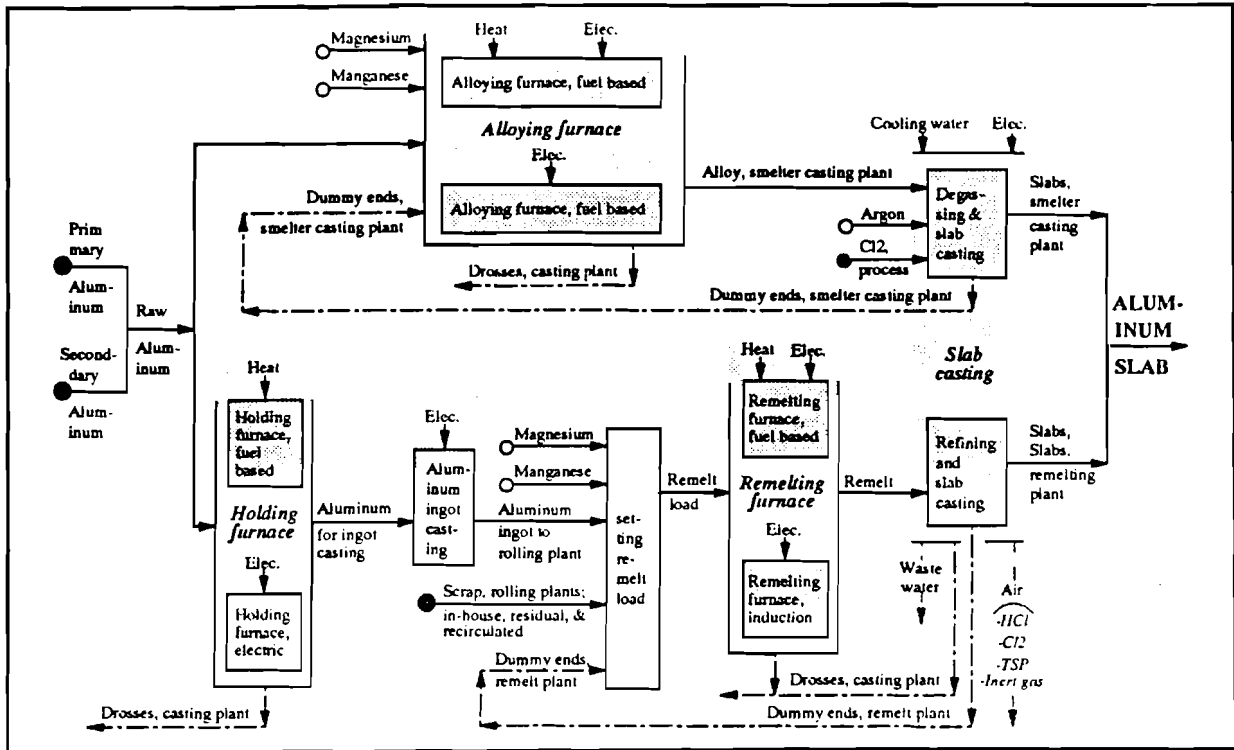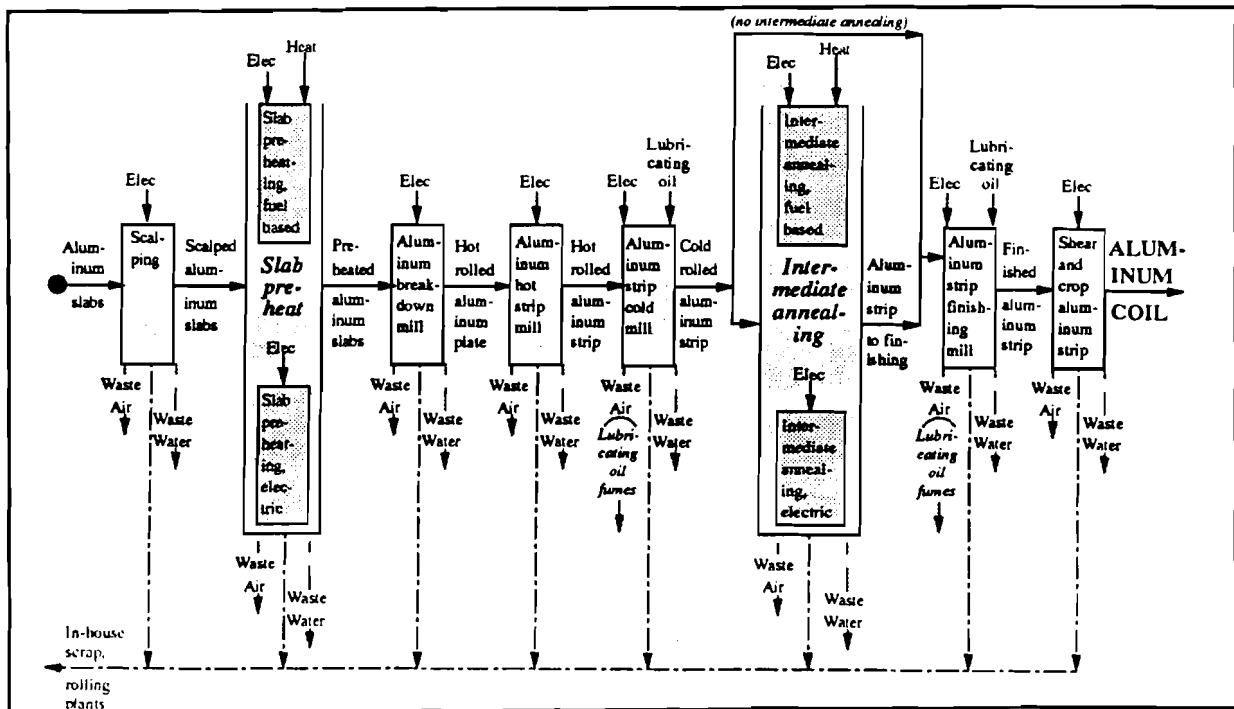**FIGURE 8.3:** Aluminum slab casting

FIGURE 8.4: Aluminum coil production

Bleaching processes can be used to remove the cyanide and to stabilize the fluoride content in the stable form of calcium fluoride. Because of the carbon and fluoride content of the solid waste, current research is directed toward recovering or utilizing these valuable components. To date, the principal economic application for spent pot linings is the reuse of the carbon constituents in steel converters where their fluoride content fulfills part of the flux material requirements.

In IDEA, no treatment processes are included for spent pot linings; they leave the system classified as special wastes, but can easily be reclassified as by-product.

8.3. The Production of Aluminum Strip

End-fabricators, such as the packaging industry, need the raw metal to be transformed into semi-fabricated products (i.e., strips, profiles, wire and cables, tubes).Packagings (cans, caps, coated boards, etc.) are produced exclusively out of aluminum strips produced by rolling. In Europe, this production occurs in large plants (output > 100,000 t/year). The sequence of operation in the production of flat products (i.e. sheet, strips, etc.) consists of (Figure 8.3, 8.4):

- *Casting*: rolling plants are generally equipped with a remelting and casting unit in order to recover their own scrap, or so-called "new fabricating scrap" from end-fabricators (e.g., can makers). This unit provides the slabs ready for rolling. In IDEA, the same unit process data as in primary aluminum production are used.
- *Hot rolling*: reduces the thickness of the slabs from around 250 or 500 mm to 2.5 to 5 mm;
- *Cold rolling*: reduces the thickness down to the final, required strip thickness;
- *Finishing operations*: heat treatment, shearing, sawing, flattening, inspection, etc.

FIGURE 8.5: Production of secondary aluminum
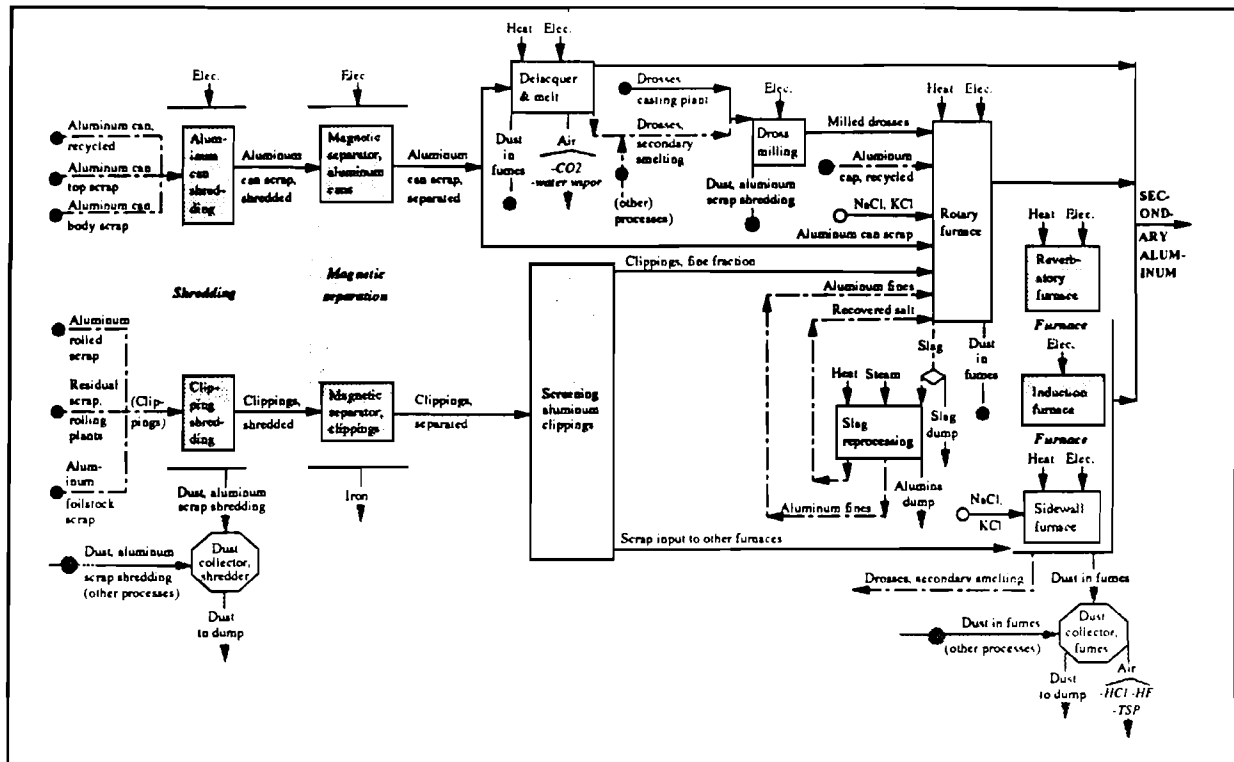
8.4. The Secondary Aluminum Industry

The role of the secondary aluminum industry is to recycle scrap aluminum. The advantages of this are that, firstly, scrap aluminum that might otherwise be discarded is reused and not dumped and, secondly, it can be shown that the energy required to recycle scrap aluminum is approximately 5% of the energy required to produce aluminum ingot of the same weight in a primary smelter.

In Western Europe, secondary aluminum is predominately used in the production of casting alloys. Other products made from secondary aluminum include wrought alloys (mainly extrusion billets) and steel-deoxidizer grade alloys.

This effectively creates a certain segregation of the primary aluminum and secondary aluminum markets. However, even if the substitution of secondary aluminum recovered from, for example, packaging systems to primary aluminum substitution is not direct, the fact that this occurs as a whole on the aluminum market constitutes the rationale for considering primary and secondary aluminum as substitutable products within our analysis. In IDEA, we therefore use a closed recycling loop.

The database includes a separate unit process for *recycled and scrap preparation*. Usually recycled clippings or new sheet scrap need to be cut and cleaned, especially iron contaminants have to be removed. They are usually run through a shredder to reduce the size of the scrap and then through a magnetic separator to remove the iron.

Also, beverage cans, before they can be remolten, need to be delacquered and there is a separate unit process for this in the IDEA database. In modern plants, this is done in a reactor where the temperature and the oxygen content of the furnace atmosphere are controlled in order to ensure a smoldering combustion of the lacquer. The contaminated flue gas is used to preheat the incoming aluminum ships and then drawn to a combustion chamber, where it is mixed with additional combustion air in order to burn hydrocarbons. The resulting flue gas is raised here to a higher temperature so that it can be further used; partly for preheating air for the melting furnace and partly in the smoldering process. This type of process is in fact suitable for preparing all types of painted or oily scrap (e.g., boring and turnings) and leads to high energy efficiencies (Lossack, 1987; Schmitz, 1987; and Twyan and Lannon, 1981.

Usually, this process is combined with the remelting of the cans as the next step. In the IDEA database, 60 % of the recycled beverage cans go first to the delacquering and subsequently to a direct remelting process. The other 40 % go directly to rotary furnaces (described later).

Before re-smelting, these drosses must be upgraded to at least 50% to make recycling profitable. This is usually done by repeated grinding, screening and magnetic separation. Being less brittle than the other dross constituents, metallic aluminum is concentrated in the coarser size fraction. The finer fraction is commonly discarded; it can also be sold for further use in exothermic reactions.

The main air pollution controls in scrap preparation are after-burners used to consume combustible black smoke generated in delacquering cans and baghouses used to collect dust from shredding and milling operations. There are usually no process-related water effluents in scrap.

Secondary aluminum slag from rotary furnaces can also be recycled (see Schmoll, 1986a,b). A unit process for *wet preparation of slag* is thus included in IDEA. Most of this is currently done in Germany where two installations, with a total capacity of 85,000t per year, treat part of the 150,000 - 200,000 t (Kirchner, 1986) of slag produced annually. Recently, another installation has been put into operation in Italy. The process allows the recuperation of salts as well as the 3 to 5% of aluminum contained in the slag.

Separate unit processes are contained in IDEA for the following furnaces for resmelting; and equal market shares of 25 % each are given in a distribution table for scrap aluminum other than recycled cans.

Rotary furnaces (or salt bath furnaces) are used for melting low grades such as dross and thin or heavily contaminated scrap; they make use of a salt bath which traps metal oxides and contaminants and avoids an over-oxidation of thin scrap, which sinks rapidly in the salt bath and is protected there from the hot air of the furnace atmosphere.

Due to their configuration (i.e., the heat from the burner can be well used inside the drum) these furnaces reach good levels of energy efficiency and values of 60% are not scarce. However, the salt consumption, which ranges from 100 to 400 kg per tonne of metal output (Erne, 1984), and the approximately one-third higher slag formation during the smelting process.

Well furnaces (i.e., sidewell furnaces or forewell furnaces) are essentially reverberator furnaces equipped with an outer well. They are convenient for melting slightly contaminated scrap. Fluxing salts (commonly 47.5% NaCl, 47.5% KCl, 5% cryolite) are used to entrain metal oxides on the metal charging surface. Once the oxides are trapped in the flux, they are removed by skimming."

Induction furnaces are most suitable for remelting fresh scrap which is not contaminated. Capacities range up to 10 t for crucible induction furnaces and up to 50t for channel induction furnaces (see Erne, 1984). The vigorous stirring action, produced by eddy current, rapidly incorporates the solid scrap into the molten metal and avoids its over-oxidation at the surface of the bath. When utilizing more contaminated scrap, extreme care must be paid to the scrap preparation in order to suppress contaminants such as oils or paints which would increase the dross formation, as well as any moisture which would cause metal explosions. In the past, such explosions led to the shutdown of induction furnaces in Italy and Germany. Switzerland is currently the only country where one induction furnace is still used for melting almost all grades of new aluminum scrap.

Reverberator furnaces may be used concurrently with induction furnace for melting fresh, non contaminated scrap. The main differences with the well furnace are that (1) the scrap is directly charged in the hearth of the furnace (i.e., no wells) where the burner flame can directly impinge the soldered scrap, and (2) there is no use of fluxing salts. The melting rate and the energy efficiency are much higher than in well furnaces.

This process (see Lossak, 1987) leads to a reduced consumption of alloying elements and to reduced metal losses. Melting is commonly done in a well furnace; the preheating of scrap and combustion air permits high melting rate and energy efficiency.

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9. Iron and Steel Production

The transformation of iron ore into steel and steel products takes place in a series of distinctly different processing steps. The four main steps are:

(1) preparation of raw materials;
(2) iron manufacture;
(3) steel manufacture;
(4) manufacture of the finished steel product.

The processes for the first four steps are described in the following sections, and are those used most commonly todate in Western Europe in steel making.

The main raw materials for iron and steel making are iron ore, coal, limestone ($CaCO_3$), or in some cases lime (CaO), ferro-manganese, natural gas and oxygen. Minor amounts of oil to provide additional carbon, and various fluxes, such as fluorspar, i.e. calcium fluoride (CaF_2), to promote fusing and prevent the formation of oxides, are also needed in certain process steps. A considerable amount of steel scrap is used in various processes to reduce the amount of virgin iron ore needed.

9.1. Preparation of raw materials

In the iron and steel industry, the following steps are necessary in extracting and preparing the raw materials:
(1) coal mining;
(2) coke production;
(3) limestone mining;
(4) lime manufacturing.
(5) iron ore preparation;
(6) iron ore agglomeration (sintering or pelletizing);

As coal, coke, limestone and lime are also used in other industries, the reader is referred to Section 1.1 for "Coal mining", Section 2.2 for "Coke production", Section 1.2. for "Limestone mining" and to Section 4 for "Lime burning". Also "Iron ore mining" has been described in Section 1.2 "Minerals Extraction and Mining".

9.2. Iron Ore Agglomeration (Sintering and Pelletizing)

The fine ore particles are agglomerated to give suitable size and strength to the material. Ore agglomeration can be achieved by various processes such as sintering, pelletizing, nodulizing and briquetting. In this study, only two processes are of interest:
(1) sintering in conventional crude steel making,
(2) pelletizing both in conventional crude steel making and in direct reduction furnaces.

In the sintering process (batch process), the finely crushed iron ore concentrate is mixed with internal steel scrap (mainly mill scale), recycled dust from both blast furnace and oxygen furnace, limestone and coal or coke breeze. The mixture is ignited and, while the coke breeze burns, the mixture is fused into a porous, but strong, sinter. This sinter is broken up and screened into suitable size before being charged into the blast furnace.

In pelletizing (batch process), the finely crushed iron ore concentrate is mixed with a small amount of binder (usually bentonite) and water, and fed into a pelletizer. This pelletizer is also continuously fed with granular dust. Through the so-called "snowball effect", the sticky mixture adheres to the granular base material and pellets are formed. Before these are transferred to the direct reduction plant or conventional steel works, they are dried and hardened.
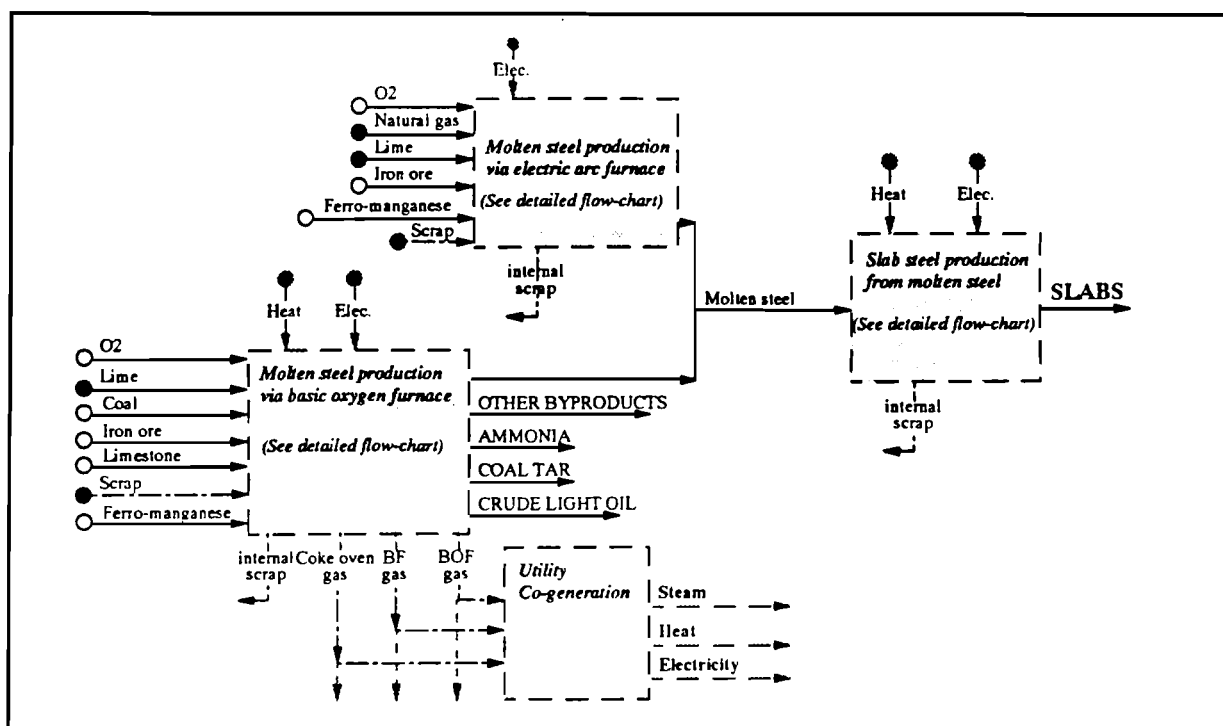
9.3. Iron Manufacture

The primary inputs to the process of iron manufacturing are sinter or pellets. Each tonne of iron requires about 1.5 t of sinter or pellets charge. Iron ore as well as both sinter and pellets contain iron primarily in the form of iron oxide, and in order to get iron, the iron oxide must be reduced. This reduction is accomplished either in
(1) blast furnaces under high temperature,
(2) direct reduction plants.

The blast furnace is charged from the top with sinter, pellets, coke, limestone and in some cases relatively small amounts of iron ore. Air, pre-heated by exhaust gases from the coke oven and the blast furnace itself, is then injected from the bottom. As the air passes through the furnace, it burns the coke, creates reducing gases (mainly CO) and sufficient heat to melt the iron, and slag (mainly oxides of calcium and ore impurities) forms on top of the molten iron (at about 1700°C). The so-called pig iron (molten iron) is withdrawn in carts and transferred to the basic oxygen furnace. The slag is periodically withdrawn and further utilized mainly by the construction industry so that there are no solid wastes from the blast furnace. Blast furnace gases are also collected and used as energy or carbon sources in some process steps in the steel plants. Pig iron has a typical composition of 93.8 % iron (Fe), 4.7 % carbon (C), 0.7 % manganese (Mn), 0.6 % silicon (Si), 0.1 % phosphorous (P) and 0.04 % sulfur (S) by weight (IISI 1982). The impurities, and in particular the carbon, make pig iron relatively brittle and difficult to form.

In the direct reduction plant, iron pellets are charged into the furnace where the oxygen content in the iron, still in its solid state, is lowered through reduction with carbon which, in Western Europe, to 97 % is supplied in the form of natural gas (the remainder is supplied as coal or coke). After the direct reduction step, the so-called sponge iron is ready to be charged into the electric arc furnace. Sponge iron contains at least 92 % pure iron (Fe), the remainder being carbon (C), manganese (Mn), silicon (Si), phosphorous (P) and sulfur (S) (UNEP 1983).

FIGURE 9.1: Alternative production lines for crude steel

9.4. Steel Manufacture

Crude steel is more formable and has higher strength than iron because of lower carbon, phosphorous and sulfur levels. It is almost exclusively manufactured in the following three types of furnaces:

(1) basic oxygen furnace;
(2) electric arc furnace;
(3) open hearth furnace.

In Western Europe in 1985 the respective shares in crude steel making were 69.7 % in basic oxygen furnaces, 29.0 % in electric arc furnaces, and 1.3 % in open hearth furnaces (IISI 1986). In the IDEA database, we therefore neglect the open hearth furnace whose share is constantly further decreasing.

Although various amounts of steel scrap are used in all furnace types, 95.3 % of the electric arc furnaces in Western Europe use exclusively steel scrap and no charge from the direct reduction plant (UNEP 1983, UNEP 1986, IISI 1983). Although the share of the electric arc furnaces that use both sponge iron from direct reduction and steel scrap is currently small, it is continuously increasing and is therefore taken into account in our study.

Figure 9.1 summarizes the different routes that we investigate in this study:

(1)   the conventional route (blast furnace - basic oxygen furnace) (70 %, as given in the mixture table.
(2)   the scrap melting route (100% scrap in electric arc furnaces) (28 %);
(3)   the direct reduction route (direct reduction - electric arc furnace) (2 %).

**FIGURE 9.2:** Molten steel via basic oxygen furnace
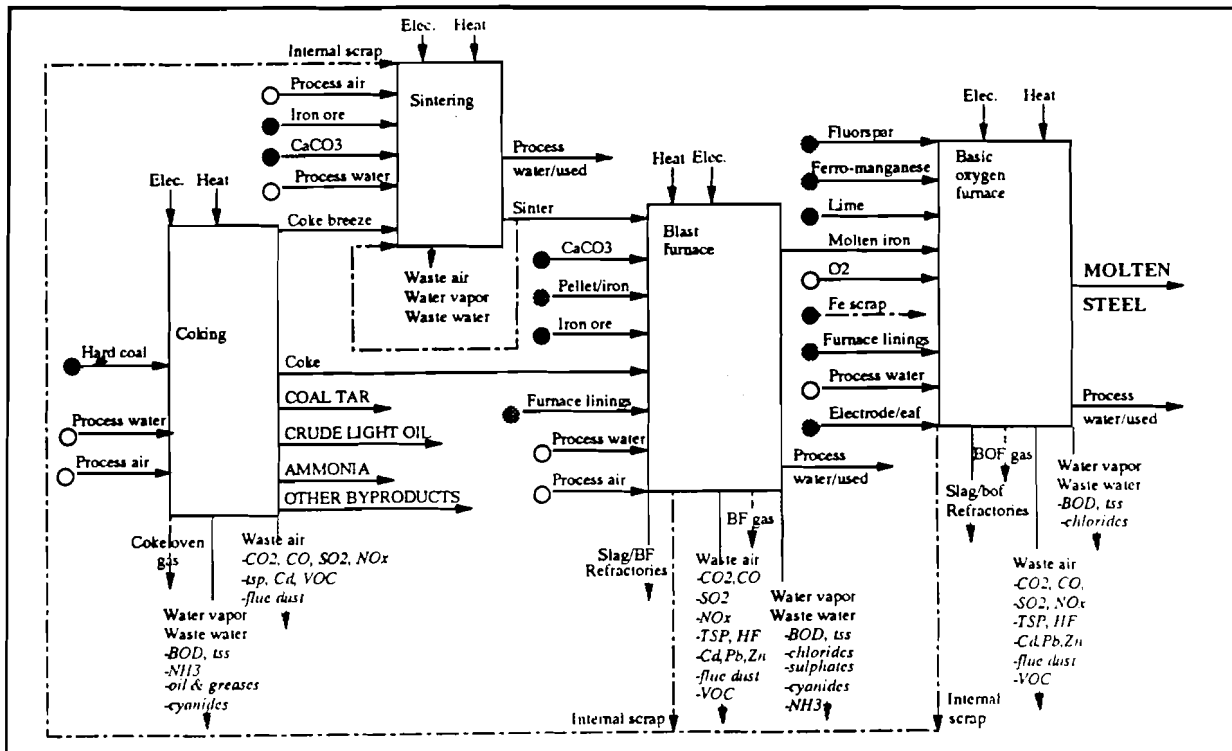
In the *basic oxygen furnace* (conventional route), the charge is a mixture of molten pig iron and scrap; in our database, we use a pig iron to scrap ratio of 3 to 1. Lime (CaO), ferromanganese, and fluxes, such as fluorspar (CaF_2), are added to the furnace in order to

(1)   reduce the carbon content of the iron,
(2)   promote fusing and prevent the formation of oxides.

The melt is heated to very high temperatures by-product gases, usually from the coke oven. The carbon in the hot metal is then reduced by oxygen lanced into furnace to make crude steel. When the oxygen and metal react under high temperatures, large quantities of iron oxides, carbon monoxide (CO) and carbon dioxide (CO_2) are formed. The iron oxides together with the calcium from the CaO form slag which is periodically withdrawn and sold to the construction industry.

The CO and CO_2 make up most of the by-product gas which is used on-site for steam-and subsequent electricity-generation. The final exhaust gases contain high levels of CO, sulfur and NO_x. The crude steel generally has a carbon content of less than 2.0 %. Figure 9.2 illustrates the process steps in the conventional route of steel making.

FIGURE 9.3: Molten steel via electric arc furnace
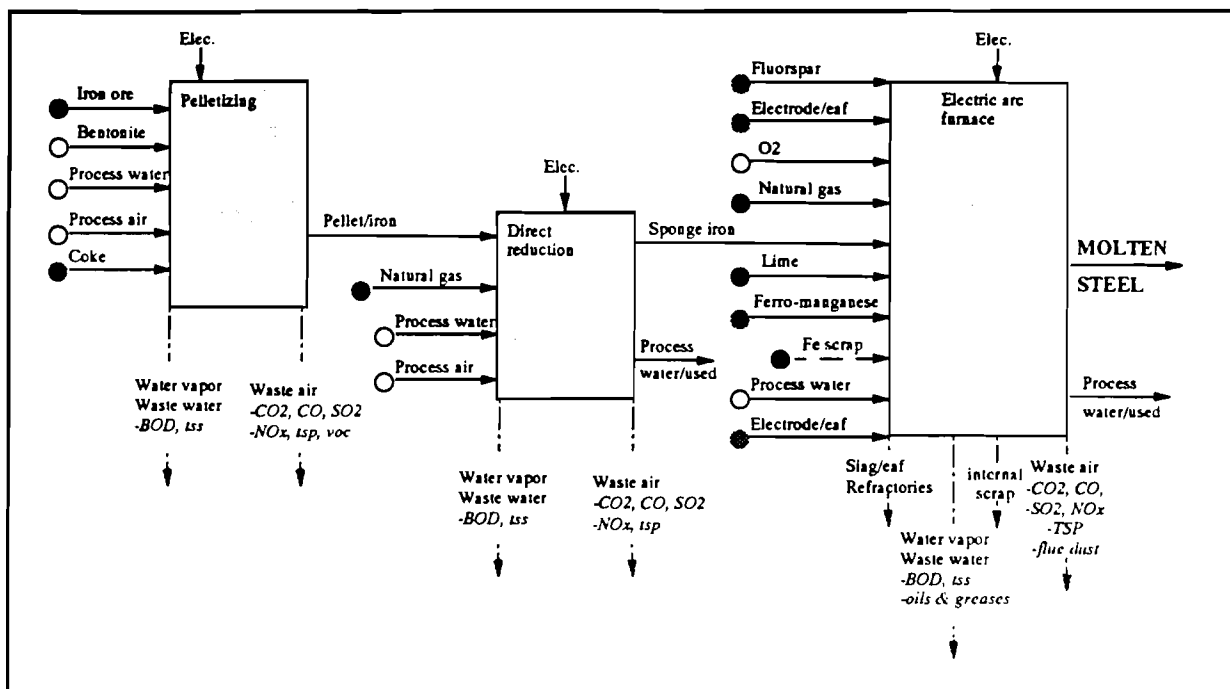
In the *electric arc furnace*, the charge is either
(1) 100 % steel scrap in the scrap melting route,
(2) a mixture of sponge iron and steel scrap (commonly, with a ratio of 7 to 3) in the direct reduction route. Again, CaO, ferromanganese and fluxes, such as CaF_2, are added to the furnace. The charge is melted by three high power graphite electrodes that descend through the furnace roof, and like in the basic oxygen process, oxygen is used to reduce the carbon level of the hot iron to make crude steel. Because of the relatively high percentage of scrap steel used as input, the slag formed on top of the molten steel is contaminated with high levels of heavy metals, and is therefore not further used, but discarded as waste material. The various process steps in both the scrap melting and direct reduction route are depicted in Figure 9.3.

FIGURE 9.4: Ingot and continuous casting for slab steel
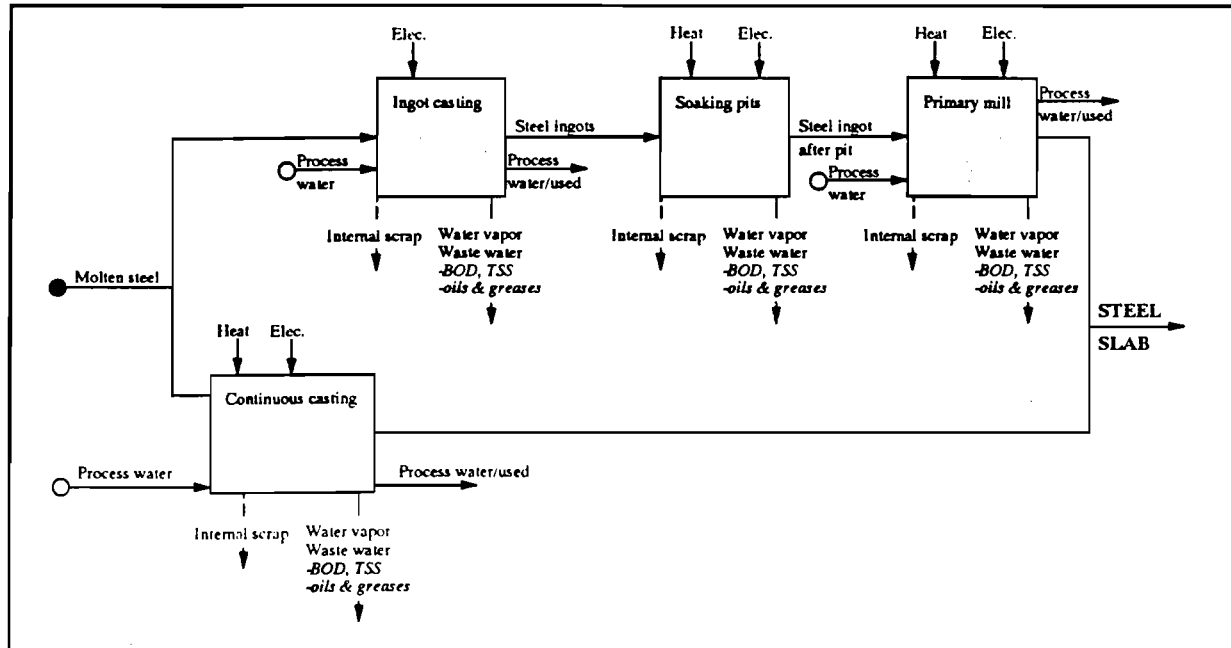
Molten steel is then casted using either continuous or ingot casting (see Figure 9.4). In Western Europe, casting is done to 70.5 % in a continuous way and to 29.5 % in ingots (IISI, 1986); these shares are therefore also used in the IDEA database. For steel ingots, soaking pits are used to uniformize the temperature within the ingots and to adjust them to the correct rolling temperature. Heated ingots are rolled in primary mills to slabs of about the same shape as continuously casted ones.

Figure 9.5 and 9.6 show the finishing section of steel making. The steel slabs are reheated, unless they are hot-charged, and rolled in the hot strip mill. Flat products are pickled (treated with acid) to remove the scale formed during cooling in previous process step and rolling oils. The next step is cold rolling, followed by annealing (reducing the temperature of the product in a controlled way in order to minimize residual stresses that might otherwise be retained), tempering (heating and subsequent quenching), steel coil preparation, and lastly, coating (electrolytic tinning for tin plate). The tin plate coil is then packed to be sold. Steel strapping, for example, which is used as a secondary packaging material, is obtained in a so-called skin pass mill which follows directly the hot strip mill.
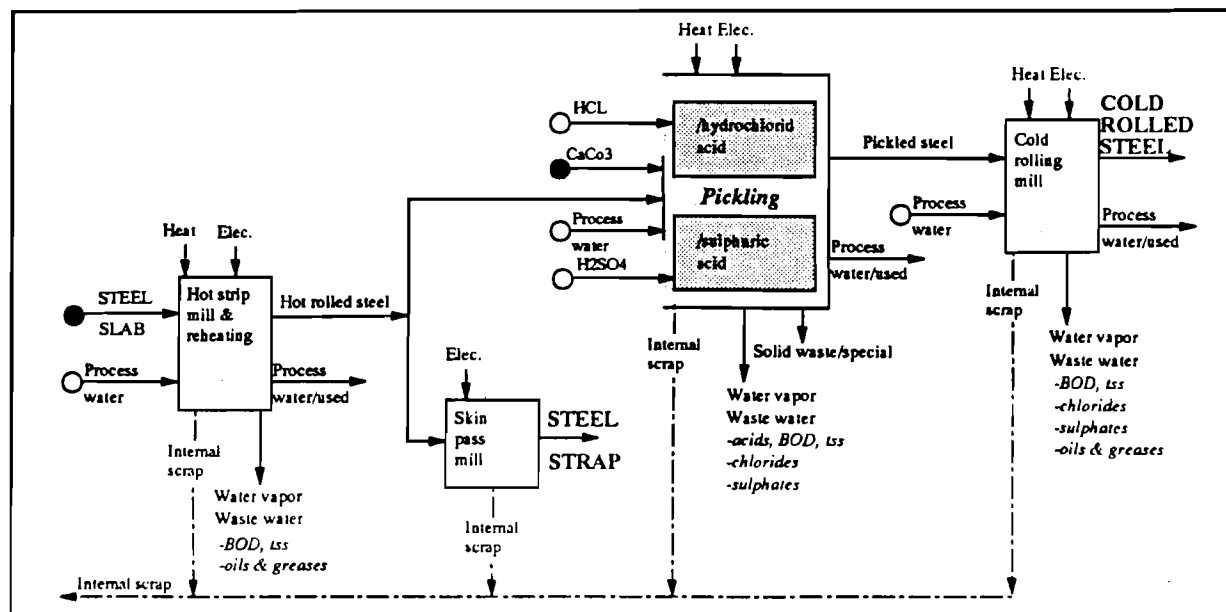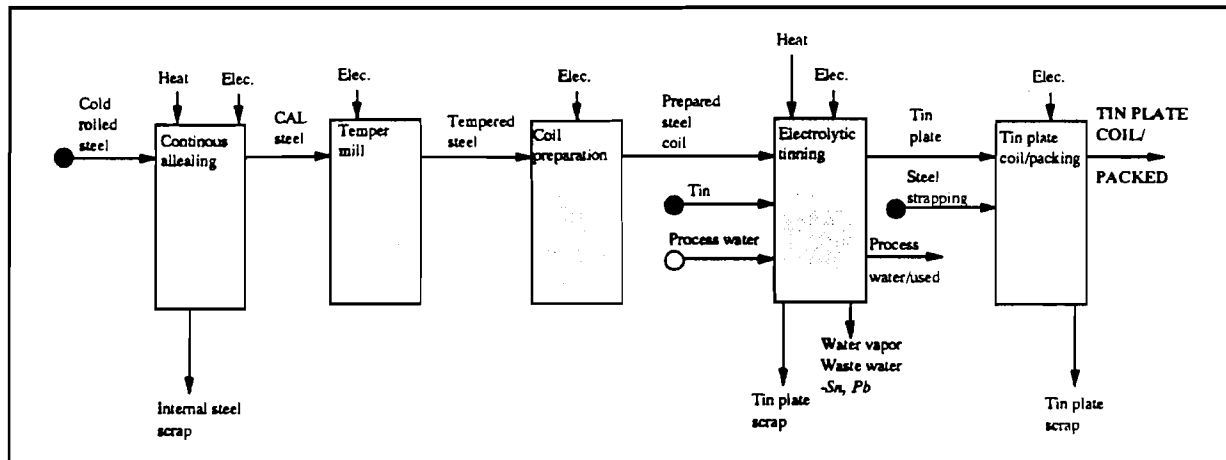
FIGURE 9.5: Steel production, finishing

FIGURE 9.7: Steel production, tin plate coil

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10. Beverage Container Manufacture

Since the methodology developed in this project was to be tested by quantitatively evaluating the environmental impacts of several beverage packages, IDEA contains the cradle-to-grave data (production, distribution, use and final disposal) for twelve different types and sizes of beverage containers. As there is a large number of different beverage packages on the market in Western Europe, we had to select several case examples.

The chosen sizes, materials and beverages represent those containers in which the largest volumes of beverages are currently being packaged, as well as those that promise to gain a significant market share in Western Europe. One container type still in frequent use in Western Europe, especially for mineral water, is the polyvinylchloride (PVC) bottle. New legislation in several countries prohibits their use, however, and there is a general trend in Europe to phase out PVC bottles. Therefore, they are not included in our analysis. The specifications and the auxiliaries (e.g., closure, label, secondary packaging, etc.) for the different packages are listed in Table 10.1.

The data are limited by several factors:

- The time available to carry out this work was limited to 14-months so that it was impossible to collect original data for all container types. We therefore had to start with published information that was carefully checked, in many instances updated and, in several cases, merged with original data from our own investigations.
- Data were aimed to reflect Western European conditions. For this purpose, we had to frequently use values that, as such, may not reflect the reality of any particular country, but only represent weighted European averages. Results as well as underlying data should therefore not be applied to a particular country or region without carefully checking their validity.
- Given the short time available, it was impossible to assess the actual technology mix as currently representative of Western Europe for manufacturing the various materials used in the beverage containers. We thus use the "state-of-the-art" manufacturing processes.

In spite of these limitations, the present data can be used to answer a number of questions on the environmental impacts of beverage containers; it allows to demonstrate how changes (e.g. increased recycling, different market shares, superior production technologies, higher trippage rates, etc.) affect the complete system. This is important as most of the studies comparing different packaging alternatives use data only of part of their life cycle. Political as well as economic decisions based on such results meant to reduce overall environmental impacts, may have only limited effects when considering the cradle-to-grave beverage container system.

TABLE 10.1: Specification for different beverage containers

Type	Size [l]	Weight [g]	Beverage	Volume [mill. l]	Closure	Labeling	Packaging
returnable glass bottle	0.5	355	beer	5215.1	crown cork	paper, glued	PE crate, pallet
	1.0	841	soft drinks	3066.2	PE twist-off alu twist-off	paper, glued	PE crate, pallet
one way glass bottle	0.75	452	wine	3188.2	crown cork	paper, glued	tray, pallet
aseptic carton	1.0	26	milk	6622.7		printed	tray, shrink film, pallet
non-aseptic carton	1.0	24	milk	1438.0		printed	tray, shrink film, pallet
gable top carton	1.0	28	milk			printed	tray, shrink film, pallet
returnable PC bottle	1.5	70	milk		PE twist-off	paper, glued	PE crate, pallet
one-way PET bottle	1.5	65	soft drinks	1743.6	PE twist-off	paper, glued	tray, shrink film, pallet
returnable PET bottle	1.5	107	soft drinks		PE twist-off	paper, glued	PE crate, pallet
HDPE bottle	1.0	28	milk	750.0	PE twist-off alu twist-off	paper, glued	tray, shrink film, pallet
steel can	0.33	31	soft drinks	1238.6	alu pull-off	printed	tray, shrink film
alu can	0.33	16	soft drinks	967.6	alu pull-off	printed	tray, shrink film

Steps towards environment-friendly packages should, for example, not only focus on the possibilities of waste minimization but also include aspects of raw material and energy consumption. Life-cycle analysis offers a good framework for such evaluations, and IDEA is a tool to estimate the consequences of proposed measures.

The following sections give a brief description of the beverage container-specific data sets, which includes:

- container manufacture,
- filling and secondary packaging,
- distribution,
- retail sale and consumption.

10.1. Glass bottles

Container Manufacture

Glass bottles manufacture is an integral part of the glass kiln. Once the glass has been adjusted in temperature so that it has a viscosity suitable for forming, the glass gob is drawn and blown into shape. Afterwards it is still finished and inspected.

Filling

The empty bottles are delivered to the bottler on reusable pallets, each layer is separated by corrugated paperboard sheets. Each pallet is strapped, or wrapped, with shrink film. At the bottler, the containers are mechanically placed on conveyors that take them to the filling line.
The filling line itself consists of:

- washing,
- filling,
- closing,
- labeling,
- packaging for shipping.

The line operates automatically, the different units are each connected by conveyors.

Labels for all bottles are assumed to be paper, glued on to the bottle with casein. Half-liter, returnable and 0.75 liter, one-way bottles are sealed with crown corks (tinplate with PVC sealing); 1.0 liter, returnable bottles, 75% are sealed with aluminum caps (with PVC sealing), and 25% with mono-component polyethylene twist-off caps. According to our assumptions, one-way bottles are packed on corrugated paperboard trays, returnable bottles in polyethylene crates. Both are placed on Europallets for shipment (see also Section on "Auxiliaries").

TABLE 10.1: Energy Consumption for Washing and Filling

Type	Size [l]	Electric power [Wh]							Heat [kJ]			
		Bottle Washing		Crate Wash	Fill	Cool	Shrink	Total	Crate Washing	Filling	Sterilization	Total
		Wh	kJ									
returnable glass	0.5	3.2	80	0.5	8.0	---	---	8.5	25	30	(200)	55
	1.0	4.0	100	1.0	10.0	---	---	11.0	50	40	---	90
one-way glass	0.75	---	---	---	9.0	---	---	9.0	---	35	---	35
aseptic carton	1.0	---	---	---		11.5	1.0		---			
non-aseptic carton	1.0	---	---	---		11.5	1.0		---			
gable top carton	1.0	---	---			11.5	---					
returnable PC	1.0	4.0	85	0.6	10.0	14.0	---	24.6	30	40		70
one-way PET	1.5	---	---	---	12.0	---	1.0	13.0	---	50	---	50
returnable PET	1.5	4.8	120	1.2	12.0	---	---	13.2	60	50	---	110
one-way HDPE	1.0	---	---	---	10.0	14.0	1.0	25.0	---	40	---	40
steel can	0.33	---	---	---	2.0	---	0.5	2.5	---	30	---	30
alu can	0.33	---	---	---	2.0	---	0.5	2.5	---	30	---	30

There are major differences in the energy requirements for one-way and reusable bottles since most of the energy is needed for washing the returned container and reusable plastic crates. Compared to these differences, the size of the container is of minor importance. It was not possible to collect new data for all container types considered. We therefore used data published by Sundström (1986), Golding (1989), Sellers (1989), Boustead (1986) as well as numbers from our interviews at filling plants to calculate the energy requirements for all systems (see Table 10.2).

The most important pollutants at the filling plant come also from the washing section. The detergents, mainly caustic soda, but also chlorine and phosphates, usually go to the municipal waste water treatment plant; sometimes they are cleaned on-site in a biological treatment plant. From the literature indicated above, we took consumption figures of 1.35 g NaOH per 1.0 liter bottle, 0.1 g anti-foam agent and 0.11 g chlorine; the demand for a 0.5 liter bottle was assumed to be 20% lower. Heavy metals, contained in printing inks and label paper, are also dissolved during the washing cycle as well as the glue of the labels, but no data on the amounts going into the waste water were available.

Solid wastes are generated when unpacking delivered container and auxiliaries (e.g., paperboard, shrink film, straps), washing returnable bottles (e.g., used caps, labels) and discarding broken bottles, crates, and pallets. Most of the waste is being sorted and delivered to recyclers (e.g., manufacturers of crates out of used plastic caps, of glass bottles with a high share of external cullets, and of paper and board from recycled pulp).

10.2. Plastic bottles

Container Manufacture

Plastic bottles are manufactured in a two-step process:

* plastic injected preforms,
* biaxial stretching blow-molding

The extrusion blow-molding technique produces a parison, i.e., a preformed gob, by extrusion. This parison is immediately introduced into a mold where it is blown with compressed air; the material is then pressed against its walls to give it the desired form. These machines can manufacture 400 to 4,000 bottles per hour and can process materials such as polyvinylchloride (PVC), polyethylene (PE), polypropylene, polycarbonate, polyester and polyacrylonitryles. Bi-orientation or biaxial stretching of the plastic material's molecular chains provides the material with physical and mechanical properties that also allow for the packaging of carbonated drinks (Hoechst, 1990; GE Plastics, 1990).

A new design of machines makes it possible to combine all operations which, so far, had to be performed in different machines:

- injection molding of the parison,
- conditioning in the thermoplastic range,
- biaxial stretching and blowing to form the container,
- removal from the mold and discharge.

By employing these machines, high-quality containers can be produced cost-effectively in a single step. The machine can also produce wide-neck containers out of special polyamides or polypropylene. Data for these machines that can be considered state-of-the-art are included in the IDEA database.

We assume that these technologies are applied for all kinds of plastic bottles. Therefore the unit processes for the different plastic bottles use the same input and output data.

Filling and Secondary Packaging

The filling operations for plastic bottles are assumed to be similar to those for glass bottles. As no specific data were available, glass data were also used for the washing and filling operations. The differences in the energy consumption for washing the bottles due to the lower heat value of the plastics was not considered here. For the auxiliaries and transport packaging used, see Section 10.

10.3 Cartons

There are two types of paper board cartons:

- Aluminum foil-coated cartons for aseptic packages (TBA) of, e.g., juice,
- Polyethylene-coated cartons for non-aseptic packages (TB) of, e.g., milk.

Starting from the outside, TB cartons are made of layers of polyethylene (13 g/m^2), paperboard (240 to 285 g/m^2) and polyethylene (50 to 52 g/m^2). TBA cartons are compound layer structures of polyethylene (13 g/m^2), paperboard (240 to 285 g/m^2), polyethylene (25 g/m^2), aluminum foil (6.5 μm) and polyethylene (35 g/m^2)

Two main types of paper board are used as raw material for both brick-type liquid packages (TB and TBA):

- duplex claycoat,
- unbleached claycoat.

Both types require chemical pulp. For rooftop-type packages (TB only), triplex claycoat paper board with a middle layer of mechanical pulp filler is used.

Duplex claycoat board consists of a thin bleached top layer and an unbleached base layer. The top layer is coated with a mixture containing kaoline and carbonates as pigments. Unbleached claycoat board is just a coated unbleached layer of pulp. For adequate brightness, its coating pigments are partly titanium oxide (TiO_2)-based. The total area weight varies for both types between 240 and 285 g/m^2, the share of coating materials being 15 to 25 g/m^2. The bleached layer of duplex claycoat board has an area weight of 65 to 80 g/m^2.

FIGURE 10.1: Packaging materials production for non-aseptic cartons
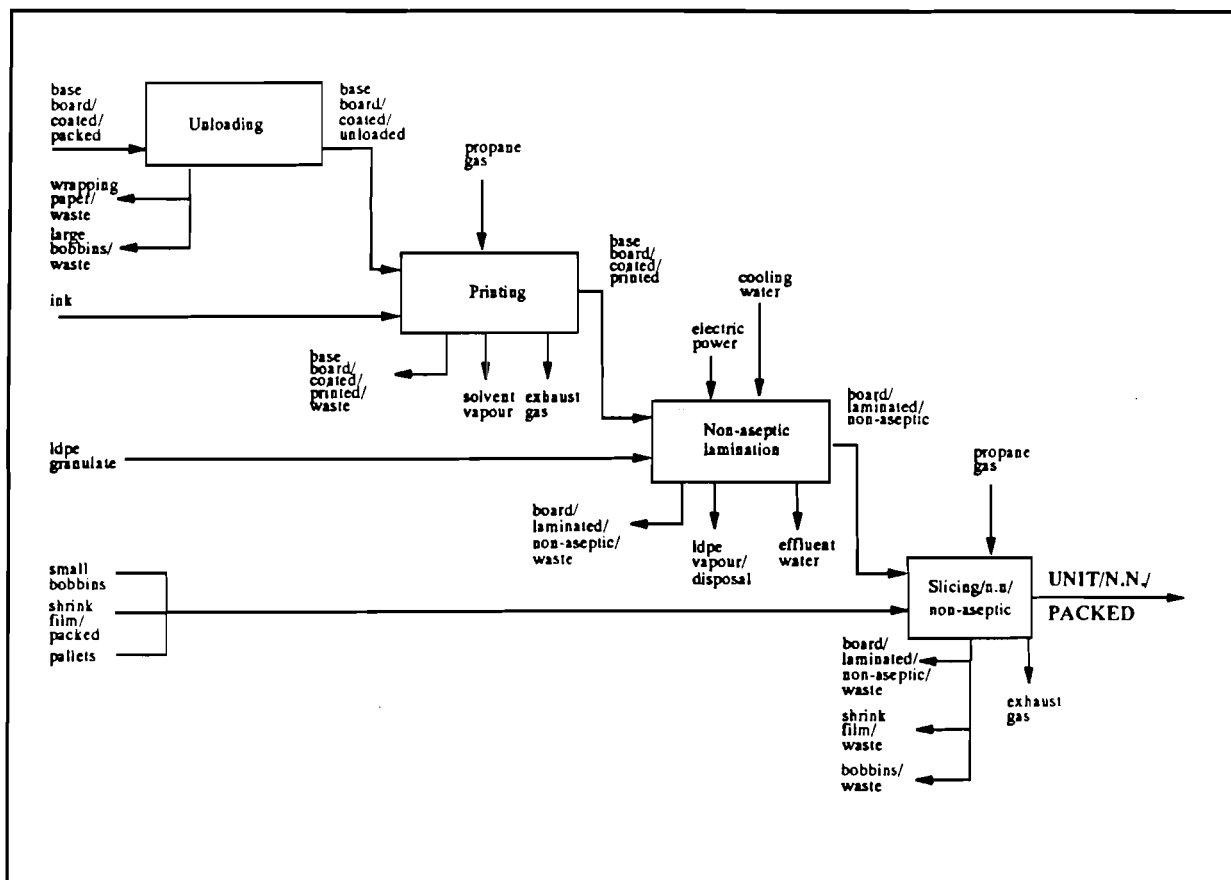
Container Manufacture

Paper board is supplied to the packaging material factory in rolls (Figure 10.1). The first stage of carton production is the printing. For this, flexography, rotogravure and offset techniques are used. Both flexography and rotogravure printing inks contain volatile solvents, like ethyl alcohol and ethyl acetate; offset printing inks contain non-volatile, greasy solvents. Solvent vapors and reaction gases are exhausted to the atmosphere.

Printed paperboard is laminated with polyethylene for TB, and with polyethylene and aluminum foil for TBA. Polyethylene is supplied to the carton manufacturer as granulate; it is then melted and extruded onto the paper board. The aluminum foil, which is supplied in rolls, is directly laminated onto the hot polyethylene which acts as a glue. Polyethylene vapors released during the process are incinerated in sand bed reactors or recovered with zeolite absorbers to be burned in high temperature incinerators.

As the final step, laminated paper board is wound in rolls, cut and packaged for transportation to the filler.

Filling and Secondary Packaging

The brick-type packages are made and filled in automatic machines. Packaging material is supplied on rolls. First, a continuous tube is formed by bending the board band and sealing the side seam. The tube is filled and the top seam is sealed continuously under the liquid level. Finally, filled packages are separated by cutting the tube at the top seam, shaped into their final form and packed for distribution. The type of package (TB, TBA or roof-top) and the pretreatment of the liquid food stock are selected according to the product's ultimate use (e.g., immediate consumption of fresh milk, and short- or long-term storage of UHT milk and juice).

Beverage cartons are first shrink film-packaged (12 cartons per tray) and then stacked on Europallets (720 l of beverage).

Distribution

The distribution of liquid foods in paper board packages from filleries to retail stores depends on the type of the packages (aseptic, non-aseptic), their contents, as well as the type of distributing and retailing organization (large food store chains, individual merchants) (Figure 10.2). The majority of packages is transported directly from filleries to retail stores. The rest is distributed via central depots, where products are stored for a varying period of time and then transported to the retail stores. A mixture table in IDEA gives a share of 50 % for the direct delivery, and 50 % for the delivery via depots.

The need for refrigeration during filling, transporting and storing varies. Whereas some aseptically packaged products, such as juice, need no refrigeration, others, such as fresh milk, require refrigeration in every step of the distribution chain. Therefore, we describe the resulting environmental impacts and energy requirements of refrigeration in dependence of the beverage to be packaged and distributed. Of those beverages packed in cartons and included in the IDEA database, only milk needs refrigeration.

FIGURE 10.2: Filling, distribution & consumption of one-way containers
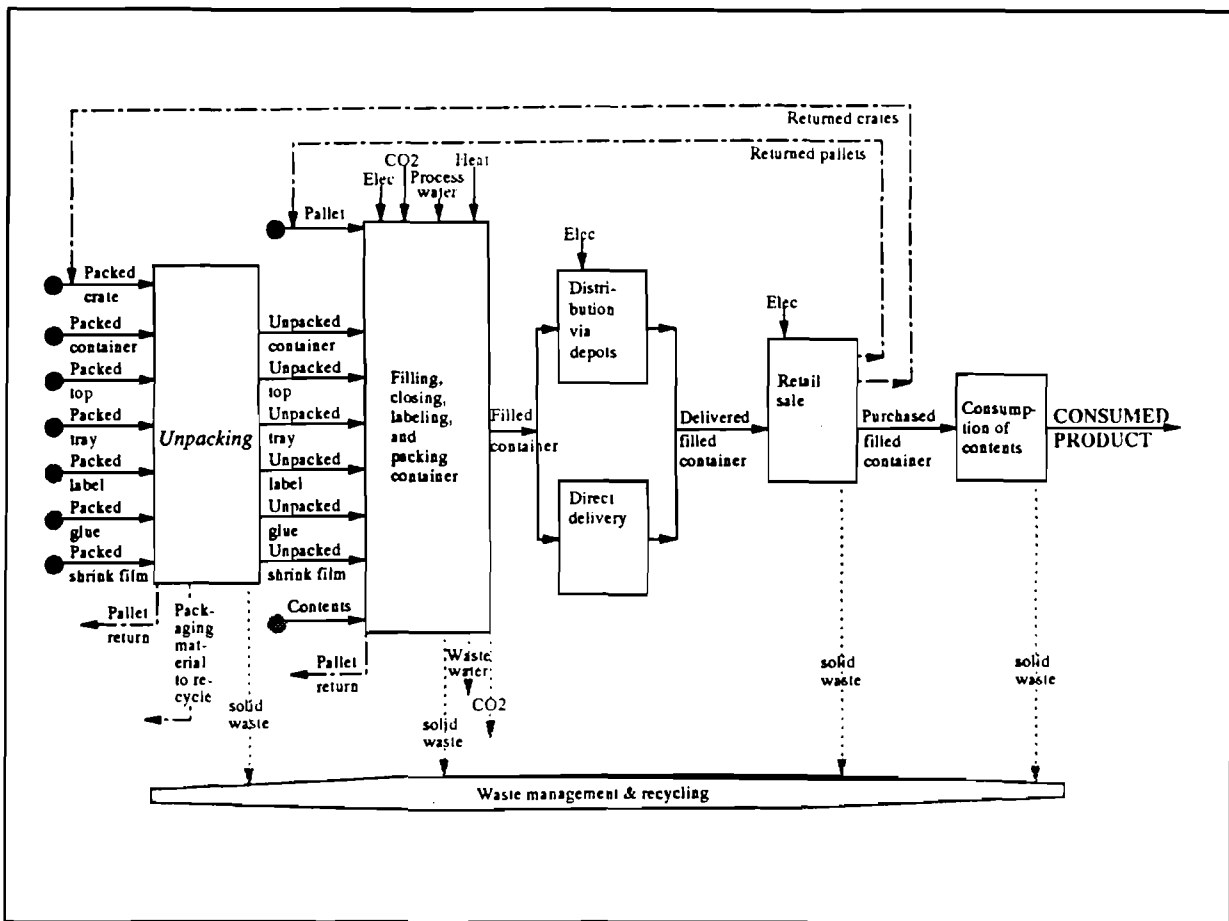
10.4. Cans

In the present study, cans have the following specifications, representing the most common ones used on the Western European market.

	Steel Can	Alu Can
content [l]	0.33	0.33
top	alu	alu
height [mm]	115.2	116
weight [g] -body -top	27.5 3.88	11.7 3.88

The tin plate for the steel can consists of 0.5 to 2.0 g/m^2 tin (Sn). The aluminum plate has a thickness of 0.3 mm and consists of the following alloys:

    body: AlMg1Mn1,
   top: AlMg5Mn.

Container Manufacture

The manufacture of the can body is a continuous process, which begins with the coil preparation and ends with palletizing (see Figure 10.3). First, the coil is fed into a cupping press which stamps discs and forms cups from the coil. These are then converted into untrimmed cans by drawing and wall ironing. Trimmers are used to remove the irregular edges of the cans and to cut them to their exact height.

Next, cans are cleaned in a washer and dried before they can be coated internally and externally. The coater covers the outside wall of the can with a base color and a protective top coat; the cans are then dried in a gas-fired hot air oven. A decorator machine applies the design on top of the protective coat of the can. Afterwards, a coat of varnish is applied to the base of the can by the so-called bottom rim coater. Next, the inside of the can is sprayed with an internal coating or protective lacquer; this internal coating is then dried in the final bake oven. For interior coatings water-based epoxy resins are predominantly used, the outside printing consists out of polyester inks.

Although the average weight of coatings and inks is only about 1 % of the total weight of the aluminum can, and half of that for the steel can, they are the main sources of volatile organic compound (VOC) emissions during the manufacture.

In order to fit the aluminum tops, the cans have to be shaped in a neck flanger. Before being palletized, all cans are run through a final high speed tester where they are checked for strength. The cans are then placed onto wooden Europallets with paperboard interlayers and a wooden board on top. Each pallet is strapped with steel strap before shipment.

FIGURE 10.3: Manufacturing of aluminum can body and top
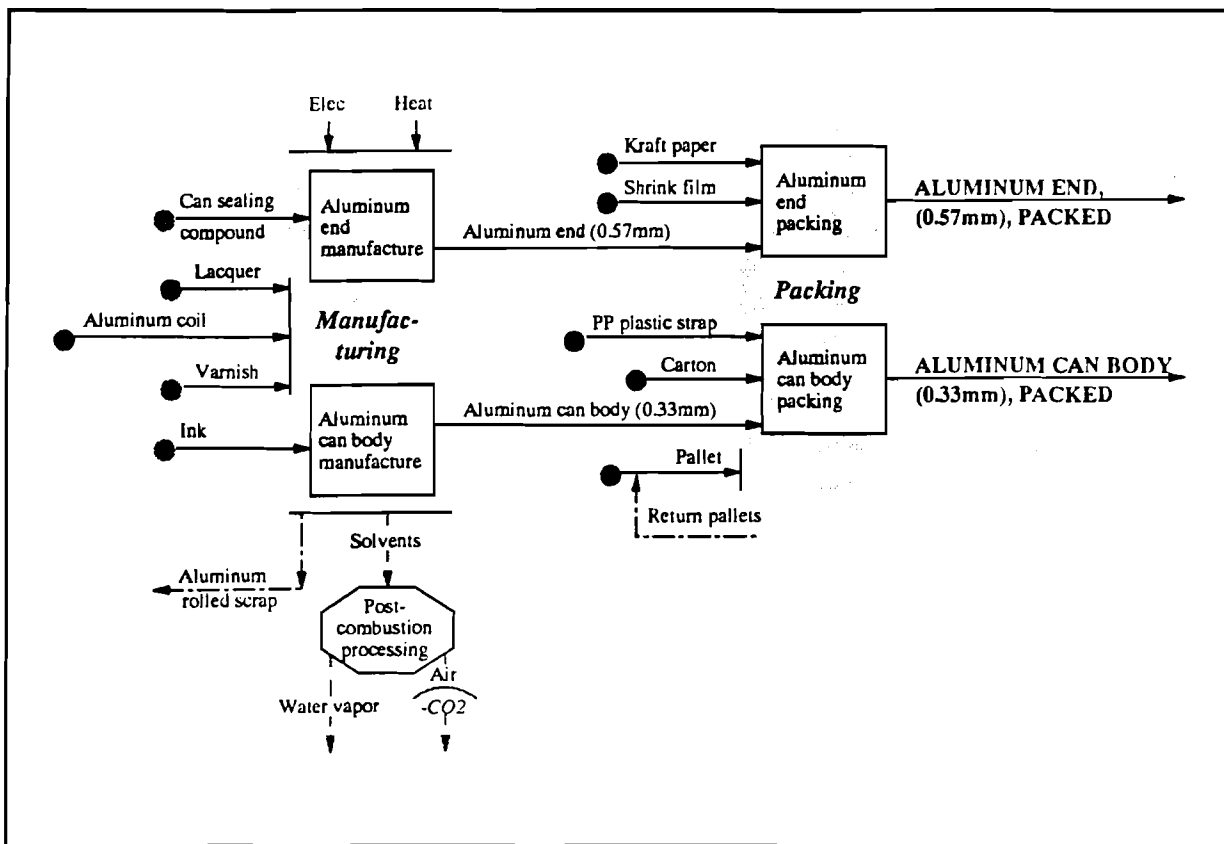
Filling and Secondary Packaging

Cans are filled in automatic filling machines. A pallet of can bodies is transferred to the beginning of the filling line. From there, cans, layer by layer, are semi-automatically guided onto a conveyer which transfers them to the filling machine. Here, cans are first rinsed with warm water, then filled, fitted with the easy-to-open aluminum tops and sealed. The ready tops, packed in a long tube, are fed into the same machine manually.

Once the cans leave the filling machine, they go onto another conveyer that takes them through rinsing and testing stages before they are packed. In the testing stage, the liquid level of the cans is checked by a light (or x-ray) beam, and those cans that do not meet requirements are rejected and go to waste. The filled cans are automatically placed on packaging board cases (usually paperboard trays with a capacity of 24 cans each), covered with polyethylene shrink film, piled up on wooden Europallets and finally taken to the warehouse by another conveyer.

10.5 Returnable container

Four bottles, contained in IDEA, are indented to be used more than one time; i.e., the 1.0 and 0.5 liter glass bottles, the 1.0 liter polycarbonate bottle, the 1.5 liter PET bottle.

Generally, reusable products have the label to be "environmentally friendly", since they reduce the amount of solid waste generated. In a comprehensive eco-profile, the environmental impacts depend strongly on how often such packages are used. The number of trips depends on:

- the number of locations where empty container can be returned,
- the deposit value,
- the misuse of the containers by consumers,
- the strength and durability of the container.

For polycarbonate (PC) bottles, the industry gives 75 trips as a reasonable estimate. Data from the United States which have a long experience with PC bottles indicate about 100 trips, whereas Swiss data indicates 75 trips. For glass bottles trip rates are much lower. They normally vary between 20 and 60. The number of trips technically possible depends mainly on the weight of the glass bottle; the heavier the bottle, the more trips are possible. On average, 25 trips seems a reasonable estimate widely used which is still applicable to lighter bottles, as is the current trend.

Only very short-term experience is available for PET bottles, since Coca Cola only brought them on the market very recently in Germany and Austria. First results show that the trip rate is comparable to those of glass bottles i.e., 25 trips (Bischoff, 1989). Trip rates are stored in the IDEA database as a substitution between waste glass or plastic and containers going back to filling.

The trip rates are converted to percentages by:

$$p = (1 - \frac{1}{x}) \times 100$$

x = number of trips,
p = percent of containers returned.

The substitution tables give the respective percentages so that different trip rates can be easily changed to calculate the influence of increasing or decreasing numbers of trips on the overall impacts of beverage containers.

11.6. Auxiliaries

In addition to the container itself, a beverage packaging system comprises a miscellaneous group of products which are used for capping, labeling and secondary packaging. These auxiliaries usually represent only a small fraction of the overall energy and materials requirements, but as they are part of the overall system, the change in an auxiliary product does not only affect its own production but influences the impacts of the entire system. For example, if you take a lighter monocomponent cap instead of one weighing 4.5 g with a PVC sealing, it reduces the total weight of the container, increases the possibility of recycling, reduces hazardous emissions in PVC incineration, etc. These effects become more and more obvious with an increasing number of trips. Since there is a great variety in the auxiliaries used for beverage containers in Western Europe we picked out the most commonly used products, or we took case examples which appeared attractive in terms of environmental effects.

Closures

There are three major types of closures used for capping bottles:
• crown corks
• aluminum caps
• plastic caps

According to Tapon France S.A., the demand for crown corks in the European Community in 1988 was 59 billions, for aluminum caps 19 billions and for plastic caps 6 millions for soft drinks, beer and mineral water. For the next years crown corks are assumed to remain stable, but the plastic closures will gain more and more market share, displacing the aluminum caps.

The plastics used are polyethylene and polyproylene. Whereas there are only little differences between the crown corks used in different areas, aluminum and plastic caps varies considerably in weight, form and sealing compounds.

We used crown corks (weight 2.2 g) for capping the 0.5 liter returnable beer bottle and the 0.75 liter one-way wine bottle. We assume that all plastic bottles are sealed with polyethylene monocomponent twist-off caps (weight 3.5 g). They can be used for all types of beverages including carbonated drinks and can easily be recycled compared with caps, for which a different sealing material is used. Their use is therefore steadily increasing. For the 1.0 liter returnable soft drink bottle, a mixture of 25% plastic caps and 75% alu caps (weight 2.1 g) was applied (see Figure 10.4).

A. Plastic Caps

Plastic caps are manufactured from high-density polyethylene (HDPE) by injection molding. For the manufacture of HDPE see Section 5.2. The HDPE granulate is mixed with the so-called masterbatch (2%), which contains pigments for coloring the cap. Finally, they are silk-screen printed.

No emission data were available for the manufacturing process, but they should be relatively low. Waste HDPE granulate occurring during or after the production is directly recycled back into raw material preparation.

Since the consumers are asked to put the twist-off cap back onto the empty bottle, a high amount is returned to the filling plant, the rest goes to the municipal waste management. At the moment used plastic caps cannot be recycled for the manufacture of new caps, but run through a cascade recycling, where they are remanufactured into plastic crates.

The caps are packed in cartons, which are partly reused up to 10 times, and transported mainly with heavy trucks to the consumer (Aichinger, 1991).

B. Aluminum Caps

Aluminum caps are punched out of aluminum coil, which is coated with lacquer and varnish. This coating is a protection and should increase the adhesion of the sealing compound. This sealing is a PVC compound, which consists of PVC, dioctyl phthalate and some additives and is injected into the cap. Finally the caps are silk-screen printed. The finished product is packed in cartons.

Data for the manufacture of aluminum caps, lacquer, varnish and the sealing compound have been taken from Boustead and Hancock (1986). The production data for PVC are contained in separate unit processes in IDEA.

Like plastic caps most of the aluminum caps are returned to the bottler, from where they are sent back to the manufacturer for recycling; the rest is thrown out and, in IDEA, becomes waste metal.

C. Crown Corks

The main production steps for crown corks are similar to aluminum caps, only the raw material is tinplate coil. We obtained data from two manufacturers in Austria and France about raw material and energy consumptions (Vandevelve, 1991; Inthaler, 1991). Lacquer, varnish and the sealing compound are assumed to be the same as for aluminum caps.

Crown corks are normally thrown away after use as household waste and, in IDEA, become waste metal.

FIGURE 10.4: Manufacturing of different closures for beverage containers
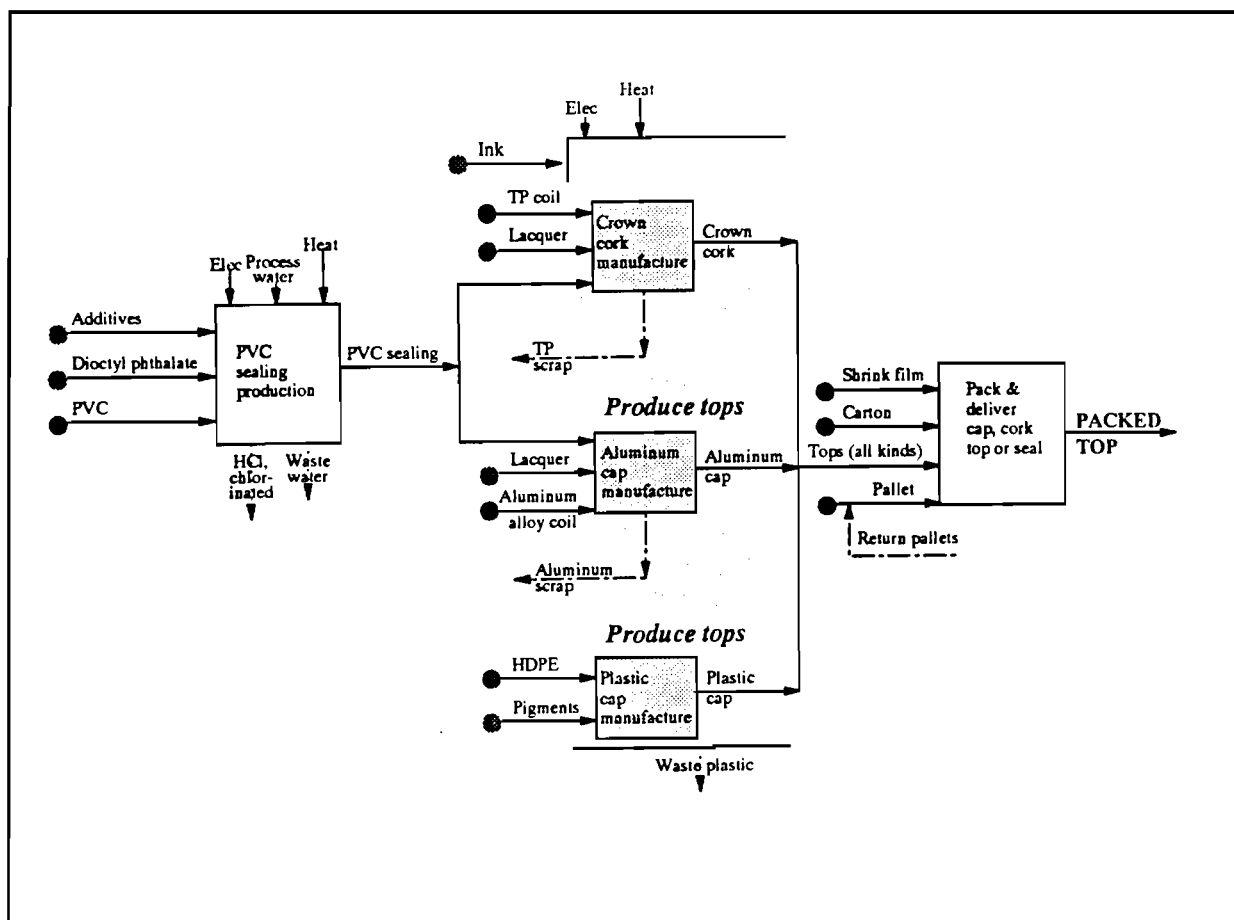
D. Can Closures

The so-called easy-to-open aluminum tops are used for both steel and aluminum cans. They are punched out of aluminum coil, which is coated with lacquer and varnish in the same way as the can body (see Section 10.4). Data for their manufacture was taken from Boustead and Hancock (1986).

Labels

To advertise the product and to inform the consumer, beverage packages are labeled. This is done by direct printing on the container, as for cartons, cans, and sometimes still for glass bottles, or by labels, attached to the package, as for all types of bottles. In IDEA, in addition to directly printed cartons and cans, we only consider paper labels, fixed with casein glue, for all the other containers. These labels, however, have different sizes, which in IDEA is accounted for by different label weights with corresponding amounts of glue consumption (compare table 10.3).

The size of the labels and the amount of glue used affect the energy and detergent consumption of the bottle washing unit. The labels removed during washing are sometimes dried and go back to recycling, or they are discarded and treated as the municipal waste. In IDEA, we assume that 50 % of the labels from returnable bottles are recycled (see Figure 10.5).

A. Printing

We assume that labels are offset (planographic) printed which, to date, is a commonly used technique. In offset printing, both the printing and non-printing parts are fixed on the printing plate in a single plane, which, in turn, is mounted around a rotating cylinder. The printing parts attract the ink which is dispersed in viscous oil and repel water, while the non-printing parts behave opposite. The ink is transferred from the printing plate cylinder to another rubber coated roll, which is in contact with the papersheets.

FIGURE 10.5.: Printing of labels for beverage bottles
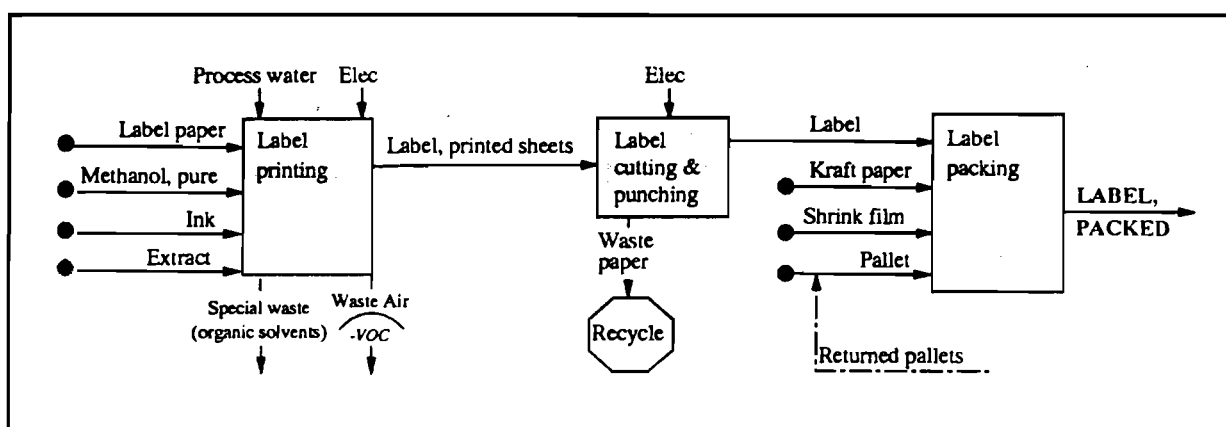
The first preparatory step is to obtain a positive or negative image on film. This film is then used to expose the printing plate, made of metal or plastics, which is finally developed and etched or washed out.

Although the chemicals involved cause some pollution, the preparation of the printing plate contributes only little when considering the overall impacts of beverage container systems. They are thus not considered in the IDEA database.

Special label paper is used which must be water- and caustic-resistent so that the labels do not decompose during the washing process. The heavy metals contained in the paper as well as in the printing inks may be harmful when dissolved during the washing of reusable bottles. There are, however, no data available about heavy metal emissions and several countries have already begun to restrict the use of heavy metals in food packaging materials.

The label paper is printed in sheets of 790 x 1020 mm or 700 x 1000 mm with a weight of 75 g/m² for small labels and 90 g/m² for large ones (e.g., wrap around labels for PET bottles). The weight of the label has been calculated via the label size. It was assumed that 90 % of the sheet area is printed.

The ink needed per color is calculated as follows (Biedermann, 1990):

$$(\frac{sheets}{1000} \times 1.7) \times c = x \ kg \ ink$$

c is the percentage of the area, covered with ink

Example: Printing of one million monocolor wrap-around labels where the color covers 80% of the printed area; 55,556 sheets needed.

$$(\frac{55556}{1000} \times 1.7) \times 0.8 = 75.52 \ kg \ ink$$

Up to four colors may be printed simultaneously in one production step. The water, circulating in the press, contains 10% methanol which evaporates during printing. The solvents of the inks also cause emissions to air. Emissions to water may occur when the press and the printing forms are cleaned, but most of them are collected and go back to the manufacturer. Caustic solutions are used to remove the rubber coating from the printing plates. We used emission factors given in Reinders (1984).

After printing and drying the labels are cut and punched into the correct format, tied in small numbers with paper strips and finally packed with kraft paper or shrink film. The waste paper is collected and goes back to paper manufacturers for recycling.

B. Inks

The manufacture of printing inks itself is so far not contained in the IDEA database.

C. Glue

At all filling plants which were visited for this study, casein glue is used to attach labels. From the data given by industry, we estimate a consumption of 10 mg glue per g of label. The manufacture of the casein glue itself is so far not contained in IDEA.
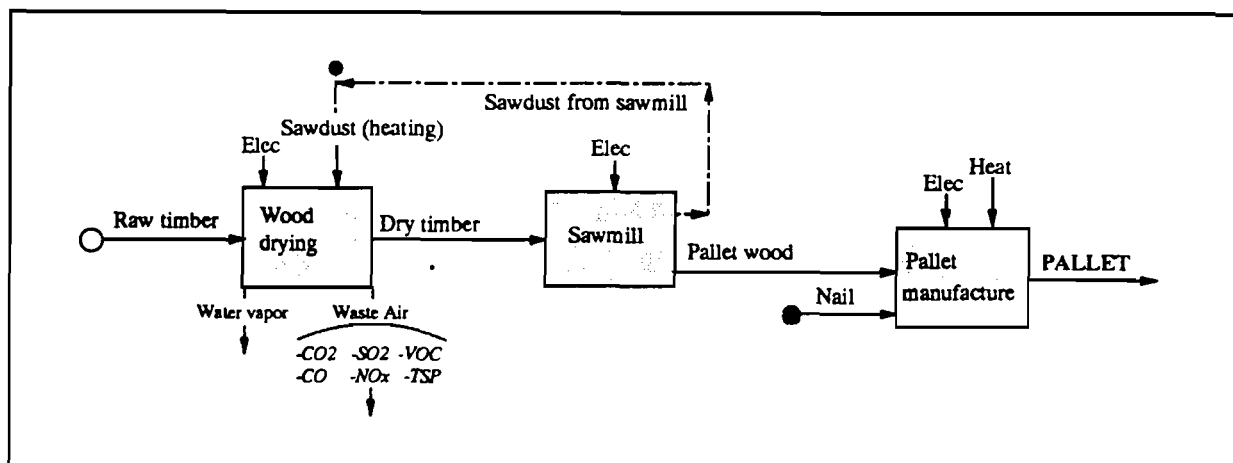
Secondary packaging

A. Pallets

Wherever goods are shipped, wooden pallets are used as a base for stacking and transporting these goods. There are still different types in use, but the standardized so-called "Europallet" is continuously gaining ground. The base of a Europallet measures 120 x 80 cm, its average weight is 25 kg. Based on information given by the beverage industry and pallet manufacturers we assume 20 trips per pallet.

IDEA contains unit processes for "pallet manufacture", "saw mill" and " wood drying" (Hofer, 1991). The planks are nailed; 0.5 kg steel nails are needed for one pallet. The production of these nails is not considered. For the heating needed for the wood drying sawdust from the sawmill is burnt (see Figure 10.6).

FIGURE 10.6: Manufacture of wooden pallets

B. Plastic Crates

Plastic crates are used as a secondary packaging container to transport filled bottles to the retail store. There is no common standard for these crates in general, only for the base area so that they fit onto the Europallet. The average weight varies between 1.8 and 2.0 kg; raw materials are polyethylene or polyproylene.

The life time of a crate is 15 to 20 years with an average number of trips of four to five each year, but may be much higher for certain beverages, as in milk distribution. Afterwards the crates are ground up and used again for the crate manufacture (this is also called regeneration). After 30 years, or two times of regeneration, the material can only be used for lower quality products.

In IDEA, we assumed that a crate weighs 2.0 kg is made of high-density polyethylene by injection molding, makes 80 trips, and then goes back to regeneration. To color the crates, pigments are mixed into the HDPE granulate which is already UV stabilized. Lastly, these crates are silk-screen printed.

FIGURE 10.6: Crates manufacture
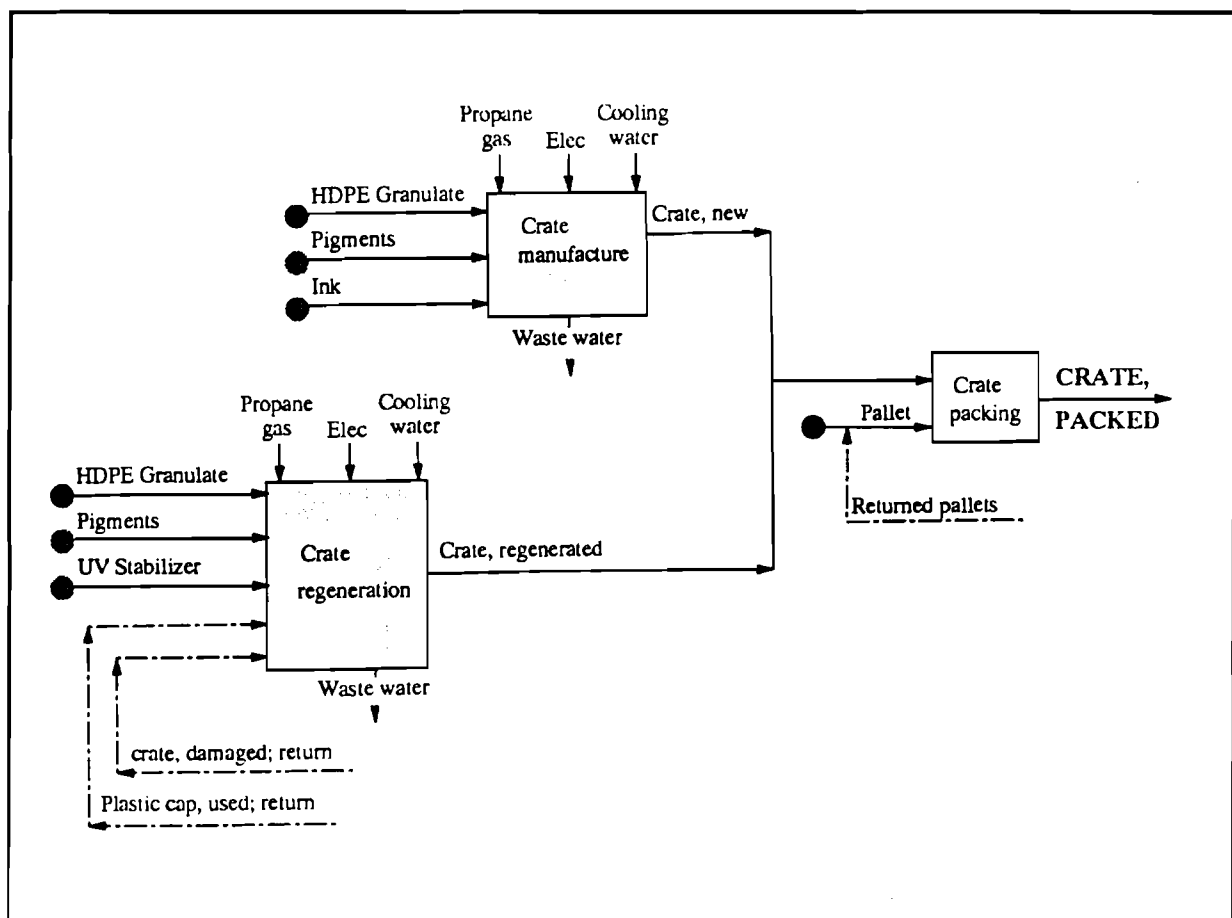
For regeneration, the damaged crates are ground up, so that the lighter damaged material settles as the top layer and can be pumped of. The material losses are approximately 5%. UV stabilizers and, if necessary, new pigments as added. As recommended by crate manufacturers we assume regenerated crates to be made only out of recycled material from damaged crates and from plastic caps (see Figure 10.6).

Production data was obtained from a crates manufacturer (Eigler, personal comm., 1990). The manufacture of pigments and UV stabilizers is currently not considered in IDEA.

C. Cardboard Trays

Cardboard trays are made from unbleached paperboard liners and an inner fluted filler of corrugated medium which is made from secondary or recycled fibers. Sellers and Sellers (1989) give a composition of 30 % unbleached linerboard and 70 % corrugated medium which are glued together with starch glue. Less than a half of the trays are printed.

Cardboard trays are used as secondary packaging for shipping the filled one-way beverage container to distributors and retailers; they are often wrapped with shrink film. At the retail store, the tray is normally removed and discarded to the household waste or collected for recycling.

We took the data from the literature (Boustead and Hancock, 1986; Sundström and Lindholm, 1985) with some additional information from industry (Plescher, personal comm., 1991; Mach, personal comm., 1991).

D. Shrink film

Shrink film is a very thin (40-60 micrometers) polyethylene foil used for wrapping boxes, trays, pallets and products. The shrink film is put around the product, e.g., the tray carrying the beverage containers, and then heated which causes the shrinking and tight fitting of the film around the tray. The amount of shrink film needed is 10 % more then the surface area of the product to be packaged; for shrinking a Europallet 0.5 to 1 kg is required. Several published data are available for shrink film consumption; we used these sources together with information from a shrinking tunnel manufacturer to derive our estimates included in the IDEA database. The data for the shrink film production in IDEA were obtained from industry (Bolum, personal comm., 1990).

TABLE 10.3: Weight specifications [g] for the different beverage containers

Type	Size	Container	Closure	Label	Glue[5]	Beverage[6]	Filled container	Tray	Shrink film[12]	Crate[14]	Pallet[20]	Total
returnable glass	0.5	355	2.2[1]	1.0	0.1	502	860.3	---	---	83.33[15]	26.04[21]	969.67
	1.0	841	2.5[2]	1.4	0.14	1000	1845.04	---	---	166.67[16]	65.1[22]	2076.82
one way glass	0.75	452	2.2[1]	1.35	0.135	747	1202.685	17.92[8]	---	---	65.1[22]	1285.71
aseptic carton	1.0	26	---	---	---	1028	1054	6.67[9]	0.86	---	34.72[23]	1096.25
non-aseptic carton	1.0	24	---	---	---	1028	1052	6.67[9]	0.86	---	34.72[23]	1094.25
gable top carton	1.0	28	---	---	---	1028	1056	---	---	100[17]	39.06[25]	1195.06
returnable PC	1.0	70	3.5[3]	1.0	0.1	1028	1102.6	---	---	100[17]	39.06[25]	1241.66
one-way PET	1.5	65	3.5[3]	3.8	0.38	1500	1572.68	6.67[9]	3.19	---	52.08[26]	1634.62
returnable PET	1.5	107	3.5[3]	1.13	0.113	1500	1611.74	---	---	200[18]	78.13[27]	1889.87
one-way HDPE	1.0	28	3.5[3]	1.0	0.1	1028	1060.6	6.67[10]	1.93	---	34.72[23]	1103.92
steel can	0.33	27.5	3.88	---	---	330	361.38	3.33[11]	0.97	---	10.52[28]	376.2
alu can	0.33	11.7	3.88	---	---	330	345.58	3.33[11]	0.97	---	10.52[28]	360.4

Notes to table 10.3:

[1] crown cork: tinplate 2.0g, PVC sealing 0.2g

[2] 25% monocomponent PE cap 3.5g, 75% alu cap with PVC sealing 2.1g

[3] monocomponent PE cap 3.5g

[5] 100g glue for 1kg labels

[6] specific weights of beverages:
   beer: 1004 g/l
   soft drink: 1000 g/l
   wine: 996 g/l
   milk: 1028 g/l

[8] weight of tray: 215g, capacity: 12 bottles

[9] weight of tray: 80g, capacity: 12 cartons

[10] weight of tray: 80g, capacity: 12 bottles

[11] weight of tray: 80g, capacity: 24 cans

[12] 110% surface area (tray+container) x thickness of shrinkfilm x specific weight of shrink film

[14] weight of crate: 2.0kg

[15] capacity: 24 bottles

[16] capacity: 12 bottles

[17] capacity: 20 bottles/cartons

[18] capacity: 10 bottles

[20] weight of pallet: 25kg

[21] capacity: 960 bottles

[22] capacity: 384 bottles

[23] capacity: 720 cartons/cartons

[25] capacity: 640 bottles?/cartons

[26] capacity: 480 bottles

[27] capacity: 320 bottles

[28] capacity: 2376 cans

10.7. Distribution

There are two main distribution routes (see Figure 10.7):

- direct delivery from the filling plant to the retail store,
- distribution via depots.

It was assumed that 50 % of the beverage packages are distributed in direct delivery and 50 % via depots. An energy consumption of 7.6 Wh per liter of beverage for storage and manipulation in the depot have been calculated based on figures obtained from a large Austrian food vender (H. Hirschberg, personal comm., 1990).

The transportation profiles for the different beverage containers, including distances and models, are contained in the transportation tables linked to the filled containers going into the unit process "depot distribution" and "retail distribution". They are based on data obtained from several filling plants in Austria, and have been extrapolated to the Western European situation.

10.8. Retail and Consumption

Data for the energy consumption in retail stores are taken from Boustead and Hancock (1986). We have assumed that all secondary packaging material is removed here and only containers themselves are sold to the consumer, although, in certain cases larger amounts are also sold together with trays and crates. The simplification seems, however, reasonable since there is a deposit on most reusable plastic crates, and one-way packaging material is in any case discarded to the municipal waste.

The transport of the containers to the homes of the consumer is not considered since no data are available. The final step is the consumption of the beverage and the discarding, or returning, of the package.

FIGURE 10.7: Filling, distribution and consumption of returnable container
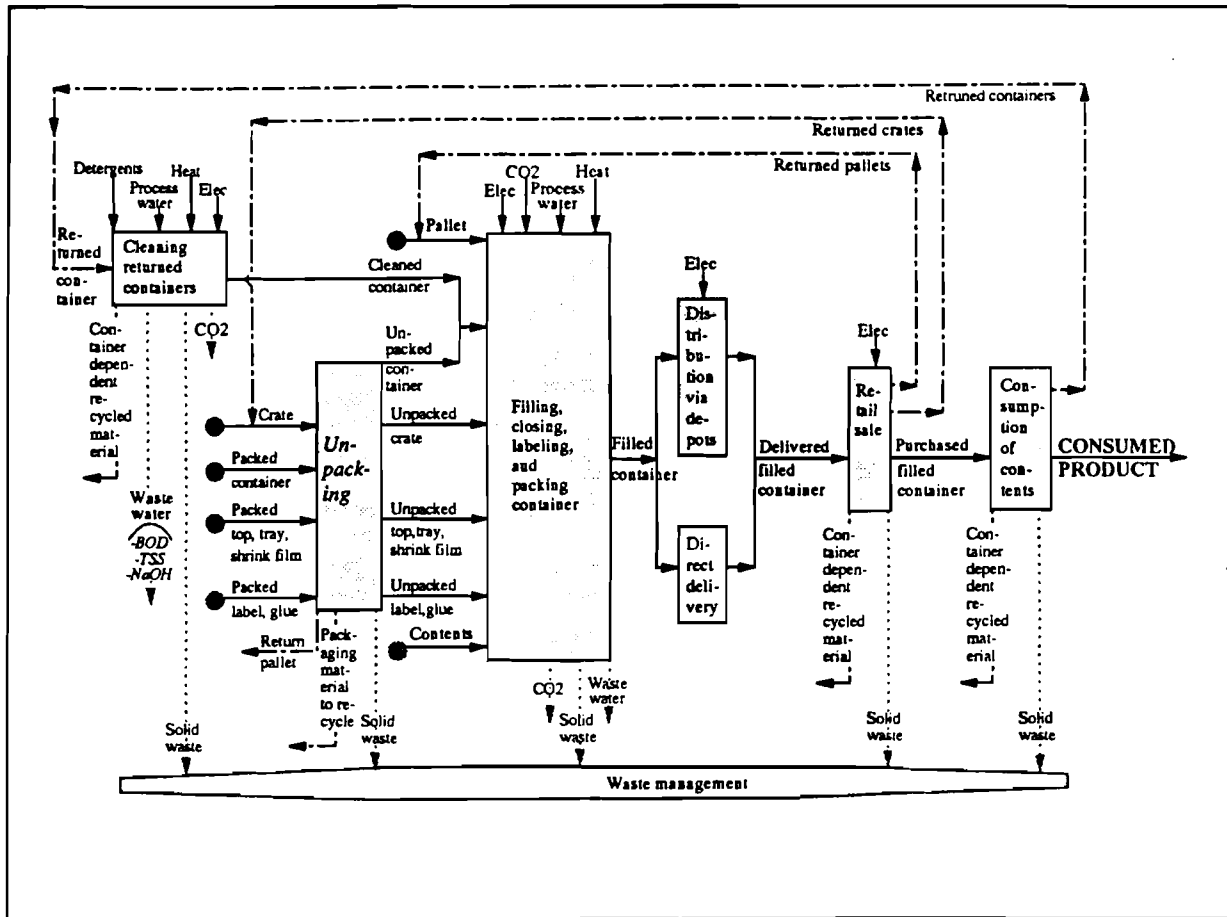
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11. Waste Management and Recycling

Waste statistics (e.g., OECD, 1987 and 1989) generally distinguish between three major *classes of wastes*:
- municipal solid waste,
- special, or hazardous, industrial solid waste,
- other large-volume industrial solid waste.

This distinction is mainly made because of the type of ultimate disposal or treatment required. Large-volume *industrial wastes* are characterized by their large amounts which are, however, chemically relatively inert; examples are mine tailings, construction debris, etc. These wastes can be relatively easily disposed of without causing leachate or ground water contamination problems, as long as the land is available; mine tailings are, for example, backstowed into the excavated mine.

Municipal solid waste can also be disposed of in landfills, or incinerated, relatively readily since much of it is organic and thus biodegradable. *Special and*, in particular, *hazardous solid wastes*, on the other hand, need special treatment before the remainder can be put back into the earth. Their treatment depends, however, on the specific type and it is difficult to generalize for all special wastes. An incinerator that takes PCBs (poly-chlorinated biphenols), for example, cannot accept any other kind of special waste.

In the IDEA database, we follow the distinction of wastes into the above three categories. For large volume industrial wastes, we only give the total quantities; also for special wastes, we do not include any further processing operation but generally try to identify the specific components of the special waste, e.g., spent sulfuric acid, cadmium, etc.

Since the composition of municipal waste, as well as the means of ultimate disposal, are relatively uniform, the IDEA database includes municipal landfilling and municipal waste incineration as two unit processes. A distribution table allocates 73% of the municipal waste generated into landfills and 27% into incinerators. This split has been derived from OECD (1989) which says that in the 17 western European countries, in 1985, 60% went to landfills, 22% to incineration, 6% to composting and 12% to other ultimate disposal (mostly open dumping). We have ignored the last two means of disposal because
- most of the waste we are concerned with in our present database cannot be composted,
- dumping is not considered a proper form of municipal waste treatment.

Also from OECD statistics (1989), we know the overall European recycling rates of waste glass and waste paper, 29% each. We have therefore added these rates in the distribution tables of waste glass and waste paper and board so that 29% are recycled, 52% go to landfilling and 19% to incineration (see Figure 11.1, 11.2).

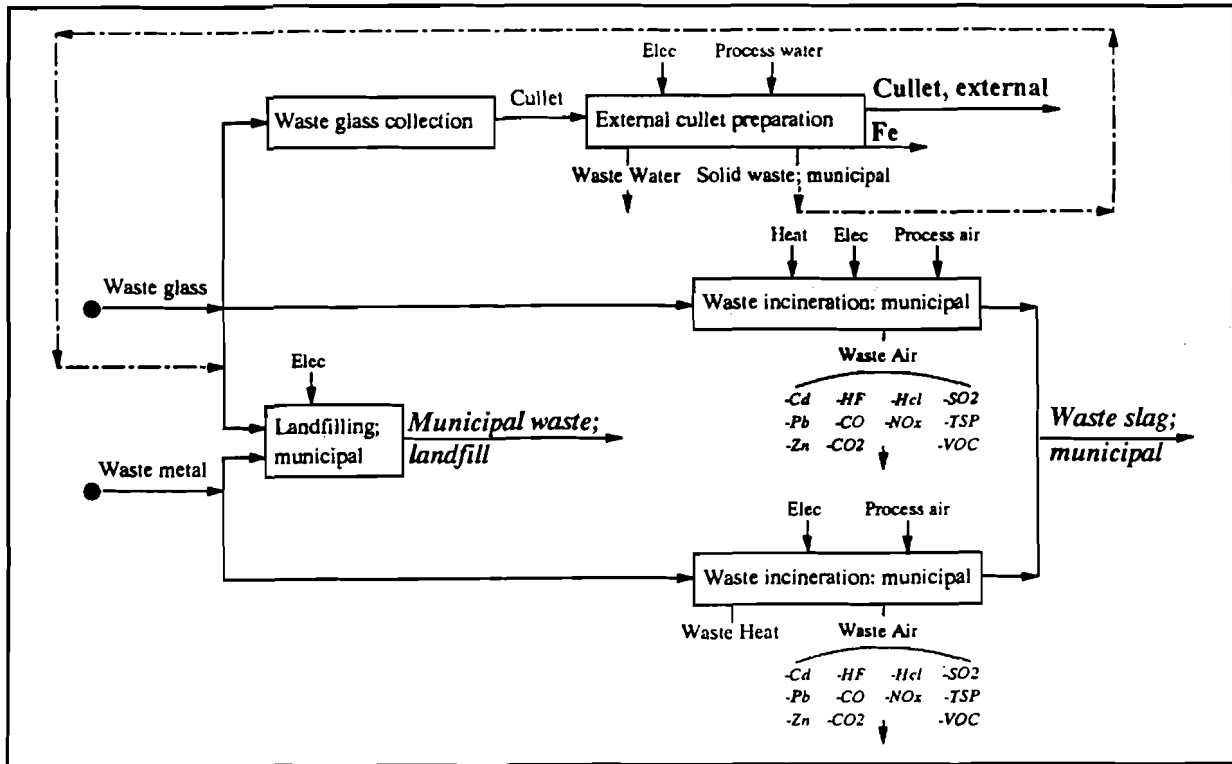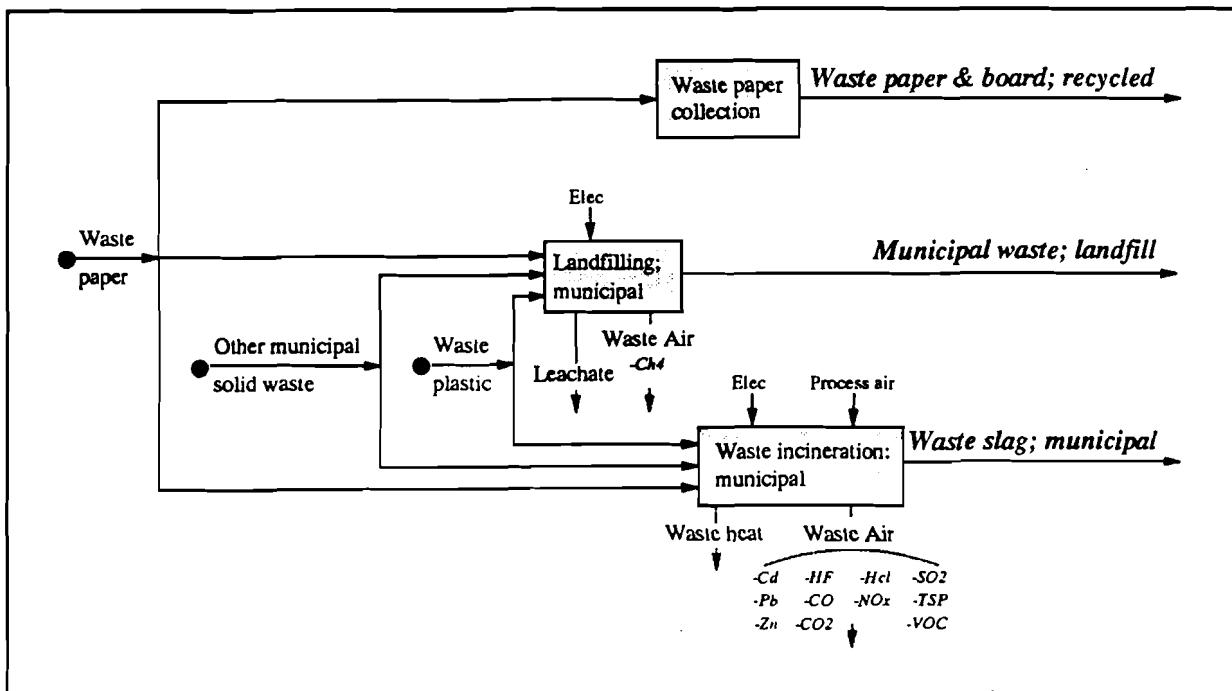**FIGURE 11.1:** Municipal waste handling for glass & metal

FIGURE 11.2: waste paper, plastic & others

The environmental effluents included for landfills are methane (CH_4) emissions
to air (BfU, 1989) and leachate to water; those for incinerators include the general
combustion emissions to air (CO_2, CO, SO_2, NO_x, and VOC) as well as process-
specific air emissions including heavy metals (Pb, Zn, and Cd) and dust (i.e., TSP),
hydrogen chloride (Hcl) and hydrogen fluoride (HF) (BfU, 1989; OECD, 1989). The
composite air emission factors for the disposal of one tonne of municipal waste in
Western Europe are given in Table 11.1.

TABLE 11.1:   Composite Air Pollution Emission Factors for Municipal Solid Waste
Disposal in Western Europe (73% landfill; 27% incineration).

Pollutant	Unit	Emission rate
CO_2	t/t	0.79
CO	kg/t	0.31
SO_2	kg/t	0.29
NO_x	kg/t	0.33
VOC	kg/t	0.07
CH_4	kg/t	43.06
TSP	kg/t	0.12
Hcl	kg/t	1.15
HF	g/t	9.72
Pb	g/t	4.2
Zn	g/t	10.61
Cd	g/t	0.24

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