Working Paper

Model-based Decision Support for Industry–Environment Interactions

A Pesticide Industry Example

K. Fedra
M. Karhu
T. Rys
M. Skocz
M. Zebrowski
W. Ziembla

November 1987
WP-87-97

International Institute for Applied Systems Analysis
A-2361 Laxenburg, Austria

Model-based Decision Support for Industry–Environment Interactions

A Pesticide Industry Example

K. Fedra
M. Karhu
T. Rys
M. Skocz
M. Zebrowski
W. Ziembla

November 1987
WP-87-97

INTERNATIONAL INSTITUTE FOR APPLIED SYSTEMS ANALYSIS
A-2361 Laxenburg, Austria

PREFACE

Applied systems analysis is – or should be – a tool in the hands of planners and decision makers who have to deal with the complex and growing problems of modern society. There is, however, an obvious gap between the ever-increasing complexity and volume of scientific and technological information and tools of analysis relevant to large socio-technical and environmental systems, and the information requirements at a strategic planning and policy level.

The Advanced Computer Applications (ACA) project builds on IIASA's traditional strength in the methodological foundations of operations research and applied systems analysis, and its rich experience in numerous application areas including the environment, technology, and risk. The ACA group draws on this infrastructure and combines it with elements of AI and advanced information and computer technology. Several completely externally-funded research and development projects in the field of model-based decision support and applied Artificial Intelligence (AI) are currently under way.

As an example of this approach to information and decision support systems, one of the components of an R & D project sponsored by the CEC's EURATOM Joint Research Centre (JRC) at Ispra, Italy, in the area of hazardous substances and industrial risk management, is described in this paper. The **PDA** (Production Distribution Area) is an interactive optimization code (based on DIDASS, one of a family of multi-criteria decision support tools developed at IIASA) and a linear problem solver, for chemical industry structures, configured for the pesticide industry of a hypothetical region.

The user can select optimization criteria, define allowable ranges or constraints on these criteria, define reference points for the multi-criteria trade-off, and display various levels of model output, including the waste streams generated by the different industrial structure alternatives. These waste streams can then be used to provide input conditions for the environmental impact models.

With the emphasis on a directly understandable problem representation and dynamic color graphics, and the user interface as a key element of interactive decision support systems, this is a step toward increased direct practical usability of IIASA's research results.

Robert H. Pry
Director

ACKNOWLEDGEMENTS

The research described in this report is being carried out by IIASA's Advanced Computer Applications (ACA) project in cooperation with the Institute for Control and Systems Engineering, Academy of Mining and Metallurgy (ICSE-AMM), Cracow, Poland. This cooperation is based on an agreement between IIASA and the Committee for Coordination of Cooperation with IIASA of the Polish Academy of Sciences (National Member Organization).

First components of the system described have been integrated in software developed under contract to the Commission of the European Communities' (CEC) Joint Research Centre (JRC), Ispra Establishment, under Study Contracts No.2524-84-11 ED ISP A and 2748-85-07 ED ISP A.

The opinions expressed in the report are those of the authors and do not necessarily reflect those of IIASA or of IIASA's National Member Organizations. Neither the collaborating institutes, the Commission of the European Communities, the Joint Research Centre, Ispra Establishment, nor any person acting on behalf of the above is responsible for the use which might be made of the information in this report.

THE AUTHORS

Kurt Fedra, Austria, is the leader of IIASA's Advanced Computer Applications (ACA) project.

Marrku Karhu, Finland, from the Technical Research Center of Finland (VTT), was a participant in the 1986 Young Summer Scientists Program (YSSP) at IIASA.

Maciej Zebrowski, Poland, is Deputy Director of the Institute for Control and Systems Engineering, Academy of Mining and Metallurgy (ICSE-AMM), Cracow.

T.Rys, M.Skocz, and W.Ziembla are staff scientists at ICSE-AMM, Cracow.

CONTENTS

Model-based Decision Support for Industry–Environment Interactions

A Pesticide Industry Example

K. Fedra, M. Karhu, T. Rys,
M. Skocz, M. Zebrowski, W. Ziembla

1. The Problem Context

Whether they appear as raw materials, as finished products, as by-products, or as wastes, hazardous substances pose risks to man and the environment which must be responsibly managed.

The annual waste generated in the countries of the EC amounts to about 2 gigatons. Somewhat less than 10% of this colossal amount is of industrial origin. Roughly 10% of these industrial wastes have to be classified as hazardous (J. Schneider, JRC/Ispra, 1984, personal communication). More graphically, this hazardous waste production amounts to approximately 20 million metric tons, that could fill a train of roughly 10,000 km in length.

The effective management of these wastes requires:

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

In addition to hazardous wastes, there is a large number of commercial products that must be considered hazardous. This is particularly true for the case of the pesticide industry discussed here.

The regulatory framework for hazardous substances within the European Community is largely defined by a number of Directives of the Council of the European Communities and the corresponding national legislation which these Directives require (see, e.g., Haigh, 1984; Majone, 1985; Baram, 1985). For example, the so-called Seveso Directive (Council Directive on the major accident hazards of certain industrial activities, 82/501/EEC) specifies that manufacturers must provide the competent authorities with information on the details of substances and processes involved in high-risk facilities. Further, people outside the establishment who might be affected by a major accident must be informed of the safety measures to be taken in the event of an emergency.

The Council Directive on toxic and dangerous wastes (78/319/EEC) calls for a comprehensive system of monitoring and supervision of facilities and operations involving hazardous wastes, specifically mentioning risks to water, air, soil, plants and animals, while also including nuisance due to noise and odors and possible degradation of the countryside and places of special interest. More recently, the Directive on the assessment of the effects of certain public and private projects on the environment (85/337/EEC, June 1985) requires comprehensive environmental assessments of projects and installations involving hazardous materials. These assessments are to include consideration of the production and storage of materials such as pesticides, pharmaceuticals, paints, etc. A broad analysis of the direct and indirect effects on people, environment, property and cultural heritage is also foreseen and the evaluation of alternatives is required. A more detailed discussion of the regulatory and institutional framework and the role computers might play in it as part of the decision-making process, is found in Fedra and Otway (1986) and Otway and Peltu (1985).

Obviously, regulation of hazardous substances and industrial risks is most effective at the source, i.e., at the industrial production process level. Options for the regulator range from the outright ban of specific products to imposing constraints (direct regulatory or possibly indirect monetary through taxes and fees) on production facilities and waste treatment and disposal options.

The model-based decision support system described here is designed to address problems that arise in the course of, for example, the analysis of regulatory options. The central component is an optimization model that describes the behavior of a chemical industry, given certain assumptions about prices for products raw materials, and labor, upper and lower limits for certain production lines or waste products, under the basic assumption that the industry will operate to maximize its net economic results while meeting the external constraints. The results of changes in these external conditions (reflecting the market as well as a set of regulatory options) will be a redistribution of production capacities, resulting in a different product mix with different effects on the environment.

In other words, the model will show what a rational industry might do given a certain set of regulations under specific market conditions. It may be worthwhile noting that the market itself is not included in the model; prices are fixed and set externally, i.e., by the user, and an adjustment of production volumes does not (within the model) affect prices.

The representation of economics in the model is certainly very simplistic, in part constrained by the linear model used. The major advantage of the model, however, is its fast and reliable bookkeeping of albeit simplified material flows and basic cost components, that allow a fast and interactive screening of regulatory options. Auxiliary databases, a conversational control over display options, coupled environmental impact analysis that translate waste streams generated directly into environmental quality indicators such as water quality, and finally a post-processor for the comparative evaluation of several optimization experiments integrate into a very powerful, but easy-to-use software tool.

1.1 The Project Background

An early prototype of the model system described here was integrated as part of an integrated software system for the management of hazardous substances (Fedra, 1985; 1986; Fedra and Otway 1986) *) for the analysis of the chemical industry, the simulation of its behavior and optimization of its structure.

The central optimization model is implemented on the basis of the PDA model (Dobrowolski et al., 1982, 1984; Zebrowski et al., 1985) and the relevant MIDA methodology (Dobrowolski et al., 1985). For the pesticide industry example, the modified version of the model and corresponding software implementation was developed.**)

The aim of the overall 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. This set of tools

*)This software system was developed by IIASA's Advanced Computer Applications (ACA) Project, under contract to the CEC's Joint Research Centre (JRC), Ispra, Italy.

**)This model and software was developed by the Joint Systems Research Department (JSRD) of the Academy of Mining and Metallurgy, Cracow, Poland, under contract to IIASA and in collaboration with the Advanced Computer Applications (ACA) Project.

is designed for a broad group of users, including non-technical users. Its primary purpose is to improve the factual basis for decision making, and to structure the decision-making process in order to make it more consistent, by providing easy access and allowing efficient use of methods of analysis and information management which are normally restricted to a small group of technical experts.

In order to design and develop an ***integrated set of software tools***, we build on existing models and computer-assisted procedures. 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 has to incorporate elements of knowledge-based or expert systems that are 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 databases, 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 design and analysis of alternative policies for the management of industrial risk.

An important element in the overall concept is the direct coupling of large databases of scientific and technical information with human expertise, of formal algorithmic methods and models with heuristics and human judgement. The expert-systems approach not only allows direct and interactive use of the computer, it is designed as a tightly coupled man-machine system where the vastly different data handling, analysis and judgement capabilities of man and computer are integrated into one coherent framework. For a fuller treatment of structure and design, and the implementation of a demonstration prototype, see Fedra (1985, 1986), Fedra et al. (1987).

1.2 A Summary Description of the Optimization Model

For purposes of this model we regard the chemical industry as being divided into a number of subsectors, each for a group of closely related chemicals. These subsectors are called Production/Distribution Areas (PDAs) because they basically comprise a network of production processes and production flows for a very specific group of chemicals. In fact, PDAs often correspond roughly to the areas of production covered by individual, large chemical companies; it makes sense for each company to deal with a particular, closely related group of chemicals because they can then coordinate the flow of intermediates, feedstocks, etc. through a set of linked processes with the minimum of dependence on external suppliers. These PDAs wish to maximize their profits by developing the most efficient production structure for a given economic, social and/or political environment; since this environment is constantly changing, the production structure must evolve to keep pace with it. One very important application of the PDA model could therefore be to help in determining the best production structure for an individual company under various operating conditions. In addition, by adjusting the boundaries of the PDA it is possible to determine how individual companies could broaden their range of activities most effectively.

To do this, a large set of technologies is considered, mapping the input resource vector onto the production goal vector (demand vector) in a given environment. The production goal may be either based on observed data or modeled according to some scenario. Using this goal and assuming that it excludes wasteful consumption, it is possible to determine the production structure for commodities that best meets this demand. Then, working backwards, and using information on the chemical precursors of each commodity, it is possible to determine the chemical production structure that underlines the production of this combination of commodities.

Therefore the general PDA model takes into account:

- the processing of flows of chemicals within the PDA,
- the flow of chemicals into and out of other areas or industries, representing the marketing or business activity of the PDA,
- the flow of investment, revenue and other resources such as energy, manpower etc.

More specifically, the model describes a set of possible modes of production, including alternative ranges of products made at a given installation, recycling of semiproducts and coupled production of a number of chemicals at one plant. Since the model is aimed at formulating decision problems concerned with the generation of efficient development alternatives for a PDA, it comprises additional constraints on resource availability as well as a set of objective functions reflecting the preferences or goals of the decision maker. The latter option generally leads to the formulation of a multiobjective optimization problem; the relative importance of various trade-offs arising in the problem can only be assessed by the decision maker. This is why it is important to use an interactive decision support system in conjunction with this model.

Despite the generality of the tool, real applications may be quite different for the various industrial sectors and case-specific assumptions. Decision problem formulations, scenarios, and subsequent numerical experiments, are different in many cases, so that the PDA model has to be tailor-made for each application.

The implementation of the extended and refined version developed for this case study of the pesticide industry is discussed below. The current issue of the model is described in detail in section 3 of the paper.

The PDA optimization module is a core of the interactive decision support system. Its aim is the selection of development alternatives in the pesticide industry with special emphasis on environmental impacts. The module comprises the data on the pesticide production technologies configured according to the structure of the optimization problem based on the PDA model. The model is solved by means of a linear programming package POSTAN, developed by JSRD, which is an extension of MINOS (Stanford, 1981). As far as multiobjective optimization experiments are concerned, the OPTIMIST package which is JSRD's enhanced version of the IIASA package MM (Kreglewski & Lewandowski, 1983) is used.

The above software has been integrated into the overall system with advanced, user-friendly graphic display, connections to various interactively accessible background databases, an environmental impact analysis (river water quality) simulation model, and a post-processor for discrete multi-criteria optimization.

For the demonstration prototype of the system, a pesticide PDA was selected. The PDA was assembled from the set of processes used by several factories. The corresponding technological network includes some synthesis and formulation processes that are carried out on the basis of active substances from domestic and external (i.e., outside the PDA) production. The pesticide PDA comprises the following installations of chemical syntheses:

- methoxychlor,
- akaritox (tetradifon),
- chlorfenvinphos,
- chlorofos (trichlorofon; dipterex),
- malathion,
- sodium trichloreacetate, and
- copper oxychloride,

out of which only the last two are pesticides which can be used directly as final products. The products of other syntheses provide interim products for the formulation process. The PDA includes the following formulation plants:

- jet mill,
- Venuleth's mixer,
- active substances spread installation,
- formulation of liquid pesticides,
- condux system.

1.3 The Pesticide Industry Case Study

For the specific implementation of this interactive decision support tool for industrial structure optimization, a case study of a pesticide industry was chosen since many of the raw materials, products, and wastes involved are hazardous substances and thus provide connections to the overall framework system with its set of risk management and impact assessment models.

The enormous increase in the use of pesticides during the past thirty years has fueled a major controversy. Proponents argue that their use is necessary to provide an adequate food supply and to protect human health. Opponents dispute this contention and claim severe damage is being done to our environment, with adverse effects on fish, wildlife, and, most worrisome, human health.

Worldwide consumption of pesticides was 4,571,000 metric tons in 1980. The annual growth rate from 1980 to 1995 is forecasted to vary between 2.3%-4.5%. This means that world production will be around 6,500,000 metric tons in 1995.

During the 1970's consumption of pesticides worldwide increased significantly, particularly in the developing regions where there was an approximately 190% increase from 1970 to 1975, implying an annual growth of 30% (Ahmed, 1985). This particular growth in the use of pesticides in the developing countries leveled to about $ 1000 M/a sales by the late 1970's in constant dollar terms. Figures for 1983 showed that there has been little change in actual sales since the late seventies. One major change occurred – the USA has become the major exporter of pesticides worldwide. Until about two or three years ago it was the second largest exporter of pesticides. The most recent figures indicate that the USA accounts for about 29.5% of the global export market, followed by West Germany (19.5%) and the UK (12.5%). The developing countries account for about 6% of the US export market and up to $ 3.8 billion worth of pesticides are exported. The developing countries import 40% for its needs.

Frost & Sullivan, Inc., in 1984 forecast 1.5% real annual growth in Western Europe's consumption of pesticides between 1982 and 1989 (Tables 1 & 2). Current sales are expected to total $ 3.8 billion in Western Europe, rising to $ 4.1 billion in 1989 (all figures are stated in constant 1982 dollars).

"Biological control methods and Integrated Pest Management (IPM) will expand their uses with the help of persuasion and trained personnel", says the report, but the increasing world need for food resources is seen insuring continued growth in use of chemical methods, though technological, regulation and environmental considerations will probably slow the rate of products innovation. One area of possible breakthroughs cited is development of highly specific agents through biotechnological techniques: piperidine derivatives have already been suggested in this connection.

Table 1. Pesticides production and consumption statistics in some European countries

Production (in thousand tons)

	1980	1981	1982	1983	1984	1989	1995	Annual Growth	Source
BUL	40	49	40	34	36				1)
CSSR	16	16	16	16					1)
GDR	51	53	53	54					1)
HUN	28	29	26	36	36		115		1)
POL	9	12	16	15	11				1)
ROM	40	43	45	48	53				1)
USSR	474	504	533	557	576		1130	2.5%	1)&2)
E.Eur	723	755	785	818	852		1344	4.2%	2)
EC	76						113	2.7%	2)
WORLD	4571	4758	4954	5157	5368		6445	4.1%	3)

Consumption (in M constant 1982 US $)

FRA			1020			490		1.0%	4)
GFR			450			490		1.1%	4)
ITA			440			490		1.4%	4)
NET			90			90		0.0%	4)
SPA			210			270		3.6%	4)
UK			430			430		0.0%	4)

1) Facts & Figures for the Chemical Industry. Section Five: Foreign Chemical Industries. Chemical and Engineering News, June 9, 1986, Vol. 64, Nr. 23, pp.83-84.

2) Predicasts, Inc. Worldcasts, 1984, pp.B114-B115.

3) Food and Agricultural Organization of the United Nations. Production Yearbook, 1985, Vol.35, p.316.

4) Frost & Sullivan, Inc. News, Report Nr. E635, May 25, 1984, p.4.

The 12 top pesticides manufacturers in order of sales volume, (listed by countries where the headquarters are situated), according to Frost & Sullivan (1984), are Bayer (West Germany), Ciba-Geigy (Switzerland), Monsanto (USA), Royal Dutch/Shell (Netherlands/UK), Hoechst, including Roussel-Uclaf (West Germany), Rhône-Poulenc (France), BASF (West Germany), Schering, including FBC (West Germany), ICI (UK), DuPont (USA), Union Carbide (USA) and Eli Lilly (USA).

Though US companies are increasingly challenging West European companies on their own turf – for instance Monsato's successful introduction of the glyphosate herbicide "Roundup" – Europe's dominance appears assured for the forecast period.

The Frost & Sullivan study also contains a special analysis of trade patterns in pesticides within Europe and between Europe and the rest of the world. It is demonstrated that West Germany is by far the biggest exporter in Europe, though Switzerland has the highest ratio of exports to imports. France is the biggest importer.

Table 2. Relative consumption of pesticides in European countries

	1974-76	1981	1982	1983
DDT	0.40	0.00	0.00	0.00
BHC (benzenehexachloride)	0.68	0.00	0.00	0.00
Lindane	1.12	0.65	0.53	0.15
Aldrin and rel. insecticides	0.23	0.01	0.01	0.00
Toxaphene	0.14	0.02	0.02	0.05
Other Chlor hydrocarbons	0.26	0.38	0.37	0.65
Parathion	1.54	1.28	1.04	0.76
Malathion	0.39	0.26	0.26	0.26
Other org. phosph. insecticides	4.27	7.08	7.10	3.64
Pyrethrum	0.01	0.02	0.02	0.06
Other horticultural insecticides	0.00	0.02	0.01	0.01
Arsenicals	0.00	0.00	0.00	0.00
Carbamates insecticide	1.41	1.01	0.99	1.03
Dinitro compounds	0.29	0.29	0.22	0.26
Mineral oils	2.54	2.47	2.78	0.54
Other insecticides	3.19	1.75	1.93	4.72
Sulphur	38.61	17.43	19.15	32.18
Lime sulphur	0.38	0.01	0.02	0.01
Copper compounds	9.04	8.74	8.21	3.13
Dithiocarbamates	5.52	5.50	5.36	4.35
Aromatic compounds	0.37	0.32	0.21	0.80
Other fungicides	8.45	16.50	12.11	10.56
Seed dress org. mercurial	0.08	0.01	0.01	0.00
Seed dressings others	0.04	0.06	0.10	0.58
2.4-D	1.40	1.04	1.23	1.89
MCPA	2.42	2.86	2.81	2.92
2.4.5-T	0.03	0.02	0.02	0.03
Triazines	3.28	4.42	3.92	3.56
Carbamates herbicide	1.45	1.85	2.41	0.22
Urea derivatives	0.12	0.99	1.00	1.42
Other herbicides	9.22	18.09	20.87	22.62
Bromides	0.38	0.88	0.97	0.04
Other fumigants	1.46	1.57	1.58	0.08
Anticoagulants	0.05	0.04	0.04	0.00
Other rodenticides	0.09	0.13	0.16	0.73
Pesticides NES	1.12	4.28	4.59	2.74

Source: FAO Production Yearbook, 1985.

Trade in pesticides within Western Europe is much larger than that between Western Europe and the USA, which in turn is greater than trade with Japan. France, West Germany and the UK are all found to be important, and approximately equal, exporters to the developing countries and the East bloc.

As regards pesticides classes, Frost & Sullivan find herbicides to have the largest market share but to be growing slowest. Spain will exhibit the fastest country growth rate through 1989. End uses are dominated by agriculture, with horticulture being comparable in consumption with industrial plus household uses.

Pesticide consumption has led to a number of problems (Ahmed, 1985):

- the problem of misleading marketing practices by both producers and distributors;
- the use of pesticides that have been banned or severely restricted in the exporting countries;
- consumer misuse and abuse;
- inadequate education and training of pesticide users and applicators.

The pesticide case study with the model-based decision support system described in this paper will not deal directly with these questions. However, it provides an important DSS type framework which may serve the purpose of solving these problems in a cooperative way between policy-making bodies and industry.

2. A Guided Tour through the Model System

The model system described here is implemented on a high-resolution color graphics workstation. Its user interface is completely menu-driven, i.e., at any point in time, all the possible options for the user are indicated by a system of hierarchical menus and associated explain functions. To give a vivid impression of how this type of interactive model works, we will structure the following description along the lines of this interface; however, since a major feature of the system is its conversational and arbitrary sequence style, any necessarily sequential description will be found wanting.

Their are several main components embedded in the system:

- a group of interrelated databases;
- the linear programming model with its interactive and hierarchically structured output control;
- environmental impact analysis (a river water quality model);
- a post-processor for scenario comparison;

all integrated within a uniform graphics-oriented user environment. The system is characterized by a high degree of connectivity, i.e., most of the modules, and in particular the databases, can be called from various places (e.g., whenever a substance listing is on the screen), and there are numerous cross-references linking the modules.

All these connections are designed to provide a "natural" extension of the information displayed in any one screen, such that the full amount of information is available to the user via one or several menus, without any of the displays being overloaded.

2.1 Getting Started

After starting the model at the command interpreter level (the shell in the UNIX environment used), the interactive program takes over and presents the start-up screen (Figure 1).

The menu on the startup page provides two standard options found in any menu of the system: STOP and EXIT, or RETURN at any lower level, that will transfer control to the next higher (previous) level, and EXPLAIN. The EXPLAIN option will darken the screen, so that the current context is only dimly visible, and display some explanatory text from a database of explanation text files, referenced by the id defined for the current position, status, or context of calling this menu option.

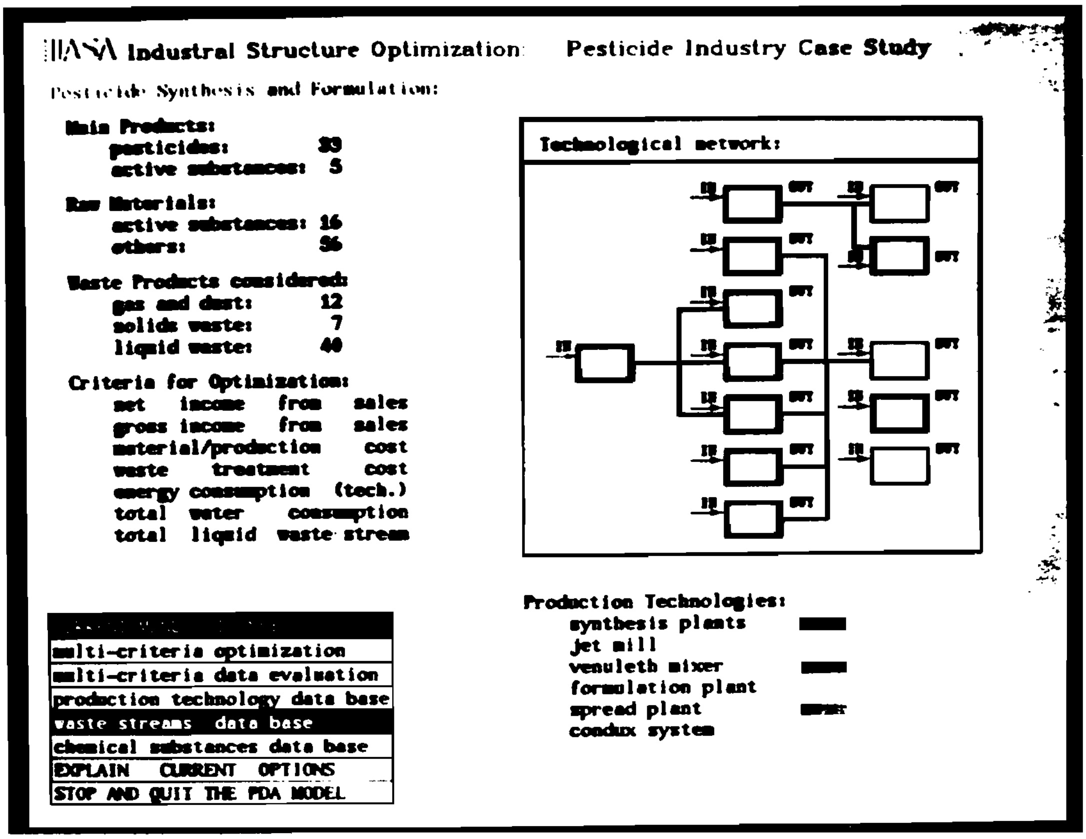


Figure 1: Start-up page with top-level menu

2.2 Databases and Background Information

The start-up page menu provides access to the three major databases of the system. These databases provide background information, in part combined with the latest results from the optimization experiments. The three databases cover:

- Production Technologies;
- Waste Streams and a related Industrial Establishments database;
- Hazardous Substances.

2.2.1 Production Technologies

The technology database contains data describing technologies that are assumed to be site independent, i.e., inputs and feedstocks, waste products and by products, trace contaminants, a qualitative hazard rating, and finally a process flow sheet or unit equipment layout. A cross-connection to the hazardous substances database (see 2.2.4) uses these listings of substances for reference.

An individual process technology can be selected from a page with process names, by picking the appropriate name with the mouse picking device. The individual process technologies are grouped by the installations they can run on (see 3.1).

In general, database structures are designed to accommodate a list or frame-oriented extension, with a DBMS implemented in LISP. Database structures are open-ended, to allow the inclusion of additional information (e.g., detailed equipment descriptions as required by the fault-tree analysis package SAFETI, Technica 1984) at a later stage without requiring a complete redesign of the databases and management software.

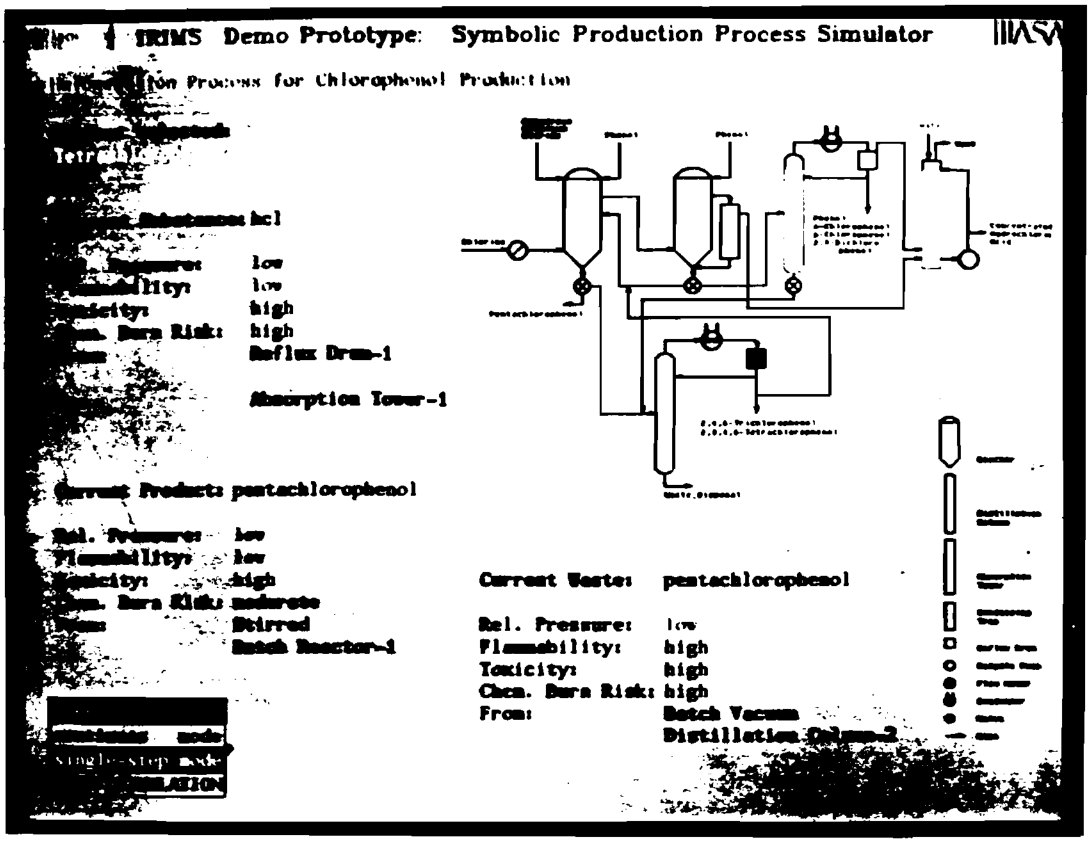


Figure 2: Production technology database: standard page display.

Also, there are several levels of individual process simulation and optimization available or under development in the framework system (Fedra, 1986; Grauer and Fedra, 1986; Winkelbauer, 1987) that could be connected to the display software for this database.

2.2.2 Process Waste Streams

The process waste stream database contains information on the 48 waste streams of the pesticide model. A specific waste stream is selected from a one-page listing of all the waste streams in the system.

This information includes:

- the name of the waste stream, including codes and acronyms where applicable;
- the number of establishments producing it, and a map displaying the individual installation location with a symbol scaled to represent production volume (since the current version of the model is spatially aggregated, allocation to individual sites is proportional, based on a fixed ratio);
- total production volume (reflecting the current status of the model, or the default *status quo* when called before an optimization experiment);
- physico-chemical waste stream characteristics such as specific gravity, water and ash content, heating value, BOD, biodegradation rate, etc.;
- substances of concern, including their mass fraction and basic physico-chemical data.

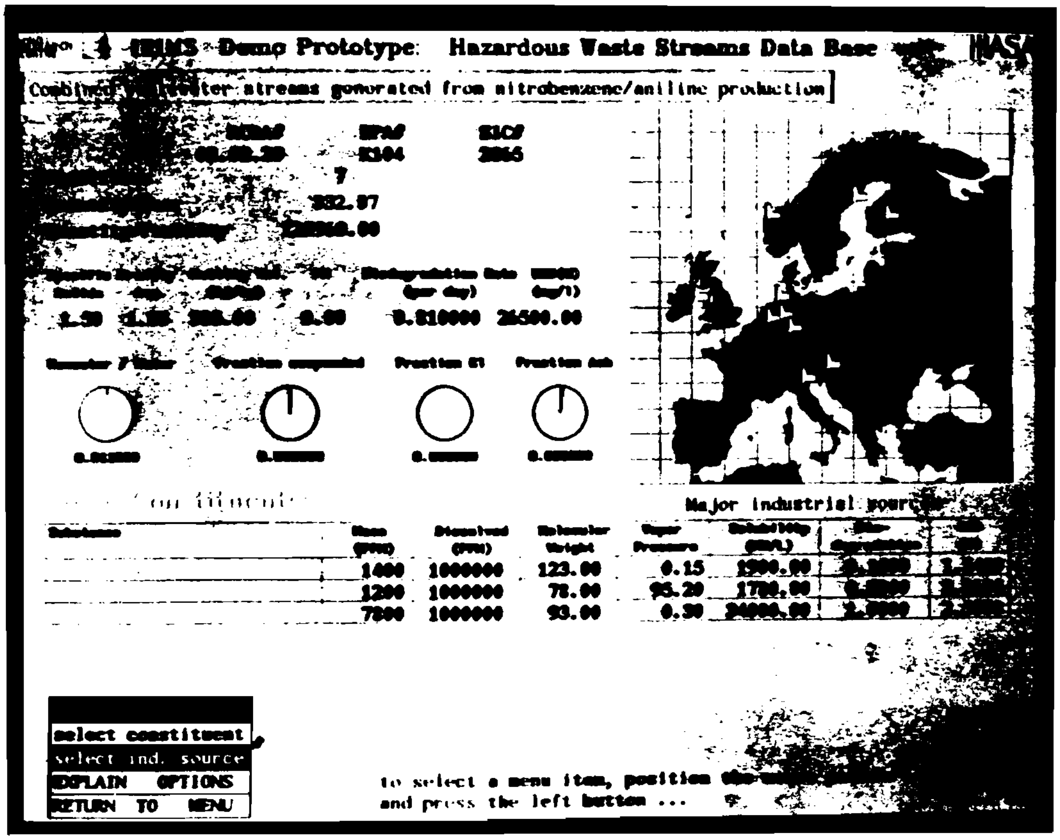


Figure 3: Waste stream database: standard page display

The waste stream database can be called from various levels; in addition to the top-level front page, the display of results on a technology level offers another entry point. Also, the substances database, in its production information window (see 2.2.4) lists waste streams that can be used as an entry point to the waste stream database.

2.2.3 Industrial Establishments Database

The map displaying the size (in terms of contributing to the waste stream in question) and location of certain industrial installations serves as an entry to the industrial establishments database. An establishment or plant is identified by picking it with the mouse pointing device from the map.

Information on a specific plant or establishment includes the name and location of the enterprise, information about its size (total production volume or number of employees), a list of major product groups, production technologies, and finally a listing of substances involved in the production that are subject to the EC Directive on the major hazards of certain industrial activities (82/501/EEC No.230).

Again, the locations database offers cross-connections to the substances database as well as the production technologies database.

2.2.4 Hazardous Substances Database

The hazardous substances database contains information on the 125 substances of the pesticide model. They may be feedstocks, interim products, products, or wastes. Access at the start-up page level is either through a multi-page listing, from which a

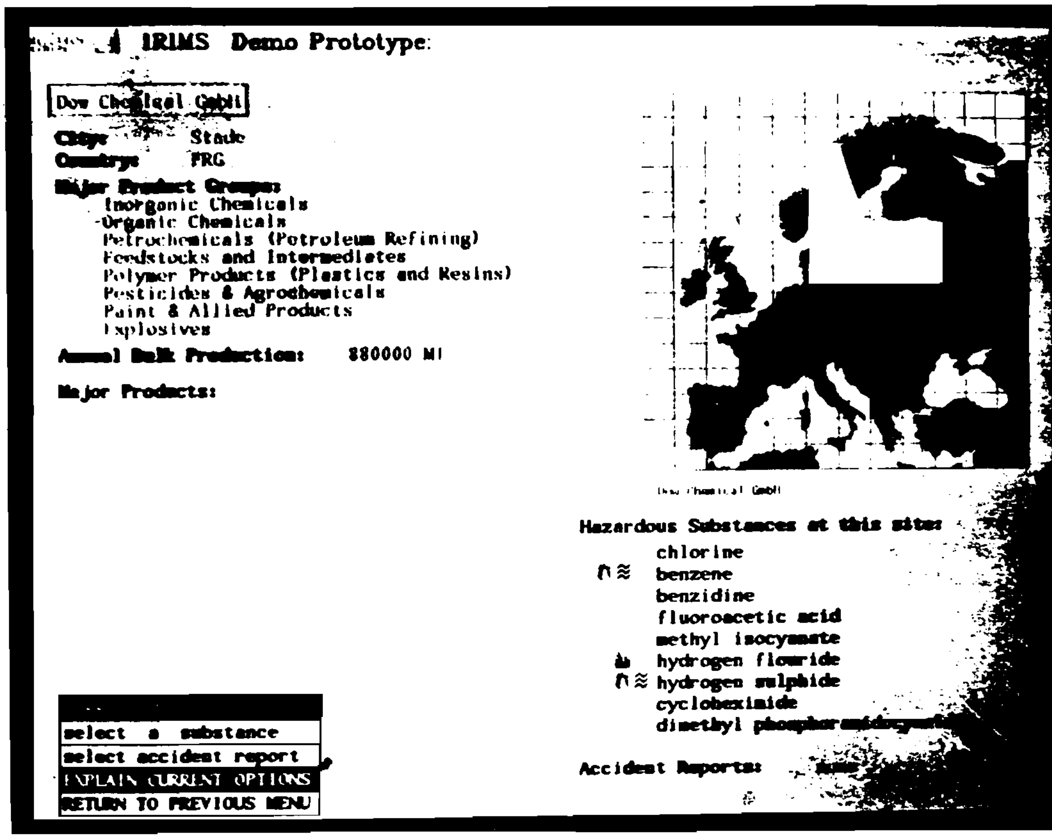


Figure 4: Industrial establishments database

substance name can be picked with the mouse pointing device, or through a parsing function that allows direct entry of substance names, or significant parts of names. The latter can result either in a single or in multiple references. In the first case, the corresponding database page will be displayed directly, in the latter, a list of all substances referred (ranked by probability, see Fedra et al., 1987) is displayed for further selection.

Substance listings are coded with a set of symbols to denote e.g., their inclusion in specific EC regulations, high toxicity, specific water pollutants, fire and explosion hazard, etc. For a more detailed treatment of the hazardous substances database implementation see Fedra et al. (1987).

The substances database can also be accessed from various other parts of the system, whenever a listing of substance names is on the screen: selecting the appropriate menu option and selecting a substance name will display the corresponding database page.

Information on individual substances includes name, synonyms, various ID numbers (CAS, UN), a summary description of state, appearance, odor, solubility and persistence in qualitative terms, health-related toxicity information, including symptoms and types of exposure; chemical formula, including a color-coded representation of chemical structure, a table of physico-chemical data, reference to legislation and regulation covering the substance, and finally production information are provided. The production information includes, in addition to average production figures, a list of production processes involving the substance (either as a feedstock, interim or by-product, or as a waste product), as well as the associated waste streams. These waste streams can be

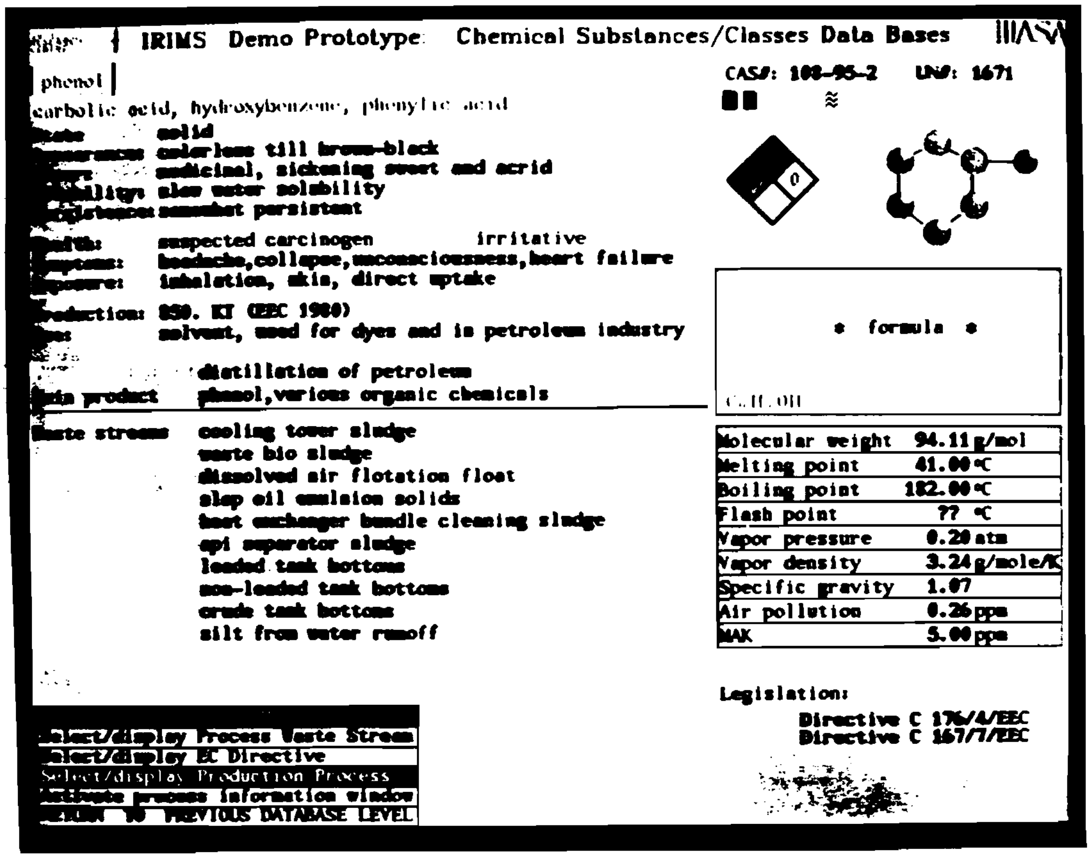


Figure 5: Hazardous substances database

used as entry points to the waste stream database described above. The production processes can be used also as references to the process technology database.

2.3 Numerical Experiments: Interactive Optimization

The final menu option of the start-up screen will initialize the optimization model, read in the data, perform an optimization run for each of the seven objectives in turn to find the respective utopia and nadir points, and finally generate results for an unconstrained simultaneous optimization of all seven criteria, with the utopia point serving as an implicit reference point. The results of this optimization run are displayed in numerical as well as in graphical form. The numerical representation is simply a list of numbers of the current and previous values for the seven criteria (which in the case of the first run are the same). In addition, these values are displayed as the position of a red arrow within the interval from original upper to lower bound for the respective criteria. In addition to the current solution, the position of the relevant bounds (upper or lower, depending on whether the criteria values are minimized or maximized) is indicated by a red bar. The utopia points are shown as yellow dots, and the reference points (in the first run coinciding with the utopia point) are marked by little blue arrowheads.

The network of installations introduced on the start-up page is displayed again. This time, the boxes representing individual production technologies are filled according to the process capacities utilized in the different installations (Figure 1).

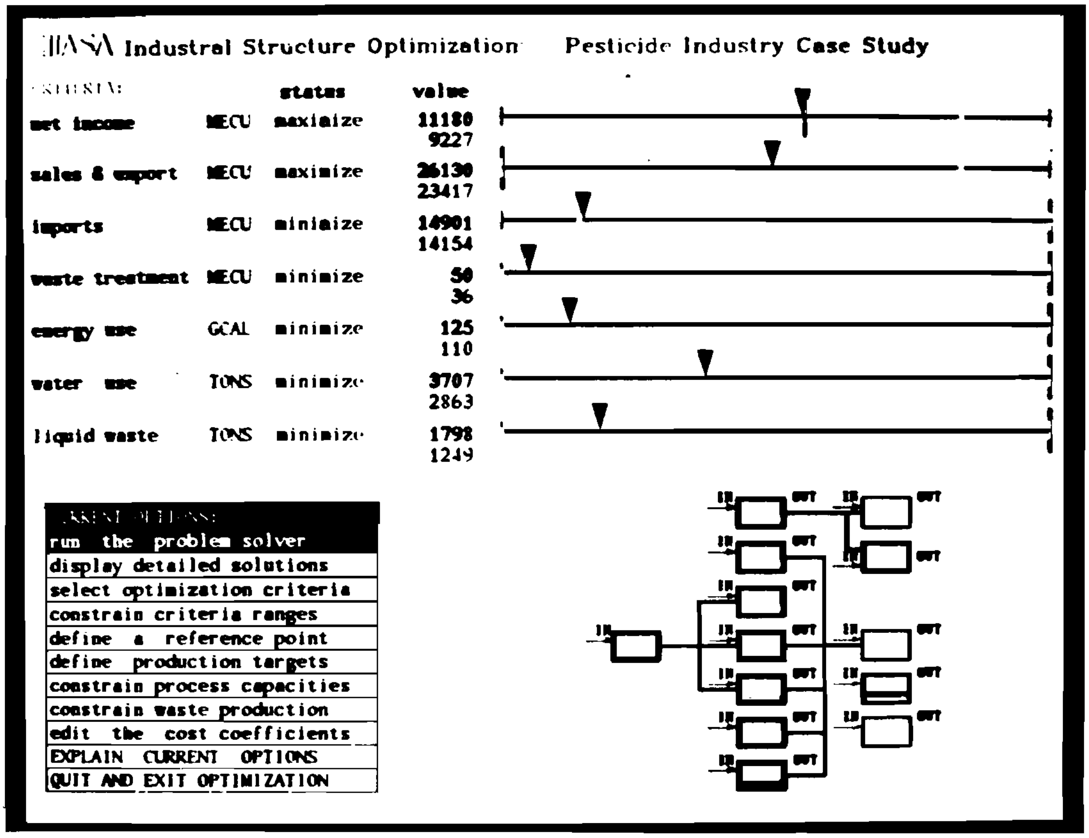


Figure 6: Top level of the interactive optimization: display of results for criteria and main control menu

The control menu, in addition to the standard EXPLAIN and STOP options, contains three types of options:

- problem formulation or scenario definition;
- output display and analysis;
- (re)run the problem solver.

To define a scenario for analysis, the user can manipulate the problem definition on the level of the criteria, by choosing to consider or ignore any subset of the criteria; he can place constraints, that is upper or lower bounds on the values of the criteria, e.g., specify a maximum amount of liquid waste; and finally, he can define a desired outcome in terms of a target or reference point, setting criteria reference values at the levels that he would prefer them to be.

The second level of problem formulation is the level of production technologies, and substances. Here the user can specify upper or lower bounds on the capacities for a production process (forcing the model to turn the respective process on or off), he can define target amounts for production (and the corresponding prices for either selling or buying the substance), and he can finally limit the amount of any specific waste the model may produce by directly putting a constraint (upper limit) on it, or by indirectly specifying a high price for treatment (which could also represent a form of waste tax).

2.3.1 Defining Scenarios for Optimization

For the problem definition at the level of the criteria, the user can choose between the following menu options:

- **select optimization criteria**
- **constrain criteria ranges**
- **define a reference point.**

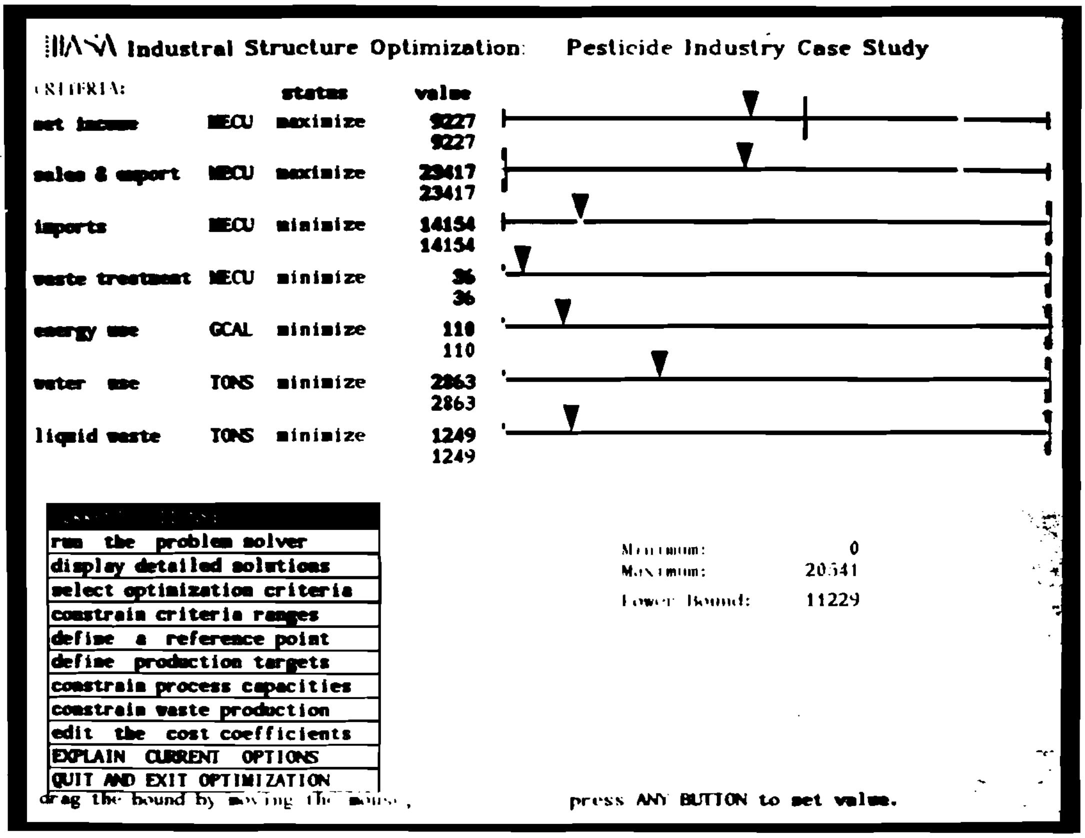


Figure 7: Setting a bound

These three menu options all directly or indirectly affect the problem definition at the criteria level. The model currently is implemented for seven criteria:

- net income;
- sales and export or gross income;
- import of raw materials;
- waste treatment costs;
- energy use;
- water consumption;
- liquid waste volume.

Select Optimization Criteria

Out of this list, the user can specify any subset by just pointing at the criterion and toggling the status indicator between minimize / maximize / ignore. The problem can thus be approached at various levels of complexity, or dimensionality.

In practice, a user could start with a small subset of the criteria that he considers to be most important. After having found a feasible solution that is satisfactory in terms of this criteria subset, additional criteria (which so far have only provided auxiliary information) can be included, one by one, to represent additional concerns requiring further trade-offs.

Constrain Criteria Ranges

For active criteria (those that have their status indicator set to either minimize or maximize), the user can set upper or lower bounds, respectively, by dragging the constraint indicator (a red bar across the displayed range) with the mouse. While the constraint is moved, the respective numerical values are indicated to provide additional information. The value is set by just clicking the appropriate mouse button, indicated by the prompt string that provides additional information after a certain menu option was selected, wherever necessary.

Define a Reference Point

Finally, the user can define a reference point (other than the default utopia point) by selecting, dragging, and positioning any of the active criteria reference point symbols with the mouse. For a description of the underlying philosophy of multi-criteria optimization, see Wierzbicki (1983). A formal description of the Reference Point Approach is given in section 3.3.

Another four menu options lead to a hierarchy of display and selection levels. These options are:

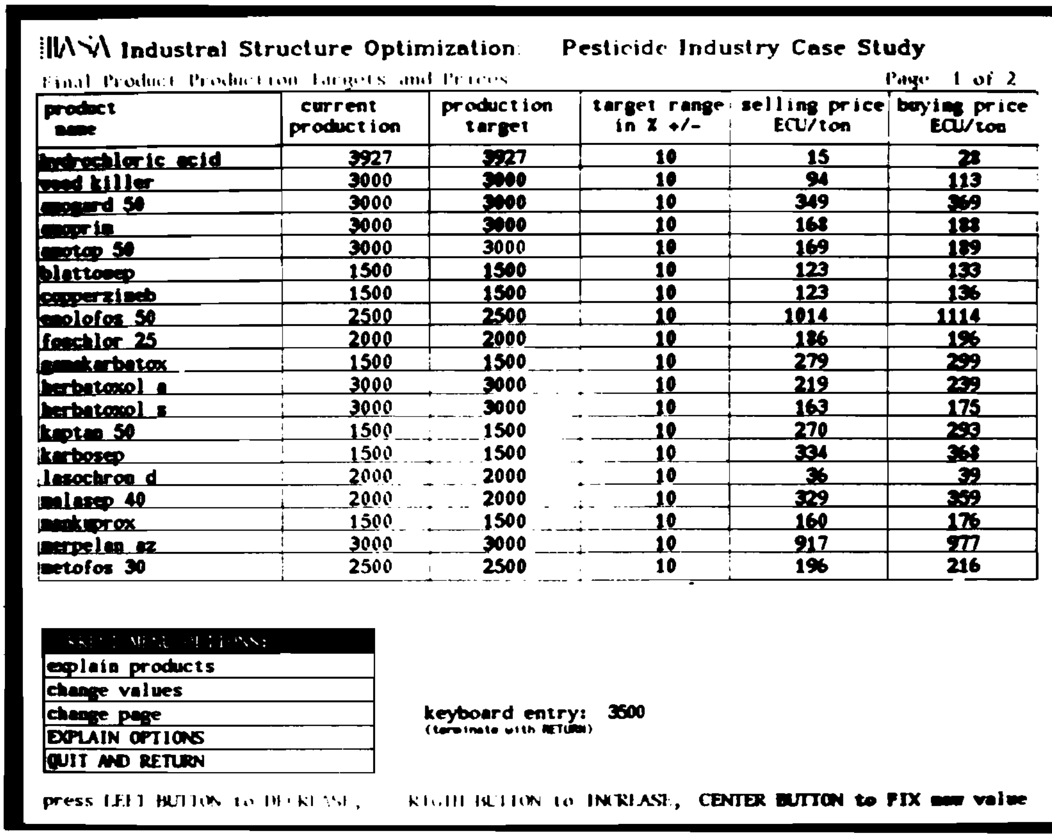
- **define production targets**;
- **constrain process capacities**;
- **constrain waste production**;
- **edit the cost coefficients**.

Define Production Targets

To define production targets, the user calls up tables listing 38 main products, together with their current production level, current target production level (which is the same as the current production for the first run), a percentage range around the target, and the import and export prices for that substance. The latter four values the user can change by identifying the selected number, and then modify it either with the mouse (pressing the left button will decrease the number with increasing speed until it reaches its allowable minimum value; pressing the right mouse button will increase the number until it reaches its upper limit; and pressing the middle button will set the number to the current value) or by direct keyboard entry.

This process can be repeated for as many numbers or as often for any number as the user chooses.

Since the model will balance any internal production deficit (due to the various constraints on processes or wastes) by imports, setting import versus export prices can considerably affect the model.



IIASA Industral Structure Optimization: Pesticide Industry Case Study

Final Product Production Targets and Prices — Page 1 of 2

product name	current production	production target	target range in % +/-	selling price ECU/ton	buying price ECU/ton
hydrochloric acid	3927	3927	10	15	23
weed killer	3000	3000	10	94	113
amogard 50	3000	3000	10	349	369
amoprin	3000	3000	10	168	188
amotop 50	3000	3000	10	169	189
blattosep	1500	1500	10	123	133
copperzineb	1500	1500	10	123	136
enolofos 50	2500	2500	10	1014	1114
fenchlor 25	2000	2000	10	186	196
gamakarbatox	1500	1500	10	279	299
herbatoxol a	3000	3000	10	219	239
herbatoxol s	3000	3000	10	163	175
kaptan 50	1500	1500	10	270	293
karbosep	1500	1500	10	334	368
lasochron d	2000	2000	10	36	39
malasep 40	2000	2000	10	329	359
mankuprox	1500	1500	10	160	176
merpelan az	3000	3000	10	917	977
metofos 30	2500	2500	10	196	216

explain products
change values
change page
EXPLAIN OPTIONS
QUIT AND RETURN

keyboard entry: 3500
(terminate with RETURN)

press LEFT BUTTON to DECREASE, RIGHT BUTTON to INCREASE, CENTER BUTTON to FIX new value

Figure 8: Defining production targets

In the worst case, it turns into a trading model, and, given stringent constraints on waste production and waste treatment prices, will resort to importing increasing amounts.

Constrain Process Capacities

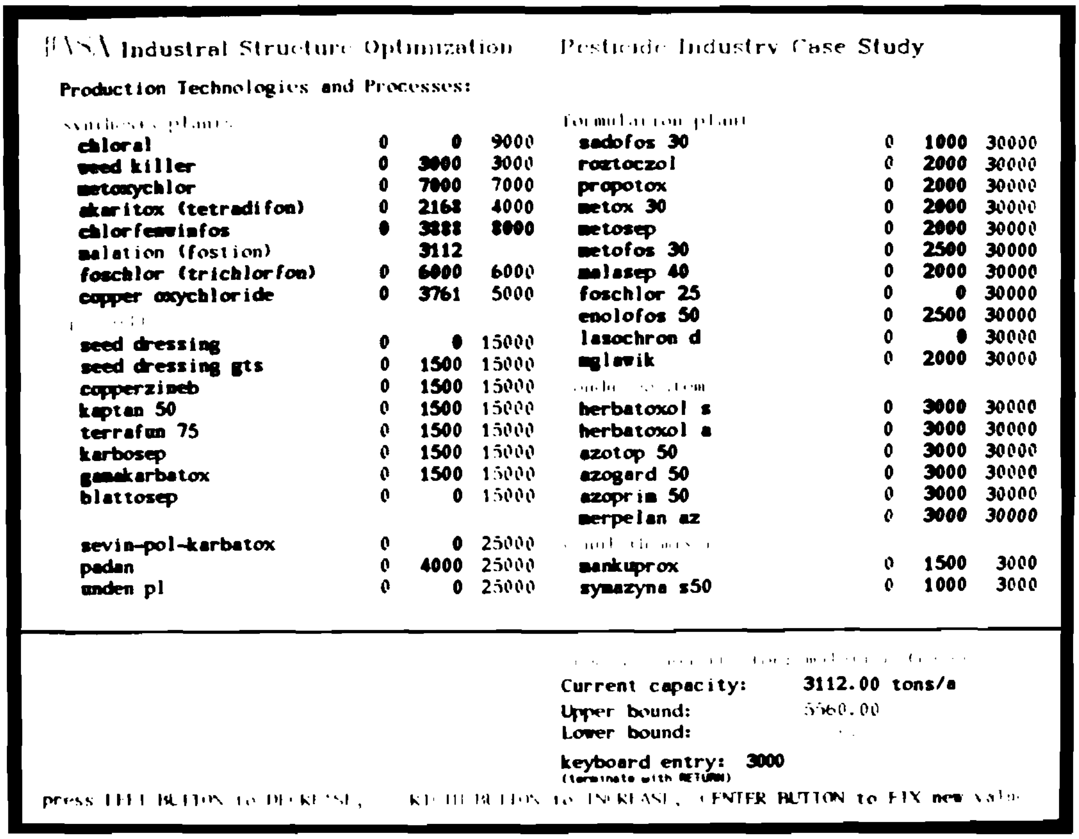
The next menu option allows one to constrain process capacities. For the 38 major production technologies of the model, a table with the current production level (in tons per year) and the upper and lower bounds around that level is displayed (Figure 9).

The constraints on the production capacities serve a dual purpose: on the one hand, they can restrict or even completely ban certain production technologies. A possible example might be high-risk technologies involving super-toxins such as various forms of furan or dioxin.

Alternatively, the lower bound can be used to force a certain minimum level of production for strategically important substances, no matter what the costs involved, or represent the situation of a subsidized industry where production capacity is held artificially high for socio-political, e.g., employment reasons.

Constrain Waste Streams

An important option is the constraining of wastes. Here the model offers two different forms of control: direct constraints, and indirect economic control via waste treatment prices (which could also represent a waste tax).



IIASA Industral Structure Optimization Pesticide Industry Case Study

Production Technologies and Processes:

chloral	0	0	9000
weed killer	0	3000	3000
metoxychlor	0	7000	7000
akaritox (tetradifon)	0	2168	4000
chlorfenwinfos	0	3888	8000
malation (fostion)		3112	
foschlor (trichlorfon)	0	6000	6000
copper oxychloride	0	3761	5000
seed dressing	0	0	15000
seed dressing gts	0	1500	15000
copperzineb	0	1500	15000
kaptan 50	0	1500	15000
terrafun 75	0	1500	15000
karbosep	0	1500	15000
gamakarbatox	0	1500	15000
blattosep	0	0	15000
sevin-pol-karbatox	0	0	25000
padan	0	4000	25000
unden pl	0	0	25000

formulation plant			
sadofos 30	0	1000	30000
roztoczol	0	2000	30000
propotox	0	2000	30000
metox 30	0	2000	30000
metosep	0	2000	30000
metofos 30	0	2500	30000
malasep 40	0	2000	30000
foschlor 25	0	0	30000
enolofos 50	0	2500	30000
lasochron d	0	0	30000
mglawik	0	2000	30000
herbatoxol s	0	3000	30000
herbatoxol a	0	3000	30000
azotop 50	0	3000	30000
azogard 50	0	3000	30000
azoprim 50	0	3000	30000
merpelan az	0	3000	30000
mankuprox	0	1500	3000
symazyna s50	0	1000	3000

Current capacity: 3112.00 tons/a
Upper bound: 5560.00
Lower bound:

keyboard entry: 3000
(terminate with RETURN)

press LEFT BUTTON to DECREASE, RIGHT BUTTON to INCREASE, CENTER BUTTON to FIX new value

Figure 9: Setting constraints on process capacities

For the 40 major substances in liquid waste streams, a table which includes substance name, current level of generation, maximum allowable level (upper bound), and a treatment price (and/or waste tax) per ton of product is displayed. Again the latter two values can be set for each substance by mouse buttons or by direct keyboard entry.

Edit Cost Coefficients

Finally, a few global cost coefficients (unit cost of labor, energy prices for electrical and technological (steam) energy, price of water, etc. can be set, in particular to analyze the system's reaction to changes in labor costs and energy. However, since a change in energy prices would in all likelihood also trigger a change of the product prices (defined above), it would be extremely difficult to formulate a consistent scenario including massive changes in energy prices. Currently, no mechanism other than simple upper and lower bounds on the values the user can change are implemented to ensure scenario consistency. This, however, would be a challenging extension of the current model.

2.3.2 Running the Problem Solver

After a scenario for analysis has been defined, the menu option **run the problem solver** will rerun the optimization package with the newly specified objectives, constraints, and coefficients.

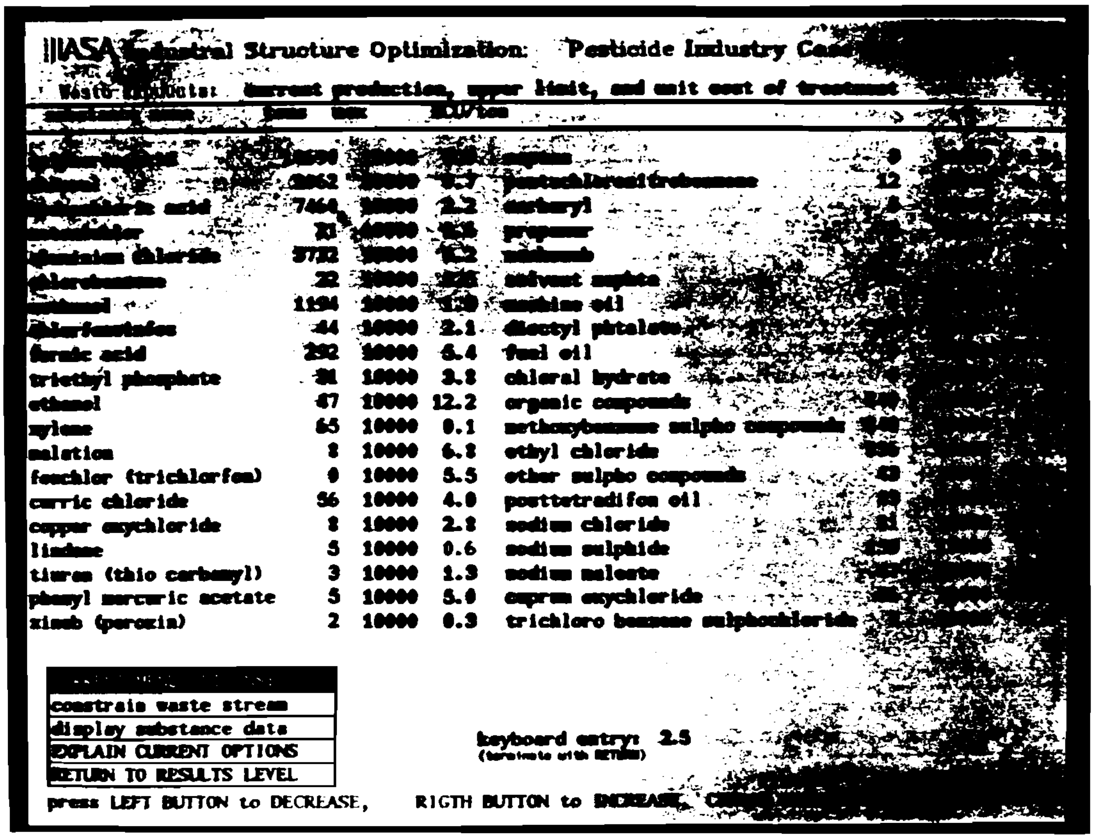


Figure 10: Setting constraints on waste products

The new results will be indicated by a shifting of the red results arrows, and the updating of the corresponding numbers (compare Figure 6).

If however, the user has made excessive changes to the scenario definition, or defined too narrow or even contradictory constraints, no feasible solution can be found. The problem solver will indicate this with a short diagnostic message, after which the main control menu for scenario definition will be offered again. If the user has made only one or a few changes since the last feasible run, the necessary modifications of the scenario definition will be obvious and easy. As an emergency escape, however, the user can restart the entire process, re-loading the default data, and thus overwrite the current (infeasible) status of the system. All completed interim solutions, however, will still be available for analysis with the post-processor (see section 2.6).

2.4 Model Output and Evaluation

The top level for the interactive optimization displays the current results for the seven criteria, and the values from the last run in numerical terms as well as graphical representation (Figure 6). It also indicates the position of bounds, utopia point, and reference point in graphical form.

The menu option **display results** will call up a more detailed representation of a run's results, together with a new menu for further control of the hierarchically organized model output.

The screen summarizes the results at the industry level. A table with a breakdown of the industries' economics is provided together with a pie chart, in parallel, summarizing the major cost components. In addition, basic resource consumption and summary

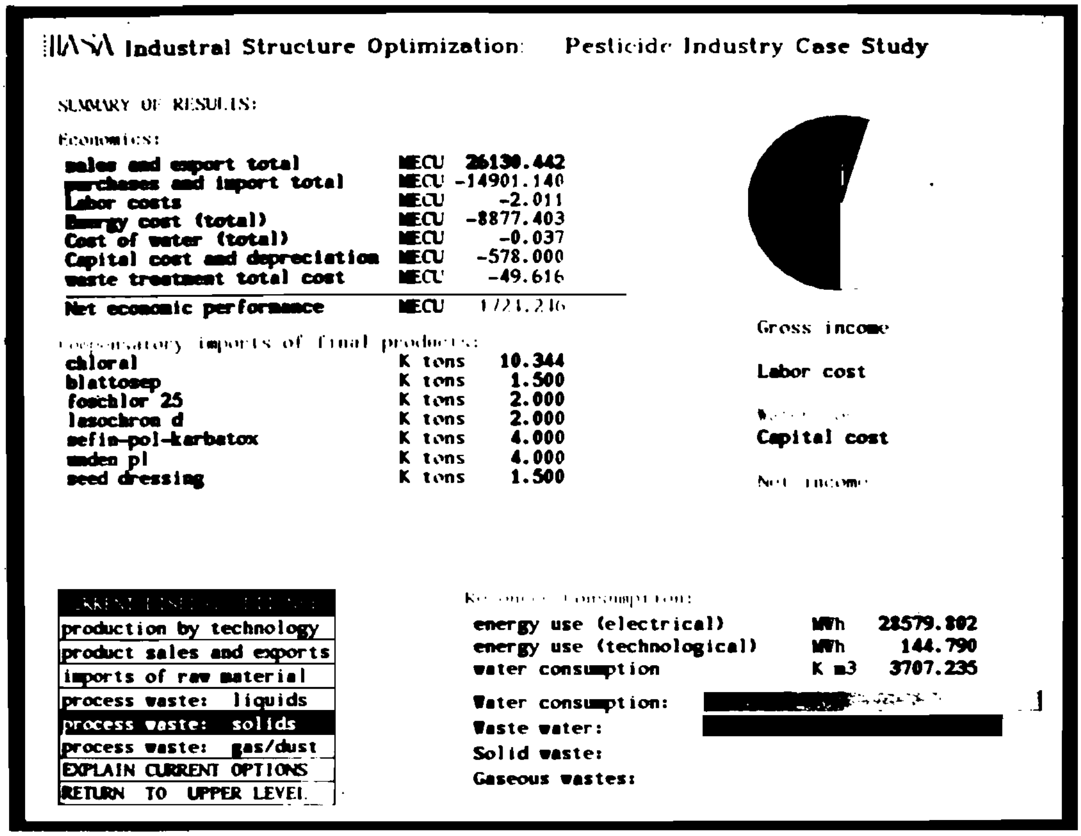


Figure 11: Display of general results and menu for the detailed results output

waste production is indicated in numeric as well as graphical form.

We also display a listing of those products, that were imported (at least in part) in order to fulfill the required target production levels.

The output control menu contains the following options:

- results by technology;
- product sales and exports;
- imports and raw materials;
- process waste: liquids;
- process waste: solid;
- process waste: gas/dust.

2.4.1. Results by Technology

This option calls up the table of production technologies, grouped by installations (see Figure 9). The user can select any of the technologies by picking it with the mouse, and either retrieve the corresponding technologies database page for background information, or call up a screen with the current optimization results summarized for this technology (Figure 12).

The page indicates the technology chosen and the current production level together with an indication of the relative capacity utilization. It also provides the same economic breakdown as the overall results page, including more detailed production costs.

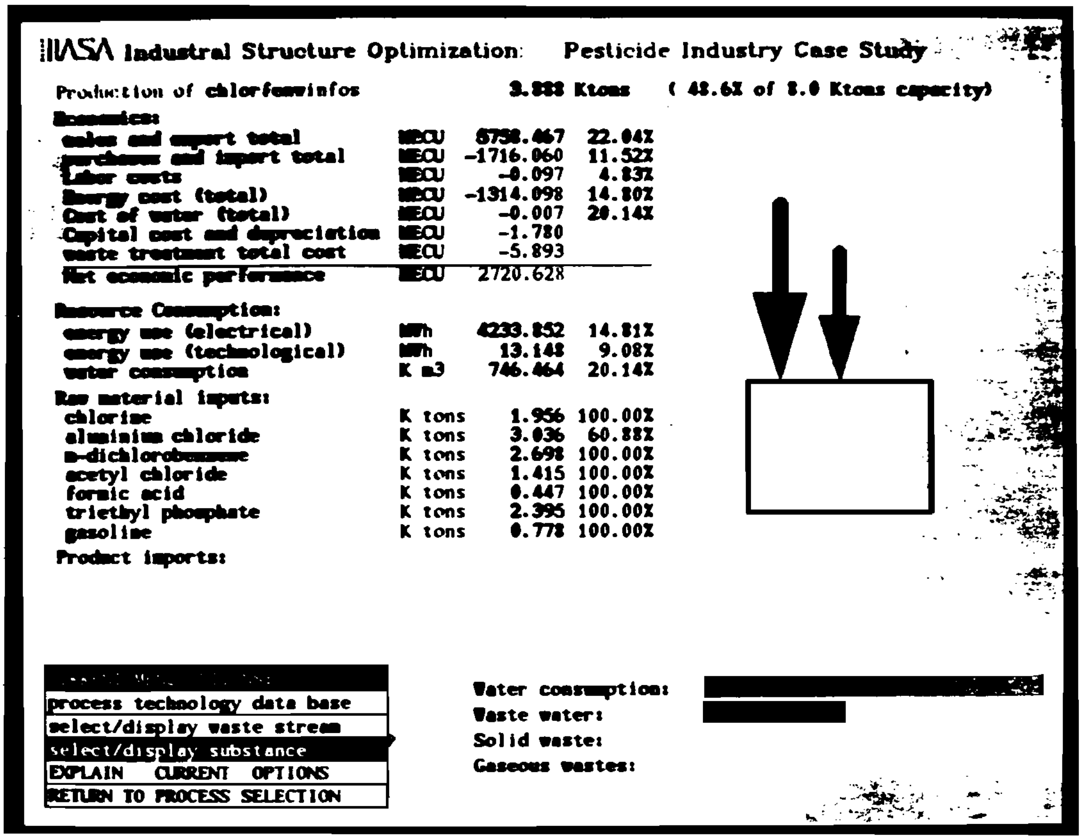


Figure 12: Detailed results output for individual technologies

The screen then includes a list of the raw materials used (which is also an entry point to the substances database), as well as of any complementary purchase of the main product. A parallel graph symbolizes the process as a box, with three arrows indicating input (electricity, steam, and water), three arrows for the output (for the three waste streams), and a graphical representation of capacity utilization.

A third table summarizes resource consumption in terms of energy and water. Finally, water consumption, total substances in liquid, solid, and gaseous waste streams are summarized by a set of color-coded bars. The module provides connections to the substances, technology and waste streams database.

2.4.2 Listing of Waste Stream Constituents

On activating any of the three available options by clicking the mouse button, a listing of the substances in the respective waste streams is displayed, sorted by amount, together with parallel pie charts which show the relative proportions of the top 10 substances (Figure 13).

The listing of the substances again serves as an entry point to the hazardous substances database.

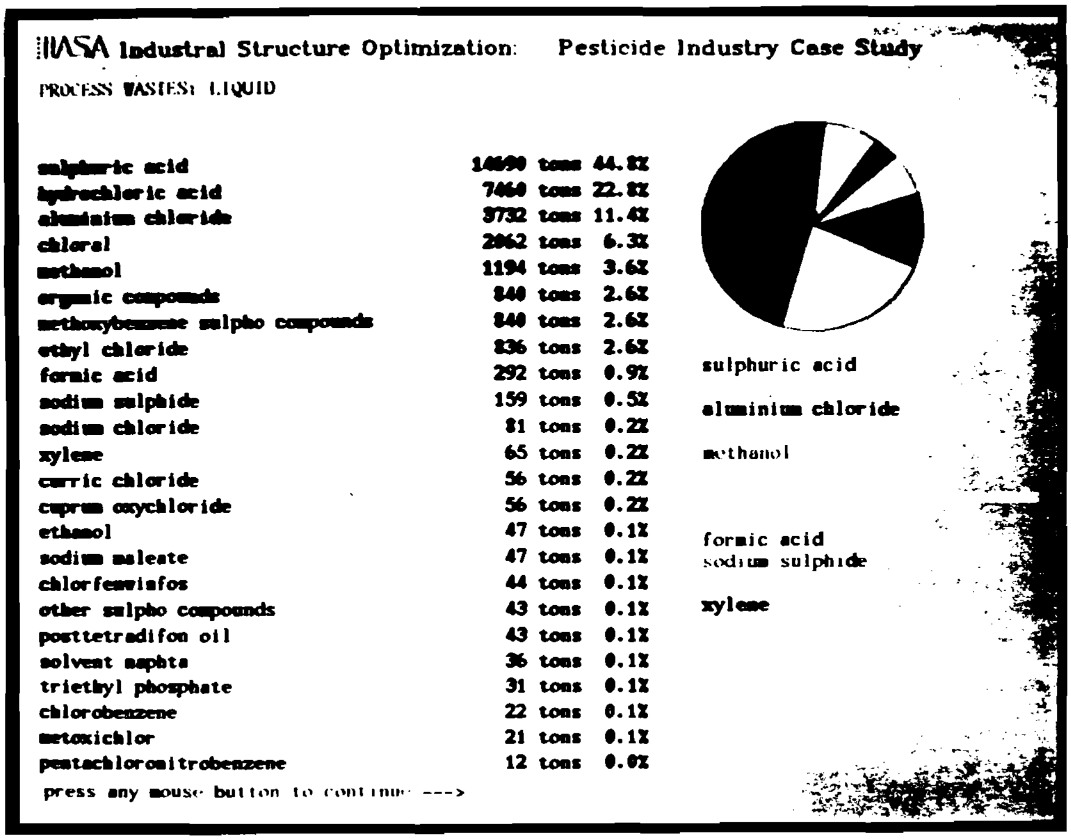


Figure 13: Process waste stream listings

2.5 Environmental Impact Simulation

The by far largest waste stream in the model is the liquid waste stream, i.e., wastewater. The primary environmental impact considered is therefore for rivers. The effect on water quality depends on the amount and mixture of substances discharged into as well as on the characteristics of the receiving water body. Substance-specific data as well as the characteristics of the river reach affected at any site are automatically retrieved from the databases.

The water quality model used is based on the river component of TOX-SCREEN (McDowell-Boyer and Hetrick, 1982). An equation similar to the one used in EXAMS (Smith et al., 1977; Burns et al., 1981) is used to estimate the pollutant mass in each time step in each reach. Instantaneous mixing of pollutants upon entry into each reach is assumed; pollutant concentrations are computed for dissolved neutral, dissolved ionic, and adsorbed forms, according to chemical equilibria. Adsorption on sediment is also described. A number of first-order rate constants (e.g., biodegradation, hydrolysis, volatilization) are used to simulate decay phenomena (Figure 14).

The necessary waste stream parameters (the model used employs five first-order rate constants to characterize a pollutant) are automatically retrieved from the hazardous substances database. The model is then solved for all constituents of the mixture simultaneously, resulting in a concentration vector in space and time. The basic simplifying assumption is that there are no interactions between substances.

The model simulates one yearly cycle in (output) time steps of one day. The option for the user include the selection of various hydrographic conditions, representing average, dry, extremely dry, and wet years. The user can also select certain levels of

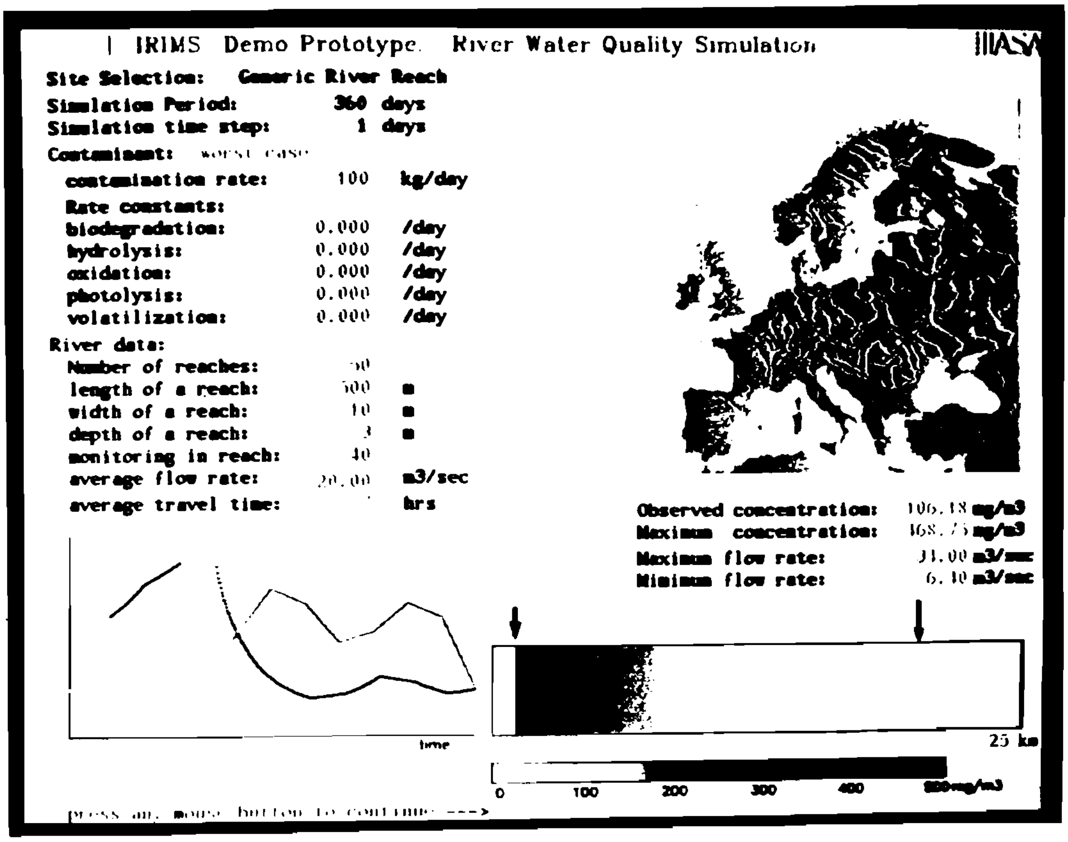


Figure 14: River water quality simulation

treatment, which will reduce the amount of substance reaching the water body, as well as the composition of the waste stream, depending on the original mixture as well as the treatment technologies employed*). For the treatment level selected, and depending on the waste stream volume, treatment costs are estimated from a two-component (fixed and operational) non-linear cost function.

Finally, the user can determine the position of the monitoring site along the river segment simulated. At this site, the concentrations for the pollutant vector are monitored, and the maximum and average concentration are recorded.

2.6 Scenario Evaluation: a Discrete Post-processor

The output from any individual run of the optimization model offers a very large amount of information. Any of the optimization runs present a feasible solution to a specific scenario definition, reflecting the user-defined set of assumptions, constraints, values, and preferences. Moving from one solution to the next, it becomes virtually impossible to keep track of previous solutions, and the user has little guidance as to how he is moving in this maze of control and performance variables.

*)The treatment component is currently under development. The reduction in waste volumes is therefore a simple proportional reduction, affecting all components in the same way.

To assist the user in analyzing a set of runs, to filter emerging patterns at the level of run comparison, we have extended the interactive optimization model with a discrete post-processor for multi-criteria selection.

For every run successfully completed, part of the performance information (e.g., the seven criteria and a few additional output variables) is stored together with the corresponding input or control information necessary to regenerate this run. As soon as at least three such data sets are available, the user can call upon the discrete post-processor for comparison.

Implementation and User Interface

The discrete post-processor can be used from the start-up level (before any optimization experiment is performed), or from within the interactive optimization. If used at the top level, the program first examines its data directory and lists all data sets (sets of experiments with a common user-defined identifier, usually performed for the same set of criteria) by a one-line identification in a sequence depending on modification dates, i.e., the data set generated last is offered as the first choice. The user then simply points at the desired data set, which is then loaded for further analysis.

Whenever the multi-criteria optimization package is used as an intergrated post-processor, this step is not necessary, since only one data set, namely the one generated with the current model, will be examined.

This data-set includes:

- the number of alternatives;
- the number of criteria considered;
- a listing of criteria, together with their status information (default settings for the three possible status indicators *minimize, maximize, ignore*), and basic statistical information (*average, minimum, maximum*) for the individual criteria.

At that level, the menu offers the following choices:

- *select criteria:* this allows the user to modify the status characterization, i.e., change the dimensionality of the problem by ignoring or including additional criteria from the list;
- *display data set:* this invokes the second level menu for the display options, discussed below;
- *constrain criteria:* here upper and lower bounds for the individual criteria can be defined, based on a graphical representation of the range and distribution of the criteria values; setting these constraints results in the reduction of the set of alternatives considered; the bounds are defined by dragging, with the mouse graphical input device, a vertical bar within the range of criteria values, and cutting off alternatives left or right of the bar. The system displays the current value of the constraint, and indicates how many alternatives will be deleted whenever the user sets a constraint. If the constraint setting is verified by the user, the alternatives excluded are deleted from the data set and new values for the descriptive statistics are computed.
- *find pareto set:* this option identifies the set of nondominated alternatives, and indicates how many nondominated alternatives have been identified; in our specific case, where the set of alternatives has been generated by an optimization model, all alternatives are non-dominated, as long as the user has not changed the set of criteria considered.
- another feature at this, as well as any other, level in the system is an explain function that provides a more detailed explanation of the menu options currently available.

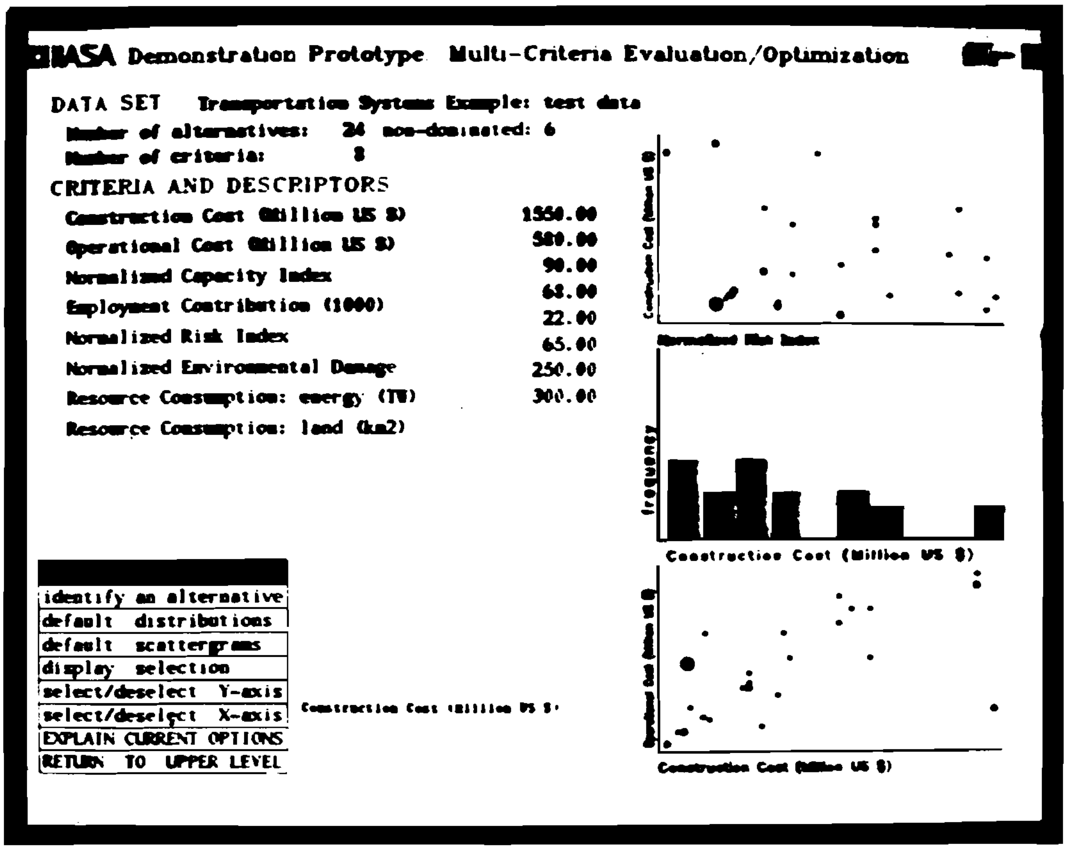


Figure 15: Standard display of scenario data projections

The option: *display data set* generates a new menu of options. The display options are:

- *default scattergrams:* the default scattergrams provide 2D projections of the data set, using pairwise combinations of the relevant criteria (Figure 15). The first three combinations are displayed in three graphics windows. If the set of nondominated alternatives has already been identified, the pareto-optimal points will be displayed in yellow and will be larger than the small, red, normal (dominated) alternatives;
- *default distributions:* this option displays the first three relevant criteria as discretized frequency distributions; again, three criteria distributions can be displayed simultaneously;
- *display selection, select x-axis, select y-axis:* these three options are used to display criteria combinations other than the default selections. Defining the x-axis only, by identifying one of the criteria lines by pointing at it, and then selecting one of the graphics windows for display, a frequency distribution will be displayed; if x and y axis are identified, a scattergram will be produced. Thus, any combination of distributions and scattergrams can be generated, allowing the user to gain some insight into the geometry and structure, e.g., dependencies of criteria, of the data set. Also, on the basis of the graphical display, it is much easier to define constraints (by returning to the previous level and invoking the appropriate menu option), if solutions are obviously clustered, i.e., distributions are multi-modal;
- *identify alternative:* one individual alternative can be identified by pointing at one of the dots in either of the graphics windows. The dot will be marked by a large blue dot in all the scattergrams currently on display. Repeating this identification

process several times, changes in the relative position of these identifiers along the individual axes support some intuitive impression of trade-offs among criteria. Parallel to marking the selected alternative on the scattergrams, numerical values for the individual criteria are displayed.

A powerful option in this system is the selection of a reference point and the resulting identification of an efficient point. To support the definition of the reference point, the (extended) range for each of the criteria is displayed beside the listing of the criteria. Thus, while all criteria as well as the utopia points and the possible ranges for a reference point are in view, the user can specify the desired level (aspiration level) for each or a few of the criteria by selecting the respective criterion and then entering either a number or pointing at an appropriate position within the interval displayed. For the dimensions (i.e., criteria) not explicitly specified by the user, the reference point value defaults to the utopia point's value.

Once all or a subset of the criteria dimensions deemed important by the user have been defined, this reference point will then be used to find an efficient point as the solution to the selection procedure. Several rounds of iteration, however, may be used to find a satisfying solution. With each efficient point, the user has the option of returning to the model that generated the alternative selected. There he can re-simulate the alternative, and thereby generate additional descriptive information on his choice. This may lead to yet another setting for the reference point, another efficient point and so on.

In summary, the discrete optimizer or post-processor is a tightly coupled option of several simulation models used for scenario analysis and/or generating a larger set of alternatives to be evaluated. Providing a combination of analysis and display options, powerful decision support can be made available to a non-expert user in a very efficient and effective way. Due to the ease of use, the high degree of flexibility and responsiveness, and the immediate understanding of results based on symbolic and graphical display combined with numerical information, the system invites a more experimental style of use. Complex models, which usually produce a confounding amount of output, can thus be made available as a direct information basis for decision making.

3. Basic Concepts underlying the DSS Development

The basic linear programming model used is a type of input-output model. The model is solved by means of a linear programming package POSTAN, developed by JSRD, which is an extension of MINOS (Stanford, 1981). As far as multiobjective optimization experiments are concerned, the OPTIMIST package which is JSRD's enhanced version of the IIASA package MM (Kreglewski & Lewandowski, 1983) is used.

3.1 PDA Model Formulation

Before describing the PDA network we define its links with the environment. The following equation describes the outflow of any chemical j:

$$y_j = y_j^{ms} - y_j^{mp} + y_j^{cs} - y_j^{cp} , \quad j \in J \quad , J \supset J_h \tag{1}$$

y_j^{ms} - market sale of chemical j,

y_j^{mp} - market purchase of chemical j,

y_j^{cs} - coordinated sale of chemical j,

y_j^{cp} - coordinated purchase of chemical j,

J - set of indices representing chemicals of the PDA,

J_h - set of indices of hazardous substances under consideration.

The variables are defined as follows:

z_k - production level of PE_k,

$\hat{z}_k$ - production capacity of PE_k,

$a_{jk}\, z_k$ - quantity of chemical j consumed by PE_k,

$b_{jk}\, z_k$ - quantity of chemical j produced by PE_k,

$d_{lk}\, z_k$ - quantity of waste l produced by PE_k,

$q_k(z_k)$ - necessary resources,

$e_k\, z_k$ - quantity of energy consumed by PE_k,

$s_k\, z_k$ - quantity of water consumed by PE_k,

$l_k\, z_k$ - quantity of labor utilized by PE_k,

$n_k\, z_k$ - investment for PE_k,

K_h - the set of indices of hazardous chemical processes.

Within K_h subsets of indices corresponding to kinds of hazards or accidents which may possibly occur during a process (fire hazard, explosion, etc.) might be distinguished.

For the balance nodes the following equations are satisfied:

$$y_j = \sum_{k \in K} b_{jk}\, z_k - \sum_{k \in K} a_{jk}\, z_k \quad .$$

$$w_l = \sum_{k \in K} d_{lk}\, z_k \quad , \quad l \in L$$

By combining the above results with (1) we obtain:

$$y^{ms} - y^{mp} + y^{cs} - y^{cp} = (\ B - A\ )\ z \tag{2}$$

$$w = D\ z \tag{3}$$

To complete this description of the network we have to add the constraints imposed on production capacity:

$$z \le \hat{z} \tag{4}$$

For multi-process installations, where processes run simultaneously, instead of the latter equation we use the following constraint:

$$\sum_{k \in K_i} z_k \leq \hat{z}_i \quad , i \in I \tag{4a}$$

where I, K_i denote respectively the sets of indices of installations and processes run on i-th installation. In addition, the model describes redevelopment of installations, i.e., substitution of an old process by a new one run on the same installation. For a given k-th process it is formulated as follows:

$$\frac{1}{\hat{z}_k^o} z_k^o + \frac{1}{\hat{z}_k^n} z_k^n \leq 1 \tag{5}$$

where:

$\hat{z}_k^o$, $\hat{z}_k^n$ denote capacities of an old and new k-th process,

z_k^o , z_k^n denote production levels of an old and new k-th process.

The idea of new technologies is fundamental to this approach, as it opens the way to technological restructuring of the PDA.

3.2 The Linear Programming Problem

It is obviously necessary to add some additional constraints on resource availability or waste production limits and a set of criteria which reflect the preference or goals of the decision maker.

First, it is assumed that for a fixed production goal only efficiency (or revenue) will be maximized. This leads to the problem:

$$Q_{rev} = \sum_{j \in J} c_j^s (y_j^{ms} + y_j^{cs}) - c_j^p (y_j^{mp} + y_j^{cp}) \quad \rightarrow \quad \max \tag{6}$$

with constraints given by market conditions and production capacities.

Following another decision strategy, resource consumption may be minimized, which results in the set of criteria:

$$Q_{ener} = \sum_{k \in K} e_k z_k \quad \rightarrow \quad \min \tag{7a}$$

$$Q_{inv} = \sum_{k \in K} n_k z_k \quad \rightarrow \quad \min \tag{7b}$$

$$Q_{labor} = \sum_{k \in K} l_k z_k \quad \rightarrow \quad \min \tag{7c}$$

One of the four objectives implemented is minimal cost of waste treatment i.e.,:

$$Q_w = \sum_{l \in L} t_l w_l \quad \rightarrow \quad \min \tag{8}$$

where t_l denotes unit cost of treatment of waste l.

From the above objective functions one may derive another useful optimization problem based on linear fractional functions (e.g., Q_{rev} / Q_{ener}) as well as various multiobjective problems. Of course, any objective (6) - (8) can be transposed onto a corresponding constraint.

Structural Correctness Control Module

This module is aimed at automatic analysis of the PDA network structure for the sake of formal correctness of the model. The module checks, for instance, whether a given constraint exists in the MPS file regardless of a value of the constraint, hence the analysis is only qualitative.

3.3 The Discrete Post-processor*)

The problem of comparing the alternative model outcomes is a well known discrete, multiobjective decision problem, in which all feasible alternatives are explicitly listed in the finite set

$x^0=\{x_1,x_2,\ldots,x_n\}$,

and the values of all criteria of each alternative are known and listed in the set

$Q=\{f(x_1),f(x_2),\ldots,f(x_n)\}$.

There are many tools which could be employed to solve this problem (e.g., Korhonen, 1985, Majchrzak, 1984). We have drawn on the method developed by Majchrzak (1985).

Usually, the procedure of problem solving is divided into two stages. The first stage is the selection of elements of a nondominated set from all the alternatives of set x^0. In the second stage, the "best" solution is identified as the decision maker's final solution to the problem under consideration, in accordance with his preferences, experience etc., as the basis for his decision.

In the discrete, multicriteria optimization module of the overall system, at the first stage of problem solving, the dominated approximation method is used to select the elements of the pareto set, because of its calculation efficiency and its ability to solve relatively large-scale problems. For instance, this method can be used to solve a problem with 15-20 criteria and more than a thousand alternatives, which is sufficient for processing the data arising from scenario analysis in the framework system.

In the second stage, an interactive procedure based on the reference point theory is employed to help the user to find his final solution. This approach combines the analytical power of the "hard" computer model with the qualitative assessments of the decision maker in the decision process. It makes the decision process more reasonable and closer to the human thinking process.

3.4 Implementation

The software system is implemented on a dedicated 32-bit color graphics workstation under the UNIX operating system.

The models are coded in FORTRAN77 and C, the graphics are based on the ACM Core graphics standard plus selected low-level raster routines, introduced for performance reasons.

*) This section is based on Zhao et al., (1985), and describes the the Reference Point Approach developed by Wierzbicki (1979, 1980) and the DISCRET package developed by Majchrzak (1984, 1985).

4. References and Selected Bibliography

Ahmed, K.A. (1985) Pesticide Consumption and Problems in the Third World: Towards Development of Marketing Guidelines to Reduce Misuse. In Chemistry & Industry, September 16, 1985 pp.610-612.

Baram, M. (1985) Implementation and evaluation of regulations. In H. Otway and M. Peltu [eds.] Regulating Industrial Risks. Science, Hazards and Public Protection. Butterworths, London. 181p.

Burns, L.A., Cline, D.M. and Lassiter, R.R. (1981) Exposure Analysis Modeling Systems (EXAMS): User Manual and Systems Documentation. USEPA Environmental Research Laboratory, Athens, GA. 460p.

Changkong, V., Haimes, Y.Y.(1983) Multiobjective Decision Making: Theory and Methodology. North Holland, New York.

Chemical & Engineering News (1986) Facts & Figures for the Chemical Industry. Section Five: Foreign Chemical Industries. June 9, 1986, Vol.64, Nr.23, p.83-84.

Dobrowolski, G., Kopytowski, J., Lewandowski, A. and Zebrowski, M. (1982) Generating Efficient Alternatives for Development in the Chemical Industry. CP-82-54. International Institute for Applied Systems Analysis, A-2361 Laxenburg, Austria. 32p.

Dobrowolski, G., Kopytowski, J., Wojtania, J. and Zebrowski, M. (1984) Alternative Routes from Fossil Resources to Chemical Feedstocks. RR-84-19, International Institute for Applied Systems Analysis, A-2361 Laxenburg, Austria. 53p.

Dobrowolski, G., Kopytowski, J., Rys, T., Zebrowski, M. (1985). MIDA (Multiobjective Interactive Decision Aid) in the development of the chemical industry. In: Theory, Software and Testing Examples for Decision Support Systems [eds.] A.Lewandowski, A.Wierzbicki, WP-87-26, International Institute for Applied Systems Analysis, A-2361 Laxenburg, Austria.

Gomide, F., Tarvainen, K., Haimes, Y.Y. (1984). Iterative Negotiations on Multiple Objectives in Large Scale Systems, IFAC 9th World Congress, Budapest.

Fedra, K. (1985) Advanced Decision-oriented Software for the Management of Hazardous Substances. Part I: Structure and Design. CP-85-18, International Institute for Applied Systems Analysis, A-2361 Laxenburg, Austria. 61p.

Fedra, K. (1986) Advanced Decision-oriented Software for the Management of Hazardous Substances. Part II: A Demonstration Prototype System. CP-86-10, International Institute for Applied Systems Analysis, A-2361 Laxenburg, Austria. 98p.

Fedra, K. and Otway, H. (1986) Advanced Decision-oriented Software for the Management of Hazardous Substances. Part III. Decision Support and Expert Systems: Uses and Users. CP-86-14, International Institute for Applied Systems Analysis, A-2361 Laxenburg, Austria. 44p.

Fedra, K., Weigkricht, E. and Winkelbauer, L. (1987) A Hybrid Approach to Information and Decision Support Systems: Hazardous Substances and Industrial Risk Management. Proceedings of the First IFAC/IFORS/IFIP/AFCET Conference on Economics and Artificial Intelligence, Aix-en-Provence, France, September 2-4, 1986. IFAC Publications, Pergamon.

Gorecki, H., Dobrowolski, G., Kopytowski, J. and Zebrowski, M. (1982) The quest for a concordance between technologies and resources as a multiobjective decision process. In M. Grauer, A. Lewandowski, and A.P. Wierzbicki [eds.] Multiobjective and Stochastic Optimization. Collaborative Proceedings CP-82-S12, International Institute for Applied Systems Analysis, A-2361 Laxenburg, Austria.

FAO (1985) Production Yearbook, Food and Agricultural Organization of the United Nations. Vol.35 p.315.

Frost & Sullivan Inc. (1984) News, Report Nr. E635, May 25,1984. 4p.

Grauer, M. and Lewandowski, A. (1982) The reference point approach - methods of efficient implementation. WP-82-26, International Institute for Applied Systems Analysis, A-2361 Laxenburg, Austria.

Grauer, M. and Kaden, S. (1984) A non-linear dynamic interactive decision analysis and support system (DIDASS/N). Users Guide. WP-84-23, International Institute for Applied Systems Analysis, A-2361 Laxenburg, Austria.

Grauer, M., Lewandowski, A. and Wierzbicki, A. (1984) Multiple-Objective Decision Analysis Applied to Chemical Engineering. RR-84-15, International Institute for Applied Systems Analysis, A-2361 Laxenburg, Austria. 40p.

Grauer, M. and Fedra, K. (1986) Intelligent Decision Support for Technology Assessment: The Chemical Process Industry. Paper presented at the VIIth International Conference on Multiple Criteria Decision Making, August 18-22, 1986, Kyoto, Japan.

Haigh, N. (1984) EEC Environmental Policy and Britain. Environmental Data Services Ltd., London. 324p.

Hay, A. (1982) The Chemical Scythe. Lessons of 2,4,5-T and Dioxin. Plenum Press, New York. 264p.

Hetrick, D.M. and McDowell-Boyer, L.M. (1978) TOX-SCREEN: A multimedia screening level model for assessing the potential fate of toxic chemicals released to environmental media. In Proceedings, 1983 Summer Computer Simulation Conf., Simulation Councils, Inc., La Jolla, CA., pp.464-469.

Hetrick, D.M. and McDowell-Boyer, L.M. (1984) User's Manual for TOX-SCREEN: A Multimedia Screening-level Program for Assessing the Potential Fate of Chemicals Released to the Environment. ORNL-6041, Oak Ridge National Laboratory and EPA-560/5-83-024, USEPA, Washington, D.C., 301p.

Korhonen, P. (1985) A Reference Direction Approach to Solving Discrete Multiple Criteria Problems. Paper presented at the Seventh European Congress on Operations Research, Bologna, Italy, June 16-19, 1985.

Kreglewski, T. and Lewandowski, A. (1983) MM-MINOS--An Integrated Interactive Decision Support System. Collaborative Paper, CP-83-63, International Institute for Applied Systems Analysis, Laxenburg, Austria.

Lave, L. [ed.] (1982) Quantitative Risk Assessment in Regulation. Studies in the Regulation of Economic Activity. The Brookings Institution, Washington, D.C. 264p.

Majchrzak, J. (1984) Package DISCRET for multicriteria optimization and decision making problems with discrete alternatives. IIASA conference on Plural Rationality and Interactive Decision Processes, 16-26 August, 1984, Sopron, Hungary.

Majchrzak, J. (1985) DISCRET--An Interactive Package for Discrete Multicriteria Decision Making Problems. Report, June 1985. Systems Research Institute, Warsaw, Poland.

Majone, G. (1985) The international dimension. In H. Otway and M. Peltu [eds.], Regulating Industrial Risks. Science, Hazards and Public Protection. Butterworths, London. 181p.

McDowell-Boyer, L.M. and Hetrick, D.M. (1982) A Multimedia Screening-Level Model for Assessing the Potential Fate of Chemicals Released to the Environment, ORNL/TM-8334. Oak Ridge National Laboratory.

Otway, H. and Peltu, M [eds.] (1985) Regulating Industrial Risks. Science, hazards and public protection. Butterworths, London. 181p.

Predicasts Inc. (1984) Worldcasts, pp.B114-B115.

Saxena, J. (1983) Hazard Assessment of Chemicals. Current Developments, Volume 2. Academic Press, New York. 361p.

Schmucker, K.J. (1984) Fuzzy Sets, Natural Language Computations, and Risk Analysis. Computer Science Press, Rockville, MD. 192p.

Smith, J.H., Mabey, W.R., Bohonos, N., Holt, B.R., Lee, S.S., Chow, T.W., Bomberger, D.C. and Mill, T. (1977) Environmental Pathways of Selected Chemicals in Freshwater Systems. EPA 600/7-77-113, US Environmental Protection Agency.

Sol, H.G. (1983) Processes and Tools for Decision Support. North-Holland, Amsterdam. 259p.

Technica (1984) The SAFETI Package. Computer-Based System for Risk Analysis of Process Plant. Vols.I-IV and Appendices I-IV. Technica Ltd., Tavistock Sq., London.

Weigkricht, E. and Winkelbauer, L. (1987) Knowledge-based Systems: Overview and Selected Examples. WP-87-xx, International Institute for Applied Systems Analysis, A-2361 Laxenburg, Austria. Forthcoming.

Winkelbauer, L. (1987) Symbolic Simulation of Chemical Production Processes. WP-87-45. International Institute for Applied Systems Analysis, A-2361 Laxenburg, Austria. 55p.

Wierzbicki, A.P. (1979) The Reference Objectives in Multiobjective Optimization – Theoretical Implications and Practical Experience. WP-79-66, International Institute for Applied Systems Analysis, A-2361 Laxenburg, Austria.

Wierzbicki, A.P. (1979) A Methodological Guide to Multiobjective Optimization. WP-79-122, International Institute for Applied Systems Analysis, A-2361 Laxenburg, Austria.

Wierzbicki, A.P. (1980) A Mathematical Basis for Satisficing Decision Making. WP-80-90. International Institute for Applied Systems Analysis. A-2361 Austria.

Wierzbicki, A. (1983) A Mathematical Basis for Satisficing Decision Making. Mathematical Modeling USA 3:391-405. (IIASA RR-83-7).

Zebrowski, M., Rys, T., Skocz, M., and Ziembla, W. (1985) Modeling the Chemical Industry for Management of Technological Hazards and Wastes. Academy of Mining and Metallurgy, Cracow and International Institute for Applied Systems Analysis, Laxenburg, Austria. Unpublished.

Zhao, Ch., Winkelbauer, L., and Fedra, K. (1985) Advanced Decision-oriented Software for the Management of Hazardous Substances. Part VI: The Interactive Decision-support Module. CP-85-50, International Institute for Applied Systems Analysis, A-2361 Laxenburg, Austria. 39p.