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Advanced Decision-Oriented Software for the Management of Hazardous Substances. Part 1: Structure and Design

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ADVANCED DECISION-ORIENTED SOFTWARE FOR THE MANAGEMENT OF HAZARDOUS SUBSTANCES

Part I
Structure and Design

Kurt Fedra

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ADVANCED DECISION-ORIENTED SOFTWARE FOR THE MANAGEMENT OF HAZARDOUS SUBSTANCES

Part I: Structure and Design

Kurt Fedra

1. PROJECT SUMMARY DESCRIPTION

1.1 Background

Many industrial products and residuals such as hazardous and toxic substances are harmful to the basic life support system of the environment. In order to ensure a sustainable use of the biosphere for present and future generations, it is imperative that these substances are managed in a *safe and systematic* manner. The aim of this project is to provide software tools which can be used by those engaged in the management of the environment, industrial production, products, and waste streams, and hazardous substances and wastes in particular.

1.2 Project Objectives

The objective of the project is to design and develop an *integrated set of software tools*, building on existing models and computer-assisted procedures. This set of tools is designed for non-technical users. Its primary purpose is to provide easy access and allow efficient use of methods of analysis and information management which are normally restricted to a small group of technical experts. The use of advanced information and data processing technology should allow a more comprehensive and interdisciplinary view of the management of hazardous substances and industrial risk. Easy access and use, based on modern computer technology, software engineering, and concepts of Artificial Intelligence (AI) now permit a substantial increase in the group of potential users of advanced systems analysis methodology and thus provide a powerful tool in the hand of planners, managers, policy and decision makers and their technical staff.

To facilitate the access to complex computer models for the casual user, and for more experimental and explorative use, it also appears necessary to build much of the accumulated knowledge of the subject areas into the user interface for the models. Thus, the interface will have to incorporate a knowledge-based expert system that is capable of assisting any non-expert user to select, set up, run, and interpret specialized software. By providing a coherent user interface, the interactions between different models, their data bases, and auxiliary software for display and analysis become transparent for the user, and a more experimental, educational style of computer use can be supported. This greatly facilitates the alternative policies and strategies for the management of industrial risk.

1.3 A Structure for the Integrated Software System

The system under design combines several methods of applied systems analysis and operations research, planning and policy sciences, and artificial intelligence into one fully integrated software system (Figure 1.1). The basic idea is to provide direct and easy access to these largely formal and complex methods for a broad group of users.

Conceptually, the main elements of the system are:

- **an Intelligent User Interface,** which provides easy access to the system. This interface must be attractive, easy to understand and use, error-correcting and self-teaching, and provide the translation between natural language and human style of thinking to the machine level and back. This interface must also provide a largely menu-driven conversational guide to the system's usage (dialog - menu system), and a number of display and report generation styles, including color graphics and linguistic interpretation of numerical data (symbolic/graphical display system);
- **an Information System,** which includes the system's Knowledge and Data Bases (KB, DB) as well as the Inference Machine and Data Base Management Systems (IM, DBMS), which not only summarize application- and implementation-specific information, but also contain the most important and useful domain-specific knowledge. They also provide the information necessary to infer the required input data to run the models of the system and

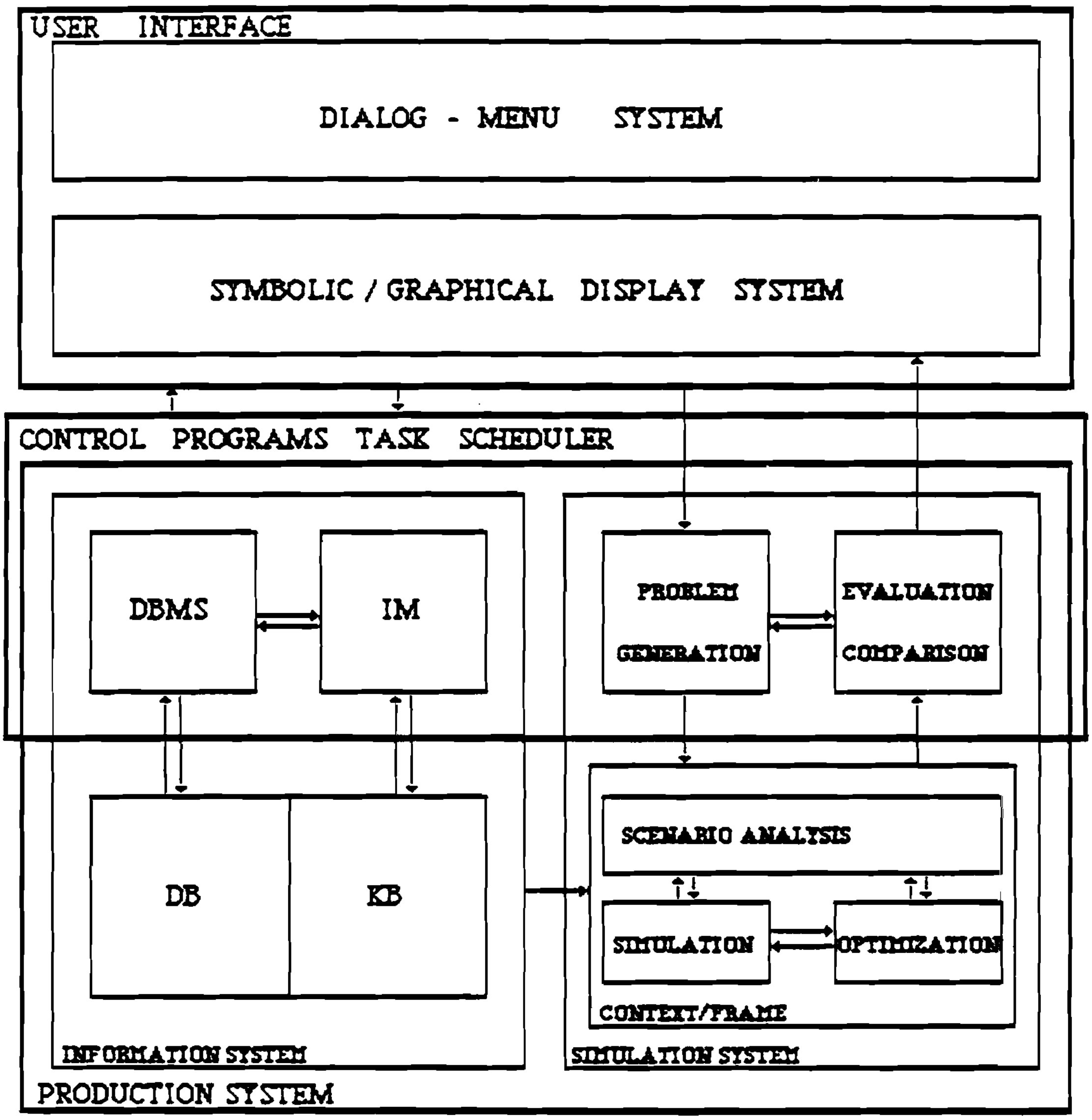

Figure 1.1: Elements of the Integrated Software System

interpret their output. The Inference and Data Base Management Systems (which are at the same time part of the Control Programs and Task Scheduler level) allow a context- and application-oriented use of the knowledge base. These systems should not only enable a wide range of questions to be answered and find the inputs and parameters necessary for the models, but must also be able to explain how certain conclusions were arrived at. For a given application, the data base systems must also perform the more trivial tasks of storing and organizing any interim or final results for display and interpretation, comparison, and evaluation;

- **the Simulation System**, which is part of the Production System and consists of a set of models (simulation, optimization), which describe individual processes that are elements of a problem situation, perform risk and sensitivity analyses on the relationship between control and management options and criteria for evaluation, or optimize plans and policies in terms of their control variables, given information about the user's goals and preferences, according to some specified model of the systems workings and rules for evaluation.

These elements are transparently linked and integrated. Access to this system of models is through a conversational, menu-oriented user interface, which employs natural language and symbolic, graphical formats as much as possible. The system must be error-correcting and self-teaching, and provide not only a low-cost entry for the casual user, but also have the potential to be custom configured for day-to-day use by users of growing expertise.

2. MANAGEMENT OF HAZARDOUS SUBSTANCES AND INDUSTRIAL RISK

About 2 gigatons of waste are produced annually in the countries of the EC. Somewhat less than 10% of that is from industrial sources. Roughly 10% of these industrial wastes have to be classified as hazardous (B.Risch, CEC, Brussels 1984, personal communication). More graphically, this amounts to 20 million metric tons, or a train of roughly 10,000 km length.

The effective management of these wastes calls for:

- a minimization of waste production by process modification and recycling;
- the conversion to non-hazardous forms;
- finally, a safe disposal of whatever is left.

In addition to hazardous wastes, there is a large number of commercial products that are considered hazardous. Their production, transportation, and use – before they enter any waste stream – is also of concern. Industrial production processes that involve hazardous interim products which may reach the environment on account of an accident and cause direct health risks to man, are also considered.

As a special category, although implied in the above, transportation of hazardous substances (including, of course, hazardous wastes), is included in the system.

The entire life-cycle of hazardous substances, from their production and use to their processing and disposal, involves numerous aspects and levels of planning, policy and management decisions (Figure 2.1). Technological, economic, socio-political and environmental considerations are required at any given stage of the management of these life cycles, and they involve various levels, ranging from site or enterprise to local, regional, national and even international scales, and from immediate operational decisions to long-term planning and policy problems.

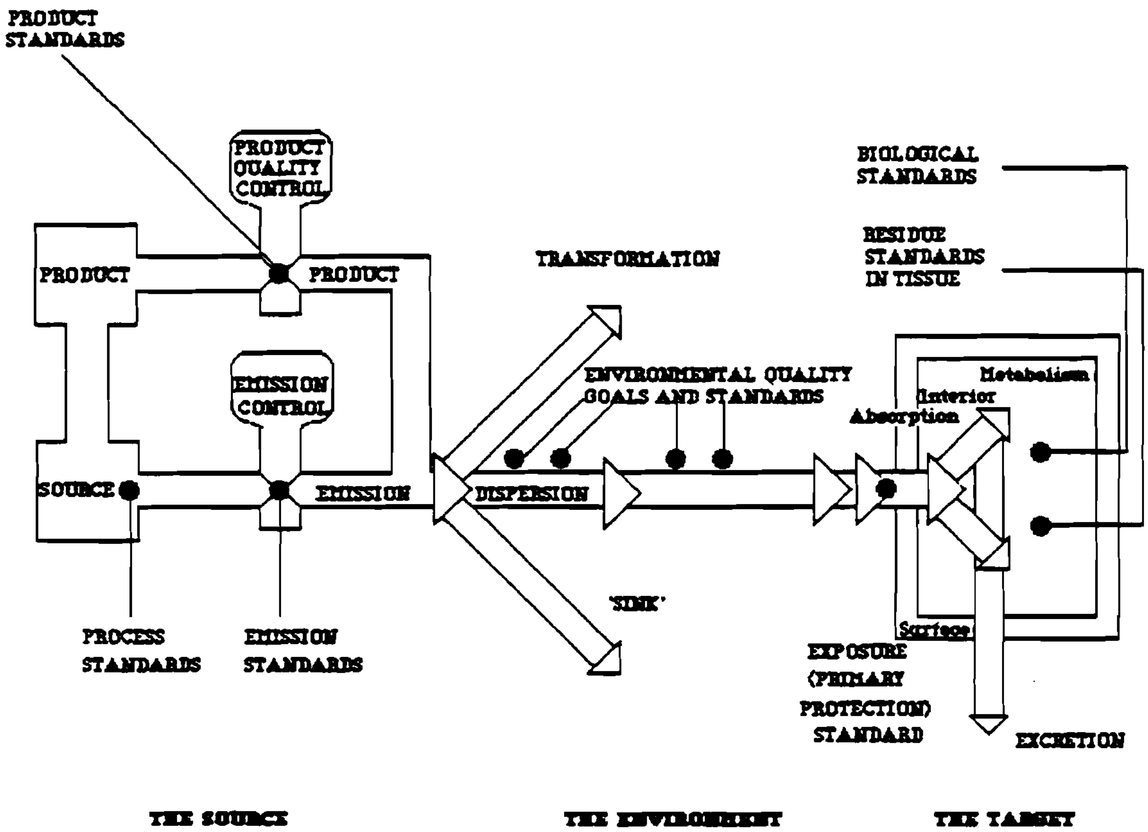

Figure 2.1: Life Cycle of Hazardous Substances.
(after Holdgate, 1979)

While uncertainties, perceptions and subjective values play an important part in management and decision making processes, scientific methodology and evidence can also contribute by providing a sound information basis in a useful and readily accessible format. Applied systems analysis and modern, computer-based information technology can provide the tools and methods to accomplish this.

2.1 Methods for Comprehensive Assessment

The problems of managing hazardous substances are neither well defined nor reducible to a small set of relatively simple subproblems. The complexity and ill-defined structure of most problems makes any single method or approach fall short of the expectations of potential users. The classical, mathematically oriented, but rigid, methods of Operations Research and Control Engineering alone are certainly insufficient.

Thus, while only the combination of a larger set of methods and approaches holds promise of effectively tackling such problems, the subjective and discretionary human element must also be given due weight. This calls for the direct and interactive involvement of users, allowing them to exert discretion and judgement wherever formal methods, by necessity, are insufficient.

We propose to design and construct an integrated and interactive computer-based decision support and information system. Recognizing the potentially enormous development effort required and the open-ended nature of such a project, we argue for a well-structured cooperative effort that takes advantage of the large volume of scientific software already available. A modular design philosophy enables us to develop individual building blocks, which are valuable products in their own right, in the various phases of the project, and interface and integrate them in a framework which, above all, has to be flexible and easily modifiable with growing experience of use.

With a functional and problem-oriented, rather than a structural and methodological design for this framework, working prototypes that allow the freedom to explore the potential of such systems can be constructed at relatively low cost and with only incremental effort.

Any comprehensive assessment of the management of industrial risk, and hazardous substances in particular, requires the consideration of technological, economic, environmental, and socio-political factors. Every scenario (defined interactively with this system) must ultimately be assessed, evaluated, and compared with alternatives in terms of a list of criteria (Table 1).

Clearly, only a small subset of these criteria may be expressed in monetary, or even numerical terms. Most of them require the use of linguistic variables for a qualitative description. Using fuzzy set theory, qualitative verbal statements can easily be combined with numerical indicators for a joint evaluation and ranking. In the systems' design, the use of programming languages like

TABLE 1: Comprehensive Assessment Criteria (after Wilson, 1984)

CRITERIA FOR THE ASSESSMENT OF WASTE MANAGEMENT PLANS	
ECONOMIC:	Capital costs
	Land costs
	Operating costs
	Revenues:
	Sales and market share
	Stability of market
	Net cost per tonne
	Net present cost
	Sensitivity of costs to market or other fluctuations
	Uncertainty in cost estimates, i.e., financial risk
	Financing arrangements, taxes, subsidies
TECHNICAL:	Adequacy of the technology:
	Feasibility
	Operating experience
	Adaptability to local conditions
	Reliability
	Interdependency of components
	Safety
	Potential for future development
	Flexibility to cope with changes in:
	Waste quantities
	Waste composition
	Source separation of materials
	Dependence on outside systems:
ENVIRONMENTAL:	Public health
	Water pollution
	Air pollution:
	Dust
	Noxious gases
	Odors
	Quality and quantity of residual wastes
	Noise
	Transportation
	Aesthetics
RESOURCE CONSERVATION & USE:	Products recovered:
	Market potential
	Net effect on primary energy supply
	Energy requirements
	Net effect on supply materials:
	Raw materials consumption
	Land use:
	Volume reduction
	Land reclamation
	Water requirements
SOCIO-POLITICAL:	Equity between communities or interest groups
	Flexibility in location of facilities
	Public acceptance
	Number of jobs created
	Employee acceptance

LISP or PROLOG gives one the freedom to manipulate symbols and numbers in a coherent framework.

2.2 Information Management and Decision Support

The sheer complexity of the problems related to the management of hazardous substances and related risk assessment problems calls for the use of modern information processing technology. However, most problems that go beyond the immediate technical design and operational management level involve as much politics and psychology as science.

The software system described here is based on *information management* and *model-based decision support*. It envisions experts as its users, as well as decision and policy makers, and in fact, the computer is seen as a mediator and translator between expert and decision maker, between science and policy. The computer is thus not only a vehicle for analysis, but even more importantly, a vehicle for communication, learning, and experimentation.

The three basic, though inseparably interwoven elements, are

- to supply *factual information, based on existing data*, statistics, and scientific evidence,
- to assist in *designing alternatives* and to assess the likely consequences of such new plans or policy options, and
- to assist in a systematic *multi-criteria evaluation and comparison* of the alternatives generated and studied.

The framework foresees the selection of criteria for assessment by the user, and the assessment of scenarios or alternative plans in terms of these criteria. The evaluation and ranking is again done partly by the user, where the machine only assists through the compilation and presentation of the required information, and partly by the system, on the basis of user-supplied criteria for screening and selection.

The selected approach for the design of this software system is eclectic as well as pragmatic. We use proven or promising building blocks, and we use available modules where we can find them. We also exercise methodological pluralism: any "model", whether it is a simulation model, a computer language, or a knowledge representation paradigm, is by necessity incomplete. It is only valid within a small and often very specialized domain. No single method can cope with the full spectrum of phenomena, or rather points of view, called for by an interdisciplinary and applied science.

The direct involvement of experts and decision makers shifts the emphasis from a production-oriented "off line" system to an explanatory, learning-oriented style of use. The decision support and expert system is as much a tool for the expert as it is a testing ground for the decision maker's options and ideas.

In fact, it is the *invention* and definition of options that is at least as important as the estimation of their consequences and evaluation. For planning, policy and decision making, the generation of new species of ideas is as important as the mechanisms for their selection. It is such an evolutionary understanding of planning that this software system is designed to support. Consequently, the necessary *flexibility and expressive power* of the software system are the central focus of development.

2.3 Model Integration and User Interface

The basic elements of a decision support and information system as outlined above are:

From a user perspective, the system must first and foremost be able to assist in its own use, i.e., explain what it can do, and how it can be done. The basic elements of this self-explanatory system are the following:

- *the interactive user interface* that handles the dialog between the users(s) and the machine; this is largely menu driven, that is, at any given point the user is offered several possible actions which he can select from a menu of options provided by the system;
- *a task scheduler or control program*, that interprets the user request – and, in fact, helps to formulate and structure it – and coordinates the necessary tasks (program executions) to be performed; this program contains the "knowledge" about the individual component software modules and their interdependencies;

  the control program can translate a user request into either:

  – a data/knowledge base query;

  – a request for "scenario analysis"

  the latter will be transferred to

- *a problem generator*, that assists in defining scenarios for simulation and/or optimization; its main task is to elicit a consistent and complete set of specifications from the user, by iteratively resorting to data base and/or knowledge base to build up the *information context or frame* of the scenario. A scenario is defined by a delimitation in space and time, a set of (possibly recursively linked) processes, a set of control variables, and a set of criteria to describe results. It is represented by
- *a set of process oriented models*, that can be used in either simulation or optimization mode. The results of creating a scenario and either simulating or optimizing it are passed back to the problem generator level through a
- *evaluation and comparison module*, that attempts to evaluate a scenario according to the list of criteria specified, and assists in organizing the results from several scenarios. For this comparison and the presentation of results, the system uses a
- *graphical display and report generator*, that permits selection from a variety of display styles and formats, and, in particular, to view the results of the scenario analysis in graphical form. Finally, although not directly realized by the user, the system employs a
- *systems administration module*, which is largely responsible for housekeeping and learning: it attempts to incorporate information gained during a particular session into the permanent data/knowledge bases and thus allows the system to "learn" and improve its information background from one session to the next.

It is important to notice that most of these elements are linked recursively. For example, a scenario analysis will usually imply several data/knowledge base queries in order to make the frame and necessary parameters transparent. Within each functional level, several iterations are possible, and at any decision breakpoint that the system cannot resolve from its current goal structure, the user can specify alternative branches to be followed.

It is also important to note that none of the complexities of system integration are obvious to the user: irrespective of the task specified, the style of the user interface and interactions with the system are always the same at the user end.

2.4 System Implementation

To be of practical use, the software system as outlined above has to be implemented on affordable hardware. Recent developments in microprocessor technology and the computer industry in general (Fedra and Loucks, 1985) make it possible to configure and implement the above ideas on a desk-top workstation (Figure 2.2).

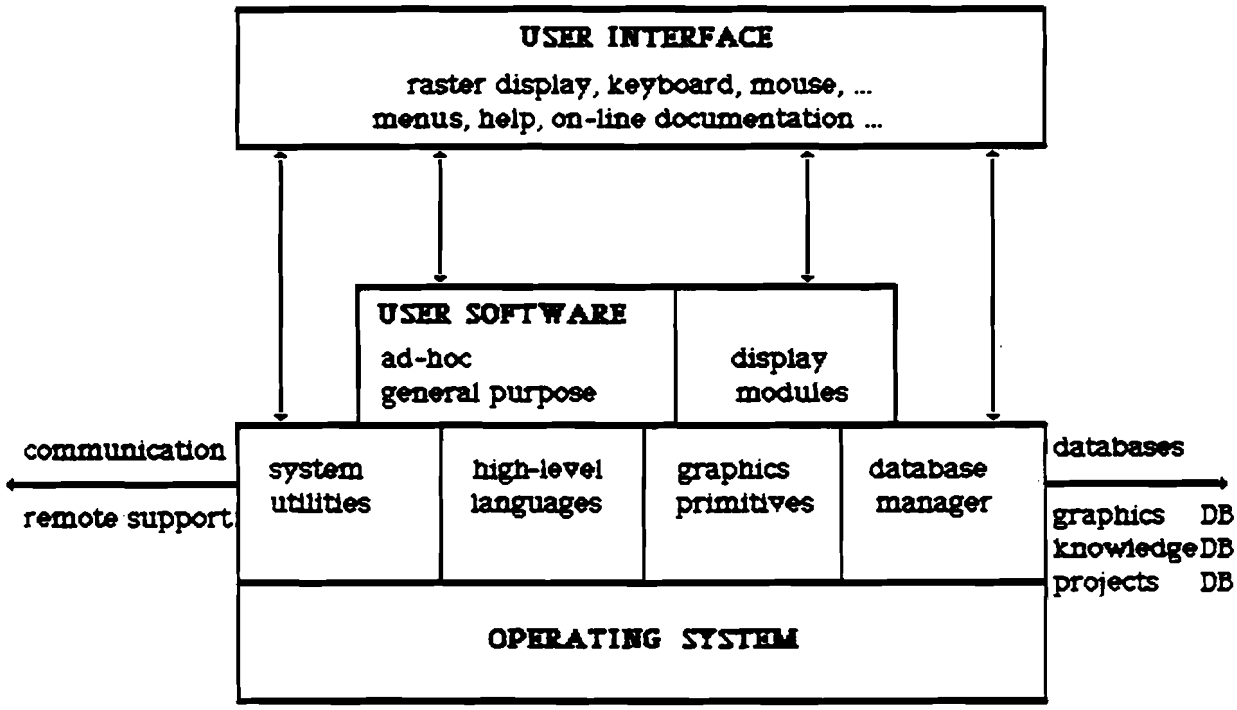

Figure 2.2: Implementation on a Super-micro Workstation.
(from Fedra & Loucks, 1985).

The super-micro workstation is based on a 32 bit microprocessor, supporting virtual memory management, thus freeing the programmer from the onerous task of storage optimization for large engineering applications. It also supports fast floating point operations, to make the interactive use of larger engineering programs feasible. The workstation offers sufficient and fast mass storage for large data bases and their interactive management.

The user interface is based on a high resolution (1 Mega-pixel) bit-mapped color screen (256 simultaneous colors or up to eight individual drawing planes) and a window-management technique that encourages the use of several virtual terminals in parallel.

The software system, based on UNIX (4.2 bsd) supports several languages to allow the integration of already existing software. This also makes it possible to select the most efficient language for a given task. In this particular application, C, FORTRAN 77, Pascal, LISP and PROLOG are used.

When developing a complex software system, like the one outlined in this report, rapid prototyping is very important. Therefore, the first implementation will be on a **prototype demonstration system** level. Its main purpose is to implement several working examples of methods and approaches proposed and discussed in this report, and thus provide a practical starting point for prospective users to work with. Only by being exposed to an operational prototype will users and co-developers be able to specify in greater detail the features they want supported by the system.

From the entire range of applications, a small, but sufficiently realistic and interesting, subset has therefore to be chosen for this implementation. For the industrial origin of hazardous substances, the sector or group of substances chosen is **the chlorination of phenols**. Here many toxic compounds are involved, including the ill-famed 2,3,7,8-tetrachlorodibenzo-*p*-dioxin (2,3,7,8 TCDD), a reaction by-product in the production of 2,4,5-trichlorophenol (2,4,5 T).

At the same time, realistic first prototype implementation can only involve a certain **small subset of simulation models** from the set discussed in the report that would ultimately be integrated in a real production system. For example, only a few environmental distribution models, some with multi-media capabilities, will be implemented in the first phase (see section 3.4).

Further, the data and knowledge bases to be implemented will not be extended to the level necessary for a real production system. Data collection and verification is a major task in itself, undoubtedly beyond the scope of this study. The prototype implementation will use fictional data for a **hypothetical, medium-sized region**. However, this region will include all major geographical features that need to be represented in any fully configured system. The data used will be taken from or based upon historical data from various existing regions, rescaled wherever necessary. The prototype implementation will also be restricted to a **local to regional level only**.

The production system and information bases of the prototype implementation will be thus reduced to a **minimum set of functional elements** that still allow the description of the entire coupled system as outlined in Figure 3.1. The structure and framework, the style of the user interface, and the basic principles of the system's operation, are those of a fully configured production system. The development of this fully configured system, implemented in several regional to national versions, and eventually in a compatible European version, is the ultimate long-term goal of the project.

3. COMPONENTS OF THE SIMULATION SYSTEM

The structure and basic elements of the simulation system are shown in Figure 3.1. A review of existing software modules that could be used to describe these elements, and a more detailed discussion of the models selected for integration into the simulation system or as the basis for further software developments, is given in Fedra et al. (1985 a).

The simulation system is always applied to a specific regional context, and the transboundary flows are specified to obtain the necessary material balances. The system represents a life-cycle approach, that traces substances from their origin and point of release to their impact. For most of these functionally specified elements, several models can be used in parallel or alternatively. The selection of the appropriate model(s) depends on the required scope and resolution in time and space, the emphasis on a certain process within a specific problem, and the available data. Wherever possible, the system will select the appropriate model automatically, or switch from one model to another automatically, if, for example, the emphasis changes from a short-term near-field to a long-term far-field problem.

The main components of the simulation system are:

1) **The Industrial Production System**, that describes the generation of hazardous substances as products, byproducts, interim products, or waste of the industrial production process.
2) **Use and Market**, a module that acts as a gateway for the industrial products, diverting them into different pathways according to their use (dispersive or non-dispersive) and waste streams (industrial, domestic). For non-dispersive use, the compartment also serves as an interim storage according to the life time of the product.

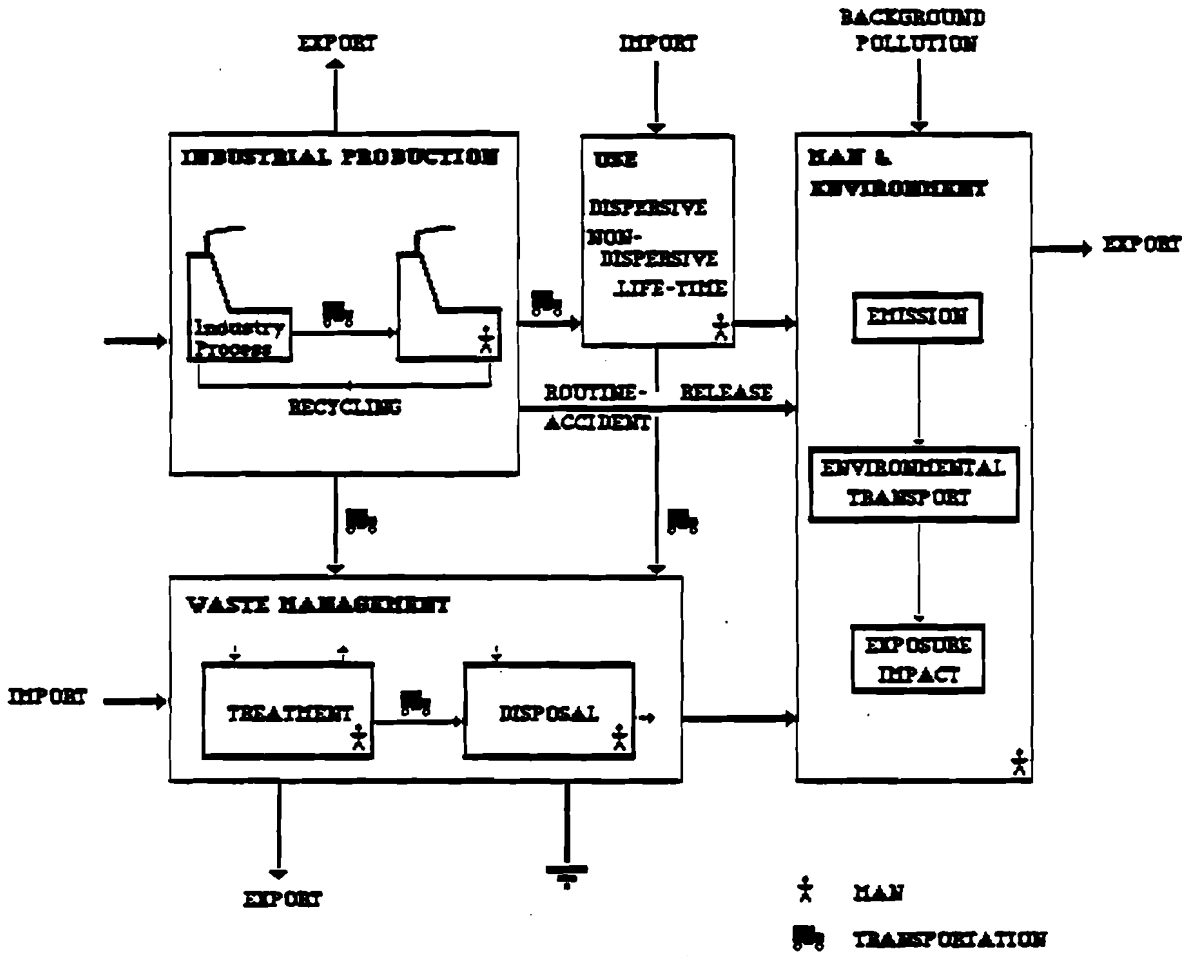

Figure 3.1 Elements of the Simulation System.

3) **Waste Management**; this module simulates treatment and disposal of wastes arriving from either the industrial production or the use/market compartments.

4) **Man and Environment**, a set of models that simulate, starting from the emissions coming from either the industrial production sector, the use compartment, transportation (see below), or the waste management block, the transport of substances through the environment (atmospheric, aquatic, soil, biological pathways), as well as impacts on man and the environment.

5) **Transportation** models interconnecting several of the above blocks. The transportation model estimates costs and risk of various transportation alternatives, and provides input to the emission gateway in the environmental sector.

6) **Cost Accounting and Evaluation** is another cross-cutting element that is used for each of the sectoral models. This evaluation comprises monetary as well as non-monetary indicators (e.g., McAllister, 1980; Tietenberg, 1984).

3.1 Industrial Production System

The Industrial Production System generates products, wastes, and interim products; it uses up raw materials, energy, manpower, etc. (Figure 3.2).

In its normal operation mode, it would estimate the amount of waste of different types for a certain set of end products, using a certain production technology or process; the waste products generated enter an industrial waste stream, and are moved to the *Waste Management Sector* for further processing, treatment, and ultimately, disposal. In part, the waste products are released into the environment on a routine basis (through stacks and chimneys, as waste water, or in the normal domestic waste stream).

In addition to this normal mode, the industrial production module can also simulate an "accident" or gross mismanagement situation. Here a large portion of raw materials, interim products in the production process, or final products can be released – more or less uncontrolled – to the environment. Explosion or fire can aggravate this release.

According to a 1980 study of the USEPA, the four industrial sectors indicated below, together with several subsectors, contribute 82% of the hazardous waste generated in the U.S. (Putnam, Hayes, and Bartlett, Inc. (PHB) 1980). Similar results were obtained in a 1983 survey of the EPA's Office of Solid Waste (Westat Research, 1984). For these industrial sectors, the USEPA study (ICF 1984a,b) identifies and provides data for 154 industrial waste streams, each characterized by 30 data elements.

The specific *Industrial Production Sectors* considered include *(List based on ICF (1984)):*

- Chemical
    - Alkali and chlorine
    - Inorganic pigments
    - Synthetic organic fibers
    - Gum and wood chemicals
    - Organic chemicals
    - Agricultural chemicals
    - Explosives
- Petroleum and Coal Products
    - Petroleum
- Primary Metals
    - Iron and steel
    - Secondary nonferrous metals
    - Copper drawing and rolling
- Fabricated Metals
    - Plating and polishing

Emphasis will be on the chemical industry; a specific sector organized around a specific set of processes (chlorination of phenols) will be the focal point for the models described below.

An alternative *Classification Scheme for Process Plants* (Zanelli et al., 1984) is currently being developed at the JRC. It is an attempt to develop a multi-level taxonomy that should allow the linking of Accident Reports, Safety Information, and the Component Reliability Parameters to their relevant industrial area or sector, plant, system, and unit.

For the description of the industrial production sector in the system outlined here, a three-level hierarchical decomposition approach is proposed (Figure 3.3). The three levels are defined and represented as described below.

3.1.1 Production Process Level

The *Production Process Level* focuses on individual product or substance-oriented production processes and unit processes (e.g., Herrick et al., 1979). The description is process-oriented and represents a mass budget, based on the physical and chemical-stoichiometric properties of the substances involved. In addition to specifying output, waste, and interim products, the model also includes process

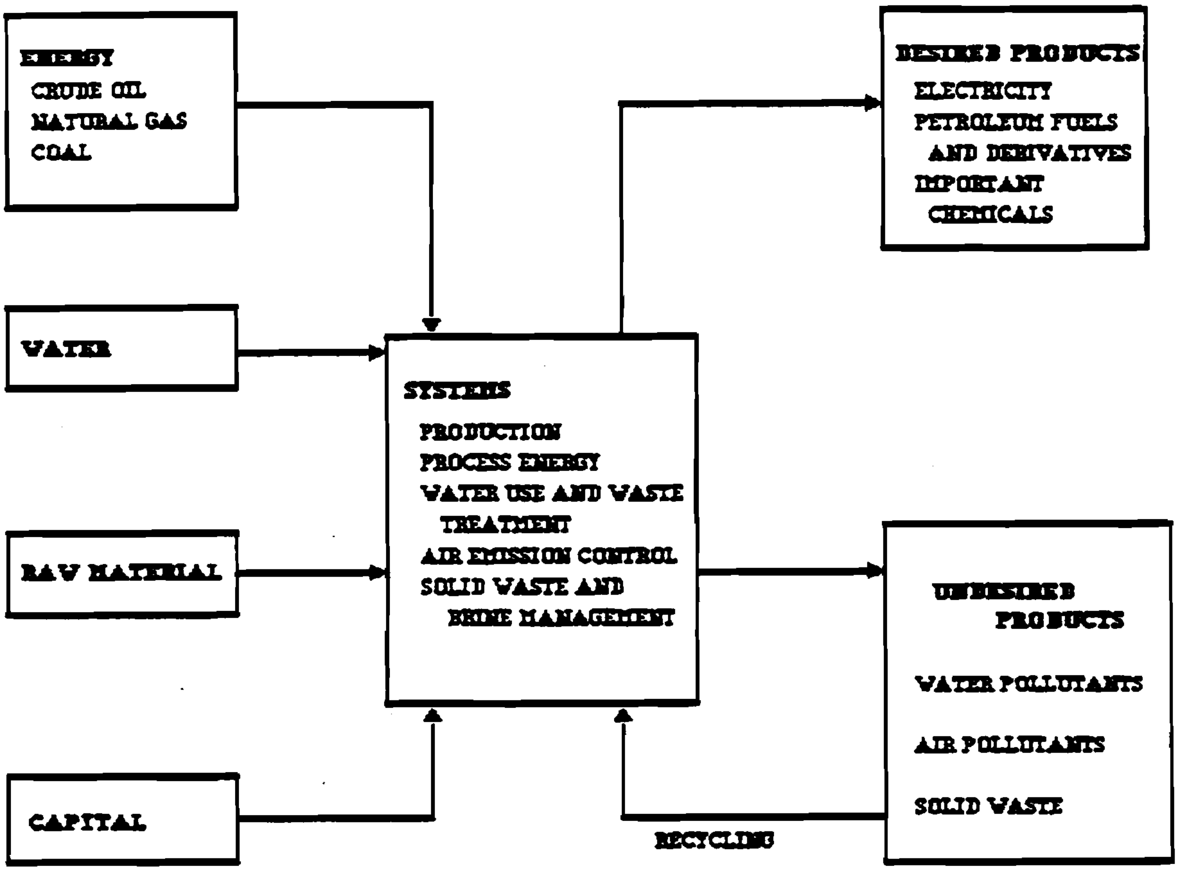

Figure 3.2: Generalized Industrial Production System.
(after Bridgewater & Mumford, 1979)

streams as its basic elements. Process streams are characterized by:

- the major substances (feedstocks, products, wastes) involved,
- typical temperature and pressure conditions,
- the plant components or equipment involved (e.g., type of reactor, see Zanelli et al., 1984),
- hazard ratings (AICE,1973 and NFPA, 1977) for the process stream.

The hazard rating allows the identification of high risk process streams for the simulation of possible accidents. The technologically-oriented process stream description provides the parameters necessary for the emission interface to the environmental distribution and transport models (substance(s), amounts, temperature, pressure).

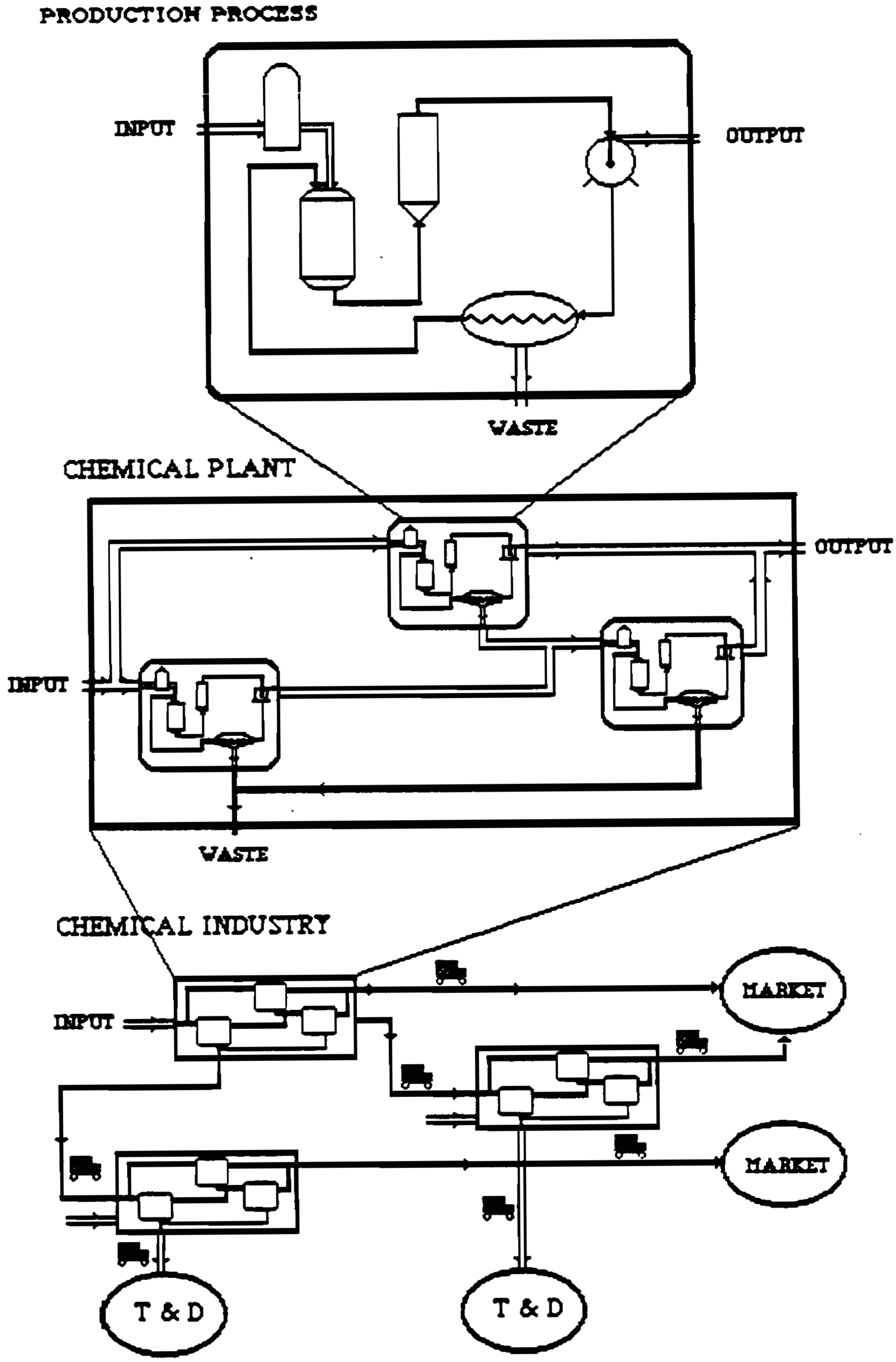

Figure 3.3: Industrial Production System Decomposition

Approaches to modeling chemical production processes are usually based on mass conservation principles (e.g., Crow et al., 1971). They can be extremely complex, involving detailed numerical models of flow processes, thermal processes, and the chemical transformations involved (see, for example, the SAFIRE model system, FAI, 1984). Since the specific data of a given process in a specific plant will rarely be known in every detail, modeling is usually based on a more or less standardized *unit process* concept (Herrick et al., 1979). Alternatively, a mixed quantitative/qualitative description, again based on unit process transformations but leaving out the physical and chemical details, may be used (Figure 3.4), (Goldfarb et al., 1981).

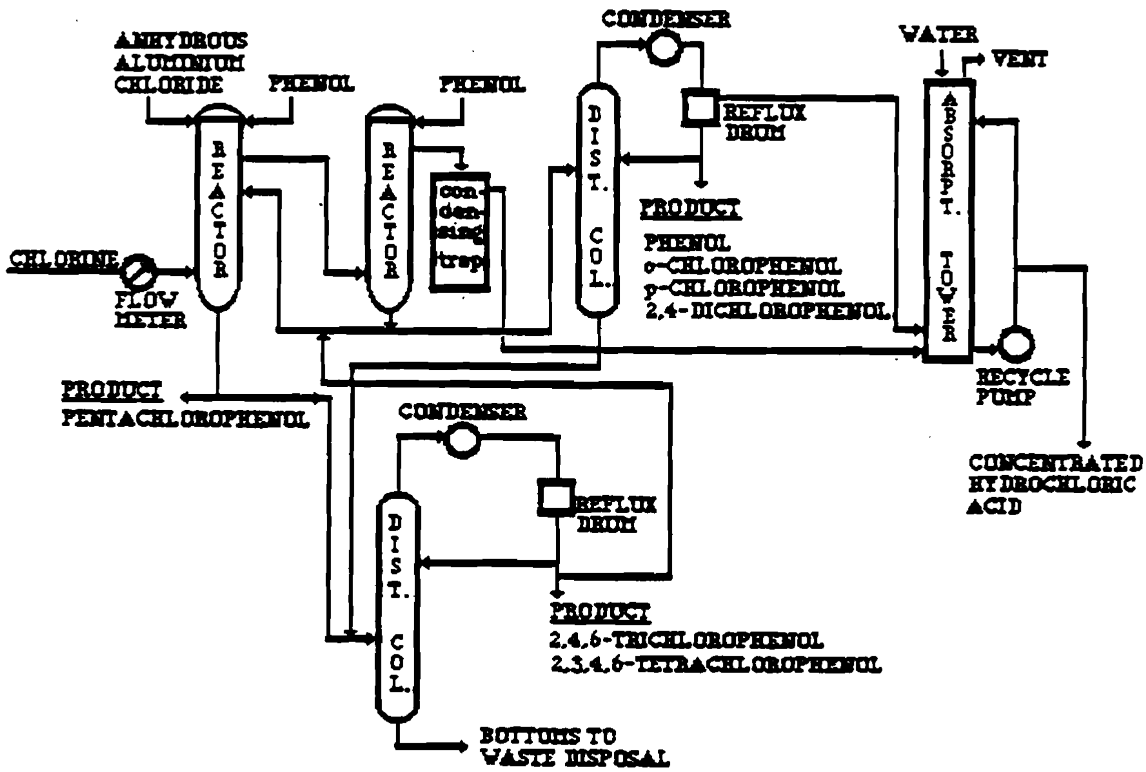

Figure 3.4: Production Process Description: Chlorination of Phenols.
after: Goldfarb et al., 1981.

3.1.2 Chemical Plant Level

The *Chemical Plant Level* looks at chemical plants as an assembly of production processes, aggregated to simple production functions. These production functions describe the relationship between inputs (including raw materials, feedstocks, energy, labor, and capital), output products, wastes, interim products, costs and revenues. While based on an aggregation of the process level descriptions, the production functions defining chemical plants are black box models. Chemical plants may be configured to represent the structure of known production sites.

Alternatively, based, for example, on the minimization of the cost function components subject to constraints on wastes, regulations of certain production processes, and the mass balance problems inherent in the production process linkages, they are composed by an optimization routine to supply a certain product mix at a certain production level (Dobrowolski et al., 1982; Grauer et al., 1984).

3.1.3 Chemical Industry Level

The *Chemical Industry Level* describes a spatially disaggregated production system, i.e., a set of chemical plants and their interrelationships. Again, they can be composed and structured to describe an existing industrial structure. Alternatively, a feasible industrial structure can be generated in response to a spatially disaggregated demand structure at, for instance, minimum cost considerations. This demand driven model would again treat chemical plants as aggregated black box models, based on the next lower level's disaggregated description (e.g., Liew and Liew, 1984).

3.2 Use and Market

The Use and Market Sector acts as a gateway for industrial products, diverting them into different pathways according to their use (dispersive or non-dispersive) and waste streams (industrial, domestic). For non-dispersive use, the compartment also serves as an interim storage point according to the life time of a product. An example showing the relationships of production, market, and the waste management sector (including various recycling options) for an unspecified metal is shown in Figure 3.5.

Ultimately, the Market Sector could also determine demand for and prices of products. In particular, any major change in either the spatial distribution of production sites (e.g., relocation of facilities) or changes in production

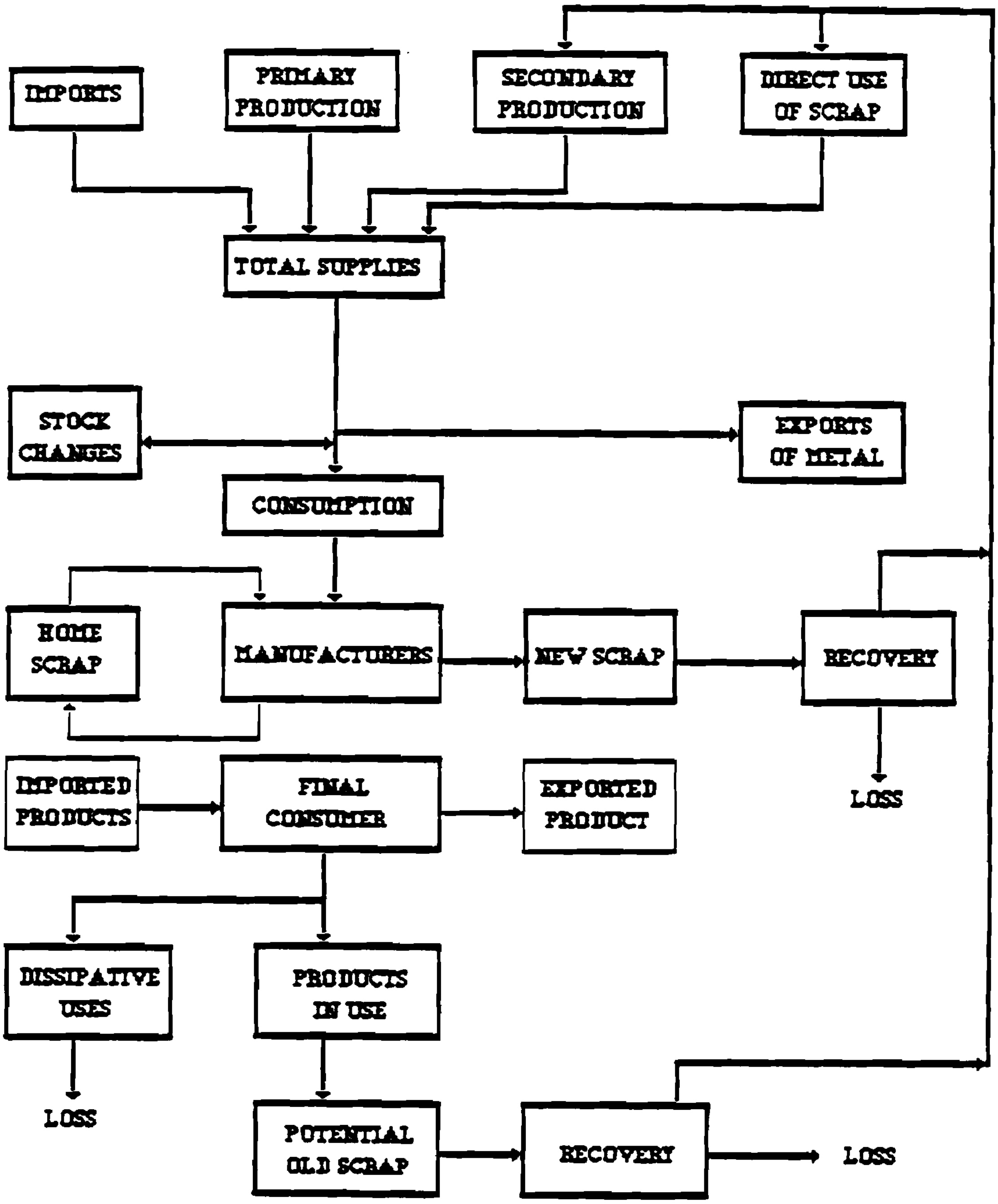

Figure 3.5 Use/Market System Example: Metal.
(from Bridgewater & Mumford, 1979)

technologies that lead to a change in product mix or alternative recovery and recycle routes, are likely to influence prices if implemented on a large scale. This, however, would require a complete economic model which is beyond the scope of the first phase of system development.

3.3 Waste Management: Treatment and Disposal

The Waste Management, or Treatment and Disposal Sector, receives the waste streams from the *Industrial Production Sector* and the *Use/Market Sector* (industrial and domestic waste). The models describe processing and treatment, potential recovery and recycling, and disposal of hazardous substances (Figure 3.6). As in the case of the industrial production sector, the models can describe several alternative technologies, and estimate costs for alternative waste management schemes. Apart from a normal operation mode, "accident" or mismanagement scenarios are possible.

In the estimation of costs and risks, a provisional selection of 15 treatment technologies is considered:

01) Vacuum filtration
02) Centrifugation
03) Sludge drying beds
04) Chemical precipitation
05) Oxidation/reduction
06) Evaporation drying
07) Steam stripping
08) Solvent extraction
09) Leaching
10) Distillation
11) Carbon adsorption
12) Biological treatment
13) Chemical stabilization/fixation
14) Asphalt solidification
15) Containerization

Each of these technologies has different characteristics with regard to key design and operating features, feasible waste streams, the effectiveness of the technology in altering the hazardous nature of the waste, and finally the amount and probability of any environmental release of hazardous constituents generated by the technology.

The second set of technologies in the waste management sector is *Disposal Technologies*. Again, a provisional list of six alternative technologies (from ICF, 1984a,b) is used as the basis for our design:

01) Landfills
02) Land treatment
03) Surface impoundment
04) Deep well injection
05) Waste piles
06) Incineration

This basic set of technologies is further divided into several subgroups (Table 2), where special emphasis is placed on new and emergent technologies (e.g.,

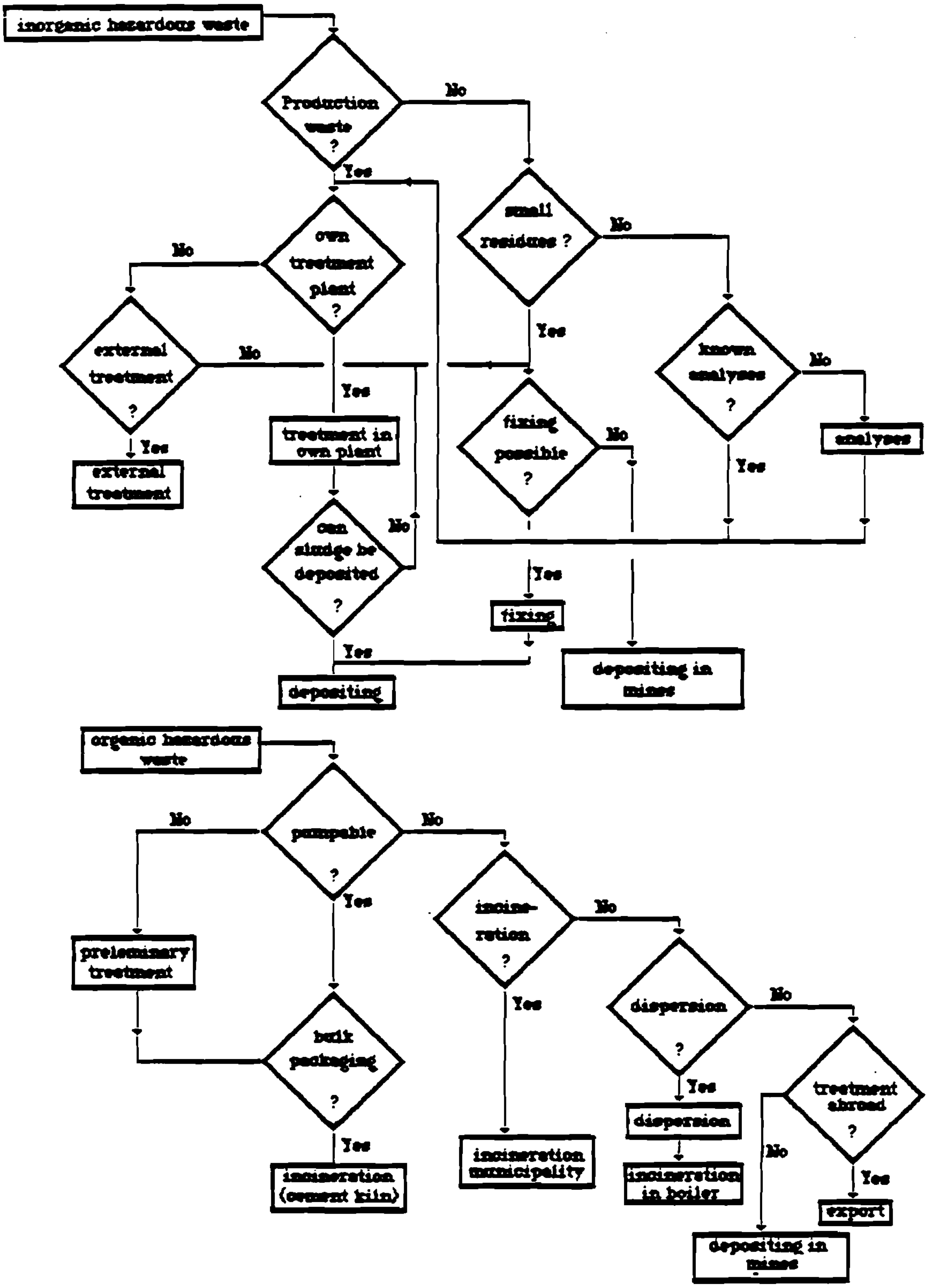

Figure 3.6: Waste Management System: Treatment and Disposal. (after Lehman, 1983).

Edwards et al., 1983). Similar to the treatment technologies, disposal technologies differ in terms of feasible waste streams, the release of constituents to the environment, and the cost and resource consumption for operation. Cost estimates for each technology are given in ICF (1984b).

TABLE 2: Waste Treatment/Disposal Techniques: Incineration (after Francis and Auerbach, 1983; Edwards et al., 1983).

Process Type	Application	Temperature (°C)	Residence Time
At-Sea Incineration	Any solid or liquid organic waste	650 - 1650	seconds - hours
Cement Kilns	Liquid organic (chlorinated) waste	1500 - 1650	<10 sec (gases) hours (liquids)
Fluidized Bed	organic liquids, gases, granular solids	800 - 900	seconds (gases) minutes (liquids)
High-Temperature Fluid Wall	liquids, granulated solids	2200	milliseconds
Molten Salt	low ash liquids/solids	800 - 1050	seconds (gases)
Multiple Hearth	sludges, granulated solids	800 - 1000	up to hours
Plasma Arc Torch	liquids and solids	50000	< 1 sec
Rotary Kilns	any combustible waste	850 - 1650	seconds (gases) hours (liq./solid)
Single Chamber/ Liquid Injection	liquids, slurries	750 - 1650	< 1 sec
Starved Air Combustion/Pyrolysis	purely organic	150 - 650	seconds (gases) hours (solids)

A possible approach to describing the waste management system is a rule based system, using, for example, the data of the IRPTC waste management file (UNEP/IRPTC, 1984), or INFUCHS (developed and maintained at the Umweltbundesamt, UBA, FRG), or the waste stream treatment and disposal technology linkages of the RCRA (W-E-T) Model (ICF 1984).

Several recent books cover treatment and disposal technologies for hazardous wastes in considerable technical detail (e.g., Edwards et al., 1983; Francis and Auerbach, 1983; Lehman, 1983; Kiang and Metry, 1982; Brown et al., 1983; Peirce and Vesilind, 1981).

3.4 Man and Environment: Emission, Transport, Impacts

The Man and Environment Sector has as its entry point an emissions compartment. It is linked to the above three sectors as well as to the cross-cutting transportation sector.

From the emission point, which specifies the nature of a pollutant (liquid, gaseous, dust, solid, etc.) and the point of release (chimney, canal, dump site, etc.) the substances are moved through one or more of the environmental transport pathways (Figure 3.7). These are: atmospheric, aquatic (surface/groundwater), terrestrial (soil system and biological food-chain); In most cases, different models for the short-term near-field, and the long- term far-field are used. A typical example would be atmospheric transport, where a singular accidental release could be handled by a Gaussian model, whereas long-term long-range transport could be handled by a Lagrangian particle-in-cell model (e.g., based on Eliassen 1978).

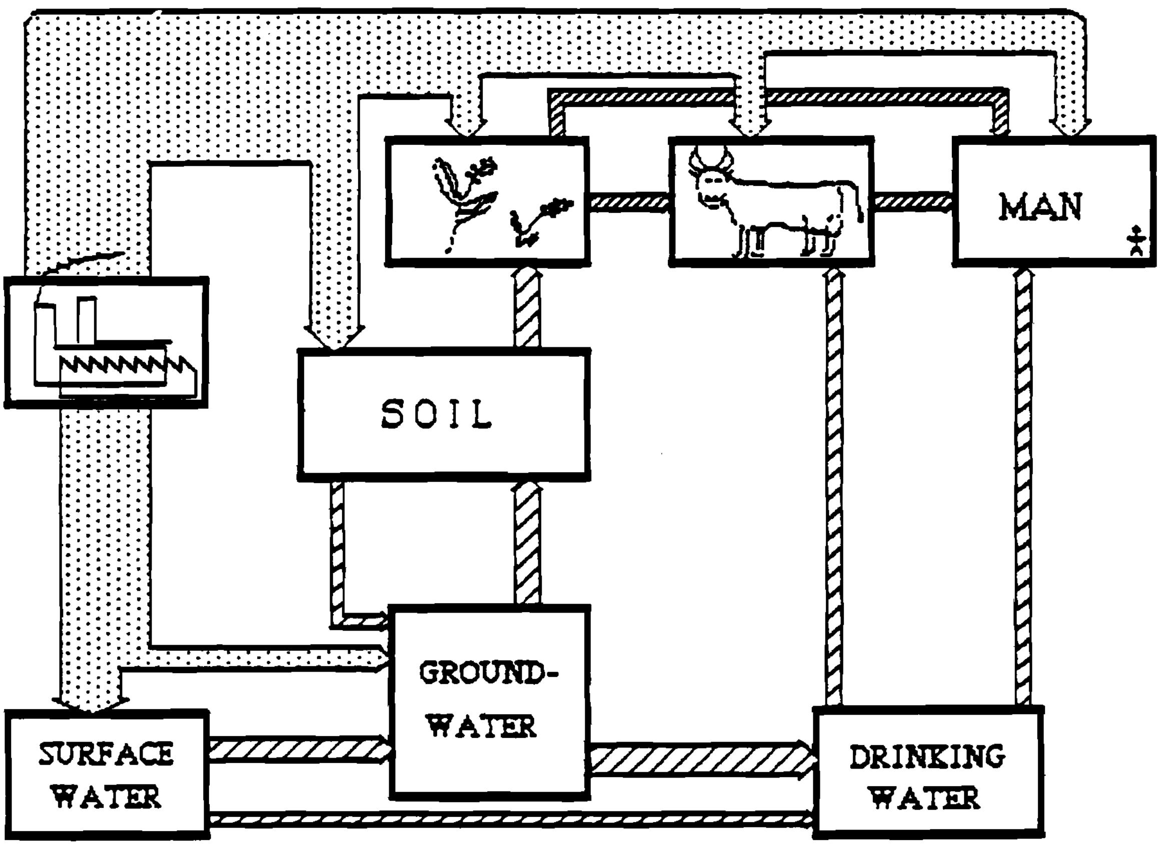

Figure 3.7: Generalized Pollutant Pathway in the Environment.

A multi-media framework is provided by TOX-SCREEN (Hetrick and McDowell-Boyer, 1979, 1984). TOX-SCREEN, developed at Oak Ridge National Laboratory, is designed to asses the potential environmental fate of toxic chemicals released to air, water, or soil. It evaluates the potential of chemicals to accumulate in environmental media and is intended for use as a screening device. The model makes a number of simplifying assumptions and operates on a monthly time step. Assumptions include a generic positioning of surface water bodies relative to atmospheric pollutant sources and contaminated land areas. The data used are typical of large geographic regions rather than site specific. This multimedia screening tool will therefore be augmented by a second layer of more detailed and site-specific models for the individual environmental media. This results in a hierarchically organized system of models of various degrees of resolution in time and space as well as in the complexity of the model equations.

In TOX-SCREEN, the physical/chemical processes which transport chemicals across air-water, air-soil, and soil-water interfaces are simulated explicitly. Deposition velocities, transfer rate coefficients, and mass loading parameters are used. Monthly pollutant concentrations in air, surface waters, and soil reflect both direct input to any or all of the media from a specified source or sources, and subsequent interaction via processes such as volatilization, atmospheric deposition, and surface runoff. Methods for estimating bioaccumulation in the food chain are also included.

3.4.1 Atmospheric Dispersion

Atmospheric dispersion from point sources is described by a modification of the original Gaussian plume equation of Pasquill (1961). Modifications include plume depletion due to wet and dry deposition, gravitational settling, and chemical degradation. Sector averaged and maximum concentrations are calculated on a monthly average basis, assuming a constant Pasquill Stability Class D (.i.e., neutral conditions). Also assumed is a constant wind direction over the period of model application.

To describe atmospheric dispersion in a more detailed, dynamic, and possibly site-specific way, the Industrial Source Complex Model (ISC) developed by the U.S. Environmental Protection Agency (EPA) is used as an alternative or extension to the TOX-SCREEN model. It is again based on an extended Gaussian model, describing the concentration/deposition of substances in time and space.

The *ISC Long-Term Model* (ISCLT) is designed to calculate the average seasonal and/or annual ground level concentration or total deposition from multiple continuous point, volume and/or area sources.

The *ISC Short-Term Model* (ISCST) is designed to calculate ground-level concentration or deposition from stack, volume or area sources (Figure 3.8). The receptors at which the concentration or deposition are calculated are defined on a x-y, right-handed cartesian coordinate system grid. Discrete or arbitrarily placed receptors may be defined. Average concentration or total deposition may be calculated in 1-, 2-, 3-, 4-, 6-, 8-, 12-, and/or 24-hour time periods. An 'n'-day average concentration (or total deposition) or an average concentration (or total deposition) over the total number of hours may also be computed. Concentrations (depositions) may be computed for all sources or for any combination of sources the user desires. Other options include input of terrain heights for receptors, tables of highest and second highest concentrations or depositions at each receptor and tables of the fifty maximum values calculated.

Other extensions of the Gaussian Model include:

- the influence of urban or rural area on the weather;
- plume rise (Briggs 1971, 1975);
- variable topography of the area, influencing the variation of wind and temperature;
- the influence of buildings close to the source (Huber and Snyder, 1976; Huber 1977), affecting the coefficient of dispersion;
- the exponential decomposition of chemicals;
- a simple deposition model (Dumbauld et al., 1976; Cramer et al., 1972).

For long-range transport on medium- to long-term time scales, the Gaussian models referred to above are not well suited. At larger distances, depending on the atmospheric stability conditions, results become more and more uncertain. Also, the variability of wind directions over the run time of a simulation will result in complex trajectories. Therefore, for long-range transport, a Lagrangian model (e.g., Eliassen 1978) will be used instead of the Gaussian models.

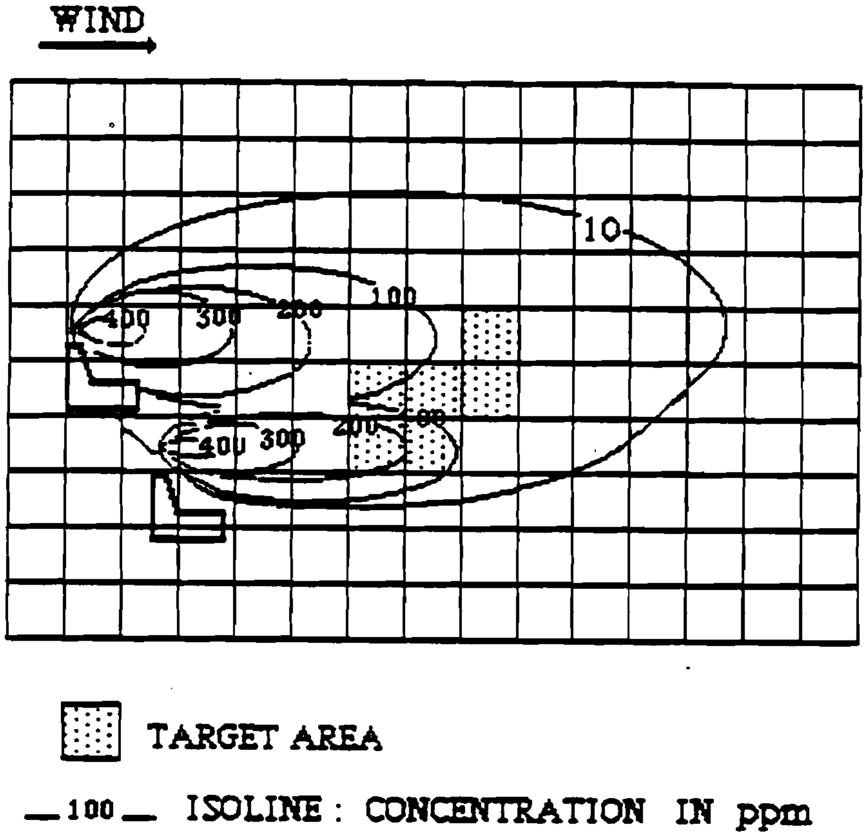

Figure 3.8: Atmospheric Transport and Diffusion Model Output.

3.4.2 Aquatic Systems

The importance of aquatic systems as the recipients of hazardous waste is obvious from the proportions reported in the 1983 CMA Hazardous Waste Survey (CMA, 1983): In the US, 99% of the hazardous waste generated (by industrial sources of the Standard International Classification 2800 group, Chemicals and Allied Products) was wastewater. These wastewaters are dilute streams defined as hazardous by the RCRA mixture rule.

In the TOX-SCREEN framework, chemicals introduced into surface water bodies, either directly or indirectly due to runoff from soil, or deposition from air, are dispersed in water and sediment according to the respective flow regime and the characteristics of the chemical. Using simplified assumptions to simulate dispersive processes underlying the dilution mechanism, TOX-SCREEN estimates concentrations in rivers, lakes, estuaries, and coastal marine systems.

Rivers: To simulate dispersion in rivers, a river is split into a number of geometrically equivalent reaches which all have the same flow rate. An equation similar to the one in EXAMS (Smith et al., 1977; Burns et al., 1981) is used to estimate the monthly pollutant mass in each reach. Instantaneous mixing in each reach upon introduction of a pollutant is assumed. Pollutant concentrations are calculated for dissolved neutral, dissolved ionic, and adsorbed forms, according to chemical equilibria. Adsorption onto sediment is also described.

For a more detailed treatment, alternative codes include WQRRS, developed by the U.S.Army Corps of Engineers (HEC 1978), or QUAL-II, developed by the Texas Department of Water Resources. With a much shorter time step, they can simulate individual spills on a higher spatial resolution and considering numerous biotic and abiotic variables together with a limited set of chemicals.

Lakes: Lakes are treated in a manner similar to that used for rivers. Again, the mass balance approach of EXAMS is used. For more detailed treatment and a shorter time step, numerous alternative models do exist. EXAMS is specifically designed for toxic chemicals (Smith et al., 1977; Burns et al., 1982). EXAMS describes the behavior of synthetic organic chemicals in aquatic environments. From the chemistry of a compound, and the relevant physical/chemical and transport characteristics of the system, EXAMS computes:

- the ultimate steady state environmental concentration resulting from a specified pattern of loading;
- the distribution of the chemical in the system and the fraction of the loadings consumed by each transport and transformation process;
- the time required for effective purification of the system via export and transformation processes once inputs cease.

The model combines loadings, transport, and transformations into a set of differential equations based on mass conservation. This accounts for all chemical mass entering and leaving the system due to

1) external loadings,
2) transport processes that export the compound from the system,
3) transformation processes that convert the parent compound to daughter products.

Concentrations are described as the balance between increases originating from external and internally recycled loadings, and decreases resulting from transport and transformations. Environmental data consist of a concise description of the aquatic system, represented by a set of n compartments or zones with specified geometry and connectedness. EXAMS also accepts standard water quality and limnological parameters.

A lake model of high complexity, MS.CLEANER (Park et al., 1979) (Figure 3.9) has been extended into the pesticide accumulation model for aquatic ecosystems, PEST (Park et al., 1977). Estimates of the required rate constants and partition coefficients are largely based on the octanol:water partition coefficient of a substance. Special emphasis is given to the accumulation of toxics in fish; examples given are DDT and Methoxychlor (Leung 1978).

Estuaries: In TOX-SCREEN, a one-dimensional steady-state model that assumes constant cross-sectional area, a constant tidally and sectionally averaged longitudinal dispersion coefficient, and a constant fresh water velocity is used for simulating dispersion of pollutants in estuaries.

Coastal Marine Systems: A steady-state Gaussian type linear diffusion model is used for discharges to coastal waters (Brooks 1960). Assumptions of the model include offshore discharge via an outfall terminating in a multipoint diffuser, movement of the resulting pollutant field at the same rate as the prevailing current, negligible vertical and longitudinal mixing and steady flow.

Groundwater: Not covered within the TOX-SCREEN framework is groundwater. While the soil subsystem model SESOIL (see below) includes groundwater recharge, no specific groundwater model is included. Groundwater, however, is an extremely important medium due to its high value as a high-quality potable water resource.

Causes and consequences of qualitative changes in groundwater regimes can be separated by decades or centuries. Once contaminated, groundwater resources may be permanently impaired. Groundwater contamination, particularly from hazardous wastes, has been recognized as a very serious national problem in many countries (Wood et al., 1984).

A survey of management-oriented groundwater models is given in Bamachmat et al., 1980. Only few field-tested models, that could be incorporated into the decision support framework are available. FEEFLOW is a sophisticated two-dimensional finite element model for the simulation of contaminant transport in porous media (Diersch, 1980; Diersch and Kaden, 1984). It has been used successfully in several case studies. Alternatively, SWIFT, the Sandia Waste-Isolation Flow and Transport Model (Reeves and Cranwell, 1981), is a fully transient three-dimensional model which solves the coupled equations for transport in geological media.

The processes considered are:

- fluid flow,
- heat transport,
- dominant species (e.g., brine) miscible displacement,
- trace species (e.g., radionuclides) miscible displacement.

The first three processes are coupled via fluid density and viscosity. Together they provide the velocity field on which the fourth process depends.

3.4.3 Terrestrial Systems

Chemicals applied to surface or subsurface soils, or deposited on the ground from the atmosphere, are dispersed in soil as a result of processes associated with the hydrological cycles and with physical and chemical phenomena. This dispersion may lead to contamination of adjacent surface waters and air, depending on chemical, soil, and climatic conditions. Uptake by plants is referred to below in the discussion of the human exposure model TERMOD.

In TOX-SCREEN, the soil system is represented by the one-dimensional model SESOIL (Bonazountas and Wagner, 1981). The model describes the unsaturated soil zone in a simple mass balance approach for a multi-layered soil compartment of arbitrary size. The simulation is structured around three cycles:

- *Hydrological Cycle*, which includes rainfall, infiltration, soil moisture, surface runoff, exfiltration, evapotranspiration, groundwater runoff, capillary rise;
- *Sediment Cycle*, which includes sediment resuspension due to wind, and sediment washload due to rain storms (not operational in the version described by Bonazountas and Wagner (1981).
- *Pollutant Cycle*, which includes advection, diffusion, volatilization, adsorption and desorption, chemical degradation and decay, biological transformation and uptake (see TERMOD-II below), hydrolysis, photolysis, oxidation, cation exchange, and complexation chemistry.

A special case of a model linking terrestrial and aquatic system is a hydrological simulation model for solid waste disposal sites (HSSWDS), Perrier et al., (1980), describing leachate behavior.

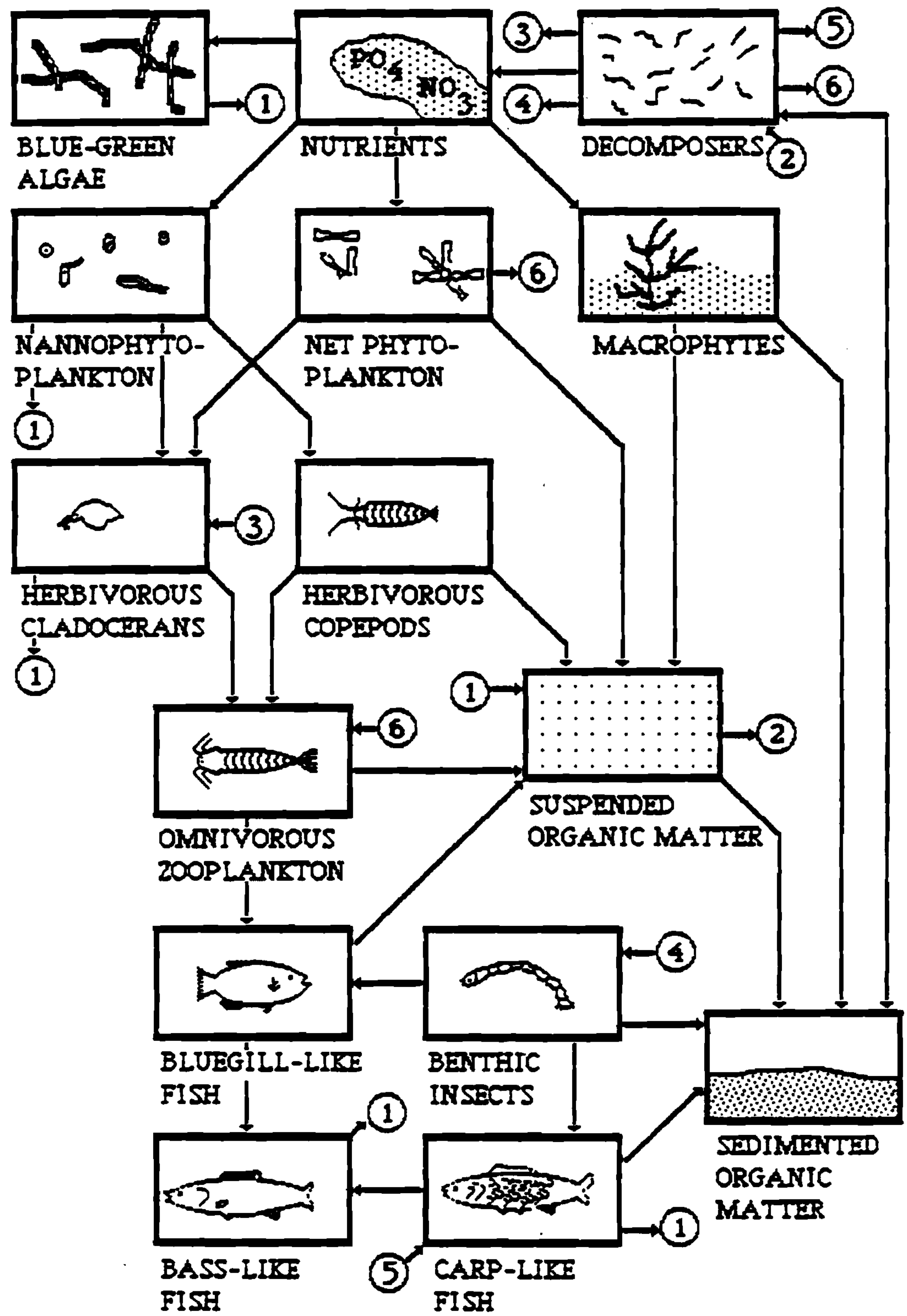

Figure 3.9: Flow Diagram for MS.CLEANER and its Extension, PEST. (after Park et al., 1977, and Leung, 1978.)

3.4.4 Impacts and Human Exposure

Impacts in the Man and Environment sectors are either human health risks or ecological risks. Obviously, they are closely linked. For the most important class of hazardous substances, i.e., toxic substances, human health risks are estimated from *exposure* and *toxicity*. They are evaluated for the individual as well as for the affected population. The toxicity of a substance or substance class determines the type of adverse effects that exposure or intake of the substance can cause (e.g., cancer, birth defects, kidney damage) and the relationship between exposure and/or intake and the magnitude of the effect. Exposure depends on the concentration in the environment and the environmental media affected (i.e., water, air, food) and the related probabilities of exposure and/or intake.

A possible model to describe these effects in detail could be based on TERMOD-II (Zach, 1978). Originally developed for radionuclides, the model calculates the time-dependent input of a substance through terrestrial pathways to man following an acute or accidental release. The model calculates daily input rates and the total intake over specified periods. The model includes three types of food, which can be contaminated by deposition. Food crops and grass can be contaminated by direct foliar deposition and via root uptake. Beef, and consequently milk, can be contaminated by uptake of contaminated grass.

An extended version will have to include direct human uptake and exposure through inhalation and skin contact as well as uptake via drinking water (Figure 3.10). The original radiation concept will be extended into a description of toxicity, considering oral and dermal toxicity (measured as LD_{50}) for acute toxicity. Long-term effects have to consider toxicological effects such as mutagenicity, carcinogenicity, teratogenicity, embryotoxicity, neurotoxicity, hepatotoxicity, renal toxicity, and pulmonary toxicity. Extended data on such effects are available for selected substances in quatitative form, for example, the Environmental Chemicals Data and Information Network (ECDIN) developed and maintained at JRC, Ispra, or in qualitative form (e.g., Epstein et al., 1982).

3.5 Transportation: Costs and Risks

The transportation model determines costs and risks for transporting certain amounts of certain substances from one location to another. This estimation is done for various transportation alternatives (e.g., air, rail, road, ship), and possible alternative routes. According to studies of the USEPA (ICF 1984a,b) 90% of hazardous waste in the US is currently transported by truck. Rail and ship

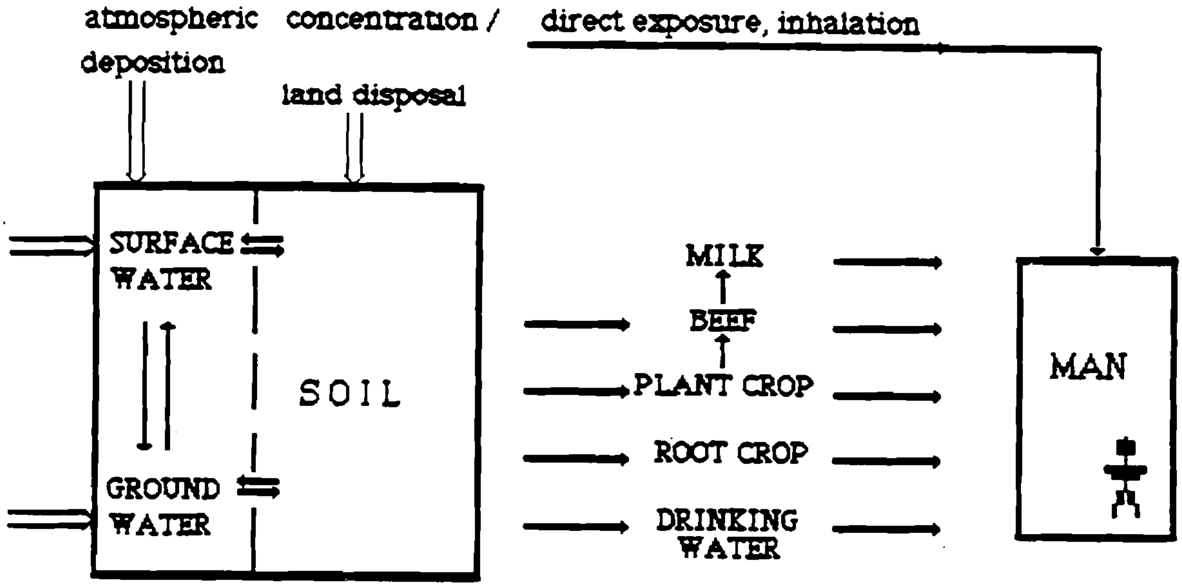

Figure 3.10: An Extended Human Exposure Model Based on TERMOD-II.

transport are of considerable importance for the transportation of ***hazardous goods***.

Examples of models for the estimation of risks and costs of the transportation of hazardous materials include INTERTRAN (IAEA, 1983), which was developed for assessing the impact from transportation of radioactive material. Several models for hazardous substances transportation are summarized and discussed in Posner (1984), including approaches developed by:

- Simmons et al. (1973), which examines the risk associated with spills of volatile, toxic chemicals, primarily chlorine;
- U.S.Coast Guard (National Science Council, 1976), a simple model based on conditional probabilities, but requiring data rarely available in practice;
- Garrick et al., (1969), based on fault-tree analysis and a spatial decomposition of the route in a system of nodes and arcs;
- Jones and Barrow (1973), developed as part of an integrated risk assessment system, the model combines estimates of likelihood of several types of incidents involving hazardous materials and a number of severity classes with the potential cost of an incident. Data for this approach were taken from HMIRS (Hazardous Materials Incident Reporting System).

- Kloeber et al., (1979), used for the assessment of air versus other modes of transportation of explosives and flammable cryogenic liquids;
- Battelle-Pacific Northwest Laboratories (Rhoades, 1978) which again uses the product of the probability of occurrence of release and the consequence of that release to describe risk; this simple model has been used to examine a wide range of hazardous materials generally transported by rail and truck.

For the decision support system under development, a model will be selected that estimates costs for each of the feasible mode/route alternatives, and also estimates the risks of possible accidents, depending not only on the substances and the mode of transportation, but also on the time of transportation (season, weather conditions, time of the day) and the exposure (population, environment, infrastructure) along a given route.

Using the model in an optimization framework makes it possible to determine a minimum cost, risk or exposure transportation/route alternative. In a multi-objective setup, a satisfying compromise solution trading costs against risks can be found.

3.6 Cost Accounting and Evaluation

Cost accounting and evaluation routines must, for each module in the simulation system, attempt to derive values (symbolic or numerical) for the applicable (sub)set of criteria (see section 2.1 and Table 1).

For the monetary value, accounting problems are aggravated by the large variety of time scales in the time streams of costs and benefits from individual actions. In most cases, only incremental costs that must already assume a certain infrastructure to be available, can be considered. The specification of the infrastructure is part of the frame problem referred to above.

Since several of the component models do some cost accounting or evaluation of impacts of their own, this module must combine, scale, and aggregate these individual contributions to an overall budget and evaluation sheet.

4. THE INFORMATION SYSTEM: DATA AND KNOWLEDGE BASES

An important element in the overall design is the information system. The information system includes data bases with their management software, and knowledge bases with their respective "inference machines".

The four main components of the information system are:

1) *organizing tools and documentation* (model descriptions, bibliography);

2) *general, cross-cutting information* (substances, regulations);

3) *process-specific information* (technologies);

4) *implementation-specific information* (regional geography, meteorology).

Due to the diverse nature of the information required, we have chosen a hybrid approach to data/knowledge representation, combining traditional data base structure and management concepts (e.g., relational data bases), with knowledge representation paradigms developed in the field of AI. While most of the "hard" and often numerical or at least fixed format data are organized in the form of relational data bases (using a relational data base system developed at IIASA, see Ward, 1984), the knowledge bases again use a hybrid representation approach.

Hybrid Knowledge Representation implies that within our information system, multiple representation paradigms are integrated. A knowledge base might therefore consist of term definitions represented as frames, object relationships represented in predicate calculus, and decision heuristics represented in production rules.

Predicate Calculus is appealing because of its general expressive power and well defined semantics. Formally, a predicate is a statement about an object:

((property_name) (object) (property_value))

A predicate is applied to a specific number of arguments, and has the value of either TRUE or FALSE when applied to specific objects as arguments. In addition to predicates and arguments, predicate calculus supplies *connectives* and *quantifiers*. Examples for connectives are AND, OR, IMPLIES. Quantifiers are FORALL and EXISTS, that add some inferential power to predicate calculus. However, constructs for more complex statements about objects can be very complicated and clumsy.

In *Object-Oriented Representation* or *frame-based knowledge representation*, the representational objects or *frames* allow descriptions of some complexity. Objects or classes of objects are represented by *frames*. Frames are defined as specializations of more general frames, individual objects are represented by *instantiations* of more general frames, and the resulting connections between frames form *taxonomies*. Each object can be a member of one or more classes. A class has attributes of its own, as well as attributes of its members. An object *inherits* the member attributes of the class(es) of which it is a member. The inheritance of attributes is a powerful tool in the partial description of objects, typical for the ill-defined and data-poor situations the system has to deal with.

A third major paradigm of knowledge representation are *production rules (IF - THEN decision rules)*: they are related to predicate calculus. They consist of rules, or *condition-action pairs*: "if this conditions occurs, then do this action". They can easily be understood, but have sufficient expressive power for domain-dependent inference and the description of behavior.

A common characteristic of all the elements in the information system is their user interface: access to data and knowledge bases is through an interactive, menu-driven interface, which allows easy retrieval of the stored information without the need to learn any of the formal and syntactically complex query language required internally.

In addition to this direct user access, the information bases also are accessed by the control programs and scenario generator (see Figure 1.1) when specific models are invoked. Here the query is formulated automatically and transparently for the user. Only if some information required to run a given model cannot be found or inferred is the user notified and asked to supply the necessary piece of information, or to reformulate the problem.

4.1 Development Tools and Documentation

To help organize the development of the software system, and to take full advantage of the methods used for their own documentation, several data bases are constructed as development tools and to organize elements of the systems documentation. A detailed description of these data bases is given in Fedra et al. (1985b).

They include a two-level description of models — a short listing of general characteristics for all models identified, and a much more detailed one for those models studied in detail and included in the system.

Parallel to the model descriptions, an annotated bibliography is maintained on topics covered in the software implementation. In particular, it lists all the sources of information used in the construction of knowledge and data bases.

Related to this listing of sources used are data bases on information services and other relevant data bases. These serve either as part of the documentation, in case they were used as sources for our own information system, or they serve as further references in case a query cannot be satisfied within the system.

As a special case, it is our intention to establish a direct and automatic link to selected outside data bases. A prime candidate is the ECDIN data base developed and maintained at the Joint Research Centre (JRC), Ispra Establishment.

4.1.1 Models and Annotated Bibliography

A detailed discussion of the models data base, its organization and contents is given in Fedra et al., (1985). About 200 models from a preliminary screening survey are included and shortly discussed in this report. The detailed evaluation of selected models, which are candidates for inclusion in the software system described here, is ongoing. Discussions of individual models and their test implementations will form a series of additional reports in support of this document.

As part of the system's documentation, model descriptions and bibliographic references pertaining to the models and the contents of data and knowledge bases are implemented as a relational data base *(db)* (Ward, 1984). A user-friendly interface allows expert and non-expert users to retrieve information on models or documentation conveniently.

The relational data base consists of several relations in two-dimensional (row and column) format. Two relations on models have been constructed. One contains a minimal description of about 200 models related to the field of hazardous substances management, the second a more detailed description of the models actually integrated into the system. An additional auxiliary relation containing descriptive keywords on model types and applications, linking these searchable identifiers to the model ID-numbers, is provided.

The basic data base management system, *db*, provides a functionally rich, but complex query language. To facilitate access, a menu-driven interactive interface (implemented in C) was developed. The menu provides two principal pathways for model selection: keyword or keyword combinations, and model acronym or number (from a list of available models displayed on request). The amount of information displayed depends on the number of models presented simultaneously, and ranges from a single line per model to a full page per model. The basic concept of menu-driven access to data bases is used for several other data bases (see below) as well.

4.1.2 *Information Services and Data Bases*

Similar to the bibliographic and model data base, a data base on information services and on-line data bases is also constructed. Selected references are given in Fedra et al., (1985). As in the case of models and literature, these data bases are implemented as relational data bases with a menu-driven interactive user interface.

This information on data bases and other sources of information can be used as a straightforward, interactive information system. However, we also foresee an automatic referral mechanism, where the user is presented a list of potential sources of further information whenever some open question cannot be resolved from the system's information basis or directly supplied by the user. As mentioned above, as a special case related to chemical substances descriptions, this referral could be entirely automatic and transparent for the user. The system would directly establish a link to an appropriate data base or information service, collect the required information, and integrate it into its own information bases.

4.2 General Cross-cutting Information Bases

In the core of the information system is a chemical substances information system (Fedra et al., 1985 b). Of related interest is information about applicable laws, regulations and institutional procedures (Fedra et al, 1985 a), which define constraints on the physical and technological system.

4.2.1 *Substances: Classification and Attributes*

Whenever any of the models in the simulation system are used, they are used for a given substance, substance group, or mixture of substances and substance groups. The classification of substances and substance groups, and the linkage between these groups and the physical, chemical, and toxicological properties of the substances are of critical importance.

With about 70,000 to 100,000 chemical substances on the world market, and about 1000 added to this list every year, any attempts at a complete or even comprehensive coverage are illusory within the framework of this project. Rather, we must provide information about a ***representative subset*** with an access mechanism that accounts for the ill-defined structure resulting from all the chemical nomenclature, trivial and trade names, and attribute-oriented cross-cutting groupings (e.g., oxidizing substances, water soluble toxics, etc.).

The starting point for any attempts at classification is thus not organic chemistry or environmental toxicology, but a reflection on likely ways to formulate a problem. Entry points for substance identification are therefore *type of use* (e.g., agricultural chemical: pesticide) or industrial origin, i.e., production process or type of industry, implying an industrial waste stream (e.g., metal plating, pesticide formulation; a listing of 154 industrial waste streams that contain hazardous components is included in the EPA's WET model approach, ICF (1984)) rather than chemical taxonomy. A detailed description of the chemical substances data base, its design philosophy, structure, information content, software implementation, and interfacing are given in Fedra et al., (1985b).

Our approach thus foresees the use of a basic list of about 500 *substances* (or "atomic" substances, i.e., entities that do not have any sub-elements), constructed as a superset of the EC and USEPA lists of hazardous substances.

In parallel we construct a set of *substance groups* (or "lists"), which must have at least one element in them. Every *substance* has a list of properties or attributes; it also has at least one *parent substance group* in which it is a member. Every member of a group inherits all the properties of this group. In a similar structure, all the groups are members of various other parent groups (but only the immediate upper level is specified at each level), where finally all subgroups belong to the top group *hazardous substances*.

Formally, this could be represented as:

substance_group ((attribute_list),(parent_group_list),(member_list))

substance ((attribute_list),(parent_group_list), NIL)

Clearly, the nature of the attribute_list will change with a changing level of aggregation. While attributes of individual substances are by and large numbers (e.g., a flash point or an LD_{50}), the corresponding attribute at a group level will be a range (flash point: 18-30°C) or a symbolic, linguistic label (toxicity: very high).

The structure outlined above also takes care of unknowns at various levels within this classification scheme. Whenever a certain property is not known at any level, the value from the immediate parent_group (or the composition of more than one value from more than one immediate parent_group) will be substituted. The structure is also extremely flexible in describing any degree of partial overlap and missing levels in a hierarchical scheme.

In addition to taxonomic relationships and the physico-chemical and toxicological attributes of substances, the substance data base also includes references to

TABLE 3: Sample Page from the Spills/Accidents Data Base.

SUBSTANCE SELECTED:	2,4,5-T and Dioxin
Place:	Seveso, Italy
Date:	July 10, 1976
Substances:	2,4,5-trichlorphenol 2,3,7,8-tetrachlorodibenzo-*p*-dioxin, reaction by-product
Quantity Released:	240-500g (Hay 1982).
No. of Casualties:	None directly related to the accident
Estimated Damage:	67.7 billion lira paid in compensation to individuals, the Lombardy Region and the Italian government 19.7 billion lira (Hay,1982), (Roche Nachrichten 1980/82).
Area Affected:	4 million m^2 (Hay, 1982); between 150,00-500,000 m^3 contaminated topsoil (Peirce & Versilind, 1981, Hay, 1982, Saxena, 1983).

DESCRIPTION:

An explosion at the chemical factory owned by **ICMESA**, a subsidiary of Hoffmann-La Roche, released a cloud of vapor over the town of Seveso. The plant had closed for the weekend 6.5 hours earlier. At the end of the last shift the reactor operators had decided not to cool the contents of the reactor by using the thousands of litres of water required to bring down the temperature of the mix. They left it to cool over the weekend. The cloud which passed over the residential area was at first thought to contain primarily chlorinated phenol and it was only *5 days later* it was even suspected that appreciable quantities of dioxin might have been vented in the reactor discharge. Unfortuntately, there was very *little information available on dioxin* as the only literature available discussed its toxicity in animals, not humans. Local authorities were slow to react or act and the situation was further aggravated by the *insufficient communication* between the various authorities.

Dioxin is known to cause malformations in animals and it was assumed that it might also be a teratogen in humans. Women in the first trimester of pregnancy were advised to stay out of the contaminated zones and the *population* in Zone A, closest to the reactor, was *evacuated*.

During the *manufacture of 2,4,5-trichlorophenol*, dioxin formation is inevitable. The temperature at which the process is carried out depends on the solvent used in the mixture. ICMESA used *ethylene glycol* and carried out the process at 170–180°C. Any rise in temperature in the reactor results in more dioxin being produced. But the *critical temperature* is 230°C. Above this, conditions in the reactor are such that the reaction becomes *exothermic* and generates its own heat. The temperature of the whole mixture then rises rapidly. In a closed reactor, the rising temperature leads to a pressure increase, eventual rupture of the reactor, or the blowing of a pressure safety disk, as happened at Seveso. However, the ingredients in the reactor were present in the correct proportions and by themselves could not have caused the temperature of the reactor to rise.

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case histories of spills and accidents (Table 3). These narrative but structured descriptions of representative spills and accidents should serve as an alternative to the somewhat abstract derived probabilities of accidents and accident classes (e.g., Berg and Maillie, 1981), allowing a user to develop some feeling for the disaster potential of certain substances more intuitively and on the basis of directly understandable descriptive formats.

4.2.2 Institutions and Regulations

Information on Legal Provisions (e.g., the IRPTC Legal File, UNEP 1984), Regulations and Institutional Procedures are on the one hand part of the information system for purely passive use (although with multiple-path, keyword-controlled access), but on the other hand they provide constraints on the generation of alternative actions within a scenario. They are either used to check the feasibility of a user-specified option - in which case they would generate an appropriate message, but allow the user an override option - or alternatively would automatically constrain the selection of options in any internal screening or optimization mode.

The second mode of use requires an interpretation of the text of a regulation by the machine, which is only feasible if this text is reformulated in an appropriate formal language, i.e., using rule-based knowledge representation.

4.3 **Process-specific Information Base**

The parameters required for the individual simulation models used are again stored in a system of process-specific data and knowledge bases. They include physical constants, process rates or coefficients, as well as rules used to estimate such values if only an approximate description of the context, process, or substance to represent is given.

4.3.1 Industrial Production and Processes

For the industrial production sector, individual production technologies have to be described in terms of the raw material requirements, waste and interim products, and routine as well as accident release rates, probabilities and magnitudes respectively per unit output (e.g., Herrick et al., 1979; Goldfarb et al., 1983).

Part of the relevant information, organized by industrial sources, can be found in the WET model's waste stream data base (ICF 1984b), which specifies constituent composition for 154 industrial waste streams. While these data can serve as a starting point for the design of the appropriate data bases, it is important to recognize the inherent uncertainty of such data. For the prototype implementation, however, the emphasis is on the *structure* of the data base rather than on its contents. The only important constraint is that the data required must be available in principle and obtainable at reasonable cost.

4.3.2 Waste Management: Treatment and Disposal

What was said above about industrial production processes also holds for treatment and disposal technologies. Again, the implementation for the prototype demonstration system emphasizes the structure and interfacing of the information. Obviously, wherever classes of processes or technologies are considered, or where specific parameters for a specific plant are unknown, the same scheme of class-inherited attributes as was described for the substances data and knowledge bases will be applied. By mixing relational data base technology at the lowest level of resolution with a frame-based knowledge representation for a corresponding taxonomy of higher classes of aggregation, we can obtain a large degree of flexibility in knowledge representation while maintaining the necessary efficiency required for a potentially very large implementation.

4.3.3 Transportation Systems

Transportation can be viewed as just another treatment technology, so that the process specific information (e.g., capacities, speeds, fuel consumption of alternative vehicles) can be managed in the same style as elements of a cost function. Emissions are due to normal operation, in particular loading, packing and unpacking, and accidents. Probabilities of accidents are just an additional attribute (e.g.,Lobet, 1981).

Cost coefficients as well as emission and/or accident probabilities are stored in the usual relational format; more complex and derived relationships can be represented as a rule-based production system to generate the required numerical or possibly symbolic information (see, for example, Turksen, 1985).

4.4 Regional/Geographic Information

For any concrete implementation, implementation-specific or geographical data are required. They describe the world the models operate on in terms of its spatial characteristics and exogenous conditions like a region's infrastructure, land use, geomorphological features, population, or climate.

This information can conveniently be grouped into time-invariant data (e.g., for the time span of meaningful model applications, the geomorphology), and dynamic data (e.g., climatic variables). Time-invariant data are simply kept in appropriate data files, organized in a world coordinate system that allows for several layers of aggregation and zooming effects. Some of these data, e.g., on infrastructural features like roads or bridges, may have to be updated from time to time, and may be modified during a scenario definition, but they are conceptually static.

Dynamic variables clearly pose a different problem. The use of models is certainly more interesting in a prognostic rather than historical and descriptive mode. Time series of observation data however, are at best available for the past. Consequently, dynamic inputs required for simulation purposes will have to be generated as synthetic time series in any case. Historical data bases can therefore be kept at a minimum, just sufficient to serve as a basis for the generation of plausible, synthetic time series (e.g., Salas et al., 1980). There are a number of well-tested and time-proven methods to analyze historic time-series data and to synthesize time series from this analysis. Several software packages implementing these methods are discussed in Fedra et al. (1985 a).

4.4.1 Maps and Geographical/Geomorphological Data Bases

For the spatial representation of any region of concern (which should ultimately range from selected regions, to countries, to all of Europe), its basic geomorphological features, together with a pictorial representation (i.e., topographic or topical maps) must be available. For the basic world coordinate system, a resolution of 10 km^2 would be manageable on a Europe-wide scale.

For most implementations of the decision-support software, and for the demonstration prototype in particular, we expect a regional to national scale for the specific implementation data bases. Spatial resolution will accordingly have to vary hierarchically. The overall and basic ***regional background information*** will be stored on a fixed, but coarse, grid (e.g., 10m by 10 km^2). Individual subregions must be treated at a higher level of spatial resolution (i.e., anything from 100 m to the 10 km of the overall grid). Examples include possible sources of emission, e.g., industrial production facilities, or target areas of special interest, e.g., groundwater aquifers or metropolitan areas. Since aquatic systems, i.e., surface waterbodies and productive aquifers, are of particular importance as receiving environmental systems (see section 3.4), additional description of waterbodies may be included in the biotopes description files (see below).

The geographical data bases are used exclusively in a passive way, i.e., they are only queried, not updated. Any modifications during a given use of the system to represent either man-made changes (e.g., introduction of a new reservoir) or a hypothetical region for experimental simulation, are made on temporary copies of the underlying data bases only. These fixed-format data will be stored in simple random access files where a simple algorithm relates any required pair of coordinates to the respective records.

4.4.2 *Population, Land Use, Biotopes*

As a subset of the criteria described in the regional geographical data base, population centers, i.e., cities and metropolitan areas, are stored together with their population numbers and the grid elements they cover. For the overall grid, only a rough classification in population density classes will be sufficient. Similarly, land use and type of biotope are attributes for each grid element. They are used to estimate the exposure of human populations, as well as an environmental damage function depending on the "value" of the land. Land use and biotope classification will also allow for special biotopes or natural preserves.

As mentioned above, several subregions or subtopics will be treated at a higher resolution than the overall geographic background data. Individual subregions are connected with the overall grid through the same coordinate system, where the various levels of resolution always differ by powers of two. This results in a nested grid system, illustrated in Figure 4.1. Effective representation of this grid is fully supported by the proposed workstation's hardware, i.e., zooming capabilities.

4.4.3 *Infrastructure*

Infrastructure subsumes man made structures such as roads, bridges, harbors, canals, and railways. They are used for the generation of transportation alternatives, but may also be used in risk/damage assessment. Their spatial attributes are coded in the same coordinate system as the geographical information. Due to their higher variability in space, individual reaches of e.g., a river or a railway system, may be anywhere within a given grid cell of the basic geographical background data.

Using the multiple graphical planes of the workstation implementation (see section 2.4), various overlays and topical maps can thus be produced to represent

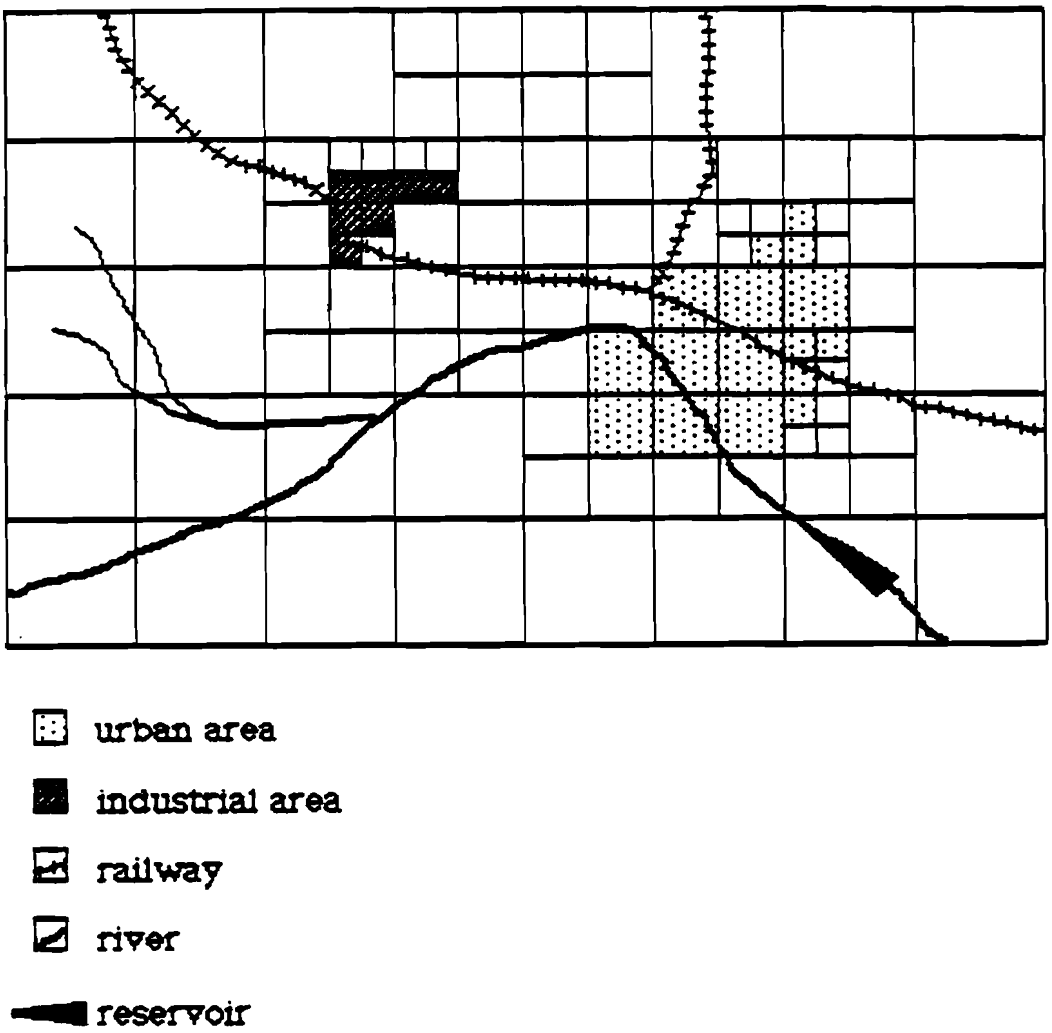

Figure 4.1: Nested Grids for Geographically Organized Data.

geographically organized data.

As a special subsection, production and treatment facilities are also organized here. Their *site-specific* attributes include e.g., size and capacity, age, and the set of applicable production, treatment or disposal technologies supported. The general and generic properties of these plants are stored in the respective technology-describing data bases which describe the technology (see section 4.3).

4.4.4 Climate and Hydrography

As mentioned above, this set of data and knowledge bases will include only selected historical data bases. Its main component is a set of synthetic time series generators used in scenario generation.

The time series required will include flow regimes for surface water bodies, precipitation, recharge/depletion time series for groundwater bodies, dynamic wind fields or sets of trajectories together with additional weather specifications (temperature, radiation, cloud cover, stability conditions of the atmosphere) etc.

Similar to the strategies for the user interface described above, these specifications will be part of the information context of a scenario. Wherever possible, they will be generated automatically. If the user has to specify certain values, he must be able to do this in common language terms, i.e., the user may specify "a sunny summer morning with low to moderate winds", from which the system will generate the required numerical weather parameters, never bothering the user with the specification of a vertical turbulence profile of the atmosphere, wet bulb temperature or the dew point.

The specific numerical values for these parameters are inferred by the system on the basis of its information in the meteorological data base and a set of rules used for data synthesis. If required, the user can certainly display any of these values as well as the basic rules used to generate them. The *backtracking* mechanism in the inference programs used provide a convenient mechanism for that.

5. APPLICATION AREAS AND MODES OF USE

The system described above can be used in many ways. These modes of operation, however, serve only as design principles. They are transparent for the user, who always interacts in the same manner through the user interface with the system. The system must, however, on request "explain" where a result comes from and how its was derived (e.g., from the data base, inferred by a rule-based production system, or as the result of a model application).

The simplest and most straightforward use of the system is as an *interactive information system*. Here the user "browses" through the data and knowledge bases or asks very specific questions. As an example, consider the substances data base, where the basic properties of a substance can be found (compare section 4.2.1). But, in addition, the system will indicate applicable regulations –

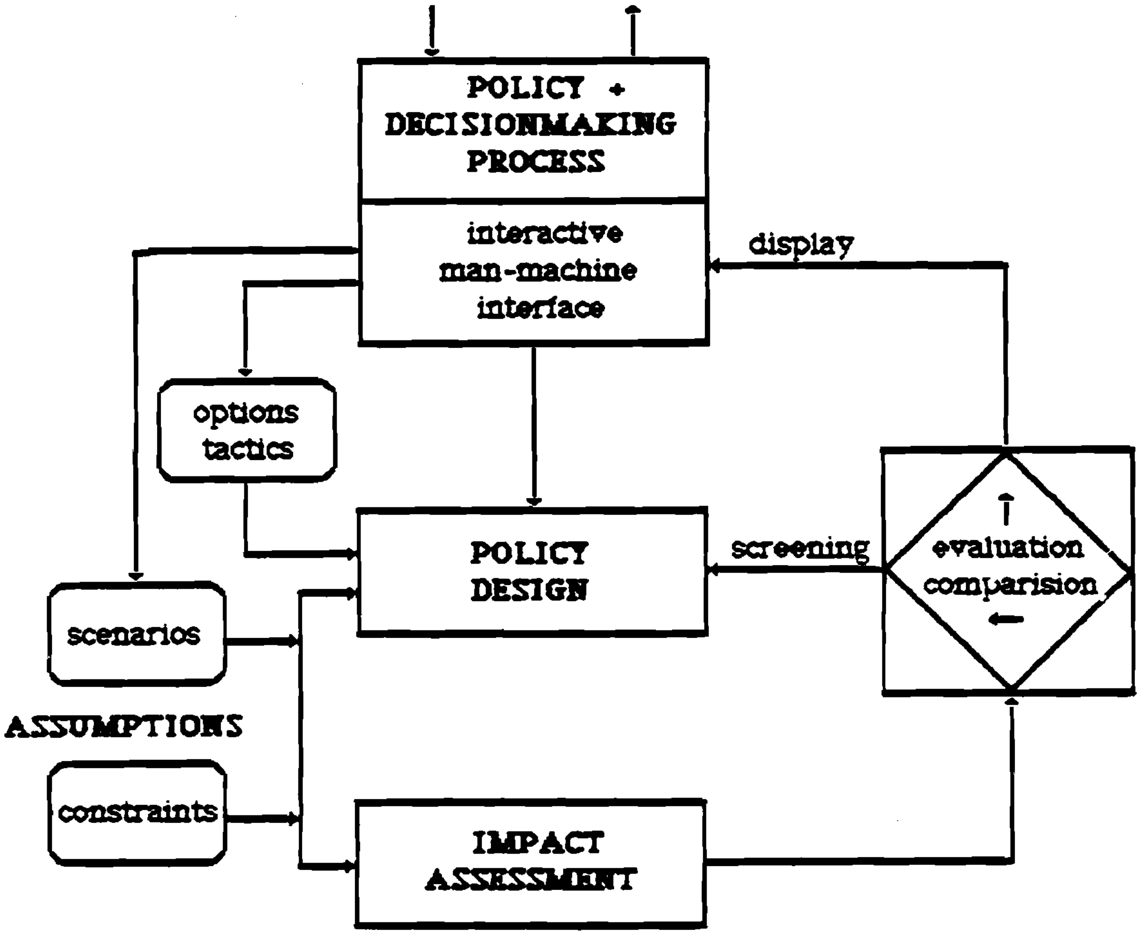

Figure 5.1: A Framework for Scenario Analysis.

which the user then can choose to read, or a history of spills and accidents the substance was involved in. The latter may serve to develop a "feeling" for the order of magnitude of possible consequences of an accident.

The second mode of use is termed *scenario analysis*. Here the user defines a special situation or scenario (e.g., the release of a certain substance from an industrial plant), and then traces the consequences of this situation through modeling (Figure 5.1). The system will assist the user in the formulation of these "What if ..." questions, largely by offering menus of options, and ensuring a complete and consistent specification.

The scenario analysis mode can use any or all models in isolation or linked together; the selection and coupling of models is transparent. The use of certain models in implied by the selection of indicators and criteria that are chosen to describe a scenario's outcome.

Two time domains for scenario analysis with different problems addressed are supported: the models can either be used to simulate medium- to long-term phenomena, with a characteristic time scale of years, or short-term events, i.e., accidents, with a characteristic time scale of days. Switching from one mode to the other, with the necessary aggregation or disaggregation of information, must be possible.

Simiiar to this switching in the time domain, a change in the space domain must also be supported. There is of course a close linkage between time and space scales, in that most short-term phenomena like spills or accidents are relevant on a local to regional scale, whereas long-term phenomena like continuous routine release of hazardous substances will usually be considered on a regional to national scale.

There are many specific problem areas that can be addressed with the system described above. A partial and by no means exhaustive list might include:

- estimation of waste streams originating from specific industrial production processes (e.g., chlorination of phenols);
- identification of process modification requirements (e.g., recycling, waste reduction, volume reduction) subject to waste output constraints (regulations);
- exploration of siting alternatives for production plants given socio-economic as well as environmental objectives and regulatory constraints;
- estimation of worst-case accident potential for given production processes or production facilities in a specific regional environment;
- simulation and evaluation of emergency plans for various types of accidents under a wide variety of meteorological conditions;
- risk/cost analysis for the transportation of hazardous materials, considering transportation mode and route alternatives, public exposure, environmental damage potential, applicable regulations, etc.;
- identification of least cost/risk treatment and disposal alternatives for given waste streams (amount, composition, transportation requirements);

- estimation of environmental and public health consequences of various emission scenarios (routine emissions to atmosphere or water, emission from waste treatment and disposal, e.g., leaching from dumpsites); such emission scenarios might be directly user-generated or result from any of the above applications;
- long-term simulation of integrated subsystems (e.g., industrial production, treatment and disposal, environment) to identify potential problem areas e.g., disposal capacity constraints, or toxics accumulations above thresholds in environmental media;
- estimation of damage potential (ambient concentrations, accumulation in the food chain, human exposure), for certain substances in specific environmental systems.

Many of these applications would require the linking of several of the component models of the system (compare Figure 3.1). The evaluation and comparison of alternatives is always performed in terms of a subset or all of the criteria listed in Table 1, including monetary as well as symbolic, qualitative descriptors.

As implied in the above listing of possible application areas, scenario analysis may be either straightforward simulation, or a combination of simulation and optimization techniques. In the latter case, the user does not have to specify concrete values for all control variables defining a scenario, but rather specifies allowable ranges on them as well as a goal structure. Using techniques like reference points in multi-objective problems, a framework such as DIDASS (Dynamic Interactive Decision Analysis and Support System, e.g., Grauer and Lewandowski, 1982) permits one to interactively modify expectations, redefine objectives and constraints, and directly incorporate the human evaluator in the optimization process.

The optimization framework usually requires certain simplifications of the substantive production models. Reformulating a preferred alternative in terms of a more detailed dynamic simulation model with finer resolution in time and space allows not only a testing of the optimization robustness and credibility, but enables a sensitivity analysis to be performed on the model.

A concrete example of the reference-point approach (Wierzbicki, 1983) applied to a policy-oriented decision support system with parallel models of different resolution is described by Kaden et al. (1985). A planning model for

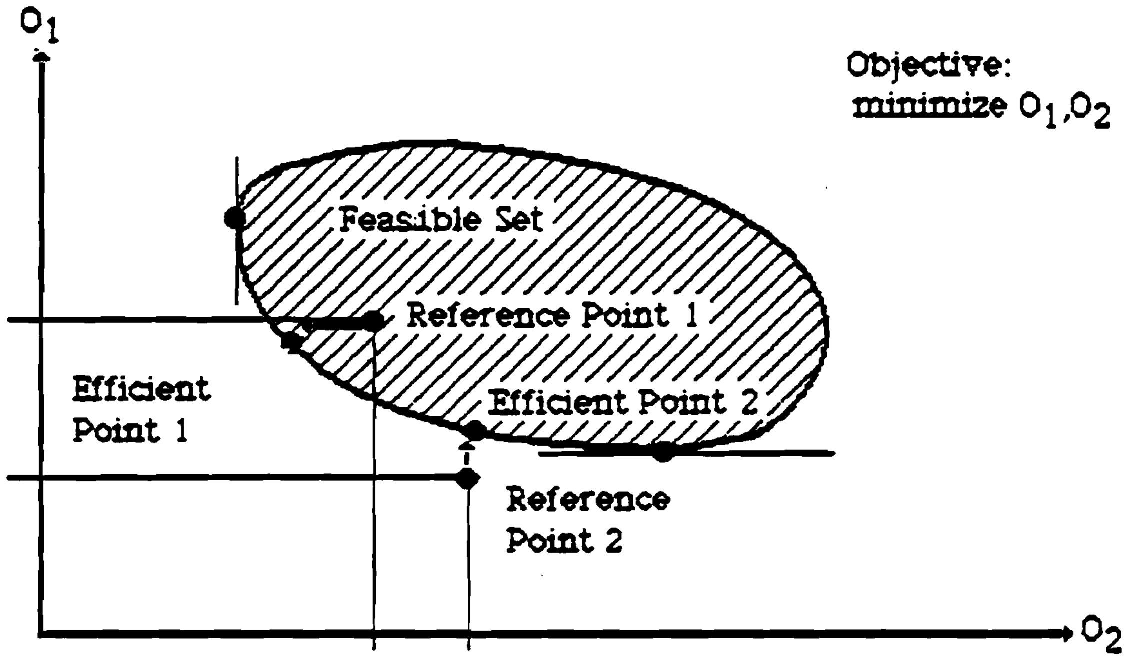

Figure 5.2: Illustration of the Reference Point Approach.
(after Kaden et al., 1985).

dynamic multi-criteria analysis can be used alternatively with a high resolution management (stochastic simulation) model. The multi-criteria nonlinear programming system is based on the idea of *satisficing* (rather than *optimizing*). Starting from the *aspiration levels* of the user, describing his preferred set of values for the indicators describing a certain scenario (reference-point or reference scenarios), efficient systems responses are generated (Pareto points "closest" to the reference points (Figure 5.2). The best-suited solution (considering the preference of the user) can be corrected by modifying the aspiration levels in an interactive procedure.

The program system is based on the nonlinear multi-criteria programming package DIDASS/N (Grauer and Kaden, 1984), coupled with the non-linear problem solver MSPN, developed at the Institute of Automated Control, Technical University Warsaw.

In the case of numerous criteria (compare Table 1, section 2.1), the reference-point procedure and the comparison of alternatives becomes rather complicated. Therefore, the interactive determination of criteria should be minimized to a smaller subset of most important ones, where the rest is considered in terms of their allowable bounds, i.e., as constraints.

All these refinements of the basic information and simulation system however must not complicate the users' interactions with the system. Ease of use, and the possibility to obtain immediate, albeit crude and tentative, answers to problems which the machine helps to formulate in a directly understandable, attractive and pictorial format are seen as the most important features of the system.

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