PHD

The environmental process performance tool

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Award date:
1998

Awarding institution:
University of Bath

THE ENVIRONMENTAL PROCESS PERFORMANCE TOOL

A tool to determine the environmental impact and environmental performance of batch chemical processes

Submitted by Heidi Aubrey for the degree of
PhD of the University of Bath
1998

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Acknowledgements

I would like to thank my supervisors Dr Bev Sowerby and Professor Barry D Crittenden for their help and guidance throughout this project. I would like to add special thanks to Dr Bev Sowerby for her continual support and encouragement throughout her time at the University of Bath and also through her own career advancement. Thank you also to Thomas Swan for permitting their process to be used in this study and particularly Ian Findley for his help. I would also like to acknowledge the Engineering and Physical Sciences Research Councils Clean Technology Unit for funding this research.

Thanks also to Claire Houghton (Dr to be!) for her help, co-operation and stress relief through the last three and a half years, and also Dr Anthony Elliott for his help during the first year of this research.

Thanks to Mum, Dad and Dan for their love, support and encouragement and also to Gran and Pop whose spirit saw me through. I would like to add one last special thanks to Iggy whom I am indebted for looking after me and keeping me sane over the last few years.

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Abbreviations

AF	Assessment Factor
BAT	Best Available Techniques
BATNEEC	Best Available Techniques Not Entailing Excessive Cost
BEO	Best Environmental Option
BOD	Biological Oxygen Demand
BPEO	Best Practicable Environmental Option
BS	British Standard
CFC	Chlorofluorocarbon
CGA	Cradle to Grave Approach
CIA	Chemical Industries Association
COD	Chemical Oxygen Demand
COSHH	Control of Substances Hazardous to Health
CoPA	Control of Pollution Act 1974
CPAS	Clean Process Advisory System
DDT	Dichlorodiphenyl trichloroethane
DoE	Department of the Environment
DOSE	Dictionary of Substances and their Effects
EA	Environment Agency
EAL	Environmental Assessment Level
EB	Environmental Burden
EC	European Community
EC_{50}	Effective Concentration to cause a defined effect on 50% of the test population
EEC	European Economic Community
EHI	Environmental Hazard Index
EII	Environmental Impact Indices
EINECS	European Inventory of Existing Commercial Chemical Substances
ELF	Environmental Load Factors
EMAS	Environmental Management and Audit Scheme
EMS	Environmental Management Systems
EniVal	Environmental Impact Valuator
ENVOP	ENVironmental OPtimisation
EPA 1990	Environmental Protection Act 1990
EPI	Environmental Performance Indicator
EPPT	Environmental Process Performance Tool
EPS	Environmental Priority Strategies
EQ	Environmental Quotient
EQI	Environmental Quality Indices

EQS	Environmental Quality Standard
ET	Environmental Theme method
F_{new}	Fisons proposed new process
F_{old}	Fisons existing process
FTSE	Financial Times Stock Exchange
GMB	Graphical Mass Balance
GWP	Global Warming Potential
HAZOP	HAZard OPerability
HEN	Heat Exchange Networks
HMIP	Her Majesty's Inspectorate of Pollution
HSE	Health and Safety Executive
IE	Industrial Ecology
IEH	Inherent Environmental Hazard
IEI	Integrated Environmental Index
IMS	Industrial Methylated Spirits
IPC	Integrated Pollution Control
IPCS	International Programme on Chemical Safety
IPCC	International Programme on Climate Change
IPPC	Integrated Pollution Prevention Control
IRIS	Integrated Risk Information System
IRPTC	International Register of Potentially Toxic Chemicals
ISI	Inherent Safety Index
ISO	International Standards Organisation
IVL	Swedish Environmental Research Institute
LC_{50}	Lethal Concentration to 50% of the test population
LCA	Life Cycle Analysis
LD_{50}	Lethal Dose to 50% of the test population
MDR	Maximum Deposition Rate
MEIM	Methodology for Environmental Impact Minimisation
MEL	Maximum Exposure Limit
MEN	Mass Exchange Network
MFAKC	Motor Fuel Anti-Knocking Compounds
MIBK	Methyl Isobutyl Ketone
MMA	Methyl Methacrylate
NEC	No Effect Concentration
NOEL	No Observable Effect Level
NRA	National River's Authority
ODP	Ozone Depletion Potential
OECD	Organisation for Economic Co-operation and Development
OEL	Occupational Exposure Limit
OES	Occupational Exposure Standards
PAH	Poly Aromatic Hydrocarbon
PCB	Polychlorinated Biphenyl

PEC	Predicted Environmental Concentration
PET	Polyethylene terephthalate
PF	Potency Factor
PNEC	Predicted No Effect Concentration
POCP	Photochemical Ozone Creation Potential
PSI	Primary Standards Index
REPA	Resource Environmental Profile Analysis
SCG	Sodium Cromoglycate
STHI	Specific Terrestrial Hazard Index
SETAC	Society for Environmental Toxicology and Chemistry
SUAQI	Standard Urban Air Quality Index
SWHI	Specific Water Hazard Index
TDA-1	Tris(3,6 Dioxaheptyl)amine
TEL	Tetra Ethyl Lead
TML	Tetra Methyl Lead
TS	Thomas Swan
UBA	German Federal Environment Agency
UK	United Kingdom
UN	United Nations
UNEP	United Nations Environmental Programme
US EPA	United States Environmental Protection Agency
VDP	Vegetation Damage Potential
VOC	Volatile Organic Compounds
WQIA	Weighted Arithmetic Water Quality Index
WQIAU	Unweighted Arithmetic Water Quality Index
WQIM	Weighted Multiplicative Water Quality Index
WQIMU	Unweighted Multiplicative Water Quality Index

Nomenclature

a	Air volume fraction
c	Concentration
d	Density
s	Soil volume fraction
v	Volume
w	Water volume fraction
F_a	Fraction of chemical in air
F_w	Fraction of chemical in water
F_s	Fraction of chemical in soil
f_{oc}	Fraction of organic carbon
K_{oc}	Organic carbon coefficient
K_{ow}	n-Octanol water partition coefficient
K_p	Soil adsorption coefficient
K_w	Inverse of Henry's Law Constant
Q_i	Quantity of pollutant *i*
Q_T	Overall production rate
wt%	Weight percent

1. Introduction

Over recent years there has been a major increase in concern for the environment. Today's consumer society has increased the demand for chemicals. As a result the chemical industry has become one of the major polluters of the modern era. The necessity to produce many chemicals is appreciated however it is of the utmost importance that they are produced in the least environmentally damaging way possible. There is an increasing need for environmental assessment techniques to determine the impact of chemical process. Until recently this has only received limited attention.

This thesis identifies the need for environmental assessment techniques, evaluates existing techniques and presents a new approach to assess the environmental impact of chemical processes. This approach is the Environmental Process Performance Tool, known as the EPPT.

This chapter provides an overview of the environment movement and the pressures from stakeholders on the chemical industry. It identifies the need for environmental assessment tools and addresses legislative measures adopted in the UK and the European Union. Strategies such as pollution prevention and waste minimisation employed by industry in response to environmental pressure are also considered.

In Chapter 2 the various types of environmental assessment and their application and limitations are discussed. The requirements for an environmental assessment tool with specific application to the chemical industry are highlighted. In Chapter 3 the focus for the Environmental Process Performance Tool is detailed. The aims and objectives of the EPPT are identified together with the concepts adopted from existing techniques and the novel aspects of the EPPT. The remaining chapters of the thesis are then outlined. They focus on the EPPT, its development, structure and application.

1.1 Concern for the environment

With public concern for the environment at an all time high, demonstrated by the UK environmental group membership rising from 1.8 million in the 1980's to almost 4 million in the mid 1990's (Hunt and Johnson, 1995), the environmental movement is going from strength to strength. This concern for the environment has escalated since the mid 1970's; some of the most significant milestones directing this move are included in Table 1.1 (adapted from Hunt and Johnson, 1995):

Table 1.1: Significant milestones in the environmental movement

Year	Milestones
1984	Accident at Union Carbide plant at Bhopal kills over 2000
1984	Liquefied natural gas plant explosion kills 452 in Mexico City
1985	Greenpeace ship *Rainbow Warrior* blown up by French agents
1985	World population passes 5 billion
1986	Chernobyl nuclear power station disaster
1986	Lead-free petrol available in the UK
1986	Sandoz warehouse fire, Basel, pollutes the Rhine
1987	Publication of *Our Common Future* (The Bruntland Report)
1987	European Year of the Environment
1988	Chico Mendes, defender of the rainforest, assassinated
1988	Publication of the *Green Consumer Guide*
1989	*Exxon Valdez* tanker disaster
1990	Shell fined £1 million for oil pollution of the Mersey
1992	Publication of BS 7750
1992	Earth Summit, Rio, Brazil
1993	*Braer* tanker disaster
1995	Massive protests over road building schemes
1996	Dumping of Brent Spar Oil Platform at sea
1997	Expansion of Manchester Airport
1997	Earth Summit +5, New York

'Green' consumerism, 'green' advertising and 'green' investment are also taking hold together with environmental reporting, environmental economics and an increased interest in 'sustainable development'. People are now genuinely concerned about the environment and there is no avoiding that this is a major issue for the latter part of the 20th Century.

1.2 Industry and the environmental movement

The attitude of industry and commerce has also evolved with public concern. Initially industry was defensive with regard to its environmental impacts. However, an acceptance is developing through to a need for environmental probity as a prerequisite for organisational survival and success. The Chairman of the Board of Management of Bayer AG stated: '.....the future success of the chemical industry .... depends on it being as environmentally compatible and safe as possible' (Strenger, 1991) and ICI's Chairman stated: 'the chemical industry does not currently enjoy a favourable reputation on its environmental performance ......' (ICI, 1992). It has become necessary for industry to adopt a sound and forward looking approach to environmental issues. Primarily this pressure has been driven by legislative and regulatory requirements. However, it has been realised that the potential benefits of sound environmental performance and attitudes could be numerous as indicated in Table 1.2 below.

Table 1.2: Benefits of sound environmental performance (Hunt and Johnson, 1995)

Legal	Avoidance of litigation, fines and legal costs, clean up costs, civil liabilities
Image	Enhanced organisational pride, corporate image/PR, attractiveness as employer
Financial	Increased financial confidence of regulators, investors and insurers
Management	Improved 'peace of mind', consistency on issues and time utilisation
Business	Enhanced performance from product differentiation, 'Eco-label' recognition, improved market share, improved margins, sound and opportune investment, improved cost control and sound acquisition and divestment

Organisations are now realising the importance of their environment performance and public image with regard to the environment, particularly the chemical industry as demonstrated by the quotes from Bayer and ICI chairmen. Companies are now adopting strategies such as environmental management systems (EMS) and environmental audits, as well as developing environmental performance indicators to demonstrate their environmental stance. These subjects will be discussed in Chapter 2.

1.3 Environmental legislation

In response to increased concern for environmental protection there has been a steady increase in environmental legislation over the last few years. Environmental legislation is not new and has been around for many years with its origins at the time of the industrial revolution. Air pollution became a major problem during the industrial revolution due to the increased use of coal to drive new machinery. The acidic emissions of hydrogen chloride from the 'alkali works' also increased air pollution. As a result, large areas of the country were severely damaged by the very highly acidic moist air burning trees, shrubs and hedges. A report from one of the centres of the alkali industry says of St. Helens, one of the centres of the alkali industry, 'there was not a single tree with any foliage on it' (Ball and Bell, 1991). This concern led to the setting up of a Royal Commission to look at the problems of alkali pollution. The recommendations from the report led to the inception of the Alkali Act in 1863. Numerous updates of this Act and additional Acts have since been implemented.

In the 1950's smog became a real problem in London. In December 1952 a smog descended on London which lasted for five days and claimed almost 4,000 lives. This immediately led to the formation of the Beaver Committee which reported on smoke pollution (Ball and Bell, 1991). Recommendations from the report led to the formation of the Clean Air Act of 1956.

Many other acts concerned with the pollution of individual media or problems with the health of the public ensued. For example, one of the first Acts to protect the aqueous environment was the Water Act of 1973. As a result, 10 water authorities were created to deal with the issue related to water supply and demand. The National Rivers Authority (NRA) was created in the 1989 update of the Water Act of 1973 with the responsibility of monitoring and controlling the pollution of Britain's controlled waters.

The Control of Pollution Act (CoPA) of 1974 was introduced to deal with municipal, commercial and industrial waste disposal. Details of these Acts and other environmental legislation can be found in Croner's Environmental Management and Case Law publication (1997).

As a result of the two World Wars and the economic depression of the 1930's, few environmental laws were enacted in the early part of the twentieth century. More environmental legislation was passed between 1950 and 1975 but it was not until after this that the real growth in environmental legislation came about. This was in response to three main elements:

1. Concern on the part of stakeholder, such as the public, media and pressure groups.
2. International conventions, agreements and protocols on environmental matters.
3. Directives and other instruments enacted by the European Union.

Concern on the part of the public has been discussed earlier. The next section looks at some international conventions and agreements that are emphasising concern for the environment. Legislation and EU Directives are then discussed in Sections 1.3.3-1.3.5.

1.3.1 International conventions and agreements

In 1973 (the same year that the UK joined the EEC), the first Environmental Action Programme was agreed between Community members. In 1985, the fifth programme 'Towards Sustainability' sets out a broad approach which the community would take on environmental matters up to the end of the millennium. The World Commission on Environment and Development (also known as the Bruntland Commission) introduced the concept of sustainable development in 1987 in its report 'Our Common Future' (World Commission on Environment and Development, 1987). This defined sustainable development to be:

> "development that meets the needs of the present without compromising the ability of future generations to meet their own needs".

This report outlined much of the debate at the UN Commission on Environment and Development conference (known as the Rio or Earth Summit) held in Rio de Janeiro, Brazil in 1992. One of the outcomes of this meeting was 'Agenda 21', an operational plan for the implementation of sustainable development in the 21st century (Prendergast, 1993).

The sustainable development strategy has significant implications as it requires a radical rethink of what is important to people, primarily in the developed world, and the signals that are being given out to developing countries. Developing countries exploit their natural resources and environment to achieve urgently needed economic growth but they must retain a healthy renewable resource base for the future. The integration of environmental assessment into economic policy and decision making of developing countries has been difficult. However the industry orientated approach and sustainable development implied by the Integrated Pollution Prevention Control (section 1.3.5), may allow a balance of immediate returns against sustainable productivity to be attained (Carpenter, 1981).

The signing of the Montreal Protocol part of the Vienna Convention, by the European Commission (a body of the European Union), also highlighted the environmental situation by acknowledging the real problem of ozone layer depletion caused from the use of chlorofluorocarbons (CFC's). The agreement by the European Commission to stabilise carbon dioxide emissions at 1990 levels by 2000 also formally acknowledged the issue of global warming.

1.3.2 Recommendations for environmental legislation

Recommendations from the Royal Commission on Environmental Pollution, the House of Commons Select Committee on the Environment and the EU underlie some of the basic principles of UK environmental law. These include:

- A move towards specific, numerical standards and away from general notions of 'harm'.
- Treatment of the environment as a whole rather than on a compartmental basis.
- Consolidation of environmental legislation and enforcing regulatory bodies.
- Requirements of potential polluters to apply for permission to operate, discharge or emit.
- Requirements for operators to demonstrate fitness to operate processes.
- Requirements of operators to demonstrate the use of specific techniques.
- Application of the 'Polluter Pays Principle' to the cost of control and clean-up.
- Growing use of public registers and greater 'transparency' of pollution control measures.
- Increases in fines, and the sanction of custodial sentences for responsible individuals.
- Increased monitoring, especially on the part of the process operators (Hunt and Johnson, 1996).

Many of these principles have been incorporated into the UK's Environmental Protection Act of 1990 which now demonstrates an integrated approach to environmental protection.

1.3.3 The Environmental Protection Act, 1990

In 1990 in the United Kingdom a major change in the way the environment is regulated came about with the creation of the Environmental Protection Act (EPA 1990). This was the first piece of legislation to allow the environment to be considered as a whole not just as individual media. The EPA 1990 allowed an integrated approach to environmental regulation under the Integrated Pollution Control (IPC) regime. The aims of IPC are 'to prevent or minimise the release of prescribed substances and to render harmless any such substances which are released .... to develop and approach to pollution control that considers discharge from industrial media in the context of the effect on the environment as a whole' (Weston and Stuckey, 1994).

IPC requires certain processes operating in the UK to have an authorisation from the Environment Agency. This requirement has been phased in over a number of years starting with the largest and most polluting industries. Now all processing industries are required to submit an application for authorisation. The application provides details of the process and emissions from that process and is required to demonstrate the selection of Best Practicable Environmental Option (BPEO).

The Best Practicable Environmental Option (BPEO) was first defined in the 12th Report of the Royal Commission on Environmental Pollution (1988) as:

> 'the outcome of a systematic consultative and decision-making procedure which emphasises the protection of the environment across land, air and water. The BPEO establishes, for a given set of objectives, the options that provides the most benefit or least damage to the environment as a whole, at acceptable cost in the long term as well as the short term'.

The EPA 1990 legislation supersedes much of the former legislation to allow for an integrated approach and introduces new requirements which adopt the recommendations detailed in Section 1.3.2. These include:

- The need to minimise pollution with regard to the Best Practicable Environmental Option (BPEO).

- The need to control emissions using the Best Available Techniques Not Entailing Excessive Cost (BATNEEC).
- An increase from £2000 to £20,000 in the maximum fine for a pollution offence which can be imposed in a magistrates' court.
- The ability of the erstwhile HMIP (Her Majesty's Inspectorate of Pollution) to seek, in the High Court, enforcement orders against persistent polluters.
- The empowerment of the HMIP to issue prohibition notices for a prescribed process in certain circumstances (Hunt and Johnson, 1996).

The Best Available Techniques Not Entailing Excessive Cost (BATNEEC) are used to minimise the release of prescribed substances to the medium for which they are prescribed. It provides a means of determining the term 'practicable' in BPEO. This is necessary as often it is found that the Best Environmental Option (BEO) is the most expensive and its cost far outweighs the benefit to the environment.

In order to determine the BPEO it is necessary to assess the environmental impact of various processes and process options. Several tools, methodologies and philosophies have been developed and applied to various often quite specific situations. These tools and methods will be discussed in Chapter 2.

1.3.4 The Environment Agency

Until 1996 Her Majesty's Inspectorate of Pollution was responsible for the implementation of IPC. Local authorities were in charge of small operators who generated emissions solely to air, the NRA was responsible for water quality and consents for emissions to controlled water and the Waste Regulatory Authorities dealt with household and municipal waste and the control of landfill sites. However on 1st April 1996 the Environment Agency was established under the conditions of the Environment Act 1995. It encompasses the responsibilities and expertise of the authorities detailed above and provides a 'one-stop shop' for improved customer service. The objectives of the Environmental Agency (EA) are:

- To adopt an integrated approach to environmental protection and enhancement which considers impacts of substance and activities on all environmental media and on geographical regions.
- To work with industry and others to develop approaches which deliver environmental requirements and goals without imposing disproportionate costs on industry or society as a whole.
- To adopt clear and effective procedures for serving its customers, including the development of single points of contact through which industry and others can deal with the Agency.
- To operate to high professional standards, based on the best possible information and analysis of the environment and of the processes which affect it.
- To organise its activities in ways which reflect good environmental practice and provide value for money for those who pay its charges and taxpayers as a whole.
- To provide clear and readily available advice and information on its work.
- To develop a close and responsive relationship with the public, local communities and regulated organisations (Environment Agency, 1995).

1.3.5 Future environmental legislation and the European Union

As is apparent from the previous sections the European Union, previously the European Community, has played a significant role providing direction for the development of environmental legislation in the UK. In 1996 the European Union adopted a Directive on Integrated Pollution Prevention and Control (IPPC). This Directive has similarities to the UK IPC system in that its aim is to prevent emissions of substances to the environment or reduce them to a minimum through the application of Best Available Technology (BAT). BAT is defined as 'being industrially feasible, in the relevant sector, from a technical and economic point of view' and is therefore equivalent to the UK BATNEEC (Munns, 1996).

The fundamental differences in IPC and IPPC lie in their focus. IPC looks at processes with a substance based approach considering releases and operational conditions, whereas IPPC has an industry based approach looking at the number of processes on a site and also the associated activities such as laboratories, canteens and truck maintenance, all of which have an environmental impact.

New installations under IPPC directive based legislation will have to demonstrate that they are a sustainable development. They must show consideration for three particular aspects of the environment:

1. Resource conservation.
2. Energy efficiency.
3. Waste minimisation.

To demonstrate resource conservation it must be shown that the process is operating efficiently, that the use of resources is as effective as possible, that is not wasteful, and that other resources have been considered. The efficient use of energy must be demonstrated and a waste minimisation strategy in the widest context must be shown (Munns, 1997). Waste minimisation in the UK is discussed in the next section. Discussions on the US approach to waste minimisation can be found in Doerr (1993), Chadha (1994) and Allen (1992).

1.4 Waste minimisation

In Section 75 of EPA 1990 the statutory definition of waste is given whereby waste: 'includes (a) any substance which constitutes a scrap material or an effluent or other unwanted surplus substance arising from the application of any process and (b) any substance or article which requires to be disposed of as being broken, worn out, contaminated or otherwise spoiled'.

Smith (1996a) defines waste as 'any material or energy which, in the eyes of the producer, arises at a rate and in a form such that it has no value'. While there is no perceived value to the producer it:

1. represents a loss of raw material or energy to the producer with the obvious financial burden associated with this together with the less obvious handling, managing and disposal costs of the waste;
2. it has the potential to cause environmental harm, directly or indirectly; and
3. waste treatment and disposal are becoming increasing regulated and expensive, an additional financial burden to the producer (Smith, 1996a).

The minimisation of these wastes has obvious benefits. Not only reduction in operating and disposal costs but also the attainment and improvement of regulatory requirements, increased health and safety to the employees and the promotion of a positive public image. From these obvious benefits the adoption of waste minimisation or pollution prevention strategies is essential for any company wanting to remain competitive into the next century.

3M was one of the first companies to give waste minimisation formal status in 1975 with its 'Pollution Prevention Pays' programme by ensuring all employees were aware of the corporate goal (Coates, 1994). Since then numerous large multinational companies such as Dow Chemical, ICI, DuPont and Exxon have all developed environmental initiatives including waste minimisation. In the UK the Chemical Industries Association (CIA) has encouraged this with the 'Responsible Care' programme started in 1989. Responsible Care pushes for improvements in environmental performance. Despite this initiative many small and medium sized companies have a lack of awareness of waste minimisation techniques and are not gaining even from the simple 'good housekeeping' approach where environmental benefits often mean short payback economic benefits (Weston and Stuckey, 1994).

The European Community Council Resolution on Waste Policy (90/C122/01) and the revised Waste Framework Directive (91/156/EEC) sets out a hierarchy of waste management options. This hierarchy is shown in Figure 1.1.

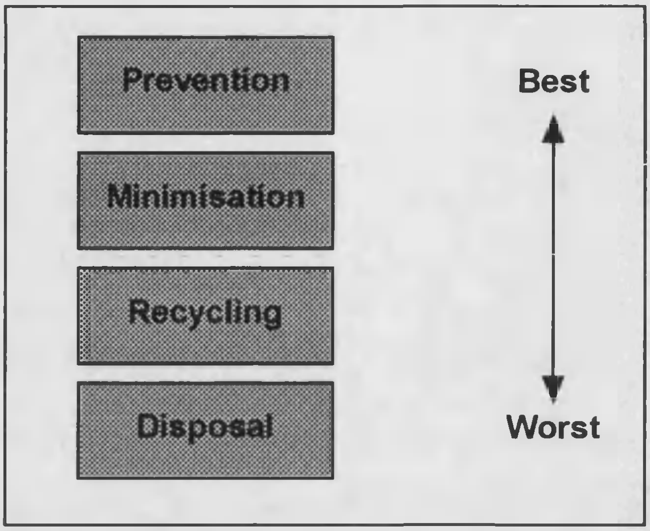


Figure 1.1: Hierarchy of Waste Management Options in EC Council Resolution on Waste Policy (91/156/EEC).

The hierarchy of waste management options can be translated into a hierarchy of waste management practices as shown in Figure 1.2.

Elimination	Complete elimination of waste.	**Highest Priority**
Reduction at Source	The avoidance, reduction or elimination of waste, generally within the confines of the production unit, through changes in industrial processes or procedures.	↑
Recycling	The use, reuse and recycling of wastes for the original or some other purpose such as input material, materials recovery or energy production.	
Treatment	The destruction, detoxification, neutralisation etc. of wastes into less harmful substances.	↓
Disposal	The release of wastes to air, water or land in properly controlled or safe ways so as to render them harmless; secure land disposal may involve volume reduction, encapsulation, leachate containment and monitoring techniques.	**Lowest Priority**

Figure 1.2: The Hierarchy of Waste Management Practices (Crittenden et al, 1995)

The aim of any waste minimisation project should be towards zero emissions and disposal. Complete elimination of waste is the ideal solution to avoid the environmental impact of the process industry, however this is a somewhat idealistic and perhaps unrealistic aim. Focus should therefore be directed towards waste minimisation at source. Several techniques to reduce waste at source are discussed later in this chapter. Recycling is perhaps the next most important approach to waste minimisation. Ideally waste streams should be recycled in the process but onsite or offsite recycling also has benefits. Waste treatment as far as possible should be carried out onsite. More realistically the disposal of wastes should be set out in the company's environmental policy indicating which type of disposal route should be carried out for which waste.

Crittenden and Kolaczkowski (1994a) adopted a more practical and accepted scheme of the waste management options and where they fit together with the focus on waste minimisation. A similar approach is adopted by the US EPA and is discussed by Hopper et al (1993). A further adaptation to Crittenden and Kolaczkowski's scheme is shown in Figure 1.3 below.

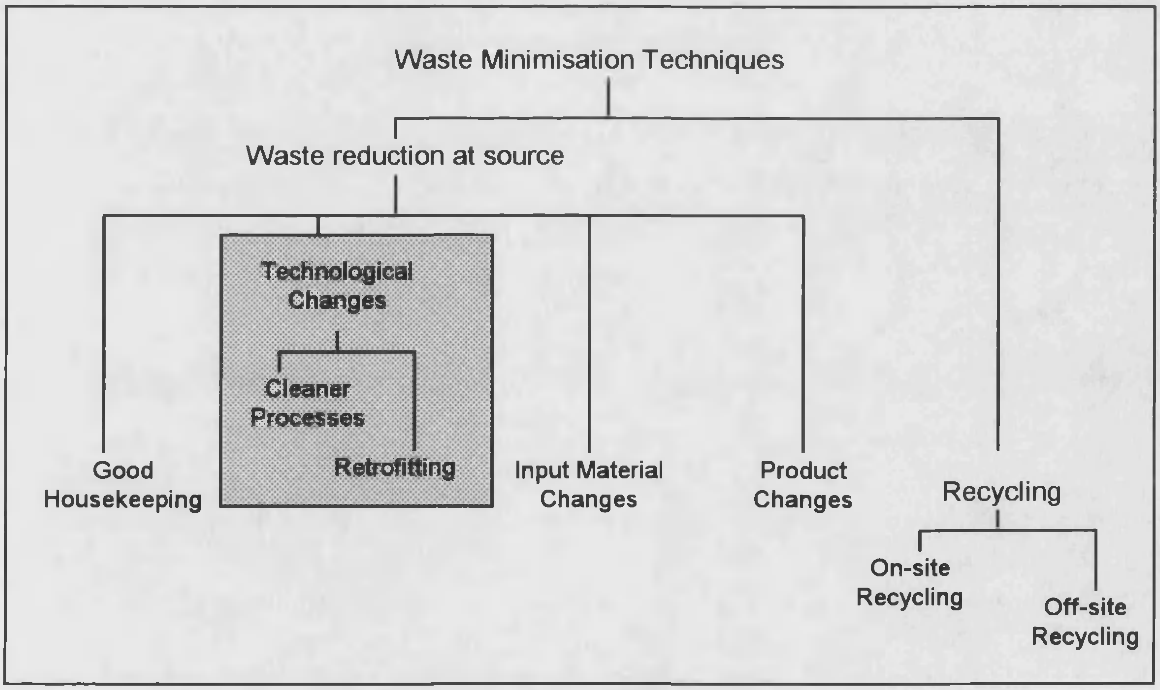


Figure 1.3: Practical Techniques for Waste Minimisation (Crittenden and Kolaczkowski, 1994a adapted from IChemE Guide).

This scheme adopts the same categories as Crittenden et al 1995. However there is an added dimension in Figure 1.3 in that the more important strategies appear near the top of the figure and the less favourable strategies appear lower on the figure.

The two main techniques for waste minimisation are waste reduction at source and recycling. Reduction at source is the most favourable as conceptually there is no need to recycle waste if it hasn't been created. However recycling is useful. It has an application to waste minimisation in its own right and also within reduction at source.

1.4.1 Recycling

In reality many processes require some form of recycling within the process due to thermodynamic or kinetic factors. Often it is a cost effective alternative to treatment and disposal. However for recycling to be effective there must be a need for the waste either as a feed for the process it came from or in another process as a raw material. In some cases it is possible to reclaim some of the constituents of the waste as a valuable material. Recycling is an approach which is also useful in technological changes (Section 1.4.2) and is considered in the design of new processes.

1.4.2 Reduction at source

There are four techniques for reducing waste at source: good housekeeping, input material changes, product changes and technological changes which include retrofitting and developing cleaner processes for the future.

Good housekeeping

Good housekeeping is perhaps the simplest and most cost effective way of reducing waste. It is easily and comparatively cheap to implement and utilises good operating practices and sound engineering such as planned maintenance (Crittenden and Kolaczkowski, 1995).

Many simple techniques are involved some of which have negligible financial outlay. These include:

- identifying and fixing leaks,
- keeping a regular audit of materials purchased against materials used,
- ensuring lids fit solvent tanks,
- changing from small volume containers to larger reusable containers,
- ensuring that staff at all levels are aware of the waste minimisation strategy, and
- encouraging process operators to suggest ways which would help.

Searle, a subsidiary of Monsanto, set targets for production line managers to reduce waste which ideally they suggested should form part of a system by which an employee's overall performance is assessed in order to determine remuneration levels (Coates, 1994).

Case studies demonstrating good housekeeping and the other techniques listed can be found in Crittenden and Kolaczkowski (1995). Larger integrated waste minimisation studies such as the Aire and Calder, Project Catalyst and the Humber Forum Waste Minimisation Projects demonstrate the growth of interest and application of waste minimisation. At least 25 waste minimisation projects are underway in the UK presently involving around 300 companies. The Humber Waste Minimisation Project has saved over £1 million since its inception in February 1995. Additional waste minimisation case studies can be found in Bradburn (1994), Hopper et al (1993) and Schmitt (1996).

Input material changes

Often hazardous materials are used in production. Changes in input material can lead to the reduction in or the avoidance of, hazardous waste production. This can be carried out by increasing the purity of the feed to reduce the amounts of hazardous components in the production system. A method of comparing these changes with respect to their environmental impact is required.

Product changes

Reformulation of products or product intermediates to reduce the amount of waste arising from production is another waste reduction at source technique. An example here would be the change from solvent based to a water based adhesive. An assessment of the impact of products and product alternatives can be carried out using life cycle assessment (LCA). LCA is discussed in Chapter 2.

Technological changes

Retrofitting and cleaner designs encompass the technological changes that result in waste minimisation. Retrofitting is the usual option open to existing processes which have exhausted other waste minimisation techniques. Cleaner designs are not usually an option for existing processes due to the excessive cost of process changes. Separation systems to allow recycling of waste stream components, or the fitting of a more effective scrubber to reduce atmospheric wastes are options which would require a sizeable financial outlay. These options are however, likely to provide benefit only over the longer term. This approach is known as second generation waste minimisation. Good results in waste reduction and often financial gain is obtained however this is generally not nearly as impressive as first generation waste minimisation (good housekeeping).

Both first and second generation techniques are reaching their limits and must make way for third generation waste minimisation. Third generation waste minimisation focuses on highly selective separation and reaction technologies specifically designed for the purpose. New methods of maximising mass efficiency and minimising effluents, and designing energy efficient processes will be developed within third generation waste minimisation (Cohen and Allen, 1992).

Clean design of processes represents the way forward for industry. In the past, chemical plants have been designed with production efficiency, cost and safety as primary considerations. However as mentioned above in third generation waste minimisation (Cohen and Allen, 1992) energy efficiency and effluent minimisation are important considerations for the future when processes will be designed with primary consideration given to the environment.

1.4.3 Clean design

There are three approaches to help designers create new processes. These are the hierarchical review including methods of structured thinking, the mathematical approach and the thermodynamic approach. Each of these methods or a combination of them encompassed in a specific method can help improve a design. They do not however provide a comprehensive, all inclusive method to solve all problems (Spriggs, 1994). It is these approaches which need to be developed further to design intrinsically clean processes and retrofits.

The hierarchical review is the most recent approach and has been applied to many design problems including pollution prevention. Douglas's hierarchical decision procedure, which has been extended to include waste minimisation, provides a simple way of identifying pollution problems in early development stages of a design (Douglas, 1992). This technique is being extended by Houghton (1998, also detailed in Sharratt, 1996) with consideration of energy recovery and focus on batch processes. Further details of the hierarchical, heuristics and related approaches for clean design and energy integration can be found in Rossiter and Spriggs (1993); Spriggs (1994); Fonyo et al (1993); Linhoff (1982) and Smith and Petela (1994).

Environmental Optimisation techniques, known as ENVOP, is a method of structured thinking used for pollution prevention. This method, developed jointly between BP and Costain, is similar to a Hazard and Operability study. ENVOP uses key words to focus a process review on effluent reduction (Potter and Isalski, 1993).

Mathematical approaches can be classified in two categories: analysis and synthesis. These approaches are potentially very powerful tools but have two main drawbacks: they are very difficult to set up and solve by the average designer and do not allow for the creativity or insight of the designer. The analytical approach includes the Graphical Mass Balance (GMB) which is a visual means of mass balance manipulation with defined environmental targets. It allows the designer to look at a range of operational conditions with both economic and environmental conditions in mind (Flower at al, 1993). The synthesis approach includes Mass Exchange Network (MEN) analysis and Heat Exchange Network (HEN) analysis. These techniques involve the 'systematic generation of a cost effective network of mass or heat exchangers with the purpose of preferentially transferring certain species or heat from a set of rich streams to a set of lean streams' (El-Hawagi and Manousiouthakis, 1989).

The two previous approaches, hierarchical and mathematical, rely on a combination of calculation and structured thinking to create new designs. The thermodynamic approaches differ as the fundamental laws and principles of physics are used to first analyse the processes as a system and then point them in the direction of good designs (Spriggs, 1994). Pinch analysis and HEN's are based thermodynamic principles. HEN's are also considered mathematical approaches. In pinch analysis the thermodynamic principles are used to construct plots and perform simple calculations which give powerful insights into heat flows through the process (Rossiter and Spriggs, 1993). Pinch analysis has been extended to wastewater minimisation reducing both effluent treatment and freshwater costs (Wang and Smith, 1994). Details of this technique can be found in Linhoff (1993) and Spriggs (1994).

Computer aided tools for designs with pollution prevention in mind are also being developed. Linninger et al. (1994, 1995) have been developing the *BatchDesign-Kit* which has two main components a *Process_Synthesizer* and a *Process_Assessor*. This, as with the other methodologies detailed above, focus on process synthesis based pollution prevention. Some simulation packages are also being developed with interactive databases which contain chemical data and regulatory information on chemicals (Shanley, 1995).

In the USA a coalition between industry, academia and government are developing 'a computer-based pollution prevention process and product design system that will put environmental design data at the designers fingertips'. This tool, the Clean Process Advisory System (CPAS), moves environmental considerations to the front of design projects (Radecki et al, 1994).

1.5 Macro-, meso- and microscale pollution prevention

Allen (1994) classifies pollution prevention on three levels: macroscale which encompasses the industry sector; mesoscale which is unit operation based; and microscale which looks at the molecular level.

Macroscale pollution prevention considers an industry wide approach and includes industrial ecology and life cycle analysis. Industrial ecology brings in the ideal of zero emissions but widens the scope from one individual process or factory to several processes or factories or any kind of establishment which feeds off other's waste (Schmidt, 1996). Industrial ecology, like the waste minimisation strategies of the UK, signals a shift from end-of-pipe pollution control towards the holistic strategies for prevention and planning of more environmentally sound industrial development (O'Rourke et al, 1996). However with scholars, consultants and environmentalists, the scope of the discipline of industrial ecology lies not only in pollution prevention and the advocation of incremental changes in existing systems but also the total transformation in industrial activity and in some cases 'a metaphor for looking at our civilisation' (Socolow et al, 1994). Details of industrial ecology can be found in Lowe and Evans (1995); O'Rourke et al (1996), Socolow et al (1994) and Graedel and Allenby (1995). Life cycle analysis is also a macroscale approach and can be used in product and process design and assessment. Life cycle analysis and industrial ecology will be discussed in more detail in Chapter 2 with a focus on environmental impact assessment.

The techniques of the UK waste minimisation strategies discussed in Section 1.4 form the basis of mesoscale pollution prevention. Mesoscale pollution prevention focuses on engineering challenges looking at individual industrial facilities where chemical processes and products can be redesigned to reduce waste.

Highly selective separation technologies relying on an understanding of adsorption and other such phenomena provide the basis for microscale pollution prevention. This third generation (section 1.4.1 technological changes) of pollution prevention techniques is discussed in Allen (1994).

Discussion of macro-, meso- and microscale pollution prevention approaches in the USA and case studies can be found in Allen (1994) and Allen and Rosselot (1994).

1.6 The need for environmental assessment

The recognition of waste minimisation by the chemical industry and the shift in emphasis from end-of-pipe technology to clean designs is a great step forward. However, there are major questions to be asked of these changes and process options that are generated - 'How do you tell which has the least environmental impact?' In some cases it is obvious with the reduction of the same emission but how do you compare changing emissions, increased energy use compared with emission reduction and the change of feed? How do you compare the relative merits of process changes?

Many researchers have identified a need for an environmental index or a quantitative tool to assess the environmental impact of process changes. Industry have also demonstrated a need for indices. Some companies, Searle, (Coates, 1994), Rhone Poulenc, (Chemical Engineer, 1993) and ICI (The Chemical Engineer, 1997) have been developing their own indices to demonstrate their environmental performance.

Allen (1992) highlighted the need for 'pollution prevention measurement tools' so that critical emissions and waste streams can be targeted for prevention. Brennan (1993) states that there is a 'pressing need for an environmental index which can distinguish between the environmental merits of alternative processes in new process development and in early phases of project development'. Crittenden and Kolaczkowski in their paper 'Stopping waste within the production process: the Research Councils' Clean Technology Unit initiative' highlights specific areas of research. They state that 'of particular interest to chemical engineers is research on waste or pollution indexing. There is a need to describe numerically the waste produced by a site in terms of both its quantity and 'quality' and an index should be a reflection of the environmental impact of the site on the environment. If properly devised and implemented, a reduction in the index should be more meaningful than simply a reduction in the total amount of waste generated since the latter could be brought about by the reduction in the quantity of the waste stream which has a low environmental impact.....'.

1.7 Summary

This chapter highlights the state of the environment and industry and provides details of the waste minimisation strategies available to reduce the environmental impact of industry as a whole and industrial processes. The need for an environmental assessment tool has been emphasised and with this need in mind the Environmental Process Performance Tool (EPPT) has been developed. The development and application of the EPPT is detailed in Chapter 3. In the next chapter, existing indices and techniques are discussed.

2. Environmental assessment - The need and the tools

Both industry and regulatory bodies have identified a need for an environmental index or a quantitative tool to assess the environmental impact of chemical processes. This chapter gives a critical review of environmental indices and tools currently available which address this need. The cradle to grave approach (CGA) adopted by life cycle analysis (LCA) and industrial ecology (IE) is also considered. The benefits and limitations of these methods are highlighted and their application to the Environmental Process Performance Tool are considered.

There are numerous indices and environmental assessment tools discussed in the literature. To provide a structured discussion on these tools it is initially necessary to classify the approaches into three categories as follows:

- Environmental Quality Indices (EQI's)
- Environmental Impact Indices (EII's), and
- The Cradle to Grave Approach (CGA)

Environmental quality indices (EQI's) are used to assess the quality of the environment. In most cases an EQI is applied to one medium and physicochemical data, measurable phenomena or public opinion are used to assess the environmental quality.

Environmental impact indices (EII's) include those which consider the whole environment and not just a single medium. An EII is used to assess impacts or waste streams rather than environmental quality. The EII category includes the Environmental Process Performance Tool and other industry based environmental indices.

The cradle to grave approach (CGA) includes life cycle analysis (LCA) and industrial ecology (IE). CGA considers the effect of a product or process over its whole life cycle. This type of assessment can be based on quantitative and/or qualitative data. Whilst CGA techniques do not encompass indices these approaches have provided useful concepts and ideas in the development of the EPPT.

This chapter initially establishes what an environmental index is. The chapter then looks at how components of an index are derived and combined. Each of the classifications previously introduced are then be discussed placing emphasis on aspects relevant to the EPPT.

2.1 What is an environmental index?

An environmental index is a tool which can be used quantitatively or qualitatively to assess environmental impact or environmental quality. An index is a single number derived from two or more sub-indices (Thom and Ott, 1976). Sub-indices are a quantitative representation of a parameter being used to assess environmental impact or quality. Two types of environmental index exist: (i) the pollution index, where the numerical value of the index increases with increasing pollution; and (ii) the environmental quality index, where numerical value of the index decreases with increasing pollution (Thom and Ott, 1976). Generally air indices have decreasing scales and are therefore pollution indices and water indices have increasing scales and are therefore quality indices.

The calculation of an environmental index consists of two steps. The first step is the calculation of the sub-indices for the pollutant parameters used in the index. The second step is the aggregation of the sub-indices to determine the overall index.

To calculate the sub-indices from the pollutant parameters determination of the relationship between the raw data and the sub-index is required. A variety of relationships exist including the following functions:

- linear functions, in which a direct proportional relationship exists between the sub-index and the pollution parameter;
- segmented linear functions, in which there is the possibility of a threshold level below which no effect occurs;
- non-linear functions, in which the rate of change varies gradually with increasing levels of pollution;
- segmented non-linear functions are used when non-linear functions become too unwieldy to use. In these cases the curve is segmented with each range being represented by a non-linear equation (Thom and Ott, 1976).

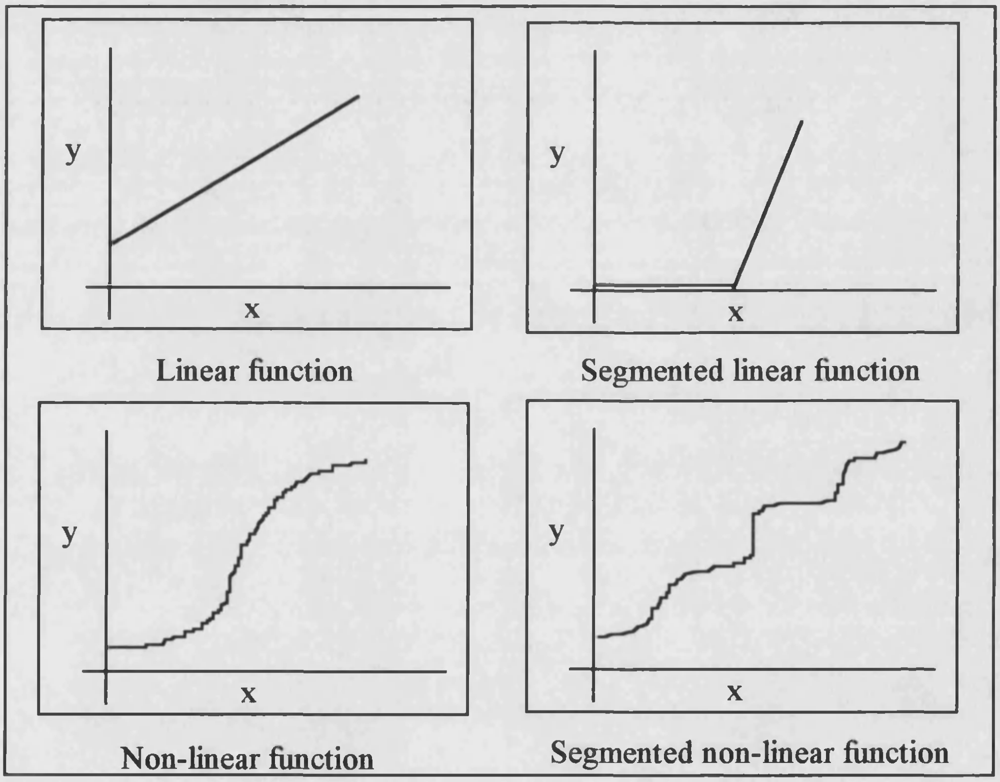


Figure 2.1: Sub-index functions

Once the functions between the parameter and the sub-index have been derived an appropriate score is assigned to the raw data. The next step is the aggregation of the scores. Aggregation is where most of the simplification and reduction of information takes place. Sub-indices can be aggregated by addition or multiplication. Unweighted addition is the simplest form of aggregation. This method simply adds the sub-indices together. Weightings are often incorporated to reflect the contribution of a parameter to an effect. This is known as weighted addition. Both weighted and unweighted parameters are also combined using multiplication.

Having looked at the general structure of environmental indices the next sections will consider the various types of indices and their applications with reference to the development of the EPPT.

2.2 Environmental Quality Indices (EQI's)

Environmental Quality Indices (EQI's) have predominantly been devised for single media usually air or water. Numerous indices have been identified and evaluated. Sections 2.2.1 to 2.2.4 give a brief summary of the main points of the indices relating to each medium with brief details of some of the indices applicable to the specific medium.

2.2.1 Air indices

Numerous air indices have been developed with various applications and assessments of air quality. The following section details the main points identified from the twelve air indices outlined in Table 2.1.

- Air indices are based on actual chemical parameters such as sulphur dioxide or nitrogen dioxide levels rather than phenomena such as Biological Oxygen Demand (BOD_5) and Chemical Oxygen Demand (COD_5) which are common criteria for water quality indices.
- All air indices identified are pollution indices and therefore have increasing scales.
- All air indices include some or all of the following variables: carbon monoxide, sulphur dioxide, total suspended particulates, nitrogen oxides, photochemical oxidants and hydrocarbons.

Table 2.1: Summary of air quality indices

Name	Variables	Scale	Subindices	Aggregation Function	Reference
Air Quality Index	CO, SO_2, TSP, NO_2, OX	Inc	Linear function	Weighted sum	Thom & Ott, 1976
PINDEX	TSP, SO_2, NO_2, CO, HC, OX	Inc	Linear function	Linear sum	Thom & Ott, 1976
Ontario Air Pollution Index	SO_2, HC	Inc	Linear function	Non-linear additive form	Thom & Ott, 1976
Oak Ridge Air Quality Index	CO, SO_2, TSP, NO_2, OX	Inc	Linear function	Non-linear additive form	Thom & Ott, 1976
Mitre Air Quality Index	CO, SO_2, TSP, NO_2, OX	Inc	Linear function	Root-sum-square	Thom & Ott, 1976
Extreme Value Index	CO, SO_2, TSP, OX	Inc	Linear function	Root-sum-square	Thom & Ott, 1976
STARAQS	CO, SO_2, TSP, NO_2, OX, HC	Inc	Linear ratio	Maximum operator	Thom & Ott, 1976
Standardised Urban Air Quality Index	CO, SO_2, TSP, NO_x, POX	Inc	Segmented linear functions	Maximum operator	Thom & Ott, 1976
Primary Standards Index	CO, SO_2, TSP, POX	Inc	Segmented linear functions	Maximum operator	Thom & Ott, 1976
Greens Combined Index	SO_2, HC	Inc	Non-linear function	Weighted sum	Thom & Ott, 1976
Measured Undesirable Respirable Contaminants	HC	Inc	Non-linear function	n/a	Thom & Ott, 1976
Combustion Products Index	Fuel Burned/Ventilating Volume	Inc	n/a	n/a ratio	Thom & Ott, 1976

CO = Carbon monoxide
SO_2 = Sulphur dioxide
TSP = Total suspended particulates
OX = Oxidants
HC = Hydrocarbons
NO_2 = Nitrous oxides
POX = Photochemical oxidants

- Generally in the calculation of the sub-indices the variables are considered to be linear with the exception of the SUAQI (Standard Urban Air Quality Index) and PSI (Primary Standards Index) proposed by Ott (Thom and Ott, 1976) which have segmented linear functions. As described in 2.1 non-linear functions are difficult and unwieldy to use. Non-linear functions have been used in the Greens Combined Index and the Measured Undesirable Respirable Contaminants Index but these have only two and one components respectively (Thom and Ott, 1976).
- No aggregation function dominates. All air indices are additive as multiplicative forms are not generally applied to increasing scale indices.

2.2.2 Water indices

Water indices have a great deal of diversity due to the various situations in which they have been used. These include the assessment of drinking water, recreational water and effluent from water treatment plants. Several water parameters are based on phenomena rather than chemical levels. The following points have been derived from the eleven water indices detailed in Table 2.2.

- Water indices tend to utilise the following parameters: faecal coliform count, pH, BOD_5, nitrates, phosphates, temperature deviation from equilibrium, turbidity, total solids and percent saturation of dissolved oxygen. With the exception of nitrates and phosphates these parameters measure phenomenon rather than chemical specific parameters.
- Water indices are generally quality indices, however McDuffies river pollution index and Prati's implicit index of pollution are pollution indices with an increasing scale.
- Water quality indices are generally comprised of more variables than air quality indices, usually around 8-10 as opposed to on average 5 for air indices.
- Sub-indices include both linear and non-linear functions within each index. Prati's index (Thom and Ott, 1976) includes segmented linear functions and non-linear functions.

Table 2.2: Summary of water quality indices

Name	Variables	Scale	Subindices	Aggregation	Reference
Hortons Water Quality Index	Diss O_2, Sew, pH, TCC, Cond, CCEx, Alk, Cl^-	Dec	Linear and Non-linear functions	Weighted sum	Thom & Ott, 1976
National Sanitation Foundations Water Quality Index (additive)	Diss O_2, TCC, pH, BOD, NO_4, PO_4 , Temp, Turb, Tot S	Dec	Linear and Non-linear functions	Weighted sum	Thom & Ott, 1976
Dinius Social Accounting System	Diss O_2, BOD, TCC, Cond, Cl^-, Hard, Alk, pH, Temp, Colour	Dec	Linear and Non-linear functions	Weighted sum	Thom & Ott, 1976
Arithmetic Unweighted Water Quality Index (WQIAU)	TCC, pH, BOD, NO_3, PO_4, Temp, Turb, Tot S, Diss O_2	Dec	Linear and Non-linear functions	Weighted sum	Landwehr et al, 1976
National Sanitation Foundations Water Quality Index (multiplicative)	Diss O_2, TCC, pH, BOD, NO_3, PO_4, Temp, Turb, Tot S	Dec	Linear and Non-linear functions	Weighted Product	Thom & Ott, 1976
Multiplicative Weighted Water Quality Index (WQIM)	TCC, pH, BOD, NO_3, PO_4, Temp, Turb, Tot S, Diss O_2	Dec	Linear and Non-linear functions	Weighted product	Landwehr et al, 1976
Multiplicative Unweighted Water Quality Index (WQIMU)	TCC, pH, BOD, NO_3, PO_4, Temp, Turb, Tot S, Diss O_2	Dec	Linear and Non-linear functions	Weighted product	Landwehr et al, 1976
Harkins Water Quality Index	TCC, pH, BOD, NO_3, PO_4, Temp, Turb, Tot S, Diss O_2	Dec	Linear and Non-linear functions	Relative index n/a	Landwehr et al, 1976
Arithmetic Weighted Water Quality Index (WQIA)	TCC, pH, BOD, NO_3, PO_4, Temp, Turb, Tot S, Diss O_2	Dec	Linear and Non-linear functions	Arithmetic mean	Landwehr et al, 1976
McDuffies River Pollution Index	Diss O_2, pH, BOD, COD, MnO_4 , Sus S, NH_4^+ NO_3^-, Cl^-, $Fe^{2/3+}$, Mn^{4+}, ABS, CCEx	Inc	Linear and Non-linear functions	Weighted sum	Thom & Ott, 1976
Prati's Implicit Index of Pollution	pH, Diss O_2, BOD, COD, MnO_4, Sus S, NH_4^+ NO_3^-, Cl^-, $Fe^{2/3+}$, Mn^{4+}, ABS, CCEx	Inc	Non-linear for sus solids, NH_4^+, NO_3^-, $Fe^{2/3+}$. Seg. linear for the others	Arithmetic mean	Thom & Ott, 1976

TCC = Total coliform count
BOD = Biological oxygen demand
Sus s = Suspended solids
Sew= Sewage treatment
COD = Chemical oxygen demand
Temp = Temperature deviation from eqm
Diss O_2 = Dissolved oxygen
Turb = Turbidity
Cond = Specific conductance
Tot S = Total solids
Alk = Alkalinity
ABS = Alkyl benzene sulphonates
CCEx = Carbon chloroform extract

- 70% of the water indices are aggregated using a weighted sum, this includes those indices which are calculated using the arithmetic mean (a form of weighting). The water pollution indices use the weighted product as the aggregation function.
- Both the unweighted multiplicative and the unweighted arithmetic water quality index devised by Landwehr (1976) correlate well with the Shannon-Weaver and Brilliouin Indices which classify species diversity and abundance, a biological reflection of water quality.

2.2.3 Land indices

No indices were found in the literature that solely assessed the quality of land although there are indices that concentrate on waste or the environmental assessment of a site. These include Shanks and McEwan's waste index (Shank's and McEwan, 1993), Rhone Poulenc's site environmental index (HMIP, 1992) and Searle's environmental index (Coates, 1994). The indices all fall into the category of Environmental Impact Indices and are discussed in section 2.3.

2.2.4 Multi-media indices

Multi-media indices, for the purpose of this discussion, are environmental quality indices that consider more than one media. The environmental quality indices include Hope, Parker and Peake's Environmental Quality Index (Hope et al, 1992) and Inhaber's National Index for Canada (Inhaber, 1974).

Hope, Parker and Peake's environmental quality index was developed using public opinion to assess environmental quality. Public opinion was used to determine the parameters for inclusion in the index and also the weighting of the parameters. The parameters are listed in Table 2.3.

Table 2.3: Parameters for Hope, Parker and Peake's Environmental Quality Index

Parameters	Units
Nitrogen dioxide emissions	'000 tonnes of NO_2 equivalent
Sulphur dioxide urban concentrations	$\mu g/m^3$
Low level ozone concentrations	average monthly 99th percentile
Carbon dioxide emissions	million tonnes of carbon
Oil spills requiring clean-up	number
Fractional length of river in poor or bad quality	percentage
Resident population	millions
Fertiliser deliveries for agricultural use	'000 tonnes
New dwellings started	'000

No attempt was made to subdivide parameters into media categories. Each parameter is considered individually with an assigned weighting factor according to the equations below:

$$Index = \sum_{i=1}^{9} q_i w_i \qquad \text{....... Equation 2.1}$$

where q_i = variable

w_i = weighting factor

Inhaber's National Index for Canada developed an air, water and land quality index. These indices were combined into an environmental quality index. The air quality index (I_{air}) is derived by calculating a specific environmental pollutant index (I_{sp}) and combining it with a regional index (I_{reg}) and an industrial emissions index (I_{ie}) as shown in Equation 3.2:

$$I_{air} = \left\{\left[5(I_{sp})^2 + 3(I_{reg})^2 + 2(I_{ie})^2\right]/10\right\}^{\frac{1}{2}} \qquad \text{....... Equation 2.2}$$

The water quality indices for the National Index for Canada are calculated by estimating the efficiencies of different types of treatment plants for different wastes.

The value of these indices can be determined from a map of Canada derived by Inhaber for this purpose. Inhaber has also developed a map which includes national parks, health and aesthetic values to determine the land index. The indices for air, water, land and miscellaneous factors (which are not detailed) are combined as follows:

$$I_{EQI} = \left\{ \left[0.3\left(I_{air}\right)^2 + 0.3\left(I_{water}\right)^2 + 0.3\left(I_{land}\right)^2 + 0.1\left(I_{misc}\right)^2 \right] \right\}^{\frac{1}{2}} \quad \text{....... Equation 2.3}$$

2.3 Environmental Impact Indices (EII's)

More recently environmental indices have focused on environmental impact rather than quality. Several companies have developed their own environmental indices with emphasis on the amount of chemicals discharged and the disposal route. Often these indices have been developed as a management tool to provide an aid to assessing and reaching emission targets. The company indices are mass rather than concentration based that is where the environmental impact is combined with the mass of the emission released. The Environment Agency has developed the Integrated Environmental Index (IEI), an environmental assessment method (Environment Agency, 1997) to determine BPEO. This method uses the concentration of released chemicals rather than mass and compares them to emission standards in order to assess the environmental impact of a process.

This section sub-divides environmental impact indices into those indices that use mass of emission released to evaluate environmental impact and those that use the concentration of emission released to evaluate environmental impact. The mass based approach will be discussed starting with the simplest load factor approach moving through chemical scoring systems. The combination of the load factor and scoring system will then be addressed followed by more specific mass based impact assessment tools. The company based environmental assessment tools will also be addressed in Section 2.3.1.3. Section 2.3.2 presents concentration based assessment tools. This will include the Environment Agency's method to assess BPEO (Environment Agency, 1997).

2.3.1 The mass based impact approach

The simplest method of assessing the reduction in waste from a process is to calculate the amount of waste produced per unit product. Caughlin (1993) was one of the first to recognise this as a parameter which he called the Environmental Load Factor (ELF) and defined as:

> 'the total amount of wastes produced by a process over a given time divided by the amount of product produced over the same time'

Sheldon (1994), renaming the ELF the environmental acceptability factor or the 'E' factor, used it to compare the relative levels of waste arising from different process industries. This is shown in Table 2.4.

Table 2.4: The 'E' factors for various industry sections (Sheldon, 1994)

Industry Section	Product Tonnage	'E' Factor (kg by-products/kg product)
Oil refining	10^6 - 10^8	~ 0.1
Bulk chemicals	10^4 - 10^6	< 1 - 5
Fine chemicals	10^2 - 10^4	5 - 50
Pharmaceuticals	10^1 - 10^2	50 - 100+

Low 'E' factors are typical of the oil refining and bulk chemical industry. This is because these processes are continuous with a large amount of recycling and have been optimised for high conversions and selectivity. As fine chemical and pharmaceutical plants are often operated on a batch system, involving several stages with numerous inefficient start-up and shut-down operations, the waste per tonne of product is high. These processes are unlikely to have been extensively optimised as with larger scale operations. There is less opportunity for recycle and more cleaning is usually required resulting in more waste.

Sheldon (1994), an organic chemist, refined this approach further and suggested that the main source of waste in organic chemistry was from inorganic salts formed from acid base neutralisations. He suggested the key to waste minimisation was selectivity in organic synthesis. He identified 'atom selectivity or utilisation' as an area often ignored by organic chemists. The assessment approach developed by Sheldon uses theoretical yields to evaluate the environmental impact of alternative routes to a single product. It is calculated by dividing the molecular weight of the desired product by the molecular weight of all substances produced. This is demonstrated below using the synthesis of chlorohydrin.

Classical route

$$C_2H_4 + Cl_2 + Ca(OH)_2 \rightarrow C_2H_4O + CaCl_2 + H_2O$$

Mol wt 44 111 18

Atom utilisation = 44/173 = 25%

Modern petrochemical route

$$C_2H_4 + {}^1/_2O_2 \xrightarrow{\text{catalyst}} C_2H_4O$$

Atom utilisation = 44/44 = 100%

This approach provides a useful method for assessing the selectivity of a reaction and the reduction of waste. However, the atom utilisation approach, like the ELF and 'E' factors, does not consider the toxicity, persistence or effects the waste may have on the environment. Sheldon (1994) states 'that to compare alternative routes solely on the basis of the amount of waste is to grossly oversimplify'. He devised the 'environmental quotient' (EQ) that considers both the amount and the nature of the waste. The EQ is calculated by multiplying the 'E' factor with an arbitrarily defined unfriendliness quotient, Q. Sheldon suggested an unfriendliness quotient of 1 for innocuous salts such as sodium chloride and 100 to 1000 for heavy metals dependent on their toxicity.

These approaches identify a basic method of assessing the quantity of waste associated with a process and are useful for waste minimisation studies. However, the major limitation of these methods lies in their omission of an environmental assessment of the waste. Sheldon identified a need to assess the impact of the waste. While he uses an arbitrarily assigned score he did recognise that 'the figure would be highly debatable and will vary from one company to another, depending partly on the ability to handle and recycle the material in question'. A scientific assessment of the environmental impact of chemicals is required to provide a more reliable method to assess process environmental performance. A chemical scoring system could provide the way forward.

2.3.1.1 Chemical scoring systems

Much of the work undertaken on scoring systems has been carried out in the USA. Scoring systems have been developed to assist in the preliminary evaluation of compounds of particular interest with respect to toxicology and the environment. The scoring system developed by the US EPA and the Oak Ridge National Laboratory (Ross and Welch, 1980, O'Bryan and Ross, 1988) combines objective guidelines with professional judgement to evaluate chemicals. This system has been designed to rapidly score chemicals with readily available information. It consists of eleven parameters, six relating to toxicity, the rest to environmental fate, occupational, consumer and environmental exposure. Each of the parameters have a scoring range of 0 to 9, 9 being the most toxic. The parameters are combined to evaluate chemicals.

An expert system to rapidly rank environmental pollutants was developed by Brown, Holt and McCaleb (1976) at the Stanford Research Institute. This system concentrates on three areas of chemical behaviour; release and distribution, transport and transformation, and effects. Parameters including threshold limits, lethal dose, partition coefficients and vapour pressure are scored and combined to rank the chemicals and assess their chemical behaviour. Nelson, Van Duuren and Goldschmidt (1975) developed a similar system for organic compounds. More recently this group have developed a scoring system with environmental indices and more emphasis on environmental parameters.

2.3.1.2 Combining mass with scoring systems

Both Elliott (1997) and Cave and Edwards (1997) have adopted the approach suggested by Sheldon (1994). Elliott (1997) has developed scoring systems which when combined with process emissions generates an overall impact score. Cave and Edwards (1997) approach has used quantitative toxicity data to determine the environmental impact of process production options.

Elliott's scoring system is based on an inverted tree structure. Level 1, the top level, is where impact score is combined with mass of the release. Level 2 considers the long-term and short-term impact of a chemical to the environment as a whole. To assess environmental impact Elliott evaluates the effects on each subsystem, air, water and soil and combines the results with environmental fate models to assess the environmental impact. Each of the short-term and long-term impacts of each chemical are assessed using parameters that represent three categories; damage, modification of the environment and persistence. Twenty eight parameters are scored using a system developed for the purpose. Elliott's scoring system has been programmed into an Windows™ based application which forms part of his Windows™ based environmental assessment tool, EniVal. EniVal requires process data to be entered and also data for the 28 parameters for each chemical. All the data entered can be stored, thus building up a chemical database for future use. EniVal then carries out distribution and impact calculations to determine the impact of the process. These calculations can be interrogated at any of the seven levels to assess where a particular impact is arising. EniVal will be discussed further with emphasis on the distribution models and impact calculations in Chapter 5 and methods of combining the mass with score in Chapter 6.

Cave and Edwards (1997) have developed the Environmental Hazard Index (EHI). The EHI is used to select process routes based on the assessment of the inherent environmental hazard (IEH). An expression has been derived which relates the EHI to an estimated fish kill. To calculate the EHI Cave and Edwards combine the potential amount of chemical that can be released with either a specific water hazard index (SWHI) or a specific terrestrial hazard index (STHI) depending on the media to which the release occurs. The SWHI and the STHI are based on three categories; toxic effects, time period and chemical distribution. The toxicity is assessed using the toxicity data for the most sensitive species. The time used for the EHI is 96 hours and the chemical distribution is assessed using Mackay's fugacity models to determine the predicted environmental concentration in each media. The SWHI and STHI are akin to Elliott's score which are combined with the amount of chemical released. The EHI has been used to assess six production routes of methyl methacrylate (MMA). Cave and Edwards compared the ranking of the MMA production routes with the EHI with the ranking obtained from the Inherent Safety Index (ISI) devised by Edwards and Lawrence (1996). In this study they found the ranking of these MMA production options very similar.

The consideration of plant safety and the environment has been highlighted by Cave and Edwards (1997). In their example there seems to be little conflict between the two. However several researchers have identified the potential conflict between plant safety and the environment. Debiel and Myren (1995) have outlined an integrated approach to solve growing safety and environmental conflicts. They suggest a four step cycle by which processes can be modified and improved to consider safety and environment. The safety and environmental assessment cycle is shown in Table 2.5.

Table 2.5: Safety and environmental assessment cycle

Step	Details
1	Select the best process(es) for safety and environmental protection
2	Estimate emissions and consumption of natural resources for selected process(es), define requirements/best available techniques (BAT) and improvements, set criteria
3	Improve process(es) by carrying out inherent safety study,
4	Design process and perform HAZard and OPerability study (HAZOP) and return to step 1

Elliott's (1997) and Cave and Edwards' (1997) methods are examples of using actual chemical data to assess the environmental impact of chemical processes be it during the design stage, during operation or evaluating potential hazards. In these methods each release is assessed based on the chemicals it contains rather than, for example, the properties of a waste stream where the constituents are unknown. This has the advantage of being able to identify particular components of the stream that are causing a significant amount of the environmental damage and focus on the real problem. These methods however do not consider any interactions between the chemicals in the waste stream which may increase or decrease the effect of the individual chemical.

2.3.1.3 Company approaches

In this section company developed approaches to the environmental assessment of processes will be presented. These approaches assign ratings to waste streams and use assessment techniques to evaluate site or process performance from year to year.

Several approaches which assess the waste streams of processes and their disposal have been developed. SmithKline Beecham's environmental impact number (EIN) combines a waste index (WI), which is essentially the same as the ELF and 'E' factor, with a difficulty factor (DF) which rates different types of waste streams (Cunningham, 1994). The difficulty factor is assigned based on a qualitative assessment of the degree or difficulty associated with treating or dealing with the stream. Cunningham (1994) defined 19 classes of generic waste and potential treatment schemes that involved 22 unit processes. The classes include, for example, aqueous waste containing >5% of toxic or priority pollutants (such as organic chlorine or pesticides) which has three treatment options; activated carbon, solvent extraction or hazardous disposal, and aqueous wastes containing no organics but containing < 5% innocuous inorganic salts (NaCl, $NaSO_4$) with the treatment options of equalisation and reverse osmosis. The cost of each of these processes was then assessed and a computer programme was developed to cost each unit and the entire train for any given waste type.

Like SmithKline Beecham, ICI adopted a similar approach of combining the quantity of each substance released (W) with its environmental impact or potency factor (PF) to establish the environmental burden (EB), where:

$$EB = \sum(W x PF) \qquad \text{....... Equation 2.4}$$

ICI hope that this method will enable them to rank the potential impact of their emissions and consequently improve their environmental management (Fell, 1997). ICI went on to identify and define seven impact categories: acidity, global warming, human health effects, ozone depletion, photochemical ozone (smog) creation, aquatic oxygen demand and aquatic ecotoxicity. Each chemical released is assessed on these categories relative to a standard chemical. The results are then judged as to their significance. The results are not aggregated due to the differing nature of the impacts.

Shanks & McEwan (1995) have developed an index to consider the treatablility of a waste stream as a measure of the environmental impact for disposal techniques. This index is used as a means of determining the BPEO for the disposal of hazardous wastes. As with the other indices discussed Shanks & McEwan's index considers the quantity of the discharge not the concentration. However the waste stream is only considered if it contains hazardous substances, that is if it contains one or more substances listed in Annex II of the EC Directive 91/689/EEC. The equation for Shanks & McEwan's index is below:

Index =

$$\frac{100}{QH} \times \left[QH - \left(Qh_{\mathrm{BAD\,(air)}} + Qh_{\mathrm{BAD\,(water)}} + Qh_{\mathrm{BAD\,(land)}} \right) - \left(\frac{Qh_{\mathrm{D\,(air)}}}{t_{1\mathrm{(air)}}} + \frac{Qh_{\mathrm{D\,(water)}}}{t_{2\mathrm{(water)}}} + \frac{Qh_{\mathrm{D\,(land)}}}{t_{3\mathrm{(land)}}} \right) \right]$$

.... Equation 2.5

where:

QH	is the quantity of the hazardous constituents with between 1 and 51 carbon atoms per molecule (C1-C51) which are contained within the waste product;
Qh_{D}	is the quantity of hazardous constituents (C1-C51) discharged over time to air, water and land during the use of the waste disposal techniques considered. This excludes discharges that are bioaccumulative or ozone-depleting which are accounted for under Qh_{BAD};
Qh_{BAD}	is the quantity of hazardous constituents which are bioaccumulative and are discharged to air, water and land during the use of the waste disposal technique under consideration; and
t_1, t_2, t_3	are the times over which the discharges to the unmanaged environmental media or air, water or land take place. For joint disposal to land, the time period begins after the waste has left any container and is in contact with the putrescible medium. Wastes which continue to discharge after two or more years are considered unsuitable for land disposal.

The discharges to air, water and land have been weighted by considering the time over which the material is discharged into the unmanaged environment. Several examples of Shanks & McEwan's index are given in their discussion document including a comparison of the disposal of 20kg of the insecticide DDT (4,4'-Dichlorodiphenyltrichloroethane). Two options were considered, incineration and landfill. Incineration was shown to be BPEO as high temperature incineration destroys

100% of the DDT with emissions of no environmental consequence. Whereas when disposed of to landfill 75% of the DDT enters the environment unchanged. This will be discussed further in Section 2.3.1.4.

Searle (Coates, 1994) have been developing an index that it is independent of production levels. This index was developed to show the public that even if the production increases waste can still be reduced. There are four sub-indices to this index: wastes to off-site disposal, discharges to sewer, discharges to atmosphere and environmental incidents. The sub-index for waste to off-site disposal is calculated by multiplying the annual tonnage rate of waste by an environmental acceptability factor in the range of 0.1 to 1.0. If materials are recovered or reused a negative number will result. The discharge to sewer sub-index is calculated as the percentage each parameter is within its control limits which have been set by the regulatory authority. Discharges to the atmosphere are listed and scored according to their severity from on-site odour to potentially harmful material being released off-site. These discharge scores range from 0 to 100 with the mean being used for the calculation of the final index. Environmental incidents are scored from 10 for a contained spillage to 100 for a hazardous spill to a watercourse. The overall index is calculated by summing the sub-indices to give a final site index. Searle has used this index to show that the aim of 10% annual reduction of waste per year has been achieved.

Rhône Poulenc Chemical Ltd (HMIP, 1992), a signatory to the Chemical Industry Associations (CIA) Responsible Care Programme, have also developed an index. Their index, part of their management system, has been developed with the guiding principles of the Responsible Care Programmes in mind. The principles are:

- to operate to the best practices of the industry
- to reflect the commitment to continuous improvement in health, safety and environmental policy

- to make available to employees, customers and the public all relevant information about activities which affect health, safety and environment (Rhône Poulenc, 1992).

Rhône Poulenc's management tool comprises three indices: the total environmental index, the special waste index and the red list substance index. The total environmental index assigns the weighting shown in Table 2.6 with the daily amounts of aqueous and non-aqueous wastes from the site. The sum of these weights multiplied by daily amounts gives the total index value which when compared with the previous years index value gives the site environmental index.

Table 2.6: Weightings for Rhône Poulenc's Site Environmental Index

Non-aqueous		Weighting Factor	Aqueous	Weighting Factor
Landfill			Chemical Oxygen Demand	1.0
Special	on-site	10.0	Total Suspended Solids	0.3
	off-site	10.0	Ammonium based compounds	0.5
Non Special	on-site	2.0	Mercury	1000
	off-site	2.0		
Inert	on-site	0.1		
	off-site	0.1		
Incineration				
Halogenated	on-site	0.5		
	off-site	5.0		
Other	on-site	0.5		
	off-site	1.0		

The special waste index and the red list substances index are the total discharge of those wastes relative to the previous year.

Robinson Brothers Ltd (RBL) index (Smith, 1996b) has been developed as part of their BS7750 standard implementation. (BS7750 will be discussed in Section 2.6). RBL had reached a point in their implementation of BS7750 where an evaluation of their environmental effects was required. They canvassed opinions from internal and external sources for ideas for inclusion in the development. With such a diverse range of chemical production by RBL, some 120 products, a decision was made to understand the relative scale of the impact of different chemicals. This allowed the company to set objectives and prioritise the future environmental management programme. RBL devised a system which evaluated the following parameters:

Quantity rating:	the amount of every raw material and product used/produced in each manufacturing process, this can be directly related to the number of batches manufactured and hence the increased level of handling risk
Consequence factors:	the chemistry of the raw materials used
Hazard factors:	the methods by which they are handled

Each of these parameters were tabulated, weighted and applied to the methodology below:

1. Understand the process
2. Establish amounts of: product produced and raw materials used (allocate a quantity rating (QR))
3. Score each material: consequence factors and hazard factors (determine an average score (X) for each of these)
4. Environmental rating for each material = ($X_{consequence}$ x X_{hazard}) x QR
5. Total environmental rating for the product = Rating of product + raw material^1 + raw material^2 + raw material^n where 1,2 ...n are the environmental rating for each raw material.

RBL felt that significant gains were made through the development of this tool. Whilst no details of the application of the tool could be found in the literature, 'the re-examination of old records educated the staff to make them consider the impact of their lives on the overall company performance' (Smith, 1996b).

Other indices have been developed including a methodology to assess the effects of a combined cycle gas turbine power station (Smith, 1996b), a regional electricity company (Smith, 1996b and Johnson, 1996) and Arthur D. Little's assessment technique (Arthur D. Little, 1995) for a company to 'measure its own performance relative to a chosen benchmark year from year to year'.

2.3.1.4 Criticisms of company indices

These company developed indices have received numerous criticisms. The Shanks & McEwan Index makes no recognition of the problems associated with carbon dioxide or PCB's (polychlorinated biphenyls) and PAH's (polyaromatic hydrocarbons) that arise from incineration. PCB's and PAH's have significant but as yet undefined environmental consequences. If a similar type of approach was undertaken by an organisation whose operations are not mainly incineration it has to be asked if the results would be the same.

Rhône Poulenc's index has been heavily criticised for the way it can be manipulated to show improved environmental performance. Greenpeace went as far as to say that the Rhône Poulenc's index is 'bizarre' and it being 'another case of industry being afraid to disclose real information'. Rhône Poulenc's chairman and managing director, Keith Humphrey's, countered that the report is not intended for public relations, he says 'the environmental index is a very important to us as a management tool' (The Chemical Engineer, 1993). In the case of these company based indices care must be taken as to their purpose and their use as a public relations tool. As more of these methods are being developed by industry and criticised, industry must be aware that their efforts to gain public approval could backfire if their methods are not credible. An independent approach applied to industry would provide a way forward but just as industry derived methods have been criticised independent methods would be criticised by industry due to the subjective nature of this type of assessment.

2.3.2 The concentration based approach

Much of the regulation of chemicals entering the environment is based on concentration data. This concentration based regulation includes discharge consents to controlled water and atmospheric releases. Discharge consents allow for local conditions such as volumetric flow rate and chemical composition to be considered. For example, the discharge consents into the River Mersey are likely to be higher than the discharge into a small river with small flow through the countryside. This is due to the volume, the flow rate and the condition and chemistry of the receiving body. The same approach is adopted for atmospheric emissions. Stacks which emit atmospheric pollution have to be high enough to have adequate dispersion so as not to breach environmental concentration levels set for the surrounding areas. Extensive dispersion modelling is required to take into account local environmental variations such as predominant wind speed and direction and the location of residential areas.

The Environment Agency has developed a method for selecting the Best Practicable Environmental Option (BPEO) for processes. This method is based on environmental concentrations (Environment Agency, 1997). The selection process involves the calculation of six parameters:

1. the Integrated Environmental Index (IEI)
2. the adverse short term effects
3. the global warming potential
4. the photochemical ozone creation potential
5. the unit hazard score, and
6. other factors related to environmental quality

The IEI compares predicted environmental concentrations (PEC) of chemicals, particularly priority chemicals, released from a process with the relevant environmental assessment level (EAL). The Environment Agency has suggested guidelines for determining priority chemicals for assessment:

$$\text{PEC} \geq 0.8\ \text{EAL}$$

$$\text{or Process contribution (PC)} \geq 0.02\ \text{EAL}$$

Releases can be considered insignificant if: $\text{PC} \leq 0.002\ \text{EAL}$

The Environmental Assessment Level (EAL) is a reference level that expresses the substances relative potential for harm. EAL's have been derived by the EA from a variety of national and international sources. Details can be found in Volume II of the Guidance Note (Environmental Agency, 1997). Environmental Quality Standards (EQS's) have been determined for some substances in some environmental medium. Where EQS's exist the EAL has been set to the same limit. In the EC a risk based approach has been adopted to determine assessment levels. This compares the concentration of a polluting substance in the environment to a reference concentration such as the no effect concentration (NEC). In 1992, the German Federal Environmental Agency (UBA) and the German Advisory committee on existing chemicals (BUA) published a comprehensive concept for the environmental assessment of existing chemicals which does just that. Further details on the German risk based approach can be found in Ahlers et al (1993 & 1994).

To determine the IEI for a process, initially, the environmental quotient (EQ) is calculated for each substance using the following equation:

$$\text{EQ}_{(\text{substance})} = \frac{\text{Process contribution}}{\text{EAL}} \qquad \text{....... Equation 2.6}$$

To calculate the EQ for each medium, air, water and land each substance EQ is combined as in the following equation:

$$EQ_{(medium)} = EQ_a + EQ_b + ...EQ_i.....$$ .... Equation 3.7

where a.....i are substances released to a particular medium.

The Integrated Environmental Index (IEI) is then calculated by combining the EQ's for each medium as shown in the following equation:

$$IEI = EQ_{(air)} + EQ_{(water)} + EQ_{(land)}$$ .... Equation 2.8

The IEI considers the long-term effects of the releases from processes on the environment. However, there is still a need to assess the short-term effects for peak releases. This assessment is carried out in the same way as the IEI except the short-term concentrations in the environment are compared with the short-term EAL's. Care must be taken that short-term concentrations are expressed on the same basis as short-term EAL's.

As well as the direct effects a substance has on the environment, addressed by the IEI and short-term assessment, consideration of the indirect effects which cause changes in environmental conditions are necessary. Of particular concern are global warming and ground level photochemical ozone creation. The calculation of the global warming effect and the photochemical ozone creation effect are carried out by multiplying the mass of the chemical released by the global warming potential or photochemical ozone creation potential of that chemical. Details of these phenomenon and the potentials can be found in Section 4.13.

The unit hazard score deals with wastes arising from process which are not released directly to the atmosphere or water. A scheme has been developed by the UK

Government-Industry Working Group on Priority Setting and Risk Assessment (Environmental Agency, 1997). The scheme is based on the following parameters:

- toxicity (to mammals or aquatic organisms)
- potential for bioaccumulation
- degradation (in soil and water), and
- other physical characteristics such as solubility, adsorption potential and volatility.

Combining scores assigned to each of these parameters gives the unit hazard score. This is then combined with the annual amount of waste produced to give an overall hazard score.

Other effects such as odours, visible plumes and unplanned releases are also assessed. The IEI, EQ's and other factors are then considered and the process options are ranked. From this information a judgement as to which is the BPEO is made.

This approach, like the industry based approaches, has had its criticisms particularly with respect to the EAL's. Many of the EAL's are based on Occupational Exposure Limits (OEL's) which have been derived for use in the work place. Despite building in a significant factor for error an accurate level for environmental assessment is still difficult to obtain. The IEI also lacks an integrated approach. Whilst the IEI considers all three media, simply adding them together doesn't provide an integrated environmental approach. Consideration of the ultimate fate of the chemicals in the environment needs to be made.

The Environment Agency's method has been derived to determine the BPEO for process options. Many of the processes are still at the design stage when the option needs to be considered and consequently emission data is not available. Concentration based emission data is also difficult to obtain from existing plants due to the expense of monitoring non-prescribed substances. Dispersion modelling can be used to obtain concentration data for new designs and existing processes. There are many dispersion models available to obtain concentration based data however the results are often inconsistent and this type of work is also relatively expensive to undertake. A mass based approach is by far the easier and more reliable option with mass data obtained from mass balances which have been determined at the design stage of a process. The IEI has also received criticism because of the limited indication of how to determine BPEO from the assessments (Elliott, 1997).

2.4 Limitations of existing environmental indices

Each index has its own limitations usually as a result of being designed for a specific purpose. Having extensively reviewed the current indices available for assessing the environmental impact the approaches, while diverse, have limited application to this study. Most indices are based on one media. The aim of each index is very specific, most considering the quality of the media rather than assessing the impact caused from process emissions. With the exception of the EniVal and the IEI there is no consideration of the effects caused by the chemicals. There is just an assessment of the amount of that chemical in the environment. A judgement as to the significance of the impact still needs to be made.

As a result of the limitations of current indices it was decided to look elsewhere for ideas on assessing the impact of chemicals released from processes. The disciplines of life cycle analysis (LCA) and industrial ecology (IE) were considered. An overview of the Cradle to Grave approach (CGA) which encompasses LCA and IE is discussed in the following section with a view to an application to the EPPT.

2.5 The Cradle to Grave Approach (CGA)

CGA differs from EQI's and EII's as it provides an holistic approach to assessing the environmental effect of a process or product. CGA provides a new way of thinking rather than an actual assessment of the environmental quality or impact although impact assessment is a component of CGA. CGA considers the inputs and outputs from a process, the energy use, recycling and transport and distribution. Several methods have been devised within the confines of the cradle to grave approach including industrial ecology and life cycle assessment also known as resource environmental profile analysis (REPA), ecobalance, ecoprofile and life cycle review (MacAlasdair, 1993). Despite the holistic cradle to grave approach there still remains much debate on the implementation and the validity of the results obtained. This section briefly discusses life cycle assessment and industrial ecology and highlights the areas of relevance for the development of the EPPT.

2.5.1 Life Cycle Assessment

LCA is an important tool for determining the environmental impact of products and processes. It is a systematic assessment of the environmental impacts of the products or processes during their whole life cycle examining energy use, resource use and environmental releases (Rethmeyer, 1993). The Society of Environmental Toxicology and Chemistry (SETAC) defines LCA as 'an objective process to evaluate the environmental burdens associated with a product, process or activity by identifying and quantifying energy and material usage and environmental releases, to assess the impact of those energy and material uses and releases to the environment, and to evaluate and implement opportunities to effect the environmental improvements' (Klöpffer, 1994).

The first applications of LCA focused around the comparison of products. Typical examples of LCA studies include the comparison of glass, aluminium cans and polyethylene terephthalate (PET) bottles as drinks containers (Crittenden, 1994b) and a comparison of disposable nappies and towelling nappies. However, the application for LCA has broadened over time and as well as comparing products it can be used to compare disposal routes and recycling (Molgaard and Alting, 1994 and Edwards and Schelling 1996a and 1996b). Moving away from traditional comparisons, more recently LCA has been used by Golonka and Brennan (1996) for pollution treatment selection and by Kniel et al (1996) for the environmental, economic analysis and optimisation of a nitric acid plant. Callahan (1994) has also used LCA to compare vapour degreasing and aqueous cleaning. Stefanis et al (1995) and Pistikopoulis et al (1995) are developing a Methodology for Environmental Impact Minimisation (MEIM) based on life cycle principles which considers the impacts of the wastes associated with inputs as well as outputs. Both Crittenden and Clift have also highlighted the importance of LCA in waste management and minimisation. Clift (1996) says that LCA should go beyond the simple reduce, reuse, recycle hierarchy and recognise the use of energy and material resources that are involved which may outweigh the apparent benefits of recycling. He uses the example of paper use and recycling in Daae and Clift to argue that newspapers should be used as a fuel and not as a recyclable material (Clift, 1996). Crittenden (1994) says of this example that 'this is not surprising as until recently analysis of environmental performance has been somewhat ringfenced and the whole of the product life cycle has not been considered'. It is important that waste minimisation should be considered beyond the confines of the boundary fence.

2.5.1.1 Life cycle assessment procedure

Life cycle assessment examines the following stages of a product or process:

- Raw material extraction
- Raw material processing
- Manufacture of the product
- Transportation of the product
- Use of the product
- Disposal, reuse or recycling of the product.

The procedure used to undertake the assessment of these stages comprises the following components.

- **Goal definition and scoping,** where the boundaries of the system are defined.
- **Inventory,** of materials use, energy use and of emissions and solid waste (known collectively as burdens).
- **Impact analysis** comprising:
    - **Classification,** in which burdens are aggregated into a smaller number of environmental impacts.
    - **Valuation,** by which the environmental impacts are reduced to a single measure of environmental performance.
- **Improvement assessment,** of the activities needed to reduce the environmental impacts.

2.5.1.2 Goal definition and scoping

Before undertaking the inventory analysis in LCA it is necessary to define the goals and scope of the study. This identifies the objectives and the purpose of the study, the product, process or activity of interest, the intended end use of the study results and the key assumptions employed (Warren and Weitz, 1994). This is a very important aspect of any assessment tool and is used in the EPPT.

2.5.1.3 Life cycle inventory

Life cycle inventory is by far the most developed component of LCA. It uses quantitative data to establish the levels and types of energy and materials inputs to an industrial system and the environmental releases that result (Graedel and Allenby, 1995). The impacts are defined in input and output terms to and from the environment without considering environmental processes (Udo de Haas, 1992). The elements of the LCA Inventory Analysis are shown in Figure 2.2.

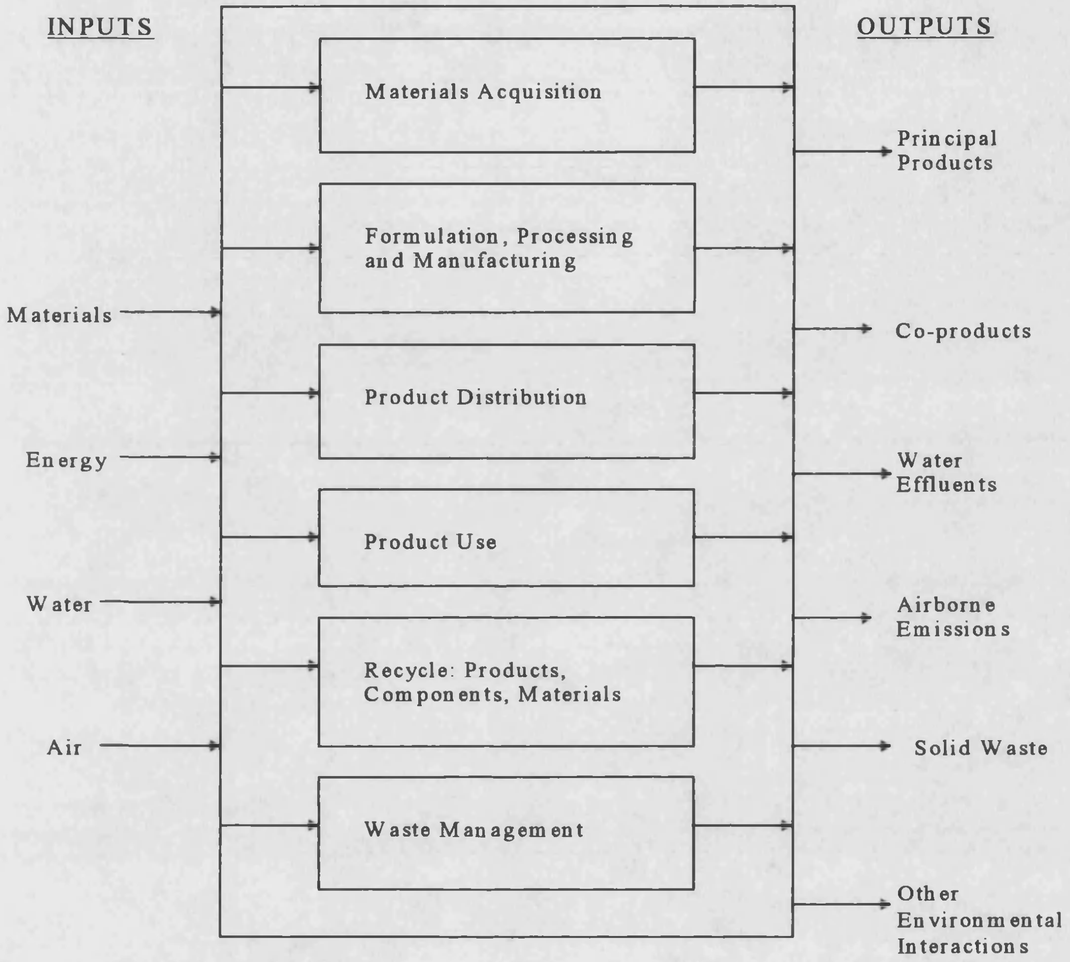


Figure 2.2: The elements of life cycle inventory analysis (Graedel and Allenby, 1995).

This extended approach to environmental assessment considering the inputs as well as outputs of a process is considered by the EPPT for process comparisons. The use of energy and water in processes is also considered by the EPPT.

2.5.1.4 Impact analysis

When the impacts have been defined in the inventory the impact analysis is carried out. Impact analysis in LCA comprises classification and valuation. Classification requires the emissions to be considered on their contribution to a certain effect. In the valuation, the effects are then reduced to determine a single measure of environmental performance. Several methods are being developed for LCA impact analysis. They can be divided into several groups:

- Qualitative methods, e.g. discussion in a panel of experts, as in the Danish PVC (poly vinyl chloride) study (Christensen et al, 1992 in Baumann et al, 1992).
- Quantitative methods:
    * grouping emissions into effect categories (Tillman et al, 1992 in Baumann et al, 1992) e.g. presenting carbon dioxide and CFC into a global effect category and sulphur dioxide, nitrogen oxides and hydrogen chloride into an acidification category.
    * low level of aggregation (Baumann et al, 1992) e.g. aggregating the different emissions into effect categories. (The weighing up of different emissions will still have to be done in the mind of the observer).
    * high level of aggregation (Ryding and Steen, 1991, Steen and Ryding, 1992 & Baumann and Rydberg, 1994) e.g. when the effects are weighted together to form a single index.

High level aggregation methods are still in their infancy. The most developed method is the Environmental Priority Strategies for Product Design (EPS) developed by the Swedish Environmental Research Institute (IVL) with the Swedish Federation of Industries and Volvo Car Corporation. Details of this method can be found in Graedel (1994), Baumann et al (1992), Ryding and Steen (1991), Steen and Ryding (1992) and Baumann and Rydberg (1994). A comparison of this method with five other methods of evaluating the environmental impact of products and processes can be found in Hertwich et al (1997).

None of the above techniques provide an ideal solution to impact analysis but they do provide guidance towards improved solutions. The weightings are always destined to be in a state of flux and must be designed in such a way as to allow for modifications in the light of new information or new perspectives.

Other methods of impact analysis exist. Most have been developed for risk assessment and require the transformation of chemical emission data into environmental exposure and environmental effect.

Environmental exposure can be expressed as:

- The dispersion of the pollutant in the biosphere - this can sometimes be described by mathematical models, and
- The breakdown of the primary pollutant - chemical reactions remove the harmful substances from the biosphere, generally expressed in terms of residence time (Baumann et al, 1992).

The effect can be calculated using a concentration-dependent response factor for the adverse effect on the environment. This model can be applied to any type of emission, but dispersion, breakdown and response equations vary from medium to medium and are generally unknown (Baumann et al, 1992).

This approach to impact assessment is akin the German approach detailed in Ahlers et al (1994). This also has a two tiered approach considering exposure assessment and effects assessment. The exposure assessment leads to the derivation of the Predicted Environmental Concentration (PEC) from the chemicals' production, use, disposal together with dispersion and degradation. The effects assessment utilises data from toxicity tests both acute and chronic to determine the Predicted No Effects Concentration (PNEC). The risk characterisation of the chemical is measured or estimated by comparing the PEC with the PNEC.

An assessment of the environmental impact of chemical emissions is required by the EPPT. However the approaches used by LCA and risk assessment whilst providing an insight into alternative methods do not provide the way forward for the EPPT.

2.5.1.5 Improvement analysis

Improvement analysis highlights the needs for reducing environmental impacts as a result of industrial activity. Improvement analysis is the ultimate goal of cradle to grave activities. Improvement analysis is where the results of the analyses are translated into the specific actions that benefit the industry-environment relationship (Graedel and Allenby, 1995). SETAC defines improvement analysis as 'a systematic evaluation of the needs and opportunities to reduce the environmental burden associated with energy and raw material use and releases to the environment throughout the life cycle of the product, process or activity. This analysis may include both quantitative and qualitative measures of improvements, such as changes in the product, process and activity design, raw material use, industrial processing, consumer use and waste management' (Udo da Haas, 1992).

Methods to assess and compare chemical processes have been developed in the EPPT. The outcome of these assessments highlights areas to reduce environmental impact and is therefore akin to improvement analysis in LCA.

2.5.1.6 The application of LCA to the EPPT

Life cycle assessment provides an interesting concept and approach detailing many aspects that could be considered in the EPPT. However, LCA as a tool is considered too complicated and detailed to assess chemical processes and process changes. The concepts of LCA rather than the methodologies are useful in the EPPT. These include the consideration of inputs as well as outputs, the consideration of energy and water use, the application of a boundary, and consideration of process improvement methods. These aspects of LCA and ideas from other approaches providing the basis for the EPPT are discussed in Chapters 3.

2.5.2 Industrial Ecology

Industrial ecology (IE) also adopts a cradle to grave approach. This relatively new ensemble concept systematically analyses the interactions between human activities and the environment. In industry, IE seeks to optimise the total materials cycle from virgin materials to finished product to ultimate disposal of waste (Socolow et al, 1994). Some of the individual elements of IE have been recognised for several years and are discussed in the following section together with the main ideas of industrial ecology.

Industrial ecology arises from the perception that human economic activity is causing unacceptable changes in basic environmental support systems. As applied to manufacturing, this concept suggests that industrial design and manufacturing processes are not performed in isolation from their surroundings, but rather are influenced by them and in turn influence them (Graedel and Allenby, 1995).

Environmental assessment procedures within industrial ecology focus on the matrix approach. Modified matrices can be used to perform and aid decisions, such as comparing designs, and to perform functions including product inventory, auditing by life stage and auditing by environmental concern. Industrial ecology can be used to compare several design options and their level of relative merit. IE is however based on qualitative assessment. This qualitative approach is somewhat controversial among engineers because of the lack of data. However, IE with its qualitative approach allow impacts which can not be quantified to be included. The systematic approach may be destroyed in a non-qualitative approach if an impact can not be quantified (Graedel and Allenby, 1995).

A specific industrial ecology analysis focuses on options for a particular process. The most common method comprises four primary matrices, each with two axes, one comprising the life stages of the product or process and the other consisting of issues categories bearing on the suitability of the option under evaluation. The matrices are detailed below:

- **Manufacturing Primary Matrix** focuses on each option with regard to manufacturing itself.
- **Environmental Primary Matrix** looks at more traditional environmental impacts of technological choices, but uses the same life-cycle stages of the product and with categories that attempt to minimise the 'single media' fixation of current approaches.
- **Toxicity/Exposure Primary Matrix** looks at toxicity and exposure issues in a systematic life cycle way.
- **Social/Political Primary Matrix** is designed to capture the broader non-technical aspects of each option (Graedel and Allenby, 1995).

The inputs to each matrix cell are based on a series of questions and answers. The cells are completed with a series of symbols and shading to represent effects, degree of effect and degree of concern. Upon completion of the primary matrices for each option being considered each matrix is given an overall degree of concern/certainty assessment. These assessments are then transferred to a summary matrix that displays the results for several alternatives. This format is suitable for easy comparison so a decision can be made. This matrix approach has been adopted by the European Ecolabelling Scheme which requires a 5 x 8 matrix to assess the cradle to grave effects of a product when deciding to award a label (Crittenden, 1994)

Industrial Ecology has limited application to the development of the EPPT. However, the checklists derived to undertake the assessment may provide a foundation on which to base the evaluation of company environmental performance, an area of future work.

2.6 Management approaches to environmental performance

Finally, it is necessary to consider the management approach to environmental assessment and to the environmental performance of companies. This includes a brief discussion of Environmental Management Systems, BS7750 and ISO 14001, environmental audits and the Environmental Management and Audit Scheme regulations. Environmental performance indicators (EPI's) are also discussed along with their uses and their possible application to the EPPT.

All methods of assessing environmental impact and performance within a company should be encompassed in the company's Environmental Management System (EMS). The aim of an EMS is to :

- help develop a proactive environmental approach
- ensure a balanced view across all functions
- enable effective, directed environmental goal setting and
- make the environmental auditing process optimally effective (Hunt and Johnson, 1995)

EMS has its origins in environmental auditing. Environmental auditing was first developed in the 1970's in North America as a management tool to examine and evaluate the compliance of facilities and operations with environmental law and regulations. Whilst the concept of environmental management systems was highlighted in papers relating to environmental auditing, very limited EMS literature was available until the inception of the Environmental Management System standard, BS7750. BS7750 has been tailored to compliment the EC's Eco-Management and Audit Regulations and the associated scheme, Eco-Management and Audit Scheme, EMAS (Hunt and Johnson, 1995). Certification for both EMAS and BS7750 became available in 1995.

In the UK many companies started environmental auditing processes in the early 1990's and found their EMS to be very weak or non-existent. BS7750, EMAS and ISO 14001 are providing a structure framework to formalise their systems. An Index of Corporate Environmental Engagement of the FTSE 100 companies has been undertaken by AEA for the Business in the Environment group which identifies the environmental consideration of the top 100 companies across all sectors. This includes details of those that have implemented an EMS (AEA Technology, 1996). Since March 1995 over 60 organisations have been awarded BS7750 certification. Six sites registered in the UK have been awarded EMAS certification, 4 in conjunction with BS7750. Convergence of all international initiatives will be encompassed in ISO14001 (Smith, 1996b).

Environmental Performance Indicators, one aspect of EMS, are analytical tools which allow comparison with respect to certain environmental characteristics between various plants in a company and various companies in an industry (Tyteca, 1996). Five driving forces for business to adopt environmental performance measurement have been identified by James (1994). These are: the biosphere, financial stakeholders, non-financial stakeholders, buyers and the public. Haines (1993) added the additional but no less importance aspect of 'the attainment of leadership in defining an industry wide environmental excellence'.

Currently the existing approaches to EPI's have focused on LCA and business specific measures. LCA is the most detailed and ideal concept for EPI's but the same problems arise with its application to EPI's as have previously been discussed. It has also been highlighted that EPI's do not tell us how to integrate the impacts of products or processes which is the goal for EPI's and that they are difficult and costly to undertake. The business specific measures include the company specific indices detailed in Section 2.3.1.3 but they do not lend themselves to inter-process or inter-company comparison. Tyteca (1996) discusses methods to quantify inputs, outputs and productive efficiency which considers the 'undesirable outputs' in parametric and non-parametric approaches. Tyteca (1996) also recognises that no attempt has been made to define or quantify pollution or environmental efficiency. This will be addressed by the EPPT and will be applied in Chapter 9. Details of EPI's can be found in Eckel et al (1992) and Azzone and Noci (1996).

2.7 Summary

The chapter has provided an overview of the environmental indices and methods available to assess environmental impact and performance of processes. It has demonstrated the limited application of many of the tools and the problems associated with certain approaches. The ideas adopted from these approaches and the areas missing relative to the application of the EPPT will be addressed in Chapter 3 where the novel aspects of the EPPT will be highlighted.

3. Development of the Environmental Process Performance Tool

This chapter presents the aims and objectives of this research and provides a focus for the discussion on the development of the EPPT that follows. Specific aspects that were considered when developing the EPPT are described. The concepts adopted from existing techniques and the novel aspects of the EPPT are also presented.

3.1 Aims and objectives

The aim of this research is to develop an environmental assessment tool for batch chemical processes. The tool is known as the Environmental Process Performance Tool (EPPT). The aims of the EPPT are to:

1. Adopt an integrated approach to environmental assessment;
2. Encompass a wider scope to environmental assessment than current environmental impact index techniques;
3. Provide a method to determine the Best Environmental Option for a process;
4. Provide a means of identifying opportunities for minimising environmental impact; and
5. Provide a method for comparing processes within and between companies.

The following objectives were set in order to achieve the aims set for the development of the Environmental Process Performance Tool.

1. To undertake a quantitative mass based assessment of the inputs and outputs of selected chemical processes;
2. To develop a method to assess the environmental impact of the chemicals to each media, from this assessment chemical scores are determined;
3. To determine a method of combining chemical scores and masses of inputs and outputs of the selected chemical processes and to determine a method of assessing the environmental impact of the utilities of selected processes;

4. To develop a method of evaluating the environmental impact of process changes and comparing different processes.

The objectives listed above provided data for process comparisons, environmental impact minimisation studies and the determination of the Best Environmental Option.

The following section identifies concepts adopted from existing techniques used in developing the EPPT.

3.2 Adoption of concepts from current techniques

When developing an environmental index it is necessary to define its scope. Specific consideration of the application of the index must be made. It is also necessary to consider impact analysis and its combination with process specific data. These aspects are discussed in the light of existing techniques.

3.2.1 The scope of the EPPT

One of the main aims of the EPPT is to assess the effect of chemical processes on the environment as a whole. Unlike existing environmental impact indices (EII's) which consider only the emissions and wastes from the site, the EPPT assesses the wider implications of emissions on the environment. In addition the EPPT assesses feedstocks to and utilities of processes.

The origin of the wider scope of the EPPT lies in life cycle assessment. LCA addresses the inputs and outputs of the process and also its energy implications. When considering inputs, LCA goes right back to the extraction of raw materials and includes the refining of those raw materials and the generation of the electricity. This complete consideration of the inputs is too detailed for the purpose of the EPPT. Therefore, the EPPT adopts an alternative approach and considers the potential environmental impact of the chemical inputs to the process. LCA also considers aspects such as the transportation of products and raw materials, and the ultimate disposal of the product. This again is beyond the scope of this research. Nonetheless, the EPPT does consider the ultimate fate of emissions from a process and not just the effects on the media to which the emissions are released. Thus the scope of the EPPT is a restricted life cycle assessment. This is demonstrated in Figure 3.1.

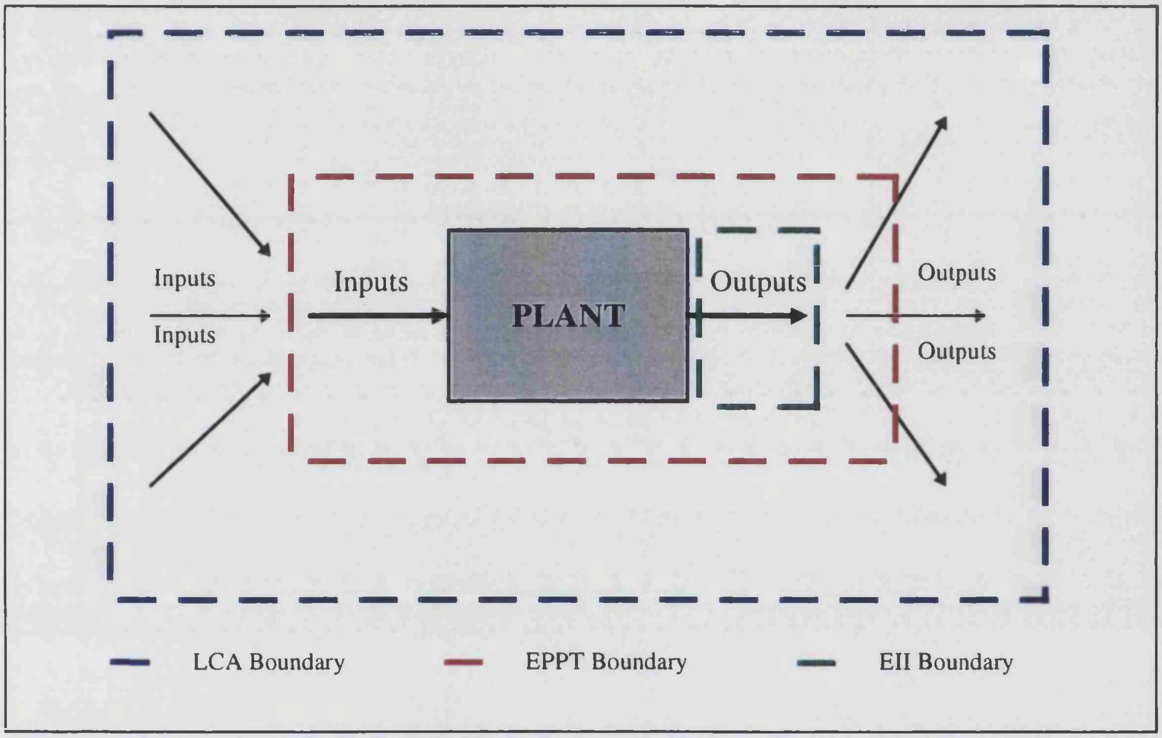


Figure 3.1: Boundaries of EPPT and comparison with LCA and EII boundaries

Having identified the boundaries of the EPPT it is now necessary to define the boundaries for its application.

3.2.2 Application boundaries

There are several boundaries that could be drawn around the application of the EPPT. For example, the EPPT could be site specific, batch specific or production unit specific. The site specific approach has been used by Rhone Poulenc (1992). In its index the amount of waste leaving the site in one year is compared with that of the previous year, regardless of the amount of production. The lack of consideration of production rate provides scope for criticism - it is easy to reduce amounts of waste reducing or not producing a product. This type of approach is not detailed enough to provide a means of comparing process changes, one of the aims of the EPPT.

The batchwise approach assesses the inputs and outputs of one batch of a product regardless of the quantity of product produced. This approach was considered for application to the EPPT as it could provide a means of comparing processes per unit operation. However, the development of comparison techniques, (discussed in Chapters 8 and 9) required a standard mass of product, which meant that the batchwise approach was unsuitable due to varying production rates. A decision on the unit amount of production was required. A unit of 1000kg of product has been selected since this is the mass on which the majority of mass balances obtained from IPC applications are based.

Having decided on a production unit of 1000kg for the application of the EPPT, it was then necessary to determine whether a qualitative or quantitative approach to impact assessment was required.

3.2.3 Qualitative or quantitative assessment procedures

Many of the existing environmental impact indices (EII's) use parameters based on qualitative assessments to ascertain the environmental impact of a process. These assessments include the categorisation assigned for waste strategies adopted by Shanks and McEwan (1994) and SmithKline Beecham (SKB) (Cunningham, 1994). In qualitative EII's the classification assigned to each of the categories are based on the waste stream and their properties. They are not based specifically on the individual chemicals contained in the stream. Quantitative assessment procedures based on the chemicals within the stream have been carried out by The Environment Agency (1997) and Elliott (1997).

In order to provide a reliable assessment tool for chemical processes, specifically for batch processes, a quantitative chemical assessment approach rather than a qualitative waste stream approach has been adopted. The main reason for a quantitative approach is that batch processes may contain many chemicals in their waste streams and, unlike continuous processes, the composition of the waste streams at any one time can vary significantly. A qualitative approach, such as SKB's, could have been applied in this situation. However, the limited variation in the overall classification for a chemical process, which is emphasised if waste streams are evaluated independently of quantity provides little scope for process comparison. Process comparisons are discussed in more detail in Section 3.3.2 and Chapters 8 and 9.

Having adopted a quantitative chemical assessment approach to determine environmental impact, a decision as to whether to combine the chemical assessment with mass based or concentration based data is required.

3.2.4 Mass or concentration

With the exception of the Integrated Environmental Index (IEI) developed by the Environment Agency (1997), indices which are production rate related are based on mass of emissions released. Using a concentration based approach has both advantages and disadvantages. As was discussed in Section 2.3.3 discharge licences and permits are based on concentration data. In order to determine the impact of chemicals based on concentration data it is necessary to establish a baseline level of the chemical in the environment. It is also necessary to establish a 'no observable effect level' (NOEL) of that chemical in the environment or to determine an environmental quality standard (EQS) or environmental assessment level (EAL). With the limited data available and the difficulty of data interpretation to determine environmental effects these levels are difficult and time-consuming to establish and are often criticised. However, applying concentration based limits in this way means a threshold limit which is deemed to damage the environment can be adhered to. This is particularly important if a chemical is known to exhibit non-linear impact effects with regard to concentration. The waste stream can be diluted or withheld to avoid exceeding the threshold limit. This is one reason for a concentration based approach in legislation.

The following simple example demonstrates the difficulty in developing EAL's or threshold levels for environmental assessment. Consider two cases: Case 1, 10kg of chemical emitted over 1 hour and Case 2, 1kg of chemical emitted each hour for 10 hours. How is the case with the least environmental impact determined? This question can only be answered with extensive testing on the chemical in question. The emission for Case 1 could provide a level which could pass the threshold and kill organisms whereas the emission for Case 2 might not effect the organism. In another situation with a different chemical, Case 2 may be worse having a cumulative effect on organisms either through bioaccumulation or steady degradation of a physiological pathway rather than a shock to the pathway as might be the case in Case 1. There is also the additional problem that the same chemical may cause a Case 1 scenario on one organism and a Case 2 scenario in a different organism which inhabit the same part of the environment. From this it may be seen that consideration of the effect of a particular chemical is difficult to establish unless extensive chemical, species and site specific studies have been carried out.

Adopting a mass based approach enables the complete mass of chemicals entering the environment to be assessed. By not comparing the emission's contribution to the environmental level the mass based approach allows the effect of chemicals to be considered on their own characteristics rather than on the characteristics of the surrounding environment. Whilst consideration of the surrounding environment may be important, if one assumes the environmental effect of chemical emissions are the same regardless of where they are released, the impact of chemical emissions can be assessed in a uniform manner. This also allows comparisons to be made between operations on different sites.

The advantages and disadvantages of mass and concentration based approaches have been described from the point of view of assessing environmental impacts. However an additional and no less important point has to be considered when deciding whether to adopt a mass or a concentration based approach, that is, the acquisition of mass or concentration data from a design study or from an existing plant. Concentration based data is hard to obtain. Extensive monitoring or dispersion modelling is required for existing plants. In some cases such monitoring or dispersion modelling already exists for legislative purposes but this is primarily for prescribed substances and sometimes uses lumped physicochemical parameters, such as BOD and pH, of streams rather than individual chemicals. In order to determine the environmental concentration of emissions from processes at the design stage relatively expensive process and dispersion modelling is required.

Mass based data is somewhat easier to acquire as mass balances are more readily available for processes and initially are set during the design stage. The EPPT can be applied to mass balance data to determine the environmental impact of the process. However, as will be seen in Chapter 8, application of the EPPT to more detailed data obtained from modelling and detailed study reveals more detailed and accurate results.

With so many chemicals involved in batch processes it is very difficult to assess the threshold limits and assessment levels required for a concentration based approach. It is also difficult to acquire the process data. For these reasons a mass based approach has been adopted for the EPPT.

3.2.5 An integrated approach

Many of the indices presented in the previous chapter, particularly the Environmental Quality Indices (EQI's) were media specific. With the exception of EniVal and IEI, none of the impact indices considered the environment as a whole. The IEI goes some way to develop an integrated approach that considers the releases to each media but then simply adds the quotients for each medium together. Elliott (1997) went further with EniVal and developed an environmental fate model to integrate the effects of each medium. Elliott also incorporated a time-based component to provide an integrated approach. These two aspects developed by Elliott have been incorporated into the EPPT to provide an integrated multi-media approach to environmental assessment.

Timescales are very important when determining the effects of chemicals on any living system, be it on micro-organisms, invertebrates, vertebrates or the environment as a whole. Simple human toxicity tests are carried out over varying time scales ranging from minutes to years. Time also needs to be considered in environmental assessment. Like EniVal, the EPPT adopts a two tier assessment of impacts on the environment, as described in Chapter 5. Elliott described these tiers as the short-term and long-term effects. The short-term effects are those which occur within hours or days of exposure and the long-term effects encompass impacts that take several years or decades to appear. The EPPT assesses the immediate release of the emissions from the process and their ultimate distribution. The persistence of a chemical is used to assess the duration over which the chemical will exhibit its effects.

Having discussed the adoption of existing techniques for possible inclusion in the EPPT, the next section highlights areas not addressed by these techniques and thereby emphasises the novel aspects of the EPPT.

3.3 Novel aspects of the EPPT

The integrated multimedia approach adopted by the EPPT has its origins in EniVal. Like EniVal the EPPT uses a scoring system which is combined with the mass of the chemicals released from the process. A two tier system of chemical assessment similar to that developed by Elliott has been applied to the EPPT. However the focus of this assessment is different. There is also a difference in the structure and the parameters of the chemical assessment. Details of Elliott's chemical assessment can be found in Elliott (1997). The chemical assessment for the EPPT is presented in Chapter 4.

The next section presents the novel aspects of the EPPT. These include the utilities assessment, the process comparisons and the EPPT as a tool to aid in the identification of impact minimisation opportunities.

3.3.1 Utilities

The environmental quality and impact indices presented in the previous chapter do not consider the environmental impact of utilities used in the chemical industry. The utilities (electricity, steam and cooling water) are assessed using the chemical assessment method within the EPPT. Often processes are changed in order to reduce the impact of chemical emissions at the expense of an increased energy use. The incorporation of an utilities assessment provides a means of comparing the environmental impact of energy use when reducing the environmental impact of chemical emissions from the process. By providing a method of assessing energy use a direct comparison between emissions and energy can be made to determine the 'Best Environmental Option'. Water use within the process, for cleaning and as a cooling medium, is also important in the chemical industry. Whilst there is a financial cost associated with water use there is also an environmental cost associated with the degradation of our waterways. Consideration of water use is therefore important in assessing the environmental impact of the chemical industry. The utilities assessment and application is discussed in more detail in Chapter 7.

3.3.2 Process comparison

Within the EPPT four methods are used to compare processes. These methods use scores derived for the input, product and emissions for a process to assess the environmental performance of the process. The four methods compare environmental impact, environmental selectivity, process conversion and impact conversion. The first method compares the environmental impact of processes based on emission scores per 1000kg of product. The second method compares the environmental impact based on the toxicity of the product. The third method compares how efficiently the process converts input score into product score and the fourth method compares how the process convert input score into emission score. Each of these methods will be discussed in detail and applied to case studies in Chapter 9.

3.3.3 Impact minimisation identification

The EPPT can also be used to identify opportunities to minimise environmental impact. It provides focus on the most polluting parts of a process which can then be used for impact and waste minimisation strategies. This will be discussed in Chapters 8 and 9.

3.4 Summary

This chapter has discussed aspects considered during the development of the EPPT in the light of existing indices and approaches to environmental assessment. Novel aspects of the EPPT have been highlighted. These will be discussed in more detail and applied to case studies in later chapters. The next section details the structure of the remaining parts of the thesis.

3.5 The structure of the thesis

The next two chapters discuss the chemical assessment used as the basis of the EPPT. Chapter 4 describes the structure of the chemical assessment. The parameters used for the chemical assessment are identified and the scoring system and assessment factors are also developed for each parameter. Chapter 5 discusses the distribution models considered for the EPPT and highlights the benefits and limitations of each model. Distribution fractions derived from the model for each chemical are then combined with the parameter scores to determine the score for each chemical in each medium. The chemical score derived for the EPPT will be compared to those derived by Elliott's scoring system.

Having now established the chemical assessment procedure, the building block of the EPPT, Chapter 6 discusses methods of combining chemical scores with mass of chemical emissions and also the assessment of utilites. Chapter 7 then outlines the processes selected for assessment using the EPPT.

In Chapter 8 process options identified for Thomas Swan's Pepton process are evaluated. The use of the EPPT to identify opportunities for impact minimisation are also discussed in Chapter 8. Both Thomas Swans Pepton process and also Fisons sodium cromoglycate process are used in this study. Chapter 9 discusses comparison techniques developed for the EPPT and describes how they are used to determine environmental performance. These comparison techniques are then applied to the processes described in Chapter 7. Finally, conclusions and future work are discussed in Chapter 10.

4. Chemical evaluation

This chapter describes the method used to assess the environmental impact of chemicals in the Environmental Process Performance Tool. Initially the subjectivity of environmental impact assessment is discussed. This discussion concludes that although environmental impact assessment is subjective some type of quantitative chemical evaluation needs to be undertaken in the EPPT. Data sources have been identified and used to provide guidance for the chemical evaluation. Within the confines of available data the structure of the chemical evaluation has been developed and justified. Thus the chemical evaluation is based on parameters that are indicative of environmental impact. A scoring system has been developed for each parameter to convert raw chemical data into comparable scores. The data used for the chemical evaluation has been stored on a database designed for the purpose. A brief discussion of this chemical database is given at the end of this chapter.

4.1 Subjectivity of impact assessment

Environmental impact assessment is subjective as it compares different and often unrelated parameters. To address this subjectivity some workers have assigned weighting factors to parameters to increase the influence of those considered to have a larger impact. Usually the weightings are applied based on the opinion of experts (Brown et al, 1970) or the opinion of the impact assessment developers. For example, the developers of the Eco-Indicator '95 (Goedkoop, 1995), which is a life-cycle approach to environmental assessment, have assigned weighting factors based on a distance-to-target method derived from scientific and political opinion. In other cases public opinion has been used to assign weightings. Weighting factors however are also subjective and compound the subjectivity of impact assessment further. For this reason weightings are not used in the EPPT and all parameters used in the EPPT are considered equal.

Subjectivity can also be introduced into environmental assessment by using toxicity data taken from one species to represent another. For example the toxicity of chemicals in rats is often used as an indicator of the effect of that chemical on humans. The factors generating subjectivity in toxicology and ecotoxicology are discussed later in Section 4.4.1. Despite such subjectivity some attempt must be made to quantify environmental impacts. It is recognised that within the chemical evaluation of the EPPT there will be areas of subjectivity as with all impact assessment methods. However, the following sections provide justification of parameter selection for impact assessment in the EPPT in an attempt to minimise criticism. The procedure presented here provides a foundation for chemical evaluation from which improvements can be made.

4.2 Data acquisition and limitations

The main problems when determining the environmental impact of a chemical is the lack of data available and the wide and disperse nature of that data. Physico-chemical data is the easiest to determine and is available in Croner's Substances Hazardous to the Environment (1997), Perry (1984) and on material safety data sheets. Toxicity data is more difficult to locate. LaGrega et al (1994) identify numerous toxicity databases including the Integrated Risk Information System (IRIS) and the International Programme on Chemical Safety (IPCS). Ecotoxicological data is the hardest to locate as this science is still in its infancy.

The Organisation for Economic Co-operation and Development (OECD) has produced guidelines detailing the data requirements for new substances dependent on their production level (West, 1993). A good range of parameters for assessing environmental impact is provided. However, this amount of data is rarely available for the majority of chemicals.

Existing chemicals, listed in the European Inventory of Existing Commercial Chemical Substances (EINECS) and hence classified as 'dangerous to the environment', have a requirement for ecological information to be detailed on material safety data sheets. This ecological information consists of:

1. Acute and chronic ecotoxicity data.
2. Environmental fate, including information on mobility, degradability and accumulation data.
3. Other adverse effects data, e.g. ozone depletion potential, photochemical ozone creation potential, global warming potential and effects on waste water treatment plants (Croner's, 1998).

However this amount of information is only available for chemicals classified as 'dangerous' and hence not available for the majority of chemicals.

The International Register for Potentially Toxic Chemicals (IRPTC) is the international clearing-house for scientific, technical and regulatory information for the assessment and control of chemical hazards (UNEP, 1990). The IRPTC has a databank of validated chemical information which can be called upon for general queries and in major disaster situations. As with the data sources already discussed, the IRPTC data profile contains several environmental components. This data source initially looked promising. However, much of the data, specifically environmentally based data for complex organics is not available.

Further detailed investigation identified data sources including Croner's Substances Hazardous to the Environment (1998) and the Royal Society of Chemistry's Dictionary of Substances and their Effects (DOSE) (Richardson, 1992). Croner's contains both qualitative and quantitative data. Numerical values for physical-chemical properties are given together with risk and safety phrases and details of pollution factors. Croner's also details the effects of chemicals on living organisms and environmental fate. Of particular relevance to the EPPT is the sections which give details of mammalian effects, ecotoxicity, bioaccumulation potential and environmental fate.

DOSE (Richardson, 1992) contains similar information to Croner's. However, DOSE contains the raw data in preference to qualitative assessments. The data given in DOSE includes physical properties, occupational exposure, ecotoxicity (subdivided into fish and invertebrate toxicity), environmental fate, mammalian toxicity, carcinogenicity and long-term effects. DOSE has been used to provide the majority of the data for the EPPT chemical evaluation. However, other data sources such as Kaiser and Palabrica (1991) and Graedel and Allenby (1995) have been used to provide data on specific parameters.

In this section the quality and quantity of data that is available in the literature and from other sources have been identified. The next section describes the type of data that have been used in the EPPT chemical evaluation.

4.3 Chemical evaluation structure

Existing environmental impact indices (Elliott, 1997 and Environment Agency, 1997) use three environmental media; air, water and soil. Other environmental compartments, such as sediment and biota, have been considered in environmental distribution models. (Environmental distribution models are discussed later in Chapter 5). Three media (air, water and soil) were considered to be sufficient for the EPPT.

Within the EPPT the environmental impact of a chemical is evaluated using a three component approach. The three components are toxicity, persistence and effect. The toxicity component evaluates the impact of a chemical on living organisms. The persistence component evaluates the duration of chemicals in the environment and consequently how long they will be exhibiting or contributing to the toxicity and the effects on the various media. The effect component evaluates the local, regional and global effects that a chemical may have on the environment.

4.4 Parameter selection

Each chemical is evaluated for its toxicity, persistence and effects on each of three media (air, water and soil). The parameters that have been used to evaluate these components in each medium are discussed and justified in the following sections.

4.4.1 Toxicity parameters

Before describing individual toxicity parameters used in the EPPT, toxicology and ecotoxicology are discussed in general terms in order to present the inherent difficulties within these sciences and the limitations of the studies.

4.4.1.1 Toxicology and ecotoxicology

Toxicology considers the adverse effects caused by the exposure of living organisms to chemicals. The discipline incorporates aspects of physiology, pharmacology, biochemistry, molecular biology and epidemiology, and unlike chemistry or physics it is not an exact science (LaGrega, 1994). As the fundamental mechanisms causing toxic responses, in for example humans, are not fully understood toxicology findings are largely based on observations and only partially derived directly from human responses. The lack of precision is not only apparent when using the evidence of one animal species to predict the effects on another, such as rat to human, but also when extrapolating from the high exposures used in animal experiments to the low dose situations actually encountered in the environment. Thus the quantification of chemical toxicity has an element of uncertainty. Despite this uncertainty it should be emphasised that toxicological evidence is sufficient to predict risks associated with the presence of chemicals in the environment (LaGrega, 1994).

Ecotoxicology is a relatively new scientific discipline which extends toxicological principles to natural systems. Ecotoxicology focuses on the effects of populations rather than individual species interacting with the physical environment. It is important to understand the indirect effects on a population and ecosystem as well as the direct effects. For example, an accidental oil spill can produce a variety of effects, including a reduction in plant productivity through the reduction in photosynthesis caused by a decreased light penetration, lethality to organisms through exposure to certain hydrocarbons, and bioaccumulation of hydrocarbons through the food chain with possible long-term implications for reproduction and other physiological systems.

LaGrega states that 'ecotoxicologists struggle to find an optimal test organism for ecotoxicity tests, akin to the white rat in toxicology' and then comments that a large variety of species ranging from primary producers (algae) through invertebrates (water fleas) to predators at the top of the food chain are used in toxicity tests. However, it should be emphasised that while it is feasible to consider mammal to mammal comparisons in toxicology, the feasibility of comparing the toxicity of a chemical to an invertebrate (such as a water flea) with that to an otter, or the toxicity to an algae with that to the toxicity of a predatory fish is questionable. Due to the lack of ecotoxicity data such extrapolations are sometimes necessary although perhaps not to the extremes suggested by these examples. Standard toxicity tests have been established by the Organisation for Economic Co-operation and Development (OECD) but there is still scientific disagreement as to the species most sensitive to a contaminant. There are also a considerable number of parameters influencing the toxicity of chemicals in the environment. Some of these parameters are shown in Table 4.1.

Despite all the elements of uncertainty in ecotoxicology, ecotoxicity data provides the best information with which to establish the environmental impact of chemicals. It is primarily ecotoxicity data that has been used to provide the toxicity evaluation of the chemical evaluation for the EPPT.

Table 4.1: Factors influencing the toxicity of trace metals in the aquatic environment (adapted from Connell and Miller, 1990)

• Form of the metal, such as:	Inorganic/organic Soluble: Ion Complex ion Chelated ion Molecule Insoluble: Colloidal Precipitates Adsorbed
• Presence of other metals or poisons, such as:	Joint action No interaction Antagonism Synergism
• Factors influencing the physiology of organisms and possibly the form of the metal in water, such as:	Temperature pH Dissolved oxygen Light Salinity
• Condition of organism, such as:	Stage in life history (egg, larva etc.) Changes in life cycle (moulting, reproduction) Age and size Sex Starvation Activity Additional protection (shell) Adaptation to metals Altered behaviour

4.4.1.2 Toxicity parameter selection

When selecting parameters to determine the toxicity of chemicals a conscious decision was made to include a representative from each of three levels in the animal and plant kingdoms. The intention was to use micro-organisms, invertebrates and vertebrates to represent the trophic levels in the animal kingdom and algae, monocotyledonous and dicotyledonous plants to represent the plant kingdom. Ideally each of these levels would be represented in each medium. The next stage was to identify data which could be used for this purpose.

OECD toxicity tests exist for crustacean species and fish, thereby representing invertebrates and vertebrates. This data is by far the most common ecotoxicity data available. *Daphnia magna,* the water flea, is used in OECD toxicity tests and is the most common species of crustacean used for this type of testing. *Lumbricus terrestris*, the earthworm, is also used although the data is more limited. *Lepomis mactochirus*, the bluegill sunfish, is the fish species selected for OECD tests. Data is fairly common for this species. However *Salmo gairdneri*, the rainbow trout is also commonly used. OECD guidelines do not exist for ecotoxicity testing of micro-organisms. However the most commonly used commercial method for toxicity evaluation using micro-organisms is Microtox™.

Plant species data for determining toxicity was more difficult to locate. Whilst OECD testing guidelines exist for algae, monocotyledons and dicotyledons the data is not common. Of the plant toxicity data that is available the focus is on herbicide toxicity tests. The chemical data which would need to be evaluated for chemical processes evaluated by the EPPT was limited. To overcome this problem plants are represented by the vegetation damage potential, an effect parameter described later in Section 4.13.5.

It became apparent that adopting parameters to represent the three levels of the plant and animal kingdom in all three environmental media would be difficult. Sufficient data exists to consider the three animal levels in water. The toxicity evaluation in the soil medium uses Microtox™ data to represent the micro-organisms. The invertebrates in soil are represented by the Earthworm. There was no vertebrate data to represent the soil medium. Therefore the maximum deposition rate (MDR), a parameter used in the Environment Agency's Integrated Environmental Index to represent soil, was selected for use in the EPPT.

Toxicity parameters to represent all animal levels in air were difficult to identify. Air based ecotoxicity tests do not exist for micro-organisms, invertebrates or vertebrates.

However standard toxicity tests are carried out on vertebrates. Inhalation toxicity tests are carried out on small mammals such as rats and mice. This data has reasonable availability. Occupational Exposure Limit data is also available and provides an indication of chemical toxicity in air. Therefore, both these parameters were selected for inclusion.

All of the parameters described above are based on acute toxicity tests. Much less data is available on the chronic toxicity of chemicals. For this reason it was decided to use carcinogenicity data to represent the chronic effect of chemicals on vertebrates. Carcinogenicity is applicable to all media.

Each of the toxicity parameters described above has a scoring system assigned to it within the EPPT. The parameters and their scoring systems will be discussed in more detail, along with assessment factors to determine the accuracy of the data, in Sections 4.5 and 4.6.

4.4.2 Persistence parameters

The duration of a chemical in the environment is determined by persistence which is evaluated using the degradation of the chemical and its bioaccumulation. Degradation is represented by half-life. In the air photo-degradation and oxidation are the main breakdown processes. Hydrolysis and biodegradation cause chemical breakdown in water. Degradation in soil occurs via biodegradation in micro-organisms, photo-degradation on the soil surface and hydrolysis in interstitial water. Bioaccumulation is represented by the bioconcentration factor (BCF). Bioaccumulation occurs when a substance moves usually from water into an organism. This can result in higher concentrations of the chemical in the organism than in the surrounding environment. This phenomenon is known as bioconcentration.

Degradation rate is used to evaluate persistence in all media. In addition bioaccumulation is used to evaluate persistence in water and soil media.

Bioaccumulation is not considered in air as it is unlikely that volatile substances will accumulate in this medium (LaGrega, 1994).

4.4.3 Effect parameters

Global, regional and local effects are evaluated in the effects component of the chemical evaluation. The global effects considered in the EPPT only concern problems in air but have implications on other media. The global effects are global warming and stratospheric ozone depletion. Regional effects such as acidification are considered for all media. In air, acidification is considered to be a problem through the production of acid rain. Acidification generates problems in the water medium through its effects on water bodies, vegetation and soil. The acidification of soil through water also has a significant effect on plants and animals and is consequently considered to be a problem in soil as well.

The other effects with implications for all three environmental media are considered to be regional or local. Photochemical ozone creation is a problem in air due to its implications on human health and damage to vegetation. Vegetation damage potential (VDP) is also considered for air and has been included to account for the toxicity to plants as discussed in Section 4.4.1. This potential has been derived by the Environment Agency for use in its Integrated Environmental Index and has been included in the EPPT in order to consider the effects on the plant kingdom. The vegetation damage potential is considered for both air and soil because there are implications for plant damage in both media. For the air the damage is caused by photosynthesis interference and for the soil by the uptake of nutrients and water through the roots.

Both the odour of a chemical and its aesthetics are considered in the air and water media. Both of these parameters have influences on local environmental quality. Aesthetics are reflected in the colour of the chemical entering the environmental medium. This is considered to be a problem in air, for example with plumes emanating from chemical works. The colour of aqueous emissions are also unsightly and often causes local concern.

4.4.4 Parameter summary

A summary of the parameters which have been selected to assess environmental impact in the EPPT is given in Table 4.2.

Table 4.2: Parameters used for chemical evaluation

	Toxicity	Persistence	Effect
Air	Mammal OEL Rat Inhalation Carcinogenicity	Degradation	Global Warming Potential Ozone Depletion Potential Photochemical Ozone Creation Potential Acidification Vegetation Damage Potential Aesthetics Odour
Water	Microtox™ Crustacean Fish Carcinogenicity	Degradation Bioaccumulation	Acidification Aesthetics Odour
Land	Microtox™ Worms Deposition Rate Carcinogenicity	Degradation Bioaccumulation	Acidification Vegetation Damage Potential

4.5 Scoring parameters

Having selected each of the parameters, the next stage was to determine a method of assessing the contribution of each parameter to the impact of the chemical on the environment. A scoring system was considered most appropriate for the EPPT. A scoring system has therefore been derived for each of the parameters listed in Table 4.2. The scores for toxicity and effect range from zero to ten, zero being the least toxic with no effect, ten being the most toxic. The scoring system for persistence ranges from one to ten. The reason for the different range is discussed in Chapter 5. The scoring systems have been devised using maximum and minimum data obtained from extensive literature reviews and the author's opinion. The scoring systems have also been cross-referenced with other work and other parameter scoring systems within the EPPT to increase the confidence of the scores assigned. If numerous conflicting data exists for any parameter the author's opinion was used to establish an appropriate score for the EPPT.

4.6 Assessment factors

Assessment factors have been used alongside the parameter scores as an indication of the certainty of the scores assigned for each parameter. This section describes how assessment factors have been applied for each parameter. The assessment factors are combined to generate the chemical assessment factor. Full details of the method for determining the chemical assessment factor are given in Chapter 5. Whilst the chemical assessment factor is not used in the environmental evaluation of the process, it does provide a means of highlighting any weakness due to lack of information in the chemical evaluation. The chemical assessment factor has been incorporated into the EPPT design in order to encourage further toxicity testing of chemicals and so to provide more accurate chemical evaluation and hence obtain better results from use of the EPPT.

The guidelines for assigning assessment factors to each parameter are described in the following sections. Where more parameter specific consideration is required the assessment factors are discussed alongside the relevant scoring system descriptions. Well documented data which has been established by the scientific community is given an assessment factor of 10. The assessment factor is reduced if variation in the test conditions or in the species of organism is found. A reduction is applied using the author's opinion and by comparison with other assessment factors in order to ensure consistency. A reduced assessment factor is also used if Croner's qualitative evaluation is used and is based on a different species. When only limited data exists for a particular chemical and a parameter score estimate has to be made using a similar chemical, then a low assessment factor of 1 or 2 is assigned. Higher assessment factor is assigned if several pieces of data are evaluated for the same parameter. This is based on the author's or expert opinion. The scoring systems and assessment factors used for the chemical evaluation are now described in the following sections.

4.7 Toxicity in Air

In the EPPT, toxicity in air is evaluated using the Occupational Exposure Limit (OEL), rat inhalation data and carcinogenicity data. These three parameters together with their scoring system and assessment factors are described in the following sections .

4.7.1 Occupational exposure limit

The Occupational Exposure Limit is aimed at limiting the exposure of employees to chemicals in the work place and is regulated by the Control of Substances Hazardous to Health (COSHH) Regulations. In the EPPT the OEL has been used as an indication of the toxicity of chemicals to humans. Long-term and short-term limits exist for occupational exposure. The long-term OEL (8 hour time weighted average) is intended to control effects by restricting the total intake inhalation over a workshift. The short-term OEL has been derived to limit effects over the short-term. The short-term OEL is also used to restrict the magnitude of excursions above the average concentrations during longer exposure (HSE, 1994). The long-term OEL's are considered to be the more appropriate for use in the EPPT since they are closer to the levels likely to be experienced outside the workplace. The scoring system has been developed by considering extremes of the OEL's and also by comparing the score with the rat inhalation score in order to ensure that the scoring system reflects the toxicity of the chemical. The scoring system has also been designed to accommodate the lower levels experienced in the environment when compared with the workplace. Table 4.3 shows the scoring system assigned for the Occupation Exposure Limit.

Table 4.3: Occupational exposure limit scores (8 hour long-term)

Score	Range (mg/m3)
10	≤ 0.005
9	> 0.005 ≤ 0.5
8	> 0.5 ≤ 1.0
7	> 1.0 ≤ 10
6	> 10 ≤ 50
5	> 50 ≤ 250
4	> 250 ≤ 500
3	< 500 ≤ 1000
2	<1000 ≤ 2000
1	< 2000
0	no effect

The accuracy of the data applied to the EPPT OEL scoring system has been assessed using the assessment factors shown in Figure 4.1.

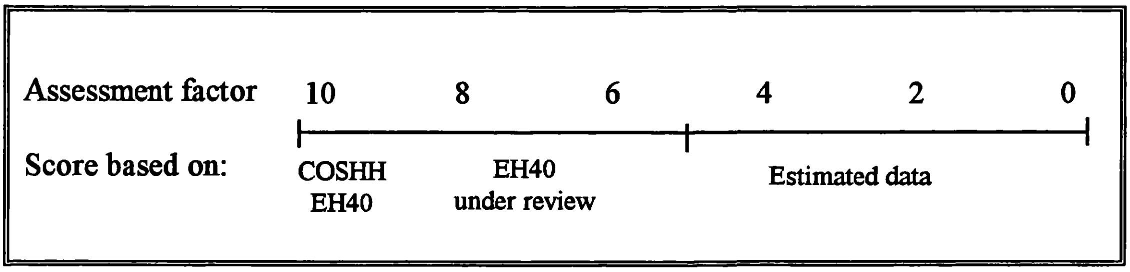


Figure 4.1: Occupational exposure limit assessment factors

4.7.2 Rat inhalation

Rat inhalation data has been used to represent the effect of atmospheric pollution on mammalian species. As the rat is the most common species for mammalian toxicity testing, rat data was selected in order to develop a scoring system since it provides a greater range of data to work with. The most common test times are between 1 and 6 hours. The majority of the rat inhalation data used in the EPPT has been obtained from Richardson (1992). Croner's (1997) mammalian toxicity evaluation based on rat inhalation and rat ingestion data has also been used but it does not provide raw data. A scoring system has been assigned to Croner's evaluation. However it has only been used when specific rat inhalation data was not available. The scoring system developed for rat inhalation data is shown in Table 4.4

Table 4.4: Rat inhalation scores based on LC_{50} in mg/m^3

Scores	Test time - 6 hours	Test time - 4 & 1 hour	Croner's evaluation
10	> 100	> 500	very high
9	$\geq 100 < 500$	$\geq 500 < 1000$	very high
8	$\geq 500 < 1000$	$\geq 1000 < 5000$	high
7	$\geq 1000 < 5000$	$\geq 5000 < 7500$	high
6	$\geq 5000 < 7500$	$\geq 7500 < 10000$	high/moderate
5	$\geq 7500 < 10000$	$\geq 10000 < 20000$	moderate
4	$\geq 10000 < 20000$	$\geq 20000 < 35000$	moderate
3	$\geq 20000 < 35000$	$\geq 35000 < 50000$	moderate/low
2	$\geq 35000 < 50000$	$\geq 50000 < 100000$	low
1	≥ 50000	≥ 100000	low
0	no effect	no effect	no effect

The accuracy of the data applied to the rat inhalation scoring system has been assessed using the assessment factors shown in Figure 4.2.

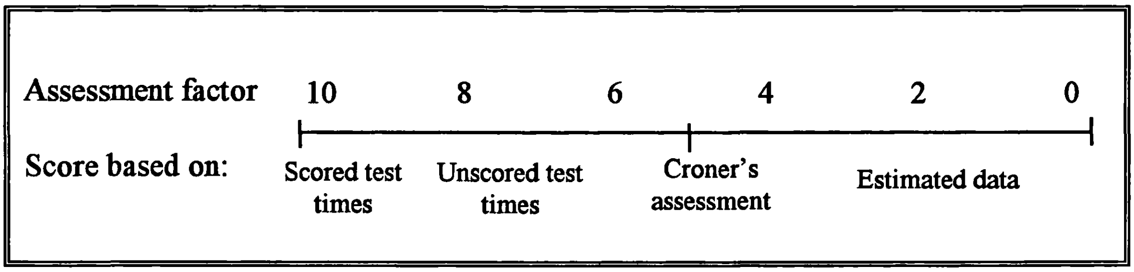


Figure 4.2: Rat inhalation assessment factors

4.7.3 Carcinogenicity

Carcinogenicity is a major factor contributing to the overall toxicity of a chemical and is considered an important factor in evaluating chronic toxicity in all media. Exact data for carcinogenicity are not generally available. The data tends towards descriptive categories. The scoring system for carcinogenicity has been developed using the classes proposed by the US EPA (LaGrega, 1994) as shown in Table 4.5.

Table 4.5: Carcinogenicity scores

EPPT Score	US EPA Class	Description
10	A	Human carcinogen - "there is sufficient evidence from epidemiological studies to support causal association between exposure to the agent and cancer".
8	B1	Probable human carcinogen - limited human data available.
6	B2	Probable human carcinogen - sufficient evidence in animals and inadequate or no evidence in humans.
3	C	Possible human carcinogen.
0	D	Not classifiable as a human carcinogen
0	E	Evidence of non-carcinogenicity in humans.

The accuracy of the data applied to the carcinogenicity scoring system has been assessed using the assessment factors shown in Figure 4.3.

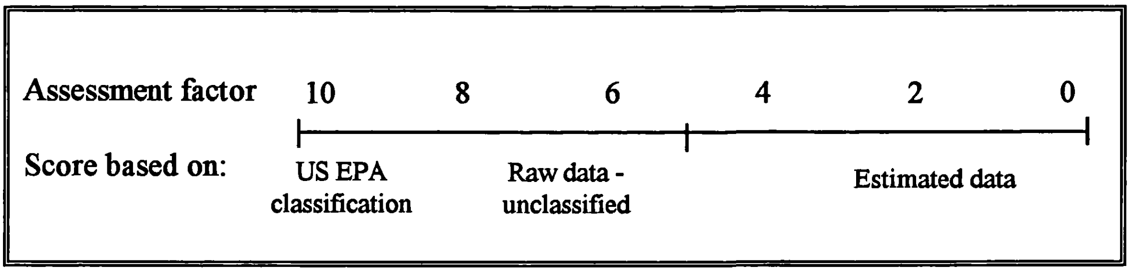


Figure 4.3: Carcinogenicity assessment factors

4.8 Toxicity in water

The toxicity of chemicals in the aquatic environment has been evaluated using ecotoxicity data from Microtox™, crustaceans, fish and carcinogenicity. A discussion of each parameter is given in this section together with the scoring system and the assessment factor derived for each parameter.

4.8.1 Microtox™

Microtox™ is a commercially available toxicity test using the light emitting bacterium *Photobacterium phosphoreum.* In this simple toxicity test the bacterial phosphorescence is first measured. The bacteria are then put into contact with the chemical. After a predetermined time the bacteria are removed and the amount of light being emitted from the bacteria is again measured. The reduction in phosphorescence is used as a measure of the toxicity of the chemical. In practice the toxicity of the chemical is measured using the EC_{50} which is the effective concentration to reduce the phosphorescence of the bacteria population by 50%. A reasonable amount of data exists for this commercially available method. The main source of Microtox™ data used in the EPPT has been obtained from Kaiser and Palabrica (1991).

The duration of Microtox™ toxicity tests is usually 30 minutes, 15 minutes or 5 minutes. For the purpose of this research the Microtox™ scoring system shown in Table 4.6 uses the 30 minute test as this provides the most common data. Evaluation of the other test times has been carried out and the data resulted in similar scoring systems. Hence data for the other times could be evaluated on the same scoring system as the 30 minute data using a lower assessment factor. Croner's (1998) have also developed an ecotoxicity evaluation based on fish and invertebrate toxicity data. This has been used with a reduced assessment factor but only if Microtox™ data was unavailable.

Table 4.6 Microtox™ scores

Score	Microtox™ data EC_{50} ppm	Croner's evaluation
10	<1	very high
9	$\geq 1 < 5$	high
8	$\geq 5 < 10$	high
7	$\geq 10 < 25$	moderate
6	$\geq 25 < 50$	moderate
5	$\geq 50 < 100$	moderate
4	$\geq 100 < 500$	low
3	$\geq 500 < 1000$	low
2	$\geq 1000 < 2500$	low
1	≥ 2500	low
0	no effect	no effect

The accuracy of the data applied to the Microtox™ scoring system has been assessed using the assessment factors shown in Figure 4.4.

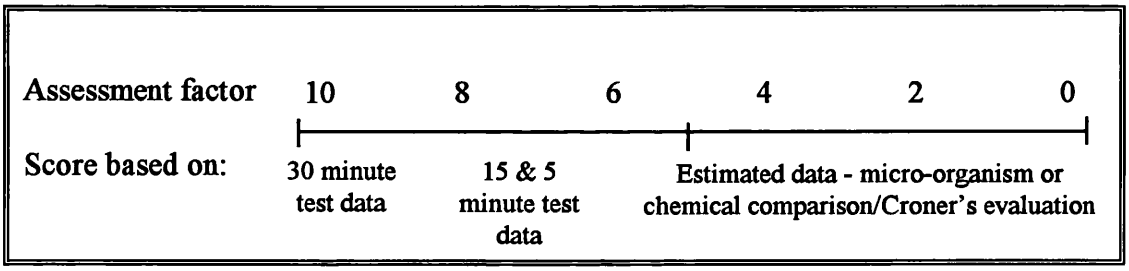


Figure 4.4: Microtox™ assessment factors

4.8.2 Crustacean

Crustaceans particularly *Daphnia* sp., the water flea, are common organisms used for toxicity tests. *Daphnia magna* is the most common species used although *Daphnia pulex* is often used. Freshwater species are much more commonly used in ecotoxicity tests than marine or estuarine species due to the difficulties in mimicking the water composition in the latter environments. Ecotoxicity tests carried out on these species measure the EC_{50} of the chemical on the species. The EC_{50} is the effective concentration to immobilise 50% of the test population over a predefined time, usually 24, 48 or 96 hours. The EC_{50} (effective concentration) rather than the LC_{50}

(lethal concentration) are used on these species because of the difficulty determining whether such a small organism is actually dead.

Scoring systems have been developed for *Daphnia pulex* and *Daphnia magna* based on data extremes and also with cross references between other crustacean species and comparison with fish and Microtox™ scoring systems. The majority of the data for crustacean species has been obtained from Richardson (1992). Croner's evaluation has also been scored and has been used if species specific data has not been available. The crustacean scoring systems are given in Table 4.7.

Table 4.7: Crustacean scores based on EC_{50} in mg/l

Score	*Daphnia magna* 24 hour	*Daphnia magna* 48 & 96 hour	*Daphnia pulex* 48 hour	Croner's evaluation
10	< 0.5	< 0.1	< 0.5	very high
9	≥ 0.5 < 1	≥ 0.1 < 0.5	≥ 0.5 < 1	very high
8	≥ 1 < 5	≥ 0.5 < 1	≥ 1 < 5	high
7	≥ 5 < 20	≥ 1 < 5	≥ 5 < 20	high
6	≥ 20 < 50	≥ 5 < 20	≥ 20 < 50	moderate
5	≥ 50 < 75	≥ 20 < 50	≥ 50 < 75	moderate
4	≥ 75 < 100	≥ 50 < 75	≥ 75 < 100	moderate
3	≥ 100 < 200	≥ 75 < 100	≥ 100 < 200	low
2	≥ 200 < 500	≥ 100 < 200	≥ 200 < 500	low
1	≥ 500	≥ 200	≥ 500	low
0	no effect	no effect	no effect	no effect

The accuracy of the data applied to the crustacean scoring system has been assessed using the assessment factors shown in Figure 4.5.

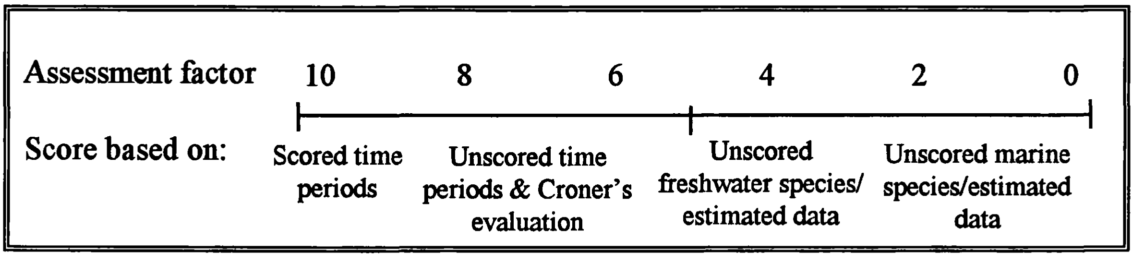


Figure 4.5: Crustacean assessment factors

4.8.3 Fish

Various species of fish are used for toxicity testing. The toxicity tests are similar to the crustacean toxicity tests with the exception that the toxicity of the chemical is measured as the LC_{50}. The LC_{50} is the lethal concentration to 50% of the test population. Rainbow trout (*Salmo gairdneri*), fathead minnow (*Pimephales promelas*), goldfish (*Carassius auriatus*) and bluegill sunfish (*Lepomis mactochirus*) are the most commonly tested species. The rainbow trout is a common UK freshwater species. The goldfish and fathead minnow are also a freshwater species although not native to the UK. The bluegill sunfish is a warm water marine species and is less likely to show the toxic responses exhibited by cold water species. However, the bluegill sunfish is the OECD guideline test species and consequently a large amount of fish toxicity data is available for this species.

A scoring system has been devised for each of these species over 24, 48 and 96 hour periods based on data primarily obtained from Richardson (1992) and Croner's (1998). Each of the scoring systems not only has been cross referenced between species using the same chemical but also has been compared with other water toxicity parameters to ensure consistent results. The fish scoring systems are based on adult fish. Juvenile fish are much more sensitive to toxins than adult fish. If only juvenile fish data has been available an increased score and a low assessment factor has been used. The data has been compared with that from other sources including Croner's evaluation and also with the scores assigned to other parameters representing toxicity in water in order to reduce misinterpretation of data. The scoring systems developed for fish toxicity data are shown in Tables 4.8 to 4.10.

Table 4.8: Rainbow trout (*Salmo gairdneri*) scores

Score	24 & 48 hours LC_{50} mg/l	96 hour LC_{50} mg/l	Croner's evaluation
10	< 0.25	< 0.1	very high
9	$\geq 0.25 < 1$	$\geq 0.1 < 0.25$	very high
8	$\geq 1 < 2.5$	$\geq 0.25 < 1$	high
7	$\geq 2.5 < 10$	$\geq 1 < 2.5$	high
6	$\geq 10 < 25$	$\geq 2.5 < 10$	moderate
5	$\geq 25 < 75$	$\geq 10 < 25$	moderate
4	$\geq 75 < 150$	$\geq 25 < 75$	moderate
3	$\geq 150 < 350$	$\geq 75 < 150$	low
2	$\geq 350 < 500$	$\geq 150 < 350$	low
1	≥ 500	≥ 350	low
0	no effect	no effect	no effect

Table 4.9: Fathead minnow (*Pimephales promelas*) and goldfish (*Carassius auriatus*) scores

Score	24, 48 & 96 hour LC_{50} mg/l	Croner's evaluation
10	< 0.25	very high
9	$\geq 0.25 < 1$	very high
8	$\geq 1 < 2.5$	high
7	$\geq 2.5 < 10$	high
6	$\geq 10 < 25$	moderate
5	$\geq 25 < 75$	moderate
4	$\geq 75 < 150$	moderate
3	$\geq 150 < 350$	low
2	$\geq 350 < 500$	low
1	≥ 500	low
0	no effect	no effect

Table 4.10: Bluegill sunfish (*Lepomis mactochirus*) scores

Score	24, 48 & 96 hour LC_{50} mg/l	Croner's evaluation
10	< 0.1	very high
9	$\geq 0.1 < 0.25$	very high
8	$\geq 0.25 < 1$	high
7	$\geq 1 < 2.5$	high
6	$\geq 2.5 < 10$	moderate
5	$\geq 10 < 25$	moderate
4	$\geq 25 < 75$	moderate
3	$\geq 75 < 150$	low
2	$\geq 150 < 350$	low
1	≥ 350	low
0	no effect	no effect

4.8.4 Carcinogenicity

Carcinogenicity in water is assessed using the same scoring system and assessment factors for carcinogenicity in air.

4.9 Toxicity in soil

Ecotoxicity data to assess the impact of chemicals on soil is less abundant than for the aquatic environment. Microtox™ and worms have been used to assess toxicity to micro-organisms and invertebrates. The maximum deposition rate (MDR), a parameter based on toxicity to soil, has also been used. Carcinogenicity has been selected to represent chronic chemical toxicity in soil.

4.9.1 Microtox™

The scoring system and assessment factors for Microtox™ have been described in Section 4.8.1. The same scoring system and assessment factors have been used for evaluating the toxicity to soil.

4.9.2 Worms

The toxicity to earthworms (*Eisenia foetida*) considers the effects on larger soil dwelling organisms. Earthworms have been selected as they are the most commonly tested soil organisms. Toxicity tests on worms can be carried out either in soil or on filter paper. Although the soil based tests are more accurate, many variables involved and the composition of the soil is a major contributor. Data using the soil test is very limited and inconsistent. The more common test is the filter paper test which is carried out by placing an earthworm on a piece of filter paper soaked in the test chemical. The test lasts for 48 hours and care must be taken to ensure that the earthworm does not dehydrate during this period. This test is carried out at various concentrations. The results are used to determine the chemical's LC_{50} for earthworms. Most of the earthworm data used has been obtained from the IRPTC database and Richardson (1992). The toxicity data for earthworms using the filter paper method and the toxicity classification for earthworms (IRPTC, 1990) (Table 4.11) have been used to determine the scoring system for worms shown in Table 4.12.

Table 4.11: Toxicity Classification for Earthworms based on LC_{50}'s (IRPTC, 1990)

LC_{50} ($\mu g/cm^2$)	Classification
< 1	Super toxic
$\geq 1 < 10$	Extremely toxic
$\geq 10 < 100$	Very toxic
$\geq 100 < 1000$	Moderately toxic
≥ 1000	Relatively non toxic

Table 4.12: Earthworm (*Eisenia foetida*) scores based on the filter paper test

Score	$\mu g/cm^2$
10	< 1
9	$\geq 1 < 10$
8	$\geq 10 < 50$
7	$\geq 50 < 100$
6	$\geq 100 < 500$
5	$\geq 500 < 1000$
4	$\geq 1000 < 2500$
3	$\geq 2500 < 10000$
2	$\geq 10000 < 50000$
1	≥ 50000
0	no toxic effects

As with other toxicity assessment factors an assessment factor of 10 has been applied if specific data based on the earthworm filter paper test is available. Any deviation from this data is reflected in a reduced assessment factor.

4.9.3 Maximum deposition rate (MDR)

The maximum deposition rate (Environment Agency, 1997) provides a method of determining the chemicals which are most toxic to soil. The MDR is defined as the quantity of pollutant which can be added daily to the soil over 50 years before the selected soil quality criteria are exceeded. MDR data is detailed in Annex C of the

Environment Agency's BPEO publication (1997). The scoring system for the maximum deposition rate is shown in Table 4.13.

Table 4.13: Maximum deposition rate scores

Score	Maximum Deposition Rates mg/m2/day
10	< 0.0001
9	≥ 0.0001 < 0.0005
8	≥ 0.0005 < 0.001
7	≥ 0.001 < 0.005
6	≥ 0.005 < 0.01
5	≥ 0.01 < 0.05
4	≥0.05 < 0.1
3	≥ 0.1 < 0.5
2	≥ 0.5 < 1
1	≥ 1
0	Not a contaminant

An assessment factor of 10 has been applied if the chemical is assigned a MDR. Generally it is assumed that if an MDR is not given then the chemical is not a problem. In this case a high assessment factor would be given. If the chemical is not given an MDR and it is thought that some effects on the soil may occur, expert opinion can be used to assign a score and an assessment factor.

4.9.4 Carcinogenicity

As with air and water, carcinogenicity is used to represent the chronic toxicity to the environment. The same scoring system and assessment factors apply to carcinogenicity in soil as in air and water.

4.10 Persistence in air

The persistence of a chemical in air has been assessed using the atmospheric degradation rate. The degradation rate has been assessed using half-life data for specific media obtained from Mackay et al (1992), Howard (1989 & 1990) and Howard et al (1991). Croner's (1998) also has a evaluation of persistence in environmental media which is shown in Table 4.14.

Table 4.14: Croner's evaluation of degradation (Croner's, 1997)

Degradation	Half-life (t)
Rapid	< 7 days
Moderate	> 7 days < 28 days
Slow	> 28 days < 6 months
Very slow	> 6 months

Croner's evaluation has been assessed together with specific half-life data. From this evaluation a scoring system has been developed to assess the persistence of a chemical in each medium. This is shown in Table 4.15.

Table 4.15: Degradation rate scores

Score	Half-life	Half-life (Hours)	Croner's evaluation
10	> 6 months	> 4320	very slow
9	> 3 ≤ 6 months	> 2160 ≤ 4320	slow
8	> 1 ≤ 3 months	> 720 ≤ 2160	slow
7	> 21 days ≤ 1 month	> 540 ≤ 720	moderate
6	> 14 ≤ 21 days	> 336 ≤ 540	moderate
5	> 7 ≤ 14 days	> 168 ≤ 336	moderate
4	> 3 ≤ 7 days	< 72 ≤ 168	rapid
3	> 1 ≤ 3 days	< 24 ≤ 72	rapid
2	> 1 hour ≤ 1 day	< 1 ≤ 24	rapid
1	< 1 hour	< 1	rapid

An assessment factor is assigned to the score based on the author's opinion of the accuracy of the data. A moderate score has been applied with a low assessment factor where no data exists for persistence.

4.11 Persistence in water

Two parameters are used evaluate the persistence of a chemical in water. They are the degradation rate in water represented by half-life and the bioaccumulation of the chemical in organisms represented by the bioconcentration factor. Degradation in water uses the same scoring system and assessment procedure as for air.

The bioconcentration factor (BCF) is used to evaluate the bioaccumulation tendency of a chemical. The BCF gives an indication of the amount of chemical that is likely to accumulate in organisms and is expressed as:

$$\text{BCF} = \frac{\text{Concentration of chemical at equilibrium in the organism (wet weight)}}{\text{Mean concentration of the chemical in the water}}$$

The bioconcentration factor is not always available. However bioconcentration can be calculated using solubilities, octanol-water partition coefficients and soil adsorption coefficients as shown in Appendix 1. The bioconcentration factor, the octanol-water partition coefficient and Croner's evaluation have been scored to provide a measure of chemical bioaccumulation. The scoring systems are shown in Table 4.16.

Table 4.16: Bioaccumulation scores

Scores	BCF	Log K_{ow}	Croner's evaluation
10	> 1000	4.33	high
9	≥ 750 < 1000	4.33	high
8	≥ 500 < 750	≥ 4	high
7	≥ 250 < 500	3.66	high/medium
6	≥ 100 < 250	3.33	medium
5	≥ 50 < 100	3	medium (no BCF data)
4	≥25 < 50	2.66	medium/low
3	≥ 10 < 25	2.33	low
2	≥1 < 10	< 2	low
1	< 1	< 1.66	low
0	0	1.66	no effect

The accuracy of the data applied to the bioaccumulation scoring system has been assessed using the assessment factors shown in Figure 4.6.

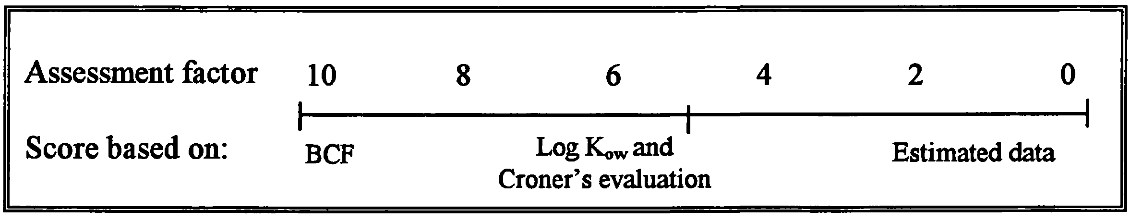


Figure 4.6: Bioaccumulation assessment factors

4.12 Persistence in soil

Persistence in soil is assessed using the chemical degradation rate in soil which is measured, like degradation in air and water, using half-life. The scoring system and assessment factors developed for degradation in air and water are applicable for soil. Bioaccumulation is also considered in the soil persistence category. The scoring system and assessment factor developed for bioaccumulation in water are also applicable for soil.

4.13 Effects in air

The parameters used to assess the impact of chemicals to air are global warming potential (GWP), ozone depletion potential (ODP), photochemical ozone creation potential (POCP), acidification, vegetation damage potential (VDP), aesthetics and odour.

4.13.1 Global warming

There is still much debate on the phenomenon known as global warming. Whilst it is apparent that the climate on the Earth is changing (as it always has done) the influence of anthropogenic emissions on this change, although recognised, has not been defined unambiguously. However there is significant concern by the public, academics and governments to justify the inclusion of global warming in the chemical evaluation of the EPPT.

The main contributors to global warming are carbon dioxide, methane, nitrous oxide and CFC's. The global warming potential, GWP, is defined as 'the cumulative radiative forcing between the present and a future time 'horizon' caused by a unit release relative to some reference gas, in this case carbon dioxide' (IPCC, 1996). The GWP ranges from 1 to 7100 and can be found in Table 7.1 of the Environment Agency's BPEO publication (1997). If a chemical is not mentioned in the Environment Agency's table it is assumed that there is no GWP for that chemical and that the chemical is not therefore considered to create a problem. The GWP's are scored in Table 4.17.

Table 4.17: Global warming potential scores

Score	GWP
10	> 13000
9	> 5000 ≤ 13000
8	> 2500 ≤ 5000
7	> 1000 ≤ 2500
6	> 500 ≤ 1000
5	> 10 ≤ 500
4	≥ 1 ≤ 10
3	< 1
2	
1	
0	no GWP

The GWP's are scored from 10 to 3. A GWP of 1, which is that of carbon dioxide, is scored 4 not 1 because carbon dioxide has a significant impact on global warming.

Chemicals with a GWP are assigned a high assessment factor. In most other cases where a chemical is not listed in the Environment Agency's Table 7.1 a score of 0 is applied along with a high assessment factor.

4.13.2 Stratospheric ozone depletion

The stratospheric ozone layer protects the Earth from the harmful radiation generated by the sun. Consequently stratospheric ozone depletion is a major concern as the hole in the ozone layer increases. The main contributors to ozone depletion are CFC's and halogenated hydrocarbons. A chemical's ability to degenerate the ozone layer is assessed using the ozone depletion potential (ODP). The ODP is defined as the effect per molecule of the specific compound on the abundance of the stratospheric ozone, referenced to the effect of CFC-11 (Graedel and Allenby, 1995). The ODP can be found in Appendix D of Graedel and Allenby (1995). ODP's range between 0 and 16. However some chemicals listed as Class I - Ozone depleting and greenhouse warming species are not assigned ODP's. It is assumed that these chemicals will have a contribution to ozone depletion but not as much as those chemicals which have been assigned an ODP. It is for this reason that the ODP scoring system ranges from 10 to 3, where the Class I chemicals score 3. The EPPT scoring system for ODP is given in Table 4.18.

Table 4.18: Ozone depletion potential scores

Score	ODP
10	> 10
9	$> 5 \leq 10$
8	$> 1 \leq 5$
7	$> 0.1 \leq 1$
6	$> 0.01 \leq 0.1$
5	$> 0.001 \leq 0.01$
4	≤ 0.001
3	
2	
1	
0	no ODP

The accuracy of the data applied to the ozone depletion potential scoring system has been assessed using the assessment factors shown in Figure 4.7.

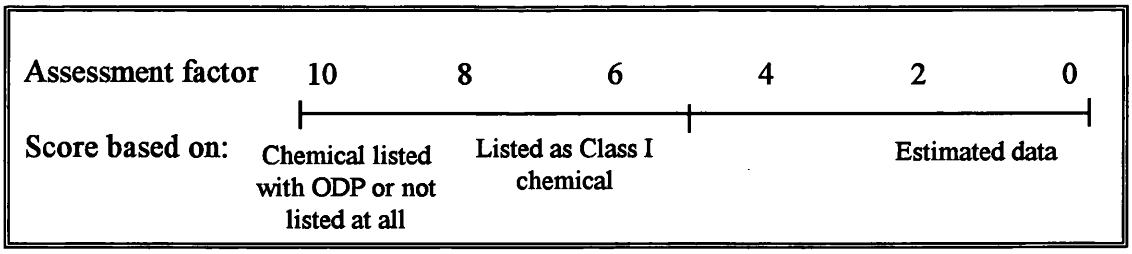


Figure 4.7: Ozone depletion potential assessment factors

4.13.3 Photochemical ozone creation

Whilst ozone is important in the stratosphere to protect the Earth it causes a significant problem at low level. Ozone is a prominent constituent of photochemical smog which causes injury to plants and animals. Chemicals with a potential to generate photochemical ozone include hydrocarbons, nitrogen oxides, sulphur dioxide and carbon monoxide. The Environment Agency (1997) have assessed photochemical ozone creation potentials (POCP) to evaluate the impact of chemicals on low level ozone creation for their Integrated Environmental Index. The EA's POCP assessment is based on data generated by Derwent and Jenkin (1991). The POCP is defined as the ratio of the change in photochemical ozone production due to an emission of a particular VOC to the ozone created by the same addition of ethylene (Derwent & Jenkin, 1991). POCP's range from 91 to -33. The EPPT scoring system developed for photochemical ozone creation potential is shown in Table 4.19.

The range of scores are from 10 to 3 for the same reasons as with the GWP and the ODP. The assessment factors assigned to the POCP scores also follow the same reasoning as for GWP and ODP systems.

Table 4.19: Photochemical ozone creation potential scores

Score	POCP
10	>90
9	$<75 \leq 90$
8	$<55 \leq 75$
7	$<30 \leq 55$
6	$<15 \leq 30$
5	$< -20 \leq 15$
4	$< -33 \leq -20$
3	≤ -33
2	
1	
0	no POCP

4.13.4 Acidification

Acidification is a significant environmental problem as it has effects in the air, water and soil media. The main chemicals involved in acidification are sulphur dioxide, nitrogen dioxide, ozone and hydrocarbons. The scoring system used for the EPPT was developed by Elliott (1997) and is based on the pollutant classes defined by the UK Terrestrial Effects Review Group (1988). Primary pollutants include sulphur dioxide, nitrogen dioxide and hydrocarbons and contribute to acid rain either by direct dry deposition or indirect wet deposition. Secondary pollutants contribute to the transformation of primary pollutants to sulphates, nitrate including NO_2 and ozone. The scores assigned to these acidification classifications are shown in Table 4.20

Table 4.20: Acidification scores

Score	Classification	Chemical
10	Primary pollutant	SO_2, NO_2, HC's containing halogens, N & S
5	Secondary pollutant	NO_2, O_3
0	Inactive	

Certain chemicals are known to cause acidification. These chemicals have an assessment factor of 10. Where uncertainty exists in the contribution of a chemical to acidification expert opinion can be used to assign scores with a significantly reduced assessment factor of no more than 5.

4.13.5 Vegetation damage potential

Damage to vegetation can be caused by chemicals in various ways. Photosynthesis, respiration and the uptake of nutrients can all be affected by chemicals. The vegetation damage potential is a classification given to chemicals and is detailed by HMIP (1994). The data to determine a chemical's capacity to damage vegetation has been derived from the World Health Organisation's Air Quality Guidelines for Europe (1987). A chemical is described either as having or not having a vegetation damage potential (VDP). There is no grading of this classification. The scores assigned to the vegetation damage potential are shown in Table 4.21.

Table 4.21: Vegetation Damage Potential Scores

Score	VDP
10	Has VDP
5	Thought to have VDP
0	Listed with no VDP
0	Not thought to have VDP

Chemicals listed with a VDP have an assessment factor of 10. Chemicals not listed are subject to the author's opinion. In this case a significantly reduced assessment factor of less than 5 is assigned.

4.13.6 Aesthetics

Aesthetics is not an obvious environmentally damaging parameter with respect to plants and animals. However, it is seen as an important parameter affecting the local environment. This parameter is also important to industry as a visible plume for example is obvious to the public irrespective of what it contains. Oily and/or coloured discharges to waterways also have aesthetic implications. To address these aspects the EPPT includes a parameter in its chemical evaluation based on colour and visibility. The data for this parameter can be found in Perry (1984), Richardson (1992) and on material safety data sheets. The scoring system for aesthetics is shown in Table 4.22.

Table 4.22: Aesthetics scores

Score	Aesthetics
10	Strong colours
5	Subtle colours
0	Colourless

This clearly is a subjective parameter and scoring system. Generally, however a plume of steam which has a subtle colour would score 5 whereas a dark plume would score 10. These are fairly obvious assignments and a high assessment factor would result. Where more subjectivity exists in scoring a chemical a reduced assessment factor of not more than 5 has been used.

4.13.7 Odour

The odour emanating from a chemical process is also important to the inhabitants of the local environment. The odour threshold of a chemical is used as the basis for the scoring system for the EPPT. Odour thresholds are detailed in Croner's (1997). The scoring system developed for evaluating odour is shown in Table 4.23.

Table 4.23: Odour scores

Score	Odour threshold mg/m3
10	< 0.005
9	$\geq 0.005 < 0.05$
8	$\geq 0.05 < 0.5$
7	$\geq 0.5 < 5$
6	$\geq 5 < 25$
5	$\geq 25 < 100$
4	$\geq 100 < 500$
3	$\geq 500 < 1500$
2	$\geq 1500 < 3000$
1	$\geq 3000 < 5000$
0	Odourless

The accuracy of the data applied to the odour scoring system has been assessed using the assessment factors shown in Figure 4.8.

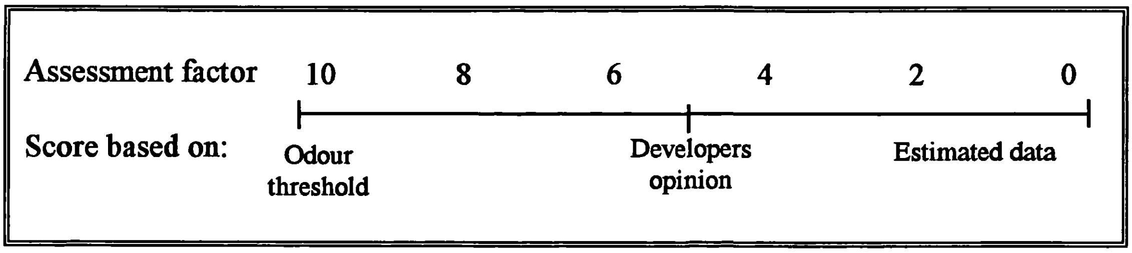


Figure 4.8: Odour assessment factors

4.14 Effects in water

The effects considered in water are acidification, aesthetics and odour. The scoring systems and assessment factors developed in the air effects category are equally applicable for water.

4.15 Effects in soil

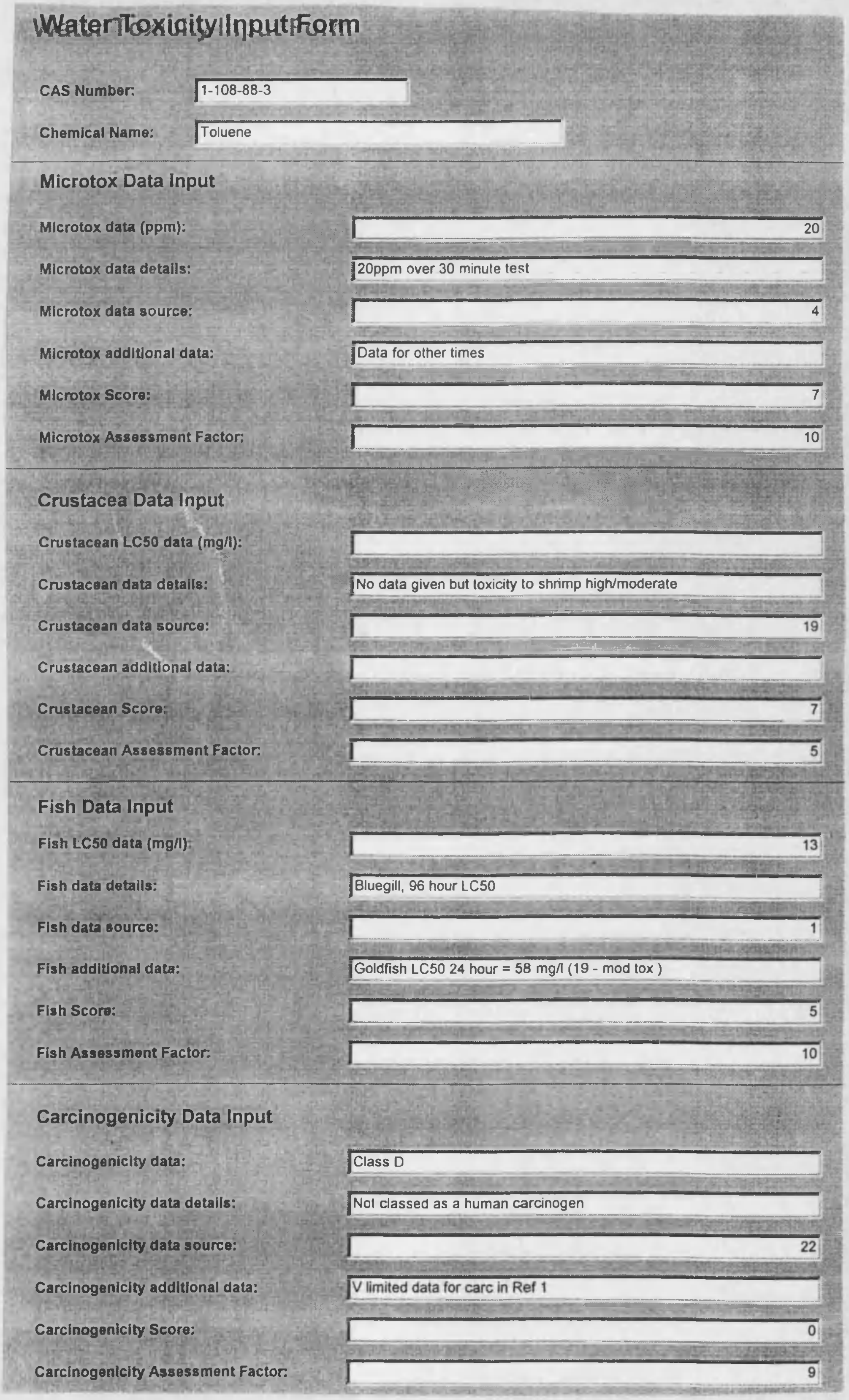
Acidification and vegetation damage potential have been selected to represent the effects of chemicals on soil. The scores and assessment factors developed in the air effects category are equally applicable for soil.

4.16 The EPPT database

It is clear from the previous sections that a substantial amount of data collection and evaluation is needed for each chemical. A chemical database has been developed to ease the data gathering, evaluation and assessment of the chemicals. This database has been designed using Microsoft Access software.

The database is subdivided into ten sections. Nine of the ten sections deal with each combination of air, water and soil with toxicity, persistence and effect (as shown in the nine elements of Table 4.2). Each section stores the data for each parameter. The raw data, source of the data (stored as a reference number listed in Appendix 2), conditions under which the data was obtained and any other relevant information are stored along with the scores and assessment factor assigned to each chemical. As an example Figure 4.9 the water toxicity section for toluene.

The tenth section consists of the chemical details, name, CAS number, organic or inorganic nature of the chemical, and also the distribution fractions of the chemical between each of the three media. The latter two aspects are discussed later in Chapter 5. Figure 4.10 shows a summary sheet of the scores and assessment factors assigned to each parameter for toluene. All of this information is saved in the database for future use. Presently there are 92 chemicals (listed in Appendix 3) on the EPPT database.



Water Toxicity Input Form

CAS Number:	1-108-88-3
Chemical Name:	Toluene

Microtox Data Input

Microtox data (ppm):	20
Microtox data details:	20ppm over 30 minute test
Microtox data source:	4
Microtox additional data:	Data for other times
Microtox Score:	7
Microtox Assessment Factor:	10

Crustacea Data Input

Crustacean LC50 data (mg/l):	
Crustacean data details:	No data given but toxicity to shrimp high/moderate
Crustacean data source:	19
Crustacean additional data:	
Crustacean Score:	7
Crustacean Assessment Factor:	5

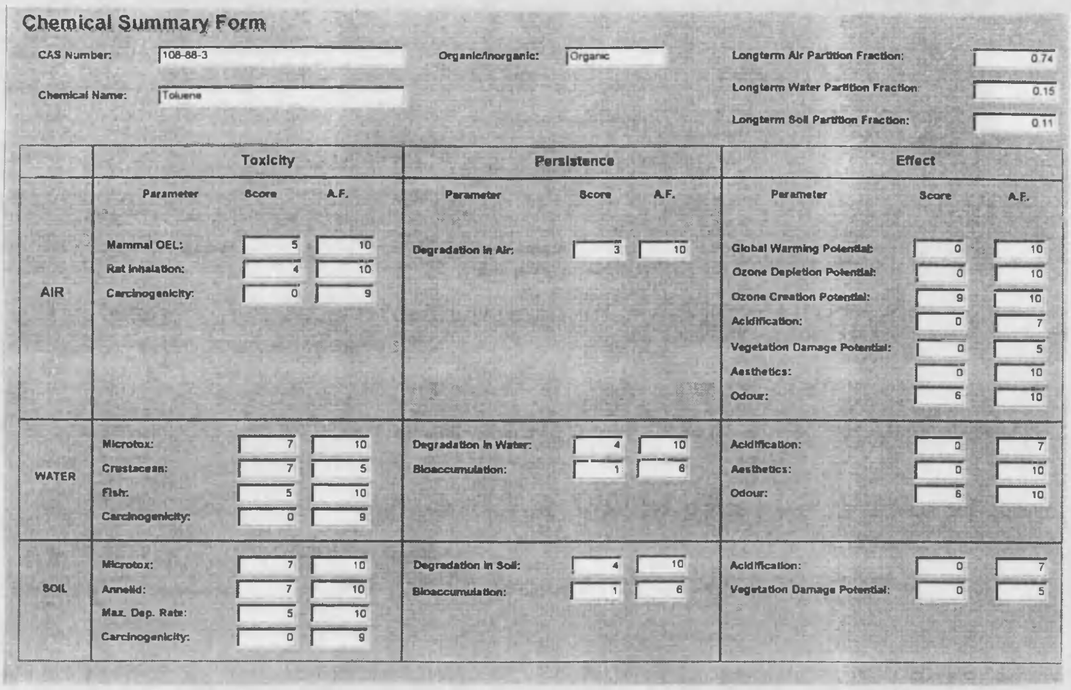
Fish Data Input

Fish LC50 data (mg/l):	13
Fish data details:	Bluegill, 96 hour LC50
Fish data source:	1
Fish additional data:	Goldfish LC50 24 hour = 58 mg/l (19 - mod tox)
Fish Score:	5
Fish Assessment Factor:	10

Carcinogenicity Data Input

Carcinogenicity data:	Class D
Carcinogenicity data details:	Not classed as a human carcinogen
Carcinogenicity data source:	22
Carcinogenicity additional data:	V limited data for carc in Ref 1
Carcinogenicity Score:	0
Carcinogenicity Assessment Factor:	9

Figure 4.9: Water toxicity input form from the EPPT chemical database



Chemical Summary Form

CAS Number: 108-88-3

Chemical Name: Toluene

Organic/Inorganic: Organic

Longterm Air Partition Fraction: 0.74

Longterm Water Partition Fraction: 0.15

Longterm Soil Partition Fraction: 0.11

	Toxicity			Persistence			Effect		
	Parameter	Score	A.F.	Parameter	Score	A.F.	Parameter	Score	A.F.
AIR	Mammal OEL:	5	10	Degradation in Air:	3	10	Global Warming Potential:	0	10
	Rat inhalation:	4	10				Ozone Depletion Potential:	0	10
	Carcinogenicity:	0	9				Ozone Creation Potential:	9	10
							Acidification:	0	7
							Vegetation Damage Potential:	0	5
							Aesthetics:	0	10
							Odour:	6	10
WATER	Microtox:	7	10	Degradation in Water:	4	10	Acidification:	0	7
	Crustacean:	7	5	Bioaccumulation:	1	6	Aesthetics:	0	10
	Fish:	5	10				Odour:	6	10
	Carcinogenicity:	0	9						
SOIL	Microtox:	7	10	Degradation in Soil:	4	10	Acidification:	0	7
	Annelid:	7	10	Bioaccumulation:	1	6	Vegetation Damage Potential:	0	5
	Max. Dep. Rate:	5	10						
	Carcinogenicity:	0	9						

Figure 4.10: Chemical summary form from the EPPT chemical database

4.17 Summary

The chemical evaluation part of the Environmental Process Performance Tool has been discussed in this chapter. The subjectivity of impact assessment has been highlighted. The data problems were addressed including the difficulty in locating the data and the problems associated with using data from an inexact science. The data was evaluated within a structure developed for the purpose. The scores resulting from the evaluation are combined in the next chapter for use in the EPPT.

5. Determination of chemical score

The last chapter presented the parameter based scoring systems that have been developed to evaluate the environmental impact of chemicals. These parameter scores need combining in order to determine the overall impact of chemicals on the environment. As discussed in Chapter 2 several methods to determine the impact of chemicals on the environment as a whole have already been developed elsewhere. The major flaw with the existing approaches is the lack of an integrated approach to represent the environment as a whole. The EPPT overcomes this limitation by considering the ultimate fate of the chemicals using a distribution model.

In this chapter existing distribution models are discussed and evaluated for application to the EPPT. The combination of distribution fractions (derived from the chosen distribution model) and the parameter scores to determine the environmental impact of each chemical is also discussed. EPPT chemical scores are derived from this combination. Three EPPT chemical scores exist for each chemical depending on whether it is released to air, water or soil. In this chapter a comparison between chemical scores derived for the EPPT and those derived by Elliott for EniVal is also undertaken and an explanation of the variations in chemical ranking is given.

5.1 Model evaluation

Literature reviews revealed numerous distribution models that are based on compartments. These compartments are used to represent environmental media. The majority of these models are rate based. However, there are simpler models based on equilibrium. Distribution models, both the traditional environmental distribution models based on mass, volume and concentration (Neely, 1981 and Trapp and Matthies, 1996) and the fugacity based models developed by Mackay (Mackay, 1979; Mackay and Paterson, 1981 & 1991; Mackay et al, 1983 and Wania and Mackay, 1995), have four levels. The levels are:

- Level 1: Equilibrium, no reaction, closed system.
- Level 2: Equilibrium with source and sink, steady-state.
- Level 3: No equilibrium partitioning, sources and sinks, steady-state.
- Level 4: Dynamic: no equilibrium partitioning, sources and sinks, transient case.

Level 1 models assume the chemical mass within the system is distributed between compartments according to equilibrium partition coefficients. In this case the chemical mass is constant, there is no movement between media and there is no source or sink. Elliott's equilibrium fate model (1997) is an example of a Level 1 model. Level 2 models make the same assumptions as Level 1 with the exception that there is a steady and equal source and sink to the system. Level 3 does not assume equilibrium between the compartments. Input and output can occur in every compartment but steady state is assumed. Level 4 is the most complex model and foregoes the somewhat unrealistic assumptions that steady-state or equilibrium exists in the environment (Trapp and Matteis, 1996).

The accuracy of these models increases in the higher levels because less assumptions are made. However, higher level models are very complex and have a large data requirement particularly kinetic data which is difficult to obtain. Neely (1981) and Schiel et al (1995) have developed Level 2 models which estimate environmental concentrations using a steady state mass balance, Henry's Law, soil adsorption data and rate constants. The requirements for these models include advection data to ascertain the rate at which the chemical moves in and out of the atmospheric media, and data on photodegradation, photolysis, hydrolysis and microbial action. Even the simplest of these models requires more data than is readily available for the chemicals evaluated by the EPPT.

The initial requirement for the EPPT was a simpler model that would provide the fractional distribution of a chemical in each medium within the environment without the need for kinetic data. As the EPPT is developed in the future, more detailed models with less assumptions could be included. However, within the time restrictions of this research a model without extensive data requirements was needed. Elliott (1997) has recently developed the equilibrium fate model which meets this purpose.

5.1.1 The equilibrium fate model

Elliott's equilibrium fate model utilises a global environmental mass balance concept to determine the long-term equilibrium distribution of pollutants. He divides the environment into three subsystems representing the air, water and soil. To maintain simplicity Elliott made the following assumptions:

- the sediments are considered as part of the soil media;
- the suspended solids and the biota are not considered;
- variation in interactions caused by one phase not in direct contact with another have been neglected to maintain simplicity. For example, air and water may not be in contact if a layer of organic material floats on the water.

Elliott (1997) initially quantified each sub-system. The air sub-system included all the matter in the atmosphere to an altitude of 50km. The water sub-system considered all surface water on the Earth including oceans, seas, rivers, lakes and anything that floats in or on the water. The soil sub-system included all organic and inorganic material to a depth of one metre and the polar ice-caps as they were considered to be a solid medium. The volume fractions of the subsystems are shown in Table 5.1.

Table 5.1: Volume fractions for the environment sub-systems (Elliott, 1997)

Sub-system	Volume fraction of sub-system
Atmosphere	0.95
Water	0.05
Soil	4.8×10^{-6}
Total	1.00

These volume fractions are used in Elliott's equilibrium fate model. A global mass balance forms the basis of the model wherein the total quantity of a pollutant in the environment is equal to the sum of the quantities in the atmosphere, water and soil sub-systems. From this global mass balance, the Henry's law constants and the linear soil adsorption isotherm, Elliott derives equations 5.1 to 5.3. The derivation of these equations is reproduced in Appendix 4.

Fraction of chemical in the air:

$$F_a = \frac{a}{(a + w K_w + s\,d\,f_{oc} K_{oc} K_w)} \qquad \text{....... Equation 5.1}$$

Fraction of chemical in the water:

$$F_w = \frac{w}{\left(\frac{a}{K_w} + w + s\,d\,f_{oc} K_{oc}\right)} \qquad \text{....... Equation 5.2}$$

Fraction of chemical in the soil:

$$F_s = \frac{s\,d\,f_{oc} K_{oc}}{\left(\frac{a}{K_w} + w + s\,d\,f_{oc} K_{oc}\right)} \qquad \text{....... Equation 5.3}$$

where:

K_w = the air-water partition coefficient (1/Henry's Law Constant)
d = the soil density
f_{oc} = the fraction of organic carbon in the soil
K_{oc} = organic carbon coefficient
a = atmosphere volume fraction
w = water volume fraction
s = soil volume fraction

Successful use of this model depends on the availability of the parameters K_{oc} and K_w. K_{oc} the organic carbon coefficient is related to the soil adsorption coefficient as follows:

$K_{oc} = K_p / f_{oc}$ .... Equation 5.4

where: K_p = the soil adsorption coefficient.

K_w, K_{oc} and K_p can be obtained by experimentation or correlation. The soil adsorption coefficient correlations have been described in Section 4.11 and can also be found in Lyman et al (1982). Henry's Law constants can be found in Howard (1989, 1991), Mackay et al (1992) and Yaws et al (1991). The latter reference gives Henry's Law constants for 362 organic chemicals.

Elliott tested forty four organic chemicals commonly used as industrial solvents using this model. Data was available for the majority of these chemicals with the exception of some K_{oc} values. Where K_{oc} values were not available correlations based on solubility were used instead. The distribution fraction of a chemical in each medium was compared with descriptive categories of the long-term terrestrial, aquatic and atmospheric fate of chemicals given in Howard et al (1991) to determine the accuracy of the results.

The derivation of the long-term distribution fractions are shown below using toluene as an example. The data (also shown below) was obtained from Elliott's model (1997).

K_W = 4.12
f_{oc} = 8% (0.08)
d = 1300g/l
K_{oc} = 100

a (air volume fraction) = 0.95
w (water volume fraction) = 0.05
s (soil volume fraction) = 4.8×10^{-6}

The distribution fractions derived for toluene in the following section have been calculated using a spreadsheet with sixteen significant figures. Consequently there is some variation between the rounded number results provided in the following equations and the accurate results used in the spreadsheet. The results derived in this example will be used later in the chapter to derive the chemical score for toluene.

Fraction of toluene in the air: $F_a = \dfrac{a}{(a + wK_w + sdf_{oc}K_{oc}K_w)}$

$$F_a = \frac{0.95}{0.95 + (0.05 \text{ x } 4.12) + (4.8 \text{ x } 10^{-06})(10400 \text{ x } 4.12)}$$

$F_a = 0.74$

Fraction of toluene in the water: $F_w = \dfrac{w}{\left(\dfrac{a}{K_w} + w + sdf_{oc}K_{oc}\right)}$

$$F_w = \frac{0.05}{\dfrac{0.95}{4.12} + 0.05 + \left(4.8 \text{ x } 10^{-06}\right) 10400}$$

$F_w = 0.15$

Fraction of toluene in the soil: $F_s = \dfrac{sdf_{oc}K_{oc}}{\left(\dfrac{a}{K_w} + w + sdf_{oc}K_{oc}\right)}$

$$F_s = \frac{(4.8 \text{ x } 10^{-06})10400}{\left(\dfrac{0.95}{4.12} + 0.05 + (4.8 \text{ x } 10^{-06})10400\right)}$$

$F_s = 0.11$

The two main sources of error in Elliott's model are the uncertainty of the data used in calculating the volume fraction and the use of data from correlations. An interest when using Elliott's model was the volumes assigned to each of the sub-systems. To address this interest an investigation of the sub-system volume fractions derived by Elliott and the volume fractions derived by Neely has been undertaken. This is discussed in Appendix 5. This investigation concluded that Elliott's volume fractions gave the most reliable results. These results were also compared with qualitative environmental fate classifications identified in Croner's (1998). Both Elliott's distribution model and Croner's evaluation identified the same significant environmental compartments for the chemicals that were evaluated.

5.1.2 Elliott's inorganic models

Elliott's equilibrium fate model was developed for organic chemicals. Due to the differing equilibrium distribution relationships exhibited by inorganic chemicals Elliott developed a series of rules that can be used to describe the ultimate fate of different types of inorganic chemicals. He categorised inorganics into the following five groups.

- Heavy metal based compounds.
- Solids.
- Aqueous solutions/liquids.
- Gases.
- Particulates.

The ultimate fate of chemicals in these groups is assessed using solubility at 20°C. This assessment procedure is given in Table 5.2 where F_A is the fraction of a chemical in the air and F_W and F_S are the fractions of the chemical in the water and soil respectively.

Table 5.2: Solubility models for inorganic groups (Elliott, 1997)

Pollutant group	F_A	F_W	F_S	Solubility (wt %)
Heavy metal based compounds	0.0	0.0	1.0	For all heavy metals
Inorganic solids and their aqueous solutions	0.0	0.0	1.0	$S < 1$
	0.0	1.0	0.0	$S \geq 1$
Gases and their aqueous solutions	0.0	0.0	1.0	$S < 0.1$
	0.8	0.2	0.0	$10 > S \geq 0.1$
	0.0	1.0	0.0	$S \geq 10$
Particulates	0.0	0.0	1.0	For all particulates

The heavy metal based compounds include aqueous solutions of metal cations, metal aerosols in the atmosphere, metal vapours in the atmosphere and heavy metal based compounds in the soil or sediments. Heavy metals have their major influence through persistence in the soils and sediments and, as quoted in Elliott (1997), Caughtrey, Martin and Unsworth (1987) write that 'metals dumped to the land are most likely to remain there with minimal leaching or vapourisation; and that subsoils have a large capacity to reabsorb metals that percolate from the top-soil'. From this, Elliott deduced that the soil sub-system was the long-term compartment for heavy metals.

To determine the distribution of inorganic solids and their aqueous solutions in the water and soil sub-systems, Elliott compared the behaviour of various inorganic solids such as sodium hydroxide, sodium chloride, calcium sulphate and alumina with their respective solubilities of 50, 36, 0.22 and 1×10^{-4} wt%. Both sodium hydroxide and chloride are very soluble. Calcium sulphate and alumina form a suspension which will settle over time. Elliott selected an intermediate solubility of 1wt% to differentiate the distribution of organic solids between water and soil. These rules also apply to solids discharged in aqueous solutions.

As with inorganic solids there is no common distribution behaviour of inorganic gases between media. Elliott compared chemicals and their known behaviour with their solubilities at 20°C. Gases such as hydrogen and nitrogen have low solubilities of 0.002 wt%. These gases usually partition in air. Gases which normally partially dissolve, such as carbon dioxide and chlorine, have solubilities of 0.16 and 0.81 wt% respectively. Gases which usually exist in aqueous solution have a high solubility, such as hydrogen chloride (72 wt%). Elliott defined three categories for the distribution of this group of chemicals. Chemicals with solubilities of less than 0.1wt% are assigned to air. Chemicals with solubilities of greater than 10wt% are assigned to water. If the solubility of a chemical exists between these extremes it is assumed that 80% of the chemical will reach equilibrium in the air and 20% will reach equilibrium in the water. Elliott assumes the adsorption of gases by soils is negligible compared with transport via aqueous solutions.

Particulates generated primarily by combustion processes are emitted to the atmosphere. Over time these particulates eventually settle to the ground. Elliott considers particulates to partition to the soil in the long-term.

5.2 Derivation of the EPPT chemical score

Each chemical evaluated in the Environmental Process Performance Tool is characterised by three chemical scores,

1. for release to air,
2. for release to water, and
3. for release to soil.

Three scores have been developed in order to distinguish between emissions to the different environmental media. The three chemical scores are comprised of a chemical release score and a long term score. The chemical release score can potentially be different for each medium whereas the long term score is the same. The structure of the EPPT chemical score is shown in Figure 5.1.

The three chemical scores range in value from zero to one hundred. This range of values are obtained by normalising each chemical score using the maximum score for each parameter. The derivation of the chemical scores are shown in the following sections.

Toluene released to air has been used throughout the following discussions to illustrate the calculation of the of the EPPT chemical score.

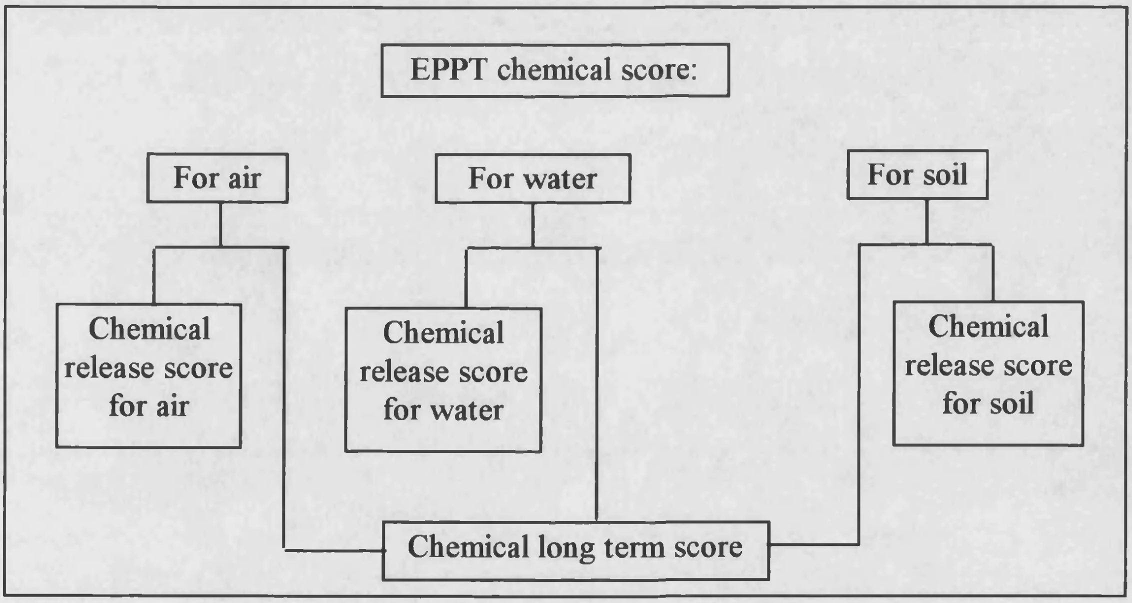


Figure 5.1: Structure of the EPPT chemical score

5.2.1 The chemical release score

The chemical release score represents the immediate impact of chemicals. The calculation of the chemical release score has three stages. Initially the intermediate release score is calculated using Equation 5.5. The second stage combines the intermediate release score with the media fraction, as shown in Table 5.3, to give the media release score as shown in Equation 5.6.

Table 5.3: Fractions for media release scores

Releases to:	Media fractions		
air	air = 1	water = 0	soil = 0
water	air = 0	water = 1	soil = 0
soil	air = 0	water = 0	soil = 1

The third stage combines the media release scores and an additional value for water (the reason for which is described on the next page), to determine the chemical release score as shown in Equation 5.7.

Intermediate release score = Σ toxicity parameter scores + Σ effect parameter scores

.... Equation 5.5

Media release score = Intermediate release score x media fraction

.... Equation 5.6

Chemical release score = (Media release score for air + Media release score for water + Media release score for soil) + 0.5*

.... Equation 5.7

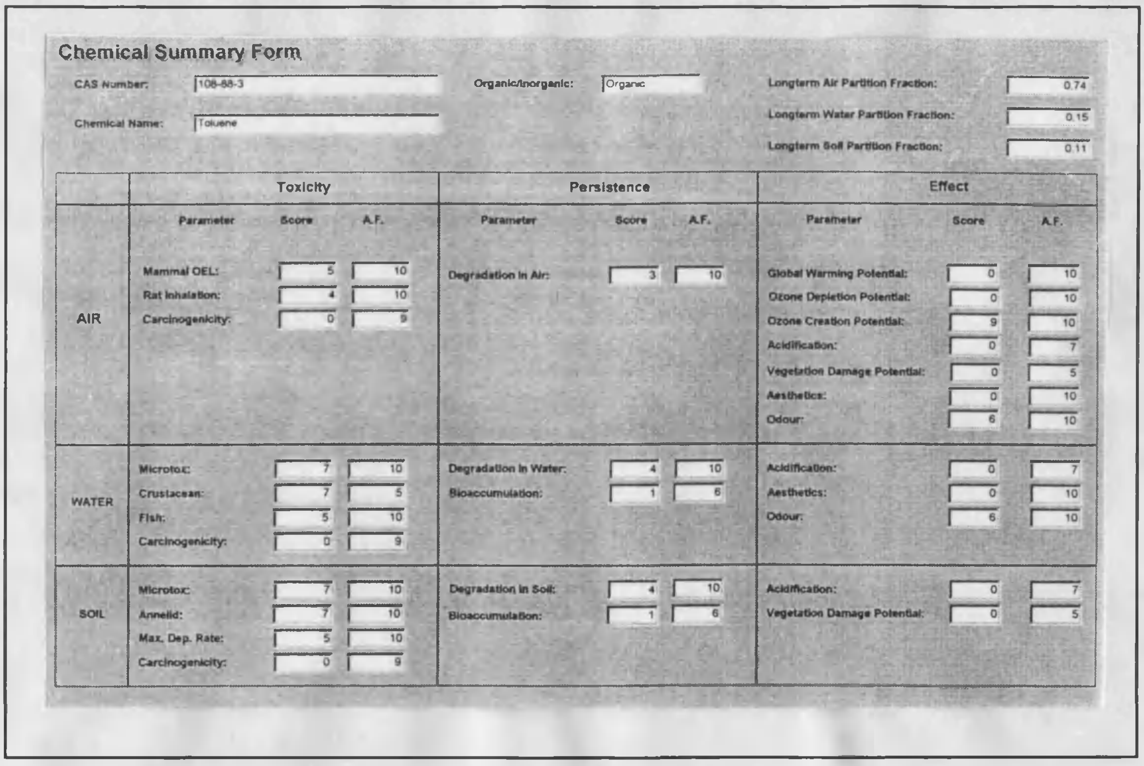
* Additional value for water

Consideration of water

Water is important in chemical processes as it has numerous applications including cooling, steam generation and heating and also in washing vessels. When evaluating water using the EPPT chemical assessment parameters no environmental impact is seen. However, the large volumes of water used by chemical processes impact on the environment. Water extraction is depleting water levels in rivers and lakes with potentially serious environmental and aesthetic consequences. In extreme cases, some smaller waterways have been known to dry up with catastrophic effects on the ecosystem. Added complications can be generated when using water as a cooling agent. Returning uncontaminated cooling water to a waterway at any deviation from the existing waterway temperature has an environmental impact by altering the biodiversity of the natural system. Assigning a score for water encourages the reduction in water use and consequent reduction in environmental impact. This is the reason for the inclusion of the value 0.5 in Equation 5.7. This small addition gives water the lowest chemical score (see Appendix 6) but clearly it could have an influence on the overall impact of a process if large amounts of water are used.

Release score calculation for toluene

The calculation of the chemical release score is demonstrated using the example of toluene released to air. The data given in Figure 5.2 are used in the calculation.



Chemical Summary Form

CAS Number: 108-88-3

Chemical Name: Toluene

Organic/Inorganic: Organic

Longterm Air Partition Fraction: 0.74

Longterm Water Partition Fraction: 0.15

Longterm Soil Partition Fraction: 0.11

	Toxicity			Persistence			Effect		
	Parameter	Score	A.F.	Parameter	Score	A.F.	Parameter	Score	A.F.
AIR	Mammal OEL:	5	10	Degradation in Air:	3	10	Global Warming Potential:	0	10
	Rat Inhalation:	4	10				Ozone Depletion Potential:	0	10
	Carcinogenicity:	0	9				Ozone Creation Potential:	9	10
							Acidification:	0	7
							Vegetation Damage Potential:	0	5
							Aesthetics:	0	10
							Odour:	6	10
WATER	Microtox:	7	10	Degradation in Water:	4	10	Acidification:	0	7
	Crustacean:	7	5	Bioaccumulation:	1	6	Aesthetics:	0	10
	Fish:	5	10				Odour:	6	10
	Carcinogenicity:	0	9						
SOIL	Microtox:	7	10	Degradation in Soil:	4	10	Acidification:	0	7
	Annelid:	7	10	Bioaccumulation:	1	6	Vegetation Damage Potential:	0	5
	Max. Dep. Rate:	5	10						
	Carcinogenicity:	0	9						

Figure 5.2: Chemical summary form for toluene from the EPPT chemical database

Using Equation 5.5 the following intermediate release scores are:

- Intermediate release score for air = (5 + 4) + (9 + 6) = 24
- Intermediate release score for water = (7 + 7 + 5) + (6) = 25
- Intermediate release score for soil = (7 + 7 + 5) + (0) = 19

Using Equation 5.6 and the following media fractions for release to air, the media release scores are calculated.

Media fractions for release to air:

- air = 1
- water = 0
- soil = 0

- Media release score to air = (24 x 1) = 24
- Media release score to water = (25 x 0) = 0
- Media release score to soil = (19 x 0) = 0

Using Equation 5.7 the chemical release score for toluene to air is calculated as,

- Chemical release score = 24 + 0 + 0 + 0.5 = 24.5

As discussed in Section 5.2 the final EPPT chemical scores need to be out of 100. Thus the maximum release score also needs to be calculated.

5.2.2 The maximum chemical release score

The maximum chemical release score is calculated using the same method as the chemical release score, the difference arising from the use of the maximum scores (10) for each parameter.

Thus using Equation 5.5 the maximum intermediate release score for any chemical is:

- Maximum intermediate release score to air = (3 x 10) + (7 x 10) = 100
- Maximum intermediate release score to water = (4 x 10) + (3 x 10) = 70
- Maximum intermediate release score to soil = (4 x 10) + (2 x 10) = 60

Using Equation 5.6 and the following media fractions for release to air, the media maximum release scores are calculated;

Media fractions for release to air
- air = 1
- water = 0
- soil = 0

- Maximum media release score to air = (100 x 1) = 100
- Maximum media release score to water = (70 x 0) = 0
- Maximum media release score to soil = (60 x 0) = 0

To calculate the maximum chemical release score for a chemical released to air Equation 5.7 is used.

- Maximum chemical release score for air = 100 + 0 + 0 + 0.5 = 100.5

Using the appropriate media fractions for release to water and soil as shown in Table 5.3, Equations 5.5 to 5.7 are used to determine the maximum chemical release score when a chemical is released to water or soil.

- Maximum chemical release score for water =

  (100 x 0) + (70 x 1) + (60 x 0) +0.5 = 70.5

- Maximum chemical release score for soil =

$$(100 \times 0) + (70 \times 0) + (60 \times 1) + 0.5 = 60.5$$

The maximum chemical release scores are used when deriving the EPPT chemical score. This is discussed in Section 5.2.6.

5.2.3 The long term chemical score

The long term chemical score represents the environmental impact of the chemical once it has distributed into its preferred environmental medium. Calculation of the long term chemical score follows a similar three stage method to the chemical release score.

Initially the intermediate long term score is calculated using Equation 5.8. The combination method of the persistence parameters is discussed in Section 5.2.6. The second stage combines the intermediate long term score with the media fraction, derived from Elliott's (1997) model, to give the media long term score as shown in Equation 5.9. The third stage combines the media long term scores and a value to consider water, to determine the chemical long term score.

Intermediate long term score for each medium = (Σ toxicity parameter scores + Σ effect parameter scores) x $\sqrt{}(\Sigma$persistence parameters$)^2$

.... Equation 5.8

Media long term score =

Intermediate long term score for each medium x medium fraction

.... Equation 5.9

Long term chemical score = (air medium long term score + water medium long term score + soil medium long term score) + 0.5

.... Equation 5.10

The calculation of the long term chemical score is demonstrated again using the example of toluene. The long term chemical score for a chemical are the same regardless of the emission media. The data given in Figure 5.2 is used in the calculation.

Using Equation 5.8 the following intermediate release scores are calculated.

- Intermediate long term score for air = $[(5 + 4) + (9 + 6)] \times \sqrt{3^2} = 72$
- Intermediate long term score for water = $[(7 + 7 + 5) + (6)] \times \sqrt{(4^2 + 1^2)} = 103.1$
- Intermediate long term score for soil = $[7 + 7 + 5) + (0)] \times \sqrt{(4^2 + 1^2)} = 78.3$

Using Equation 5.9 and the following media fractions calculated using the distribution model, the media long term scores are calculated;

Long term distribution fractions for:

- air = 0.74
- water = 0.15
- soil = 0.11

- Media long term score for air = (72 x 0.74) = 53.3
- Media long term score for water = (103.11 x 0.15) = 15.5
- Media long term score for soil = (78.3 x 0.11) = 8.6

Using Equation 5.10 the long term chemical score for toluene is calculated.

- Long term chemical score = 53.3 + 15.5 + 86.1 + 0.5 = 77.9

As discussed in Section 5.2 the final EPPT chemical scores need to be out of 100. Thus the maximum long term score needs to be calculated.

5.2.4 The maximum long term score

The maximum long term score is calculated using the same method as the long term chemical score, the difference arising from the use of the maximum scores (10) for each parameter.

Thus using Equation 5.8 the maximum intermediate long term score for any chemical is:

- Maximum intermediate long term score for air =

  $[(3 \times 10) + (7 \times 10)] \sqrt{(10)^2} = 1000$
- Maximum intermediate long term score for water =

  $[(4 \times 10) + (3 \times 10)] \sqrt{(10^2 + 10^2)} = 989.9$
- Maximum intermediate long term score for soil =

  $[(4 \times 10) + (2 \times 10)] \sqrt{(10^2 + 10^2)} = 848.5$

Unlike the maximum release score for each chemical, the maximum long term score differs for each chemical because different media fractions are calculated for each chemical. Using Equation 5.10 and the following media fractions for the long term distribution of toluene to the environment, the maximum long term scores are calculated;

Long term distribution fractions for:

- air = 0.74
- water = 0.15
- soil = 0.11

- Maximum long term media score for air = (1000 x 0.74) = 740.0
- Maximum media release score for water = (989.9 x 0.15) = 148.5
- Maximum media release score for soil = (848.5 x 0.11) = 93.3

Equation 5.6 is used to calculate the maximum long term chemical score for a chemical. This calculation is demonstrated using toluene as an example.

- Maximum long term chemical score = 740.0 + 148.5 + 93.3 + 0.5 = 982.3

5.2.5 The EPPT chemical score

The EPPT chemical score for air is calculated using Equation 5.11.

EPPT chemical score for air =

$$\frac{\text{Release score for air} + \text{Long term score}}{\text{Maximum release score for air} + \text{Maximum long term score}} \times 100$$

.... Equation 5.11

The EPPT chemical score for release to water or soil is calculated using Equations 5.12 and 5.13.

EPPT chemical score for water =

$$\frac{\text{Release score for water} + \text{Long term score}}{\text{Maximum release score for water} + \text{Maximum long term score}} \times 100$$

.... Equation 5.12

EPPT chemical score for soil =

$$\frac{\text{Release score for soil} + \text{Long term score}}{\text{Maximum release score for soil} + \text{Maximum long term score}} \times 100$$

.... Equation 5.13

The EPPT chemical scores for toluene are shown in Table 5.4.

Table 5.4: Toluene chemical scores

Media			Sum	**Chemical score**
Air	Chemical release score for air	24.5	102.3	**9.4**
	Long-term chemical score	77.8		
	Maximum chemical release score for air	100.5	1082.8	
	Maximum long-term chemical score	982.3		
Water	Chemical release score for water	25.5	103.3	**9.8**
	Long-term chemical score	77.8		
	Maximum chemical release score for water	70.5	1052.8	
	Maximum long-term chemical score	982.3		
Soil	Chemical release score for soil	19.5	97.3	**9.3**
	Long-term chemical score	77.8		
	Maximum chemical release score for soil	60.5	1042.8	
	Maximum long-term chemical score	982.3		

These EPPT chemical scores can now be used to assess the impact of chemicals on the environment. They also consider the media into which the chemical is released. The EPPT chemical scores range from 0 to 100. The chemicals that have currently been evaluated for the EPPT have chemical scores ranging from 0.09 for water, oxygen and hydrogen to 66.18 for nickel. Appendix 6 details the EPPT chemical scores for 92 chemicals that have been evaluated.

5.2.6 Persistence combination method

As mentioned in Section 5.2.3 the persistence score is a combination of the rate of degradation and the bioaccumulation of the chemical for water and soil, and solely degradation in air. With a varying number of parameters (toxicity and effect) reflecting impact to each media these persistence parameters had to be combined in such a way as to provide a similar magnitude of impact to each media. The maximum long term chemical score is required to demonstrate this. The maximum long-term score is the sum of the toxicity and effect parameter scores multiplied by the persistence scores. Multiplying the sum of the toxicity and effect parameter scores with the sum of the persistence parameter scores yields the following results:

- air 10 x 10 parameters x maximum persistence (10) = 1000
- water 10 x 7 parameters x maximum persistence (2 x 10) = 1400
- soil 10 x 6 parameters x maximum persistence (2 x 10) = 1200

Assuming water is 100%, there is variation of a almost 30 % between the maximum long term score that can be obtained for each media. To provide a maximum score with less variation the root-sum-squared combination was adopted to determine the persistence parameters for water and soil. This is shown in Equation 5.14

$$\text{Persistence score} = \sqrt{(\text{degradation score})^2 + (\text{persistence score})^2} \quad \text{....... Equation 5.14}$$

This gives maximum long-term scores of:

- air 10 x 10 parameters x maximum persistence (10) = 1000
- water 10 x 7 parameters x maximum persistence (14.142) = 989.9
- soil 10 x 6 parameters x maximum persistence (14.142) = 848.5

This method reduces the variation (assuming air is 100%) in the maximum long-term scores between each medium to 15% and has been used in the EPPT.

5.3 The chemical assessment factor

The chemical assessment factor gives an indication of the accuracy of the chemical score based on the data that has been used in the parameter score derivation. The chemical assessment factor is not however used in the impact assessment of chemical processes. The assessment factor is calculated using the same method as the chemical score but with two exceptions. The first exception is that when determining the maximum long-term score, the sum of the maximum toxicity and effect parameters is added to the maximum persistence score and not multiplied by it. This means that there is an equal contribution to the chemical assessment factor from each of the parameters irrespective of how they are used. The second exception is that the value of 0.5 for water added to the release and the long-term scores is omitted. This value is not based on parameter data and consequently is not included in the chemical assessment factor.

Like the chemical evaluation exercise, this data evaluation exercise is characterised by three assessment factors,

1. for release to air,
2. for release to water, and
3. for release to soil.

Three assessment factors have been developed to assess the three chemical scores which distinguish emissions to the different environmental media. Like the chemical scores the three assessment factors are comprised of a chemical release assessment factor and a long term chemical assessment factor. The chemical release assessment factor can potentially be different for each medium whereas the long term assessment factors are the same.

The calculation of the chemical assessment factor for toluene is given below. Equations 5.5 to 5.10 are used but the parameter scores are substituted for assessment factors. The assessment factors for each parameter score are given in Figure 5.2.

5.3.1 Release assessment factor

Using Equation 5.5 the intermediate release assessment factors for toluene released to each media are:

- Intermediate release assessment factor for air =

  (10 + 10 + 9) + (10 + 10 + 10 + 7 + 5 + 10 + 10) = 91

- Intermediate release assessment factor for water =

  (10 + 5 + 10 + 9) + (7 + 10 + 10) = 61

- Intermediate release assessment factor for soil = (10 + 10 + 10 + 9) + (7 + 5) = 51

Using Equation 5.6 and the following media fractions for release to air, the media release assessment factors were calculated;

Media fractions for release to air:

- air = 1
- water = 0
- soil = 0

- Media release assessment factor to air = (91 x 1) = 91
- Media release assessment factor to water = (61 x 0) = 0
- Media release assessment factor to soil = (51 x 0) = 0

Using Equation 5.7 the chemical release assessment factor for toluene to air is calculated.

- Chemical release assessment factor for air = 91 + 0 + 0 = 91

Using the media fractions in Table 5.3, chemical release assessment factors can be calculated for release to water and soil using Equation 5.7.

- Chemical release assessment factor for water = 0 + 61 + 0 = 61
- Chemical release assessment factor for soil = 0 + 0 + 51 = 51

Like the EPPT chemical scores, the assessment factors are also out of 100. Thus the maximum release assessment factor needs to be calculated.

5.3.2 The maximum chemical release assessment factor

The maximum chemical release assessment factor is calculated using essentially the same method as the chemical release assessment factor, the difference arising from the use of the maximum assessment factors of (10) for each parameter.

Thus using Equation 5.5, the maximum intermediate release assessment factor for any chemical is:

- Maximum intermediate release assessment factor to air =
  (3 x 10) + (7 x 10) = 100
- Maximum intermediate release assessment factor to water =
  (4 x 10) + (3 x 10) = 70
- Maximum intermediate release assessment factor to soil =
  (4 x 10) + (2 x 10) = 60

Using Equation 5.6 and the following media fractions for release to air, the maximum media release assessment factors are calculated;

Media fractions for release to air:

- air = 1
- water = 0
- soil = 0

- Maximum media release assessment factor to air = (100 x 1) = 100
- Maximum media release assessment factor to water = (70 x 0) = 0
- Maximum media release assessment factor to soil = (60 x 0) = 0

To calculate the maximum release assessment factor for a chemical released to air Equation 5.7 is used,

- Maximum release assessment factor for air = 100 + 0 + 0 = 100

Using the appropriate media fractions for release to water and soil as shown in Table 5.3, Equations 5.5 to 5.8 can be used to determine the maximum chemical release assessment factor when a chemical is released to water or soil.

- Maximum chemical release assessment factor for water =

  $$(100 \times 0) + (70 \times 1) + (60 \times 0) = 70$$

- Maximum chemical release assessment factor for soil =

  $$(100 \times 0) + (70 \times 0) + (60 \times 1) = 60$$

The maximum chemical release assessment factors are used when deriving the EPPT chemical assessment factors. This is discussed in Section 5.3.5.

5.3.3 The long term chemical assessment factor

The calculation of the long term chemical assessment factor is demonstrated using as an example the release of toluene to air. The data given in Figure 5.2 are used in the calculation.

Using Equation 5.8 the following intermediate long term assessment factors are calculated.

- Intermediate long term assessment factor for air =

  $$[(10 + 10 + 9) + (10 + 10 + 10 + 7 + 5 + 10 + 10)] + 10 = 101$$

- Intermediate long term assessment factor for water =

  $$[(10 + 5 + 10 + 9) + (7 + 10 + 10)] + \sqrt{(10^2 + 6^2)} = 72.7$$

- Intermediate long term assessment factor for soil =

$$[(10 + 10 + 10 + 9) + (7 + 5)] + \sqrt{(10^2 + 6^2)} = 62.7$$

Using Equation 5.9 and the following media fractions calculated using the distribution model, the media long term assessment factors are calculated:

- air = 0.74
- water = 0.15
- soil = 0.11

- Media long term assessment factor for air = (101.0 x 0.74) = 74.7
- Media long term assessment factor for water = (72.7 x 0.15) = 10.9
- Media long term assessment factor for soil = (62.7 x 0.11) = 6.9

Using Equation 5.10 the chemical long term assessment factor for toluene is calculated.

- Chemical long term assessment factor = 74.7 + 10.9 + 6.9 = 92.5

Like the chemical scores the EPPT chemical assessment factors are out of 100. Thus the maximum long term assessment factor needs to be calculated.

5.3.4 The maximum long term chemical assessment factors

The maximum long term chemical assessment factor is calculated using essentially the same method as for the long term chemical assessment factor, the difference arising from the use of the maximum assessment factors (10) for each parameter.

Thus using Equation 5.8 the maximum intermediate long term assessment factor for any chemical is:

- Maximum intermediate long term assessment factor to air =

$$[(3 \times 10) + (7 \times 10)] + \sqrt{(10)^2} = 110$$

- Maximum intermediate long term assessment factor to water =

$$[(4 \times 10) + (3 \times 10)] + \sqrt{(10^2 + 10^2)} = 84.1$$

- Maximum intermediate long term assessment factor to soil =

$$[(4 \times 10) + (2 \times 10)] + \sqrt{(10^2 + 10^2)} = 74.1$$

Unlike the maximum release assessment factor for each chemical, the maximum long term assessment factor differs for each chemical. This is because differing media fractions are calculated for each chemical. Using Equation 5.9 and the following media fractions for the long term distribution of toluene to the environment, the maximum media long term assessment factors are calculated:

Long term media fractions for toluene:

- air = 0.74
- water = 0.15
- soil = 0.11

- Maximum medium long term assessment factor to air = (110 x 0.74) = 81.4
- Maximum medium long term assessment factor to water = (84.1 x 0.15) = 12.6
- Maximum medium long term assessment factor to soil = (74.1 x 0.11) = 8.2

Equation 5.6 is used to calculate the maximum long term chemical assessment factor for a chemical.

Maximum long term chemical assessment factor = 81.4 + 12.6 + 8.2 = 102.2

5.3.5 The chemical assessment factor

The chemical assessment factor is calculated using Equation 5.15.

Chemical assessment factor for air =

$$\frac{\text{Release assessment factor for air} + \text{Long term assessment factor}}{\text{Maximum release assessment factor for air} + \text{Maximum long term assessment factor}} \times 100$$

.... Equation 5.15

The EPPT chemical score for release to water or soil is calculated using the Equations 5.16 and 5.17.

Chemical assessment factor for water =

$$\frac{\text{Release assessment factor for water} + \text{Long term assessment factor}}{\text{Maximum release assessment factor for water} + \text{Maximum long term assessment factor}} \times 100$$

.... Equation 5.16

Chemical assessment factor for soil =

$$\frac{\text{Release assessment factor for soil} + \text{Long term assessment factor}}{\text{Maximum release assessment factor for soil} + \text{Maximum long term assessment factor}} \times 100$$

.... Equation 5.17

The determination of the chemical assessment factor for toluene is shown in Table 5.5.

Table 5.5: Toluene chemical assessment factor determination

Media			Sum	**Chemical assessment factor**
Air	Chemical release assessment factor for air	91.0		**90.8**
	Long-term chemical assessment factor	92.5	183.5	
	Maximum chemical release assessment factor for air	100.0		
	Maximum long-term chemical assessment factor	102.2	202.2	
Water	Chemical release assessment factor for water	61.0		**89.1**
	Long-term chemical assessment factor	92.5	153.5	
	Maximum chemical release assessment factor for water	70.0		
	Maximum long-term chemical assessment factor	102.2	172.2	
Soil	Chemical release assessment factor for soil	51.0		**88.5**
	Long-term chemical assessment factor	92.5	143.5	
	Maximum chemical release assessment factor for soil	60.0		
	Maximum long-term chemical assessment factor	102.2	162.2	

As with the EPPT chemical scores, the chemical assessment factors range from 0 to 100. A score above 80 is high and suggests that reliable data has been used to determine the score which represents the impact of toluene on the environment. Chemical assessment factors lower than 10 exist for some chemicals. Appendix 6 gives the assessment factors derived for all the chemicals in the EPPT database.

5.4 Comparison of the EPPT's and EniVal's chemical assessment

Having determined the chemical scores using the EPPT the results were compared with the chemical scores derived by Elliott using EniVal. Similarities exist in both chemical assessments primarily from the use of the same distribution model and also from using some of the same parameters and data sources to assess environmental impact.

The main difference however lies in the focus of the chemical assessments. Whilst both methods include a persistence category and an effects category (named 'modification of the environment' in EniVal) the difference lies in the EPPT toxicity /EniVal damage categories. Damage to the environment, considered in EniVal, evaluates the toxicity and hazards of the chemical on the environment. Toxicity is evaluated by one toxicity parameter, and hazards to the environment are evaluated in terms of flammability and explosivity. The EPPT's toxicity category has a much greater environmental and ecological focus since it considers the toxicity of chemicals to various levels of organisms existing in environmental media. The EPPT makes no consideration of other hazard parameters as these can be evaluated using other chemical engineering techniques such as Dow and Mond's Fire and Explosion index (1987).

The other difference between the EPPT and EniVal chemical assessments lies in the weighting of parameters. The weighting of parameters and its subjectivity have been discussed in Section 4.1. Elliott adopted an opinion based approach to weighting parameters in EniVal. However, due to the subjectivity involved in applying such weightings they have not been applied in the EPPT. Each of the parameters has an equal weighting in the chemical assessment. If at a later date a reliable method of assigning weights is developed then there is an opportunity to incorporate weightings into the chemical assessment of the EPPT.

5.4.1 Comparison of the EPPT and EniVal chemical scores

The scores and ranking of 25 chemicals evaluated using EPPT and EniVal are shown in Table 5.6. EniVal's scores range from 0 to 10, 0 having the least environmental impact, 10 having the most. The EPPT scores range from 0 to 100, 0 having the least environmental impact, 100 having the most. EniVal's scores have been multiplied by ten for ease of comparison.

Table 5.6: Comparison of the EPPT and EniVal's chemical scores

EniVal			**EPPT**		
Chemical	**Medium**	**Score x 10**	**Chemical**	**Medium**	**Score**
Water	Air	2	Hydrogen	Air	0.1
Pentane	Air	10	Water (Steam)	Air	0.2
Hydrogen	Air	11	Sodium Hydroxide	Water	3.6
Particulates	Air	11	Methanol	Water	4.3
Ethane	Air	13	Ethane	Air	7.1
Aluminium Chloride	Soil	14	Pentane	Air	7.4
Ethyl Chloride	Air	14	Toluene	Air	9.4
Methanol	Water	15	Ethylene	Air	9.9
Paraxylene	Air	16	Paraxylene	Air	13.7
Chlorine	Air	17	Particulates	Air	14.9
Ethylene	Air	17	Chlorine	Air	21.9
Formaldehyde	Air	17	Ethyl Chloride	Air	22.7
Sodium Hydroxide	Water	17	Formaldehyde	Air	24.1
Sulphur Dioxide	Air	17	Sulphur Dioxide	Air	24.3
Benzene	Air	18	Aluminium Chloride	Soil	25.1
Toluene	Air	18	Benzene	Air	25.3
Nitrogen oxides	Air	19	Nitrogen oxides	Air	29.3
Nitrobenzene	Air	22	Nitrobenzene	Air	30.0
Zinc	Soil	31	Lead	Soil	41.7
Copper	Soil	33	Chromium	Soil	45.1
Mercury	Soil	42	Mercury	Soil	45.1
Cadmium	Soil	47	Zinc	Soil	46.7
Lead	Soil	47	Copper	Soil	51.7
Nickel	Soil	47	Cadmium	Soil	57.5
Chromium	Soil	48	Nickel	Soil	66.7

The EPPT and EniVal's (x10) chemical scores have been plotted on a scatter diagram against the 45° line in Figure 5.1. This highlights where the differences in scores lie .

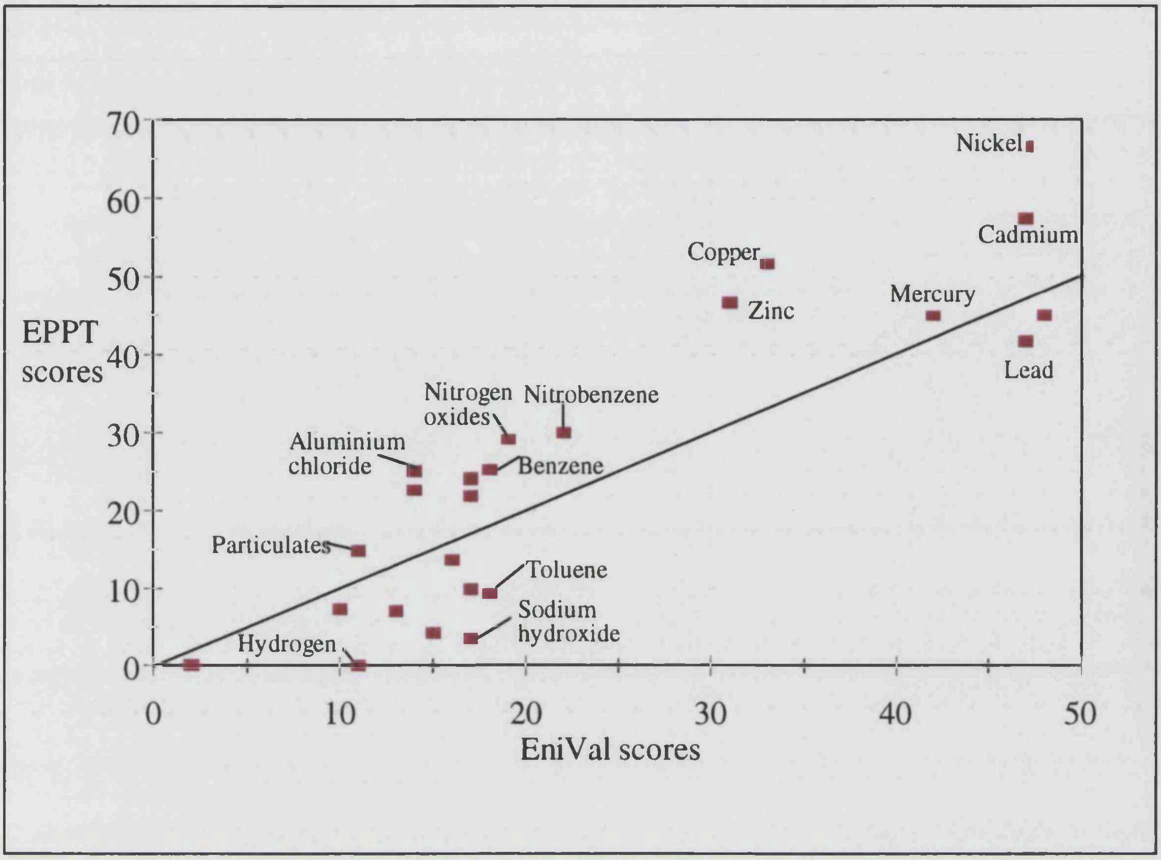


Figure 5.1: Comparison of EPPT and EniVal scores

In Table 5.7 four chemicals with significant variation in score have been identified. The reasons for the variation in scores are identified in the following discussion.

Table 5.7: Chemicals with significantly differing EniVal and EPPT scores

Chemical	EniVal score	EPPT score
Hydrogen	11	0.9
Sodium hydroxide	17	3.6
Toluene	18	9.4
Benzene	18	25.3
Aluminium chloride	14	25.1

For hydrogen, the relative environmental impact calculated by EniVal is much higher than that calculated by the EPPT. This is primarily due to the fact that EniVal includes a hazard section comprising of a flammability and explosivity score.

Hydrogen scores highly in these parameters. The EPPT does not consider hazards and thus a lower environmental impact is calculated.

For sodium hydroxide, the environmental impact calculated using the EPPT is much lower than that calculated by EniVal. The main reason for this difference is that the EPPT assigns a much lower degradation score. The lower score used in the EPPT arises because of the dissociation of sodium hydroxide into sodium and hydroxide ions.

Toluene has a lower chemical score than benzene using the EPPT. However, EniVal scores both chemicals the same. It would appear that either EniVal is not sensitive to the increased toxicity and persistence of benzene or there are limitations in the data used to evaluate these chemicals with EniVal. The latter is unlikely to be the case as assessment factors derived using the EPPT method indicates that data for assessment is good for toluene and benzene with assessment factors of around 88 and 75 respectively.

Aluminium chloride is scored more highly in the EPPT than EniVal. Again this is due to the more significant toxicity contribution. The significance of toxicity within EniVal is reduced as it is combined with hazard parameters.

The majority of the differences between the EPPT and EniVal impact calculations are due to the decreased significance of toxicity in EniVal and the inclusion of hazard parameters detracting from scoring the actual environmental impact of a chemical in a normal release situation. If hazard needs to be assessed then this should be carried out using specific tools designed for the purpose, rather than being combined into a tool like EniVal.

Having evaluated the chemical scores calculated using the EPPT a pattern has emerged based on chemical type. This is shown in Figure 5.3.

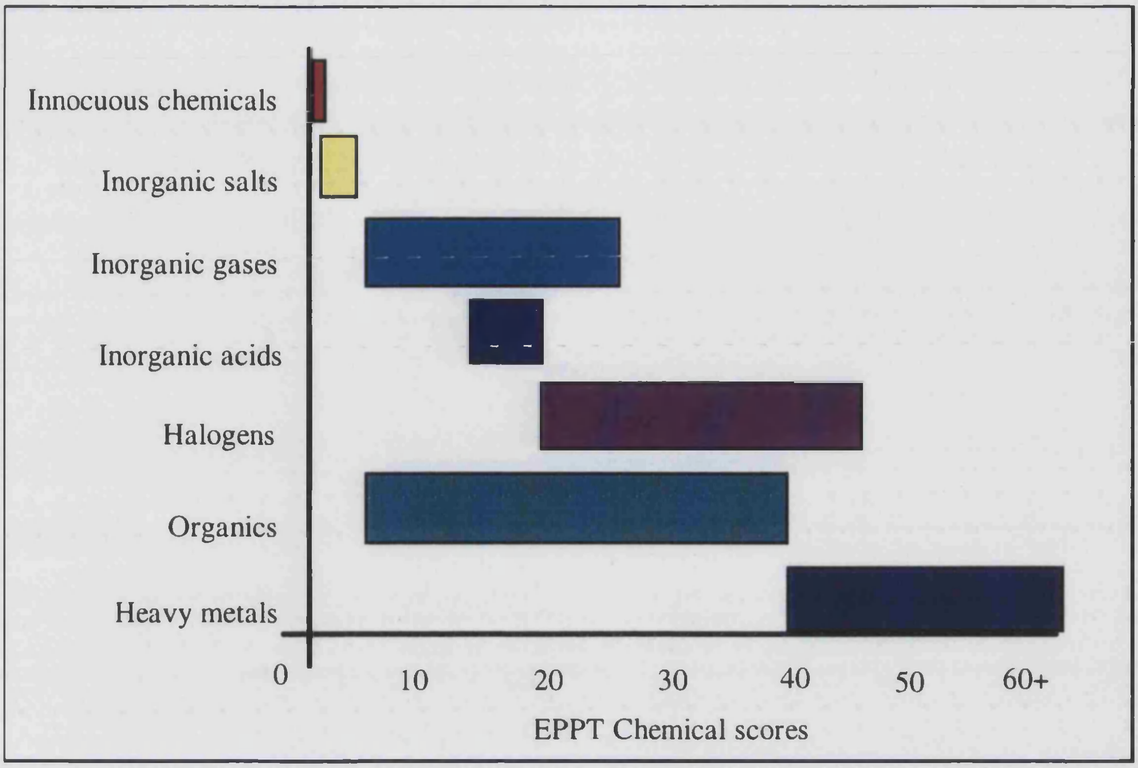


Figure 5.3: Scoring ranges for chemical types

Heavy metals have the highest scores of 40 and above. A score between 25 and 40 reflects the more toxic organics such as benzene and nitrobenzene and also some halogens. The lower and mid 20's include organics, halogens and some of the more polluting inorganic gases with global, regional and local effects. Inorganic acids have scores in the mid to high teens together with the less polluting organics and inorganic gases. Below 10 the alkanes and gases such as carbon monoxide and carbon dioxide are represented. Less than 5 includes salts, particularly sodium salts. Those chemicals which score less than 1 include the ubiquitous substances such as water and oxygen.

5.5 Summary

In this chapter the models considered for the determination of the long-term distribution of chemicals have been discussed. Details of Elliott's distribution model which was applied to the EPPT have also been discussed. The method of combining parameter scores and assessment factors assigned in Chapter 4 have also been described. The derivation of the chemical score and assessment factor for toluene has been used as an example. A comparison has been made between the chemical scores derived using EniVal and those derived using the EPPT. The similarities and differences in approach have been highlighted and used to discuss the variation in chemical ranking.

In the next chapter the several method of combining EPPT chemical scores with mass have been described. Details of the evaluation of electrical energy, cooling water and steam are also given. This chapter also presents the assumptions made with regard to pollution abatement strategies that will be used in process and process option comparisons in later chapters.

6. Determination of the EPPT process scores

The chemical scores for the EPPT have been derived in Chapters 4 and 5. In this chapter the combination of these chemical scores with the mass of emissions from a chemical process is described. This combination provides the basis for process and process option comparisons which will be discussed in Chapters 8 and 9. This chapter also introduces the utilities evaluation, a novel aspect of the EPPT, which enables the environmental impact of electrical energy use and cooling water use to be incorporated into the process assessment. Finally the assumptions made regarding emissions treated in effluent treatment plants and scrubbers, and also the final disposal to landfill are considered.

6.1 Combining mass with chemical score

To determine the environmental impact of a chemical process the mass of an emission released and the EPPT chemical score are combined. Elliott (1997) investigated five ways of combining EniVal's impact scores (akin to the EPPT chemical scores) with mass of emissions. The five methods are shown in Table 6.1.

Table 6.1: Impact-quantity combination methods (Elliott, 1997)

Method	Formula	Description
1	$\sum_i \left(I_i \times \frac{Q_i}{Q_T} \right)$	Impact score multiplied by discharge ratio
2	$\sum_i \left(I_i \times \frac{\log(Q_i)}{\log(Q_T)} \right)$	Impact score multiplied by log discharge ratio
3	$\sum_i \left(10^{I_i} \times \frac{Q_i}{Q_T} \right)$	Inverse log of the impact score multiplied by the discharge ratio
4	$\sum_i \left(10^{I_i} \times \frac{\log(Q_i)}{\log(Q_T)} \right)$	Inverse log of the impact score multiplied by the log discharge ratio
5	$\sum_i \left(e^{I_i} \times \frac{\ln(Q_i)}{\ln(Q_T)} \right)$	Exponential of the impact score multiplied by the natural log discharge ratio

EniVal, like the EPPT, includes both the quantity of a pollutant i, (Q_i) and the overall production rate (Q_T) of the process. The inclusion of the production rate allows comparison between processes with different production rates to be made. In the methods described in this chapter Q_i/Q_T is known as the discharge ratio. The log discharge ratio is defined as log Q_i/log Q_T and I is the impact score, or in the case of the EPPT, the chemical score.

Elliott (1997) compared each of the five methods by considering:

1. the range and spread of the overall score,
2. the effects of errors in raw data on the overall score, and
3. the sensitivity of the combination technique to changes in process data.

The five methods were evaluated using emission data for twelve chemical processes including nitrobenzene, paraxylene, hydrogen chloride, and speciality chemical plants together with several boilers and cement clinker plants.

6.1.1 Elliott's evaluation for range and spread of values

Initially Elliott evaluated the five different methods for the range and spread of overall scores obtained with the twelve processes. Method 1 was eliminated as a discontinuity occurred in the range of the overall scores. High overall scores were derived for the cement clinker plants caused by the high discharge levels of carbon dioxide compared with the clinker production levels. The remaining processes had a very narrow range of overall scores making process distinction difficult. Due to the limited range and uneven spread of values in Method 1, additional methods (2 and 5) that increased the contribution of the impact scores and reduced the contribution of the discharge ratio were investigated.

Method 2 decreases the contribution of the discharge ratio by using logarithms. This reduces the range of the discharge ratio from an almost limitless range to values more comparable with impact scores (Elliott, 1997). However, reducing the discharge ratio reduces the range of overall scores moreso than Method 1.

Method 3 uses the inverse logarithm of impact scores rather than discharge ratios. This method gives a greater range and more even spread of overall scores and ranks the processes in a similar order to Method 1. Elliott investigated further the more successful results of Method 3 in Methods 4 and 5.

Method 4 uses the inverse logarithm of the impact score and the ratio of the logarithm of the discharge ratio to reduce the contribution of the discharge ratio. Again a good spread of overall scores was obtained. The processes with pollutants with high impact scores had the highest overall scores which represents the worst environmental impact. However, Elliott (1997) states that Method 4 was an extreme analysis akin to simply using the impact scores due to the decreased significance of the discharge ratio. Elliott considered a fifth method using the exponential of the impact scores and the natural logarithm of the quantities. This increased the contribution of the impact score (although to a lesser extent than the inverse logarithm to the base 10) by reducing the quantity contribution. Method 5 produced results similar to Method 4. However the contribution from impact scores was slightly less. The spread of the overall scores was also reduced.

Elliott (1997) concluded that Methods 3 and 4 provided the greatest range and spread of results. He discounted Methods 1, 2 and 5 due to the disjointed and limited ranges of overall scores. Elliott then analysed Methods 3 and 4 for the effects of errors in the combination techniques and the sensitivity of the formulae to changes in emission data.

6.1.2 Elliott's error and sensitivity analysis

Elliott (1997) showed that the errors in Method 3 are significantly lower than those in Method 4. This was expected as Method 3 uses the pollutant quantities rather than the logarithm of the quantities. Elliott's sensitivity analysis showed that reducing the discharge of a pollutant with a high impact and a low emission has little effect on the overall score using Method 3. However reducing the discharge of a pollutant with a high emission and a low impact has a greater effect on the overall score. The reverse is true for Method 4.

Elliott (1997) concluded that Method 3 was most applicable for combining discharge quantity and impact score due to the spread and range of overall scores obtained, the significantly lower response to raw data errors and its sensitivity to process data changes.

In this thesis Method 3 has been adopted to combine mass and chemical score in the EPPT. However a slight modification has been introduced in order to accommodate the differing ranges of chemical scores.

Like EniVal the EPPT combination method uses the inverse logarithm of the impact score. However in the EPPT, the chemical scores lie in the range is 0 to 100. This wider range of chemicals scores provides a better range of values with which to assess chemicals and avoids numerous chemicals having the same scores (as in EniVal). However an increased scoring range causes Elliott's Method 3 to generate values biased towards an increased contribution by the chemical score and thus would generate the problems associated with Elliott's Methods 4 and 5. To avoid the problems associated with Elliott's Methods 4 and 5 the EPPT impact score is divided by 10 to reduce the contribution of the chemical score. The following example demonstrates this point.

Consider two chemicals; A and B. EniVal's scoring system assigns both chemicals a score of 3.0 whereas the EPPT assigns scores of 31.0 and 39.0. Assuming 10kg of each chemical is emitted from a chemical process (based on 1000kg production rate which has been adopted for use in the EPPT and therefore Q_i/Q_T = 10). Using the combination methods shown in Figure 6.1 the following impact scores for the process are derived:

Elliott's Method 3

$$\sum_{i}\left(10^{I_i} \times \frac{Q_i}{Q_T}\right)$$

EPPT combination method

$$\sum_{i}\left(10^{(I_i/10)} \times \frac{Q_i}{Q_T}\right)$$

Figure 6.1: Elliott's Method 3 and the EPPT combination method

Elliott's method 3:

Impact score $= (10^3 \mathrm{x}10)+(10^3 \mathrm{x}10)$
$= \mathbf{2 \times 10^4}$

EPPT method:

Impact score $= (10^{31/10} \mathrm{x}10)+(10^{39/10} \mathrm{x}10)$
$= \mathbf{9.2 \times 10^4}$

This shows that using a wider range of scores (0 to 100 rather than 0 to 10) increases the sensitivity of the impact assessment tool without increasing the problems associated with Elliott's Method's 4 and 5.

6.2 Utilities evaluation

The consideration of utilities such as electrical energy and cooling water is lacking in many environmental assessments particularly those applied to the environmental impact of chemical processes. To counter such criticism an assessment of the environmental impact of electrical energy and cooling water has been undertaken in the EPPT. The utilities evaluation is based on the EPPT chemical evaluation. Adopting the chemical evaluation approach allows direct comparison between emissions and electrical energy use and cooling water use. In this chapter the utilities evaluation for electrical energy and cooling water are described. The utility evaluations are applied to the case studies and process options described in Chapter 8.

6.2.1 Electrical energy evaluation

An evaluation of emissions associated with electrical energy generation has been used to determine the environmental impact of electrical energy production. The emissions have been determined using 1992 data obtained from the Department of the Environment's Digest of UK Energy Statistics (1994). The evaluation does not consider the production of electrical energy by nuclear power because the impact of nuclear power and nuclear waste disposal cannot be adequately evaluated using the chemical evaluation derived for the EPPT.

There are seven main pollutants associated with non-nuclear electrical energy production. They are:

- Carbon dioxide - the most important greenhouse gas responsible for 72% of global warming (DoE, 1994)
- Methane - the second most important greenhouse gas accounting for 10% of global warming.
- Sulphur dioxide - the main gas responsible for acid deposition.
- Black smoke (particulates) - a contributor to smog.
- Nitrogen oxides - also responsible for acid deposition.
- Volatile organic compounds (VOC's) - a main contributor to ground level ozone creation. (In the EPPT toluene is used to represent VOC's as it is a commonly used solvent).
- Carbon monoxide - derived from incomplete combustion of fuel, carbon monoxide oxidises to carbon dioxide.

Table 6.2 gives a summary of the mass of the pollutant associated with electrical energy production in the UK, the percentage generated from power stations in the production of energy and the mass of each pollutant generated from non-nuclear power stations.

Table 6.2: Emission summary of 1992 UK energy production

Emission	Total mass of man-made emissions (tonnes)	% release from power stations	Mass emitted from power stations (tonnes)
Carbon Dioxide	155,000,000	33 %	51,000,000
Methane	4,736,000	< 1 %	3,000
Sulphur Dioxide	3,500,000	69 %	2,427,000
Particulates	457,000	5 %	25,000
Nitrogen Oxides	2,750,000	25 %	694,000
VOC's	2,556,000	< 1 %	12,000
Carbon Monoxide	6,708,000	1 %	45,000

Water vapour is also emitted from power stations. The amount of steam released from a power station has been calculated from data available on the Ratcliffe power station that was obtained from Powergen's Environmental Report (1995). Ratcliffe power station releases 13 million cubic metres of steam to produce 13 terawatt hours of electrical energy. This is equivalent to $5.9\text{x}10^{-4}$ kilograms of steam (at 1 bar) per kilowatt hour (assuming one cubic metre of steam weighs 0.59 kilograms at 1 bar). This calculation is given in Appendix 7.

The emissions shown in Table 6.2 were generated in the production of 298,469 GWh of electricity (Department of the Environment, 1994). The breakdown of this energy production is given in Table 6.3.

Table 6.3: Energy production in the UK, 1992

Total electricity generated	320,961 GWh
Total electricity supplied (gross)	300,726 GWh
Total electricity supplied (net)	298,469 GWh

The lower figure for electricity supplied, gross and net, compared with that generated is accounted for in the pumping and working of the system.

The impact of the emissions produced per unit of electrical energy generated is calculated by dividing the emissions by the total net electricity supplied. This is shown in Table 6.4. The calculations are given in Appendix 7.

Table 6.4: Emissions per unit energy production

Emission	Emission (tonnes)	Net production (GWh)	Emission (tonnes/GWh)	Emission (kg/kWh)
Carbon dioxide	51,000,000	298,469	170.87	1.709×10^{-1}
Methane	3,000	298,469	0.01	1.005×10^{-5}
Sulphur dioxide	2,427,000	298,469	8.13	8.131×10^{-3}
Particulates	25,000	298,469	0.08	8.376×10^{-5}
Nitrogen oxides	694,000	298,469	2.32	2.325×10^{-3}
VOC's	12,000	298,469	4.02	4.021×10^{-5}
Carbon monoxide	45,000	298,469	1.51	1.508×10^{-4}
Steam				5.9×10^{-4}

The emissions per unit of electricity can then be evaluated on the same basis as the chemicals to give a comparable EPPT score per unit of electricity.

To calculate the EPPT electrical energy score the masses of emissions released to produce 1 kWh are combined with the EPPT chemical scores for these emissions. The combination of masses and EPPT chemical scores uses the method described in Section 6.1. Table 6.5 shows the derivation of the EPPT score for the production of 1 kWh of electrical energy.

Table 6.5: The derivation of the EPPT energy score

Emission	kg emission/ kWh produced	Chemical score for release to air (kg^{-1})	Mass ($kg\ kWh^{-1}$) x $10^{(Score/10)}$ (kg^{-1})
Carbon dioxide	1.709×10^{-1}	7.7	1.0
Methane	1.005×10^{-5}	11.2	1.3×10^{-4}
Sulphur dioxide	8.131×10^{-3}	24.3	2.2
Particulates	8.376×10^{-5}	15.7	3.1×10^{-3}
Nitrogen oxides	2.325×10^{-3}	29.3	2.0
VOC's	4.021×10^{-5}	10.5	4.5×10^{-4}
Carbon monoxide	1.508×10^{-4}	9.9	1.5×10^{-3}
Steam	5.9×10^{-4}	0.2	6.2×10^{-4}
EPPT electrical energy score			5.2 kWh^{-1}

Thus the EPPT electrical energy score is 5.2 kWh^{-1}. When applying the EPPT energy score to a chemical process the electrical energy score is multiplied by the amount of energy used in kilowatt hours to produce 1000kg of product. This results in a non-dimensional impact score which can be combined with the process impact score. Examples using the EPPT electrical energy evaluation are given in Chapter 8.

6.2.2 Cooling water evaluation

Cooling water is used in many process operations. In cooling a vessel or process stream the heat from the source is transferred to the water, cooling the source and causing an increase in the water temperature. The water needs to be cooled in a cooling tower or air cooler for reuse or release. In a cooling tower, warm water is sprayed into a rising air current. The difference in temperature between the water and the air causes some of the water to vapourise which causes the water to cool. 0.073kg of water vapour is produced in cooling one kilogram of water from 30°C to 20°C, assuming that air enters the system at 20°C, 20% relative humidity and leaves at 25°C. Thus 7.3% of the water is evaporated. These calculations are given in Appendix 8.

In the chemical evaluation of the EPPT, 7.3% of the water is assumed to become water vapour and is scored accordingly. The remaining mass of water is combined with the chemical score for liquid water. Table 6.6 shows the EPPT chemical scores for water, steam and cooling water. Studies of process options using cooling water are given in Chapter 8.

Table 6.6: Water, steam and cooling water comparison

	Mass released kg/1000kg product	Release media	EPPT chemical score (kg^{-1})	EPPT score Mass(kg/1000kg product) x $10^{Score/10}$ (kg^{-1})
Water	100	Water	0.1	102.3
Steam	100	Air	0.2	104.7
Cooling water	100	Water - 92.7% Air - 7.3%	0.1 0.2	94.9 + 7.6 = 102.5

6.3 Pollution abatement considerations

Having established the method of combining mass of emission and chemical score, and having incorporated the contribution due to utilites, the final step in determining the EPPT process score is to identify where the chemicals in a process become emissions. In the EPPT it is assumed that the impact of the process is determined from the emissions that arise after treatment, that is when the emissions have been sent through the pollution abatement equipment such as an effluent treatment plant or scrubber.

In the case studies addressed in this research (described in Chapter 7) most emissions are sent to an effluent treatment plant or scrubber. Any emissions arising from these pollution abatement technologies, or any other part of the process, which are released to the environment are then assessed on their impact to air, water or soil. The following sections describe the assumptions made when evaluating the emission treatment of chemical processes.

6.3.1 Effluent treatment

In many chemical processes the aqueous effluent is sent to an on-site or off-site effluent treatment plant. Often the effluent treatment plant serves more than one process and details of the inputs and outputs to the effluent treatment plant from one process are unknown. Specific effluent treatment plant data was unavailable for two process described in Chapter 7. (Thomas Swan Pepton process and Fison's sodium cromoglycate process). In these cases the following assumptions were made.

- No feeds with the exception of the waste stream are added to the effluent treatment plant. This is not generally the case as often streams are mixed to reduced/increase the pH or BOD_5 of a stream or a precipitator or flocculant is added.
- Water passes through treatment plants (on-site and off-site plants including sewage works) and is eventually released to controlled waters.
- Non metallic inorganic salts pass through the effluent treatment plant unchanged and are eventually released to controlled waters. For the Thomas Swan and Fison's process this is mainly sodium salts. Often the concentration of these salts in the streams are reduced by precipition or diluted to levels below consent limits.
- It is assumed that all metallic inorganic salts are disposed of in landfill. This is in reference to Fison's sodium cromoglycate process where low levels of aluminium salts are present.
- All organic compounds sent to effluent treatment where it is arbitrarily assumed that 90% are degraded and 10% are disposed of in landfill (for details of evaluating landfill disposal see Section 7.3.3). This is a very gross assumption and the degradation of organics, amount of organics passing through the treatment plants, and their disposal of to landfill/incineration needs to be considered in more detail
- It is assumed that there are no emissions to air from the effluent treatment plant. This is also a gross assumption as complaints are often made with regard to odours from effluent treatment plants.

These gross assumptions have been made where specific effluent treatment plant data is unavailable. Where specific effluent treatment data is available the percentage removal of each type of chemical is calculated and the percentages applied to the waste streams. This has been carried out for the Associated Octel tetra alkyl lead processes to be described in Chapter 7. For Associated Octel's effluent treatment plant it is assumed that:

- 99.5% of all lead (inorganic and organic) are recovered and reused, the remaining 0.5% are released to controlled water.
- All non-lead inorganic salts are discharged to controlled waters (these are primarily sodium salts).
- An arbitrarily assigned figure of 90% of non-lead organic liquid effluents are assumed to degrade in the effluent treatment plant. The remaining 10% is sent to landfill.
- All gaseous emissions are released directly to the atmosphere. Associated Octel do not operate a scrubber.

The above assumptions have been made to provide a way forward for the process comparisons and the more detailed analysis of this research. Modelling and evaluation of effluent treatment plants using the EPPT would provide much more reliable assumptions for situations in which process specific effluent treatment data is not available. This subject is addressed in Chapter 11 where future work is discussed.

6.3.2 Scrubbing

Scrubbing is pollution abatement technique usually used to reduce gaseous emissions. Two of the IPC applications evaluated in Chapter 7 (Fisons and Associated Octel) contain no details of scrubbers. The third application (Thomas Swan) operate a scrubber however the data given was insufficient to model the scrubber. For this reason it is assumed that all gaseous emissions are released to the atmosphere. In the future an evaluation of scrubbers is required to determine the percentage of gases that are released to the atmosphere and the percentage released to an effluent treatment plant.

6.3.3 Landfill

Effluent or waste which is sent to landfill is scored using the chemical score when released to soil. However the total value derived for the discharges to landfill are reduced to 10% of the total score. This arbitrary reduction accommodates the fact that the chemicals should be contained and therefore in theory should not affect the environment.

Again, this is a very bold assumption and has been made to provide a means of moving forward in order to undertake process comparisons. The disposal to land needs to be addressed further, as does incineration as an alternative disposal method.

6.4 Summary

In this chapter the method of combining chemical scores and quantity data has been presented together with an evaluation of utilites and the assumptions necessary with regard to emission treatment and disposal. In the next chapters these methods and assumptions are applied to process data where they are used to compare processes and process options.

7. Process descriptions

This chapter presents the four chemical processes which have been used to develop and test the EPPT. The four processes provide examples from the fine chemicals sector, the pharmaceutical sector and the bulk chemicals sector. The processes are:

1. The Pepton process operated by Thomas Swan Ltd.
2. The sodium cromoglycate process operated by Fisons plc.
3. The tetra ethyl lead (TEL) and tetra methyl lead (TML) processes operated by Associated Octel Co. Ltd.

The mass balances given in the following sections are used in Chapter 9 to evaluate and compare the environmental impact of one process with another. More detailed data is given where the process has been used for more detailed evaluation of process changes. With the exception of Thomas Swan's Pepton process, the data used from the processes has been obtained from publicly available data contained in IPC applications.

7.1 Thomas Swan - Pepton process

Thomas Swan Ltd, a fine chemicals producer based in Consett, County Durham, operates a batch process for the production of Pepton (HMIP, 1994c). Pepton is an organo-sulphur compound used as a peptiser in the manufacture of car tyres. Pepton is added to the rubber to increase malleability and to make the rubber easier to mould. Thomas Swan produces 600 tonnes per annum of Pepton in a five stage process shown in Figure 7.1.

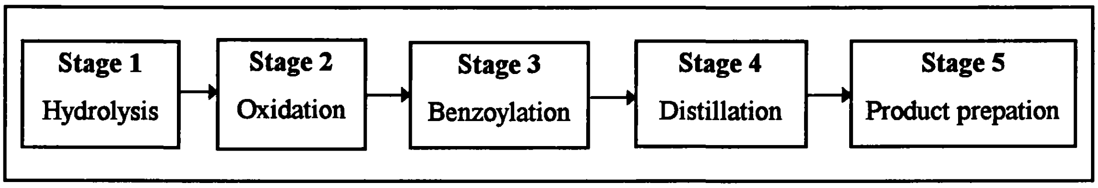


Figure 7.1: Five stages in Thomas Swan's Pepton process

The Pepton process has been used to demonstrate how the EPPT can be used to evaluate the environmental impact of process changes. Process changes have been derived and modelled for stages 1 and 2 of the process (Houghton, 1998) and are evaluated using the EPPT in Chapter 8. A detailed mass balance of stage 1 and 2 are therefore provided in this chapter. Commercial confidentiality precludes the provision of details of process operation, some chemicals and chemical reactions. To comply with confidentiality requirements some chemicals are labelled as Chemicals A, B and C etc.

7.1.1 Process details and stage mass balances

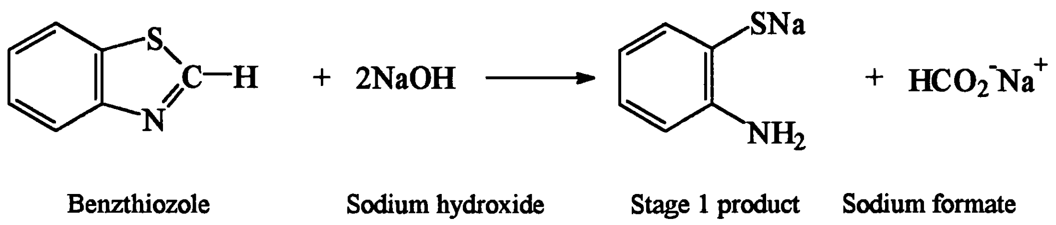
The following section describes each stage in the process and provides a mass balance for stage 1 and 2. An overall mass balance for the process is also given. Houghton (1998) derived the mass balances based on process data using the HYSYS™ modelling software.

Stage 1: Hydrolysis

Pressure hydrolysis of benzothiazole using a caustic soda solution is carried out in stage 1. Under specific operating conditions (that cannot be given because of confidentiality restrictions) the hydrolysis of benzothiazole [$C_6H_4(SN)(CH)$] by sodium hydroxide is performed and stage 1 product, sodium 2-amino thiophenate [$(C_6H_4(SNa)(NH_2))$], is formed. This is a three step process in which the vessel is:

- charged,
- heated, and
- vented.

Sodium formate is produced as a by-product of the reaction. The reaction is as follows:



The benzothiazole feed contains the following contaminants by weight:

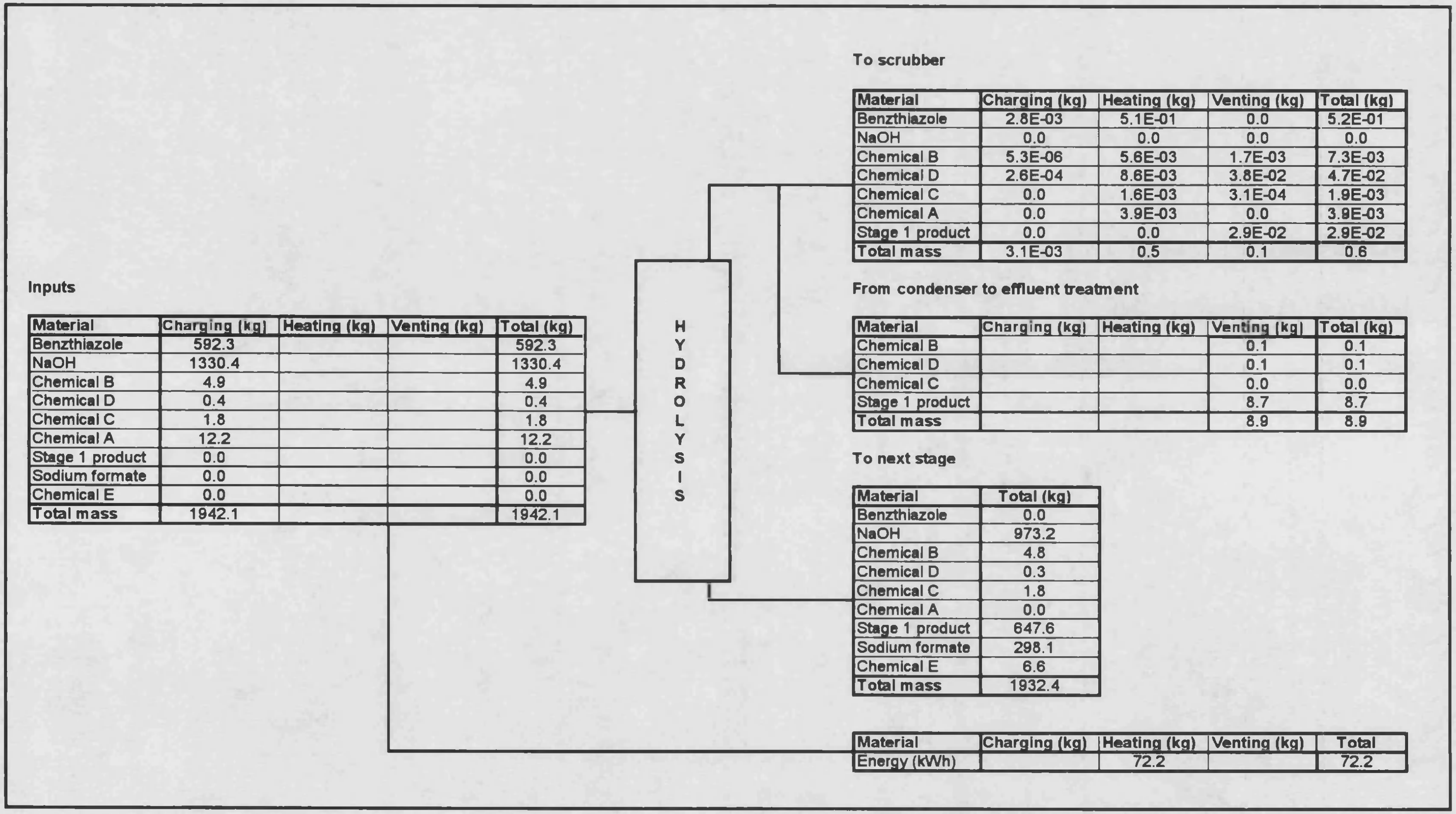
Chemical A = 2.0 %
Chemical B = 0.8 %
Chemical C = 0.3 %
Chemical D = 0.07 %

One main organic contaminant, Chemical A, reacts in a similar manner to benzothiazole producing a different sodium salt, Chemical E. The other main contaminant, Chemical B, remains unreacted in the process. Chemicals C and D appear as emissions although their mass is reduced in the reaction. The reaction mechanisms of these chemicals in the process are unknown. The sodium hydroxide is in excess (~17%) and leads to an effluent stream arising from the benzoylation stage. The benzoylation stage is operated under mild alkaline conditions to ensure that the acid by-products are neutralised. Once the hydrolysis reaction is complete the vessel is vented. Gaseous organic emissions are generated which are passed through a scrubber. The mass balance for stage 1 is shown in Figure 7.2.

Stage 2: Oxidation

The stage 1 product is oxidised using hydrogen peroxide in stage 2. This is also a three step stage which involves:

- charging,
- the addition of hydrogen peroxide, and
- venting.



Inputs

Material	Charging (kg)	Heating (kg)	Venting (kg)	Total (kg)
Benzthiazole	592.3			592.3
NaOH	1330.4			1330.4
Chemical B	4.9			4.9
Chemical D	0.4			0.4
Chemical C	1.8			1.8
Chemical A	12.2			12.2
Stage 1 product	0.0			0.0
Sodium formate	0.0			0.0
Chemical E	0.0			0.0
Total mass	1942.1			1942.1

To scrubber

Material	Charging (kg)	Heating (kg)	Venting (kg)	Total (kg)
Benzthiazole	2.8E-03	5.1E-01	0.0	5.2E-01
NaOH	0.0	0.0	0.0	0.0
Chemical B	5.3E-06	5.6E-03	1.7E-03	7.3E-03
Chemical D	2.6E-04	8.6E-03	3.8E-02	4.7E-02
Chemical C	0.0	1.6E-03	3.1E-04	1.9E-03
Chemical A	0.0	3.9E-03	0.0	3.9E-03
Stage 1 product	0.0	0.0	2.9E-02	2.9E-02
Total mass	3.1E-03	0.5	0.1	0.6

From condenser to effluent treatment

Material	Charging (kg)	Heating (kg)	Venting (kg)	Total (kg)
Chemical B			0.1	0.1
Chemical D			0.1	0.1
Chemical C			0.0	0.0
Stage 1 product			8.7	8.7
Total mass			8.9	8.9

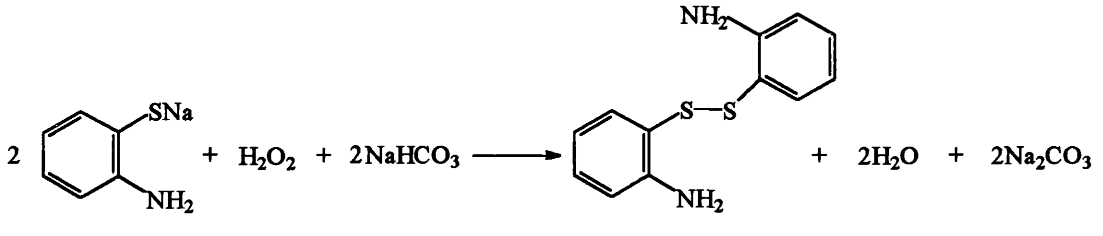
To next stage

Material	Total (kg)
Benzthiazole	0.0
NaOH	973.2
Chemical B	4.8
Chemical D	0.3
Chemical C	1.8
Chemical A	0.0
Stage 1 product	647.6
Sodium formate	298.1
Chemical E	6.6
Total mass	1932.4

Material	Charging (kg)	Heating (kg)	Venting (kg)	Total
Energy (kWh)		72.2		72.2

Figure 7.2: Hydrolysis mass balance

Initially water, sodium bicarbonate and hydrogen peroxide are added with the stage 1 product which is oxidised to the stage 2 product, 2,2'-diaminodiphenyl disulphide [$(C_6H_4(NH_2)S)_2$]. The oxidation reaction is as follows:



Stage 1 product Stage 2 product

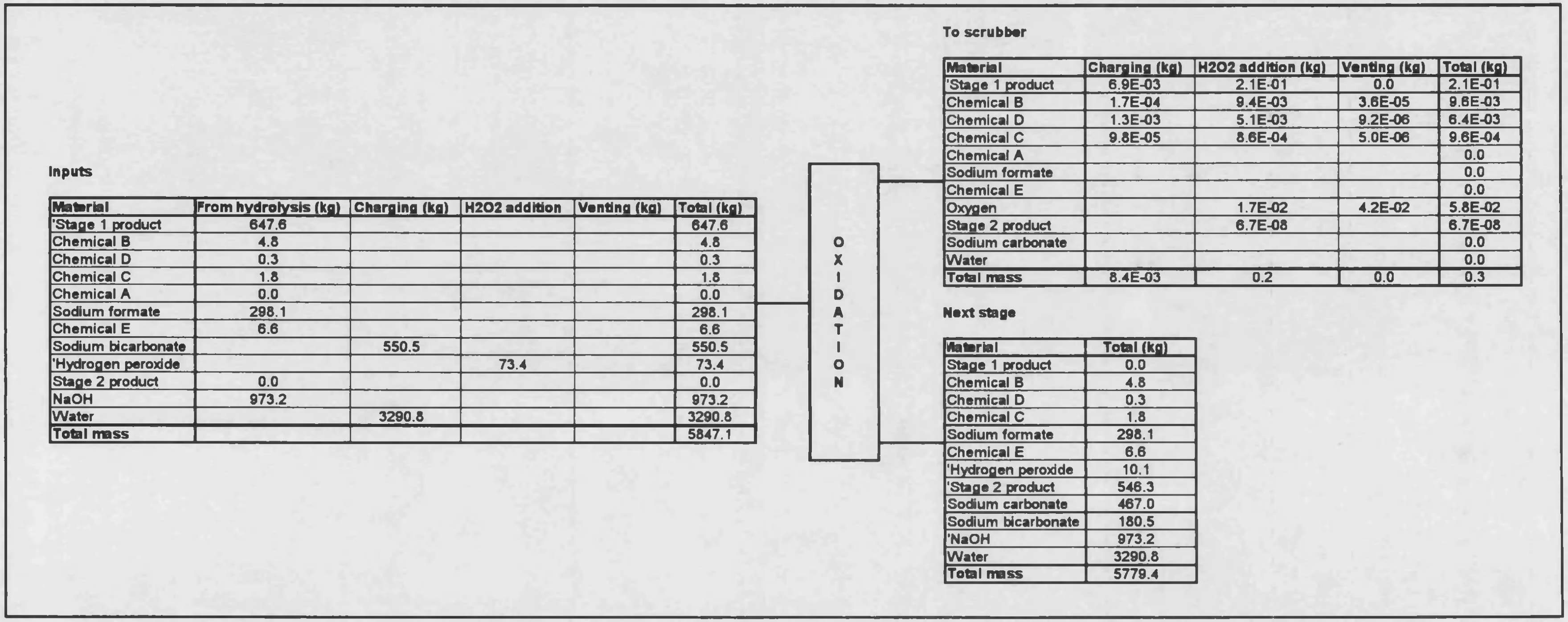
The emissions during this operation are the vents from each of the three steps. The emissions from this stage of the process are mainly organics and organic sulphurous compounds which are passed through the scrubber. The mass balance for stage 2 is shown in Figure 7.3

Stage 3: Benzoylation

The benzoylation reaction is carries out between the stage 2 product and benzoyl chloride in stage 3. This is a four step stage where the products from oxidation are then mixed with a recycled toluene stream. The four steps are:

- charging,
- the addition of benzoyl chloride and toluene,
- heating, and
- agitation.

This transfers the stage 2 product from the water (aqueous phase) to the toluene (organic phase). The benzoyl chloride [$C_6H_5(COCl)$] is added under defined (but confidential) conditions and reacts with the stage 2 product to produce Pepton (2,2'-dibenzaminodiphenyl disulphide) [$(C_6H_3S(NH)C)C_6H_5)_2$]. The benzoylation of the stage 2 product occurs by the following reaction:



Inputs

Material	From hydrolysis (kg)	Charging (kg)	H2O2 addition	Venting (kg)	Total (kg)
'Stage 1 product	647.6				647.6
Chemical B	4.8				4.8
Chemical D	0.3				0.3
Chemical C	1.8				1.8
Chemical A	0.0				0.0
Sodium formate	298.1				298.1
Chemical E	6.6				6.6
Sodium bicarbonate		550.5			550.5
'Hydrogen peroxide			73.4		73.4
Stage 2 product	0.0				0.0
NaOH	973.2				973.2
Water		3290.8			3290.8
Total mass					5847.1

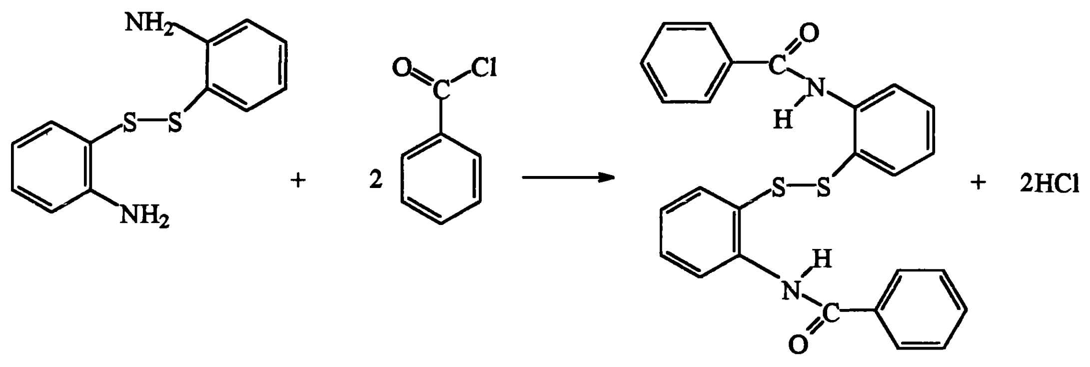
To scrubber

Material	Charging (kg)	H2O2 addition (kg)	Venting (kg)	Total (kg)
'Stage 1 product	6.9E-03	2.1E-01	0.0	2.1E-01
Chemical B	1.7E-04	9.4E-03	3.6E-05	9.6E-03
Chemical D	1.3E-03	5.1E-03	9.2E-06	6.4E-03
Chemical C	9.8E-05	8.6E-04	5.0E-06	9.6E-04
Chemical A				0.0
Sodium formate				0.0
Chemical E				0.0
Oxygen		1.7E-02	4.2E-02	5.8E-02
Stage 2 product		6.7E-08		6.7E-08
Sodium carbonate				0.0
Water				0.0
Total mass	8.4E-03	0.2	0.0	0.3

Next stage

Material	Total (kg)
Stage 1 product	0.0
Chemical B	4.8
Chemical D	0.3
Chemical C	1.8
Sodium formate	298.1
Chemical E	6.6
'Hydrogen peroxide	10.1
'Stage 2 product	546.3
Sodium carbonate	467.0
Sodium bicarbonate	180.5
'NaOH	973.2
Water	3290.8
Total mass	5779.4

Figure 7.3: Oxidation mass balance



Stage 2 product   Benzoyl chloride   Pepton   Hydrochloric acid

The hydrochloric acid formed during this reaction is neutralised via the following reaction by the sodium carbonate which is formed as a by-product of the oxidation reaction:

$$2HCl + Na_2CO_3 \longrightarrow 2NaCl + CO_2 + H_2O$$

Chemicals B and C, originating as contaminants in the benzothiazole feed, also react with the benzoyl chloride to form Chemicals F and G respectively.

The carbon dioxide released during the neutralisation reaction is saturated with toluene and is vented to atmosphere via a condenser and a glycol cooler. The sodium salts are dissolved in the aqueous stream together with the excess Pepton and soluble by-products. A small amount of toluene is also dissolved. Displaced vapours containing Chemicals B, C and D are vented during various raw materials charging steps.

Stage 4: Distillation

Toluene is distilled from the Pepton product in stage 4. The Pepton is then reslurried in water. The toluene is removed by azeotropic steam distillation at atmospheric pressure. The distilled toluene and water are condensed and seperated in a decanter. The toluene is returned to a storage tank. The water is sent back to the distillation vessel to reslurry the product.

Stage 5: Product preparation

In stage 5, the Pepton is filtered, vacuum dried, milled and sieved in preparation for packing and sale.

7.1.2 Mass balance

The overall mass balance calculated by Houghton (1998) is shown in Figure 7.4. This overall mass balance has been used to assess the environmental impact of the Pepton process and to compare different processes. Details are given in Chapter 9.

7.1.3 Emissions summary

The gaseous and aqueous emissions arising from the Pepton process are summarised in Table 7.1. No solid emissions, with the exception of packaging, arise directly from the process.

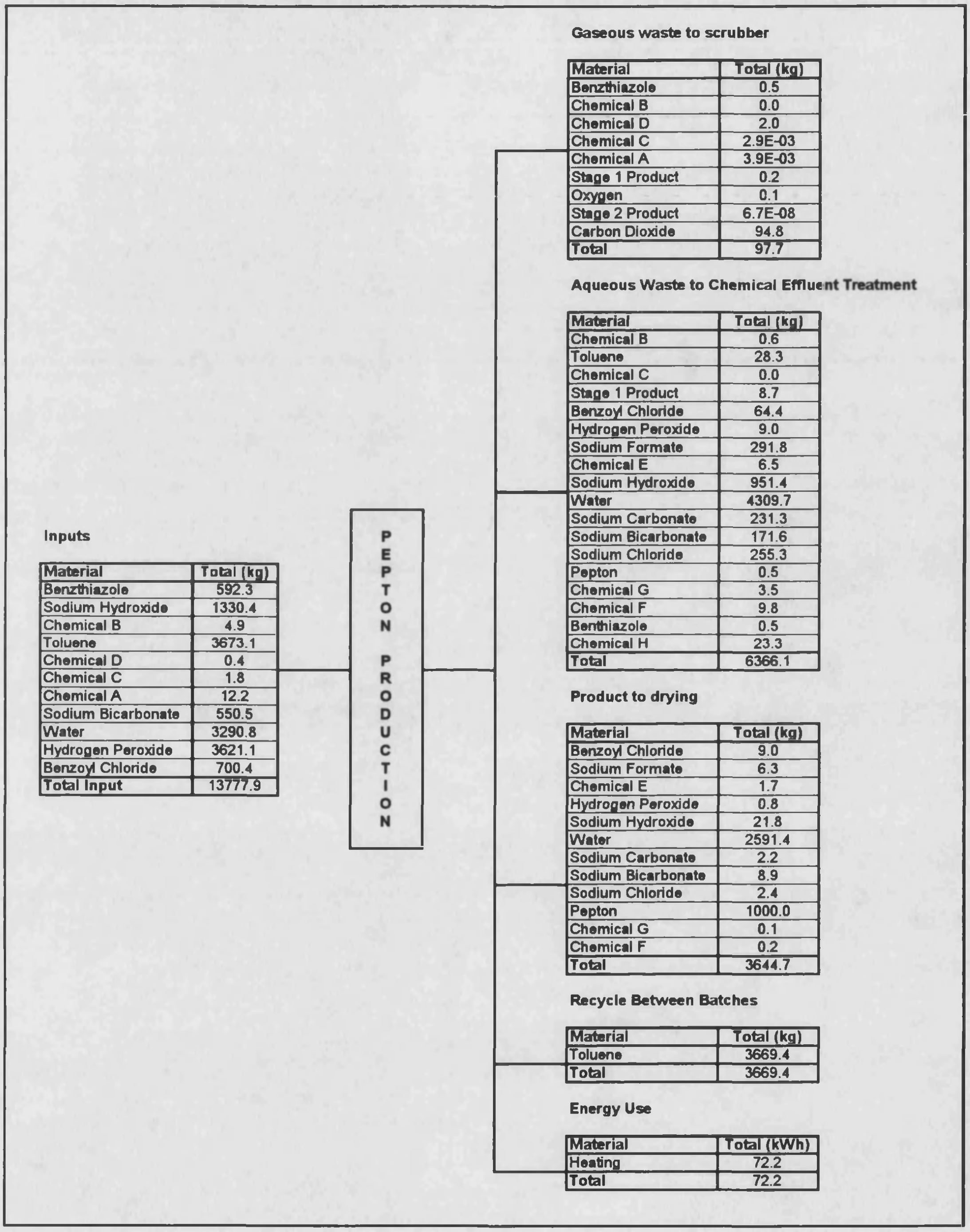
Table 7.1: Pepton emission summary

	Mass of gaseous emissions (kg)/1000kg product	Mass of aqueous emissions (kg)/1000kg product
Hydrolysis	0.61	8.86
Oxidation	0.29	0.00
Benzoylation	96.7	5290
Distillation	0.00	2620

The main emissions from the process are water and sodium salts from the benzoylation and distillation phases. The releases to air are dominated by the carbon dioxide produced in the benzoylation stage. Thus the main emissions are identified but the question arises as to whether they are the main areas of concern with regard to environmental impact. This matter will be discussed in Chapter 9.

7.2 Fisons - Sodium cromoglycate process

Fisons plc, a multinational chemical company, operates a batch process for the production of sodium cromoglycate (SCG) which is an active ingredient of the non-steroidal, anti-inflammatory drug Intal. The process includes the preparation of SCG, the recovery of solvents, the site steam raising plant and the effluent treatment plant.



Inputs

Material	Total (kg)
Benzthiazole	592.3
Sodium Hydroxide	1330.4
Chemical B	4.9
Toluene	3673.1
Chemical D	0.4
Chemical C	1.8
Chemical A	12.2
Sodium Bicarbonate	550.5
Water	3290.8
Hydrogen Peroxide	3621.1
Benzoyl Chloride	700.4
Total Input	13777.9

Gaseous waste to scrubber

Material	Total (kg)
Benzthiazole	0.5
Chemical B	0.0
Chemical D	2.0
Chemical C	2.9E-03
Chemical A	3.9E-03
Stage 1 Product	0.2
Oxygen	0.1
Stage 2 Product	6.7E-08
Carbon Dioxide	94.8
Total	97.7

Aqueous Waste to Chemical Effluent Treatment

Material	Total (kg)
Chemical B	0.6
Toluene	28.3
Chemical C	0.0
Stage 1 Product	8.7
Benzoyl Chloride	64.4
Hydrogen Peroxide	9.0
Sodium Formate	291.8
Chemical E	6.5
Sodium Hydroxide	951.4
Water	4309.7
Sodium Carbonate	231.3
Sodium Bicarbonate	171.6
Sodium Chloride	255.3
Pepton	0.5
Chemical G	3.5
Chemical F	9.8
Benthiazole	0.5
Chemical H	23.3
Total	6366.1

Product to drying

Material	Total (kg)
Benzoyl Chloride	9.0
Sodium Formate	6.3
Chemical E	1.7
Hydrogen Peroxide	0.8
Sodium Hydroxide	21.8
Water	2591.4
Sodium Carbonate	2.2
Sodium Bicarbonate	8.9
Sodium Chloride	2.4
Pepton	1000.0
Chemical G	0.1
Chemical F	0.2
Total	3644.7

Recycle Between Batches

Material	Total (kg)
Toluene	3669.4
Total	3669.4

Energy Use

Material	Total (kWh)
Heating	72.2
Total	72.2

Figure 7.4: Pepton process mass balance

The process can be operated 24 hour/day throughout the year to produce up to 60 tonnes/year of SCG. An outline description of the process is given in this section.

Fisons propose to modify the process to reduce its environmental impact. In Sections 7.2.1 and 7.2.2 the mass balances of the eight stages of the existing and proposed new plants are detailed. This data will be used in Chapter 8 to demonstrate the use of the EPPT to identify opportunities to minimise environmental impact and in Chapter 9 in a comparison of different processes.

7.2.1 Process details and stage mass balances

Sodium cromoglycate is manufactured in an eight stage process (HMIP, 1994b). Figure 7.5 gives and outline of these stages.

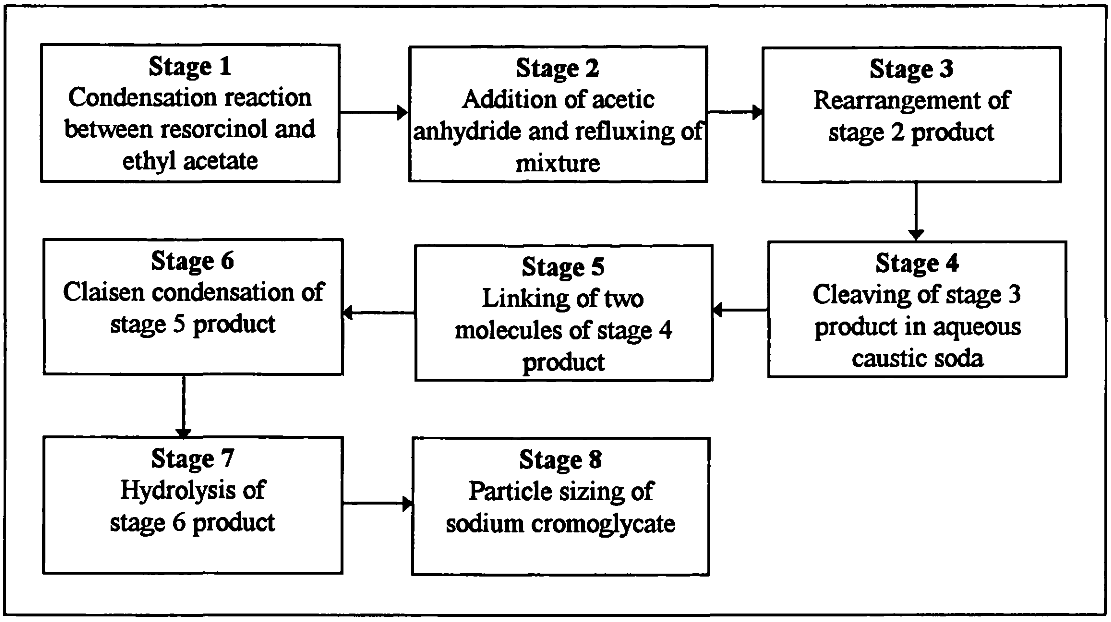


Figure 7.5: Eight stages in Fison's sodium cromoglycate process

This section describes and gives a mass balance for each stage. The data for the mass balances have been obtained from the IPC authorisation and accompanying application. The mass balance has been derived based on annual emission/production rates and has been normalised in both the existing and proposed new plants to a production rate of 1000kg of sodium cromoglycate.

Stage 1: Condensation reaction between resorcinol and ethyl acetoacetate

In stage 1, the condensation reaction between ethyl acetoacetate ($CH_3COCH_2CO_2C_2H_5$) and resorcinol ($C_6H_4(OH)_2$) is carried out to produce 7-hydroxy coumarin (stage 1 product). Sulphuric acid is used as a catalyst. The mixture is heated to effect the condensation reaction and ethanol is formed as a by-product. This ethanol is removed by vacuum distillation. The 7-hydroxy coumarin is not isolated at the end of stage 1 but is reacted directly in stage 2.

Stage 2: Acetic anhydride is added and the mixture refluxed

Acetic anhydride is added to the stage 1 vessel to start the stage 2 reaction. This produces 7-acetoxy coumarin, the stage 2 product. The reaction mixture is refluxed and the resulting molten reaction mass quenched with water. The stage 2 mixture is recrystallised by charging industrial methylated spirits (IMS). After refluxing for 1 hour the solution is cooled, centrifuged and dried. The combined mass balance for stages 1 and is shown in Table 7.2.

Table 7.2: Mass balance for stages 1 and 2

				Effluent to				
Stage 1/2	In	Product	Recovered	Water	Air	Offsite	Land	Total out
Resorcinol	4.29×10^{2}			0.00				0.00
Ethyl acetoacetate	5.84×10^{2}			7.66×10^{1}				7.66×10^{1}
Sulphuric acid	7.50×10^{-1}			7.50×10^{-1}				7.50×10^{-1}
Acetic anhydride	8.71×10^{2}				0.03			3.00×10^{-2}
IMS	4.78×10^{3}		4.78×10^{3}		1.02			4.78×10^{3}
Water	9.79×10^{3}			9.77×10^{3}				9.77×10^{3}
Ethanol				1.79×10^{2}				1.79×10^{2}
Acetic acid				7.89×10^{2}	1.07			7.90×10^{2}
Stage 2 product		8.52×10^{2}						8.52×10^{2}
Total	1.65×10^{4}	8.52×10^{2}	4.78×10^{3}	1.08×10^{4}	2.12	0.00	0.00	1.64×10^{4}

Stage 3: Rearrangement of stage 2 product

The stage 2 product undergoes a rearrangement reaction by fusing with aluminium and sodium chlorides. The fused mass is quenched by water and hydrogen chloride is evolved. The remaining hot slurry is filtered. The stage 3 product, 7-hydroxy-8-acetyl coumarin, is isolated under acidic conditions to remove the aluminium salts. The mass balance for stage 3 is shown in Table 7.3.

Table 7.3: Mass balance for stage 3

				Effluent to				Total out
Stage 3	In	Product	Recovered	Water	Air	Offsite	Land	
Stage 2 product	8.51×10^2							0.00
Aluminium chloride	2.73×10^3					2.68×10^3		2.68×10^3
Sodium chloride	3.44×10^2					3.44×10^2		3.44×10^2
Hydrochloric acid	3.86×10^2			3.86×10^2				3.86×10^2
Water	5.51×10^4	3.27×10^3		4.09×10^4		1.09×10^4		5.51×10^4
HCl	0.00			3.53×10^1	0.03			3.53×10^1
Al salts	0.00					2.58×10^1		2.58×10^1
Stage 3 product	0.00	8.52×10^2						8.52×10^2
Total	5.94×10^4	4.13×10^3	0.00	4.13×10^4	0.03	1.40×10^4	0.00	5.94×10^4

Stage 4: The stage 3 product is cleaved in aqueous caustic soda

The stage 3 product is cleaved in aqueous caustic soda to produce the stage 4 product, 2,6-dihydroxyacetophenone. The reaction mass is cooled and acidified to precipitate the stage 4 product which is then centrifuged and dried. Acetone is evolved. The mass balance for stage 4 is shown in Table 7.4.

Table 7.4: Mass balance for stage 4

				Effluent to				Total out
Stage 4	In	Product	Rec	Water	Air	Offsite	Land	
Stage 3 product	8.51×10^2							0.00
Sodium hydroxide	1.74×10^3							0.00
Sodium metabisulphate	1.17			1.17				1.17
Hydrochloric acid	2.34×10^3			1.55×10^3				1.55×10^3
Water	8.52×10^3	1.54×10^2		9.48×10^3				9.63×10^3
Acetone				2.26×10^2	2.00×10^{-2}			2.26×10^2
Carbon dioxide					1.72×10^2			1.72×10^2
Sodium chloride				1.27×10^3				1.27×10^3
Stage 4 product		5.94×10^2						5.94×10^2
Total	1.34×10^4	7.48×10^2	0.00	1.25×10^5	1.72×10^2	0.00	0.00	1.34×10^5

Stage 5: Two molecules of Stage 4 product are linked

Stage 4 intermediate is refluxed with methyl isobutyl ketone (MIBK) to remove water. Sodium carbonate, TDA-1 (catalyst) and epichlorohydrin are added and the mixture refluxed. When the reaction is complete the MIBK is distilled off causing the stage 5 product to precipitate. The stage 5 product is purified by reslurrying in IMS, centrifuging, washing and drying. MIBK is used as a solvent to prevent decomposition of the intermediates and enhance the yield of the reaction. The mass balance for stage 5 is shown in Table 7.5.

Table 7.5: Mass balance for stage 5

				Effluent to				Total
Stage 5	In	Product	Recovered	Water	Air	Offsite	Land	out
Stage 4 product	$5.93\text{x}10^2$							0.00
Epichlorohydrin	$1.81\text{x}10^2$			$9.90\text{x}10^{-1}$				$9.90\text{x}10^{-1}$
MIBK	$7.25\text{x}10^2$		$7.25\text{x}10^2$					$7.25\text{x}10^2$
Sodium carbonate	$1.15\text{x}10^2$			$1.14\text{x}10^1$				$1.14\text{x}10^1$
Carbon dioxide	0.00				$4.29\text{x}10^1$			$4.29\text{x}10^1$
TDA-1	2.97			2.97				2.97
IMS	$7.66\text{x}10^3$		$7.65\text{x}10^3$		9.27			$7.66\text{x}10^3$
Water	$5.55\text{x}10^3$			$5.57\text{x}10^3$				$5.57\text{x}10^3$
Sodium chloride				$1.14\text{x}10^2$				$1.14\text{x}10^2$
Stage 5 product		$7.03\text{x}10^2$						$7.03\text{x}10^2$
Total	$1.48\text{x}10^4$	$7.03\text{x}10^2$	$8.38\text{x}10^3$	$5.70\text{x}10^3$	$5.22\text{x}10^1$	0.00	0.00	$1.48\text{x}10^4$

Stage 6: Stage 5 product undergoes a Claisen condensation reaction

Diethyl oxalate is added to the stage 5 product to produce the Claisen condensation reaction using sodium ethoxide as a base. The sodium ethoxide is prepared by reacting dry ethanol with sodium metal. When the reaction is complete the reaction mass is extracted with chloroform and hydrochloric acid. The chloroform liquors are filtered and washed before being distilled to recover chloroform. The stage 6 product separates during distillation. The slurry is cooled, filtered, washed with IMS and dried. The mass balance for stage 6 is shown in Table 7.6.

Table 7.6: Mass balance for stage 6

				Effluent to				Total
Stage 6	In	Product	Recovered	Water	Air	Offsite	Land	out
Stage 5 product	7.03x10^{2}							0.00
Sodium metal	2.23x10^{2}							0.00
Hydrogen	0.00				9.68			9.68
Ethanol	4.31x10^{3}		2.71x10^{3}	1.76x10^{3}	1.66x10^{1}			4.49x10^{3}
Diethyl oxalate	1.65x10^{3}	1.56x10^{1}		1.06x10^{3}	0.00			1.06x10^{3}
Chloroform	5.77x10^{3}		5.36x10^{3}		4.11x10^{2}			5.77x10^{3}
Water	1.21x10^{4}			1.21x10^{4}				1.21x10^{4}
Hydrochloric acid	3.81x10^{2}							0.00
Sodium hydroxide	1.81x10^{2}			1.50x10^{2}				1.50x10^{2}
Sodium chloride				6.10x10^{2}				6.10x10^{2}
IMS	5.21x10^{3}		4.89x10^{3}		3.13x10^{2}			5.21x10^{3}
Stage 6 product		1.02x10^{3}						1.02x10^{3}
Total	3.05x10^{4}	1.04x10^{3}	1.29x10^{4}	1.57x10^{4}	7.50x10^{2}	0.00	0.00	3.04x10^{4}

Stage 7: Hydrolysis of stage 6 product

The stage 6 product is hydrolysed with caustic soda producing the stage 7 product, sodium cromoglycate. After the reaction is complete the reaction mass is filtered and clarified. The mass balance for stage 7 is shown in Table 7.7.

Table 7.7: Mass balance for stage 7

				Effluent to				Total
Stage 7	In	Product	Recovered	Water	Air	Offsite	Land	out
Stage 6 product	1.02x10^{3}							0.00
Diethyl oxalate	1.56x10^{1}							0.00
IMS	6.90x10^{3}		6.51x10^{3}		3.98x10^{2}			6.90x10^{3}
Water	3.15x10^{3}			3.16x10^{3}				3.16x10^{3}
Sodium hydroxide	1.64x10^{2}			0.00				0.00
Carbon	7.24x10^{1}						7.24x10^{1}	7.24x10^{1}
Ethanol	0.00		1.78x10^{2}		1.09x10^{1}			1.89x10^{2}
Sodium oxalate	0.00				1.43x10^{1}			1.43x10^{1}
Stage 7 product		1.00x10^{3}						1.00x10^{3}
Total	1.13x10^{4}	1.00x10^{3}	6.68x10^{3}	3.16x10^{3}	4.23x10^{2}	0.00	7.24x10^{1}	1.13x10^{4}

Stage 8: Sodium cromoglycate particle sizing

The sodium cromoglycate derived from stage 7 has a high level of purity. However certain pharmaceutical formulations require drug substances to be in a specific form with regard to particle size. This is achieved by recrystallisation of sodium cromoglycate crystals from IMS/water solutions under controlled conditions. The final crystals are isolated, dried, milled and packaged. The mass balance for stage 8 is shown in Table 7.8.

Table 7.8: Mass balance for stage 8

Stage 8	In	Product	Recovered	Effluent to Water	Air	Offsite	Land	Total out
Stage 7 product	1.00×10^3							0.00
IMS	1.38×10^4		1.18×10^4		2.08×10^3			1.38×10^4
Water	3.34×10^3			3.22×10^3	1.11×10^2			3.33×10^3
Stage 8 product		1.00×10^3						1.00×10^3
Total	1.81×10^4	1.00×10^3	1.18×10^4	3.22×10^3	2.19×10^3	0.00	0.00	1.81×10^4

The SCG process makes extensive use of organic solvents such as IMS, chloroform and MIBK. These are recovered, cleaned and reused wherever possible.

7.2.2 Proposed new plant mass balances

Fisons have proposed that the existing stages 5 to 8 be replaced by a new plant. The new plant has been designed 'to BATNEEC to prevent and mitigate releases to the environment', and 'adopts BPEO in arriving at the techniques for the disposal of wastes generated by the process' (HMIP AL4716). These changes enable an increase of 33.3% in the production capacity of sodium cromoglycate process from 60 to 80 tonnes per year. The chemistry of the process remains the same. However the plant will include the latest monitoring and control technology plus improved abatement for releases to air, notably chilled glycol condensers, carbon adsorption, nitrogen blanketing and conservation vents on storage tanks. Mass balances for each stage of the new process are given in Tables 7.9-7.16. Mass balances for Stages 1 to 4 have been included as an increase in Stage 4 product is required for the new Stage 5.

Table 7.9: Mass balance of Stages 1 and 2 of proposed new plant

				Effluent to				Total
Stage 1/2	In	Product	Recovered	Water	Air	Offsite	Land	out
Resorcinol	4.99x10^{2}			0.00				0.00
Ethyl acetoacetate	6.79x10^{2}			8.90x10^{1}				8.90x10^{1}
Sulphuric acid	8.70x10^{-1}			8.70x10^{-1}				8.70x10^{-1}
Acetic anhydride	1.01x10^{3}				3.00x10^{-2}			3.00x10^{-2}
IMS	5.56x10^{3}		5.56x10^{3}		1.19			5.56x10^{3}
Water	1.14x10^{4}			1.14x10^{4}				1.14x10^{4}
Ethanol				2.09x10^{2}				2.09x10^{2}
Acetic acid				9.18x10^{2}	1.24			9.19x10^{2}
Stage 2 product		9.90x10^{2}						9.90x10^{2}
Total	1.91x10^{4}	9.90x10^{2}	5.56x10^{3}	1.26x10^{4}	2.47	0.00	0.00	1.91x10^{4}

Table 7.10: Mass balance of Stage 3 of the proposed new plant

				Effluent to				Total
Stage 3	In	Product	Recovered	Water	Air	Offsite	Land	out
Stage 2 product	9.90x10^{2}							0.00
Aluminium chloride	3.17x10^{3}					3.12x10^{3}		3.12x10^{3}
Sodium chloride	4.00x10^{2}					4.00x10^{2}		4.00x10^{2}
Hydrochloric acid	4.49x10^{2}			4.49x10^{2}				4.49x10^{2}
Water	6.41x10^{4}	3.80x10^{3}		4.76x10^{4}		1.27x10^{4}		6.41x10^{4}
Hydrogen chloride	0.00			4.10x10^{1}	4.0x10^{-2}			4.10x10^{1}
Aluminium salts	0.00					2.99x10^{1}		2.99x10^{1}
Stage 3 product	0.00	9.90x10^{2}						9.90x10^{2}
Total	6.91x10^{4}	4.79x10^{3}	0.00	4.81x10^{4}	4.0x10^{-2}	1.62x10^{4}	0.00	6.91x10^{4}

Table 7.11: Mass balance of stage 4 of the proposed new plant

				Effluent to				Total
Stage 4	In	Product	Recovered	Water	Air	Offsite	Land	out
Stage 3 product	9.90x10^{2}							0.00
Sodium hydroxide	2.02x10^{3}							0.00
Sodium metabisulphate	1.36			1.36				1.36
Hydrochloric acid	2.72x10^{3}			1.80x10^{3}				1.80x10^{3}
Water	9.90x10^{3}	1.79x10^{2}		1.10x10^{4}				1.12x10^{4}
Acetone				2.63x10^{2}	3.0x10^{-2}			2.63x10^{2}
Carbon dioxide					2.0x10^{2}			2.00x10^{2}
Sodium chloride				1.48x10^{3}				1.48x10^{3}
Stage 4 Product		6.90x10^{2}						6.90x10^{2}
Total	1.56x10^{4}	8.69x10^{2}	0.00	1.45x10^{4}	2.0x10^{2}	0.00	0.00	1.56x10^{4}

Table 7.12: Mass balance of stage 5 of the proposed new plant

				Effluent to				Total
Stage 5	In	Product	Recovered	Water	Air	Offsite	Land	out
Stage 4 product	6.90x10^{2}							0.00
Epichlorohydrin	2.10x10^{2}			5.30x10^{-1}				5.30x10^{-1}
MIBK	8.56x10^{2}		8.56x10^{2}					8.56x10^{2}
Sodium carbonate	1.33x10^{2}			1.29x10^{1}				1.29x10^{1}
Carbon dioxide	0.00				4.99x10^{1}			4.99x10^{1}
TDA-1	3.49			3.49				3.49
IMS	5.96x10^{3}		5.90x10^{3}	6.71x10^{1}	1.41			5.97x10^{3}
Water	6.74x10^{3}	1.09	1.93x10^{3}	4.80x10^{3}	2.13x10^{1}			6.75x10^{3}
Sodium chloride			1.12x10^{1}	1.22x10^{2}				1.33x10^{2}
Impurities	3.19x10^{2}			3.19x10^{2}				3.19x10^{2}
Stage 5 product		8.17x10^{2}						8.18x10^{2}
Total	1.49x10^{4}	8.18x10^{2}	8.70x10^{3}	5.33x10^{3}	7.26x10^{1}	0.00	0.00	1.49x10^{4}

Table 7.13: Mass balance of stage 6 of the proposed new plant

				Effluent to				Total
Stage 6	In	Product	Recovered	Water	Air	Offsite	Land	out
Stage 5 product	8.17x10^{2}							0.00
Sodium metal	2.59x10^{2}							0.00
Hydrogen	0.00				1.13x10^{1}			1.13x10^{1}
IMS	4.47x10^{3}	5.43x10^{1}	4.41x10^{3}	0.00	6.45			4.47x10^{3}
Ethanol	3.70x10^{3}	4.75x10^{1}	3.86x10^{3}	0.00	5.65			3.91x10^{3}
Diethyl oxalate	1.91x10^{3}	0.00		1.25x10^{3}				1.25x10^{3}
Chloroform	7.15x10^{3}		7.14x10^{3}		7.30x10^{-1}			7.14x10^{3}
Water	1.44x10^{4}	2.81x10^{1}	4.04x10^{3}	1.05x10^{4}				1.45x10^{4}
Hydrochloric acid	4.55x10^{2}							0.00
Sodium hydroxide	4.92x10^{1}			4.9x10^{-1}				4.90x10^{-1}
Sodium chloride	0.00			7.30x10^{2}				7.30x10^{2}
Stage 6 product	0.00	1.19x10^{3}						1.19x10^{3}
Total	3.32x10^{4}	1.32x10^{3}	1.94x10^{4}	1.25x10^{4}	2.41x10^{1}	0.00	0.00	3.32x10^{4}

Table 7.14: Mass balance of stage 7 of the proposed new plant

				Effluent to				Total
Stage 7	In	Product	Recovered	Water	Air	Offsite	Land	out
Stage 6 product	1.19x10^{3}	6.55x10^{1}	2.84	0.00				6.83x10^{1}
Diethyl oxalate	6.00x10^{-1}							0.00
IMS	8.49x10^{3}		8.42x10^{3}		4.34		6.59x10^{1}	8.49x10^{3}
Water	5.29x10^{3}	4.21x10^{1}	4.83x10^{3}	3.55x10^{2}			6.47x10^{1}	5.29x10^{3}
Sodium hydroxide	1.82x10^{2}			1.04x10^{1}				1.04x10^{1}
Carbon	1.35x10^{2}						1.35x10^{2}	1.35x10^{2}
Impurities	1.32x10^{1}	1.32x10^{1}						1.32x10^{1}
Ethanol	0.00		1.96x10^{2}		1.0x10^{-1}		1.53	1.97x10^{2}
Sodium oxalate	0.00						5.5x10^{-1}	5.5x10^{-1}
Stage 7 product	0.00	1.02x10^{3}	7.27x10^{1}					1.09x10^{3}
Total	1.53x10^{4}	1.14x10^{3}	1.35x10^{4}	3.65x10^{2}	4.44	0.00	2.67x10^{2}	1.53x10^{4}

Table 7.15: Mass balance of stage 8 of the proposed new plant

				Effluent to				Total
Stage 8	In	Product	Recovered	Water	Air	Offsite	Land	out
Stage 7 product	$1.02x10^3$							0.00
IMS	$1.82x10^4$		$1.82x10^4$		$1.81x10^1$			$1.82x10^4$
Water	$3.61x10^3$		$3.61x10^3$					$3.61x10^3$
Stage 8 product		$1.00x10^3$	$2.35x10^1$					$1.02x10^3$
Total	$2.28x10^4$	$1.00x10^3$	$2.18x10^4$	0.00	$1.81x10^1$	0.00	0.00	$2.28x10^4$

7.2.3 Emission summary

Table 7.17 gives a summary of the aqueous and gaseous emissions from each stage of the existing and proposed plants based on a production of 1000kg of sodium cromoglycate.

Table 7.17: Comparison of emissions from the existing and proposed new plant

		Mass of emissions		
Stage	Plant	Aqueous	Gaseous	Disposed of to land
1&2	Existing	$1.08x10^4$	2.12	0.00
	New	$1.26x10^4$	2.47	0.00
3	Existing	$4.13x10^4$	$3.00x10^{-2}$	0.00
	New	$4.81x10^4$	$4.00x10^{-2}$	0.00
4	Existing	$1.25x10^4$	$1.72x10^2$	0.00
	New	$1.45x10^4$	$2.00x10^2$	0.00
5	Existing	$5.70x10^3$	$5.22x10^1$	0.00
	New	$5.33x10^3$	$7.22x10^1$	0.00
6	Existing	$1.57x10^4$	$7.51x10^2$	0.00
	New	$1.25x10^4$	$2.41x10^1$	0.00
7	Existing	$3.15x10^3$	$4.23x10^2$	$7.24x10^1$
	New	$3.65x10^2$	4.44	$2.68x10^2$
8	Existing	$3.22x10^3$	$2.18x10^3$	0.00
	New	0.00	$1.81x10^1$	0.00

There are increases in the emissions of the new plant from stages 1 to 4 due to the increased input of stage 4 product into stage 5. There are however significant decreases in the mass of emissions to air from stages 6 to 8 due to the introduction of the nitrogen blanket and the carbon adsorption removing the organics. Water recovery accounts for the significant decrease in aqueous emissions in stages 7 and 8 of the proposed new plant. This decrease is seen despite the new process in stages 5 to 8 (where new technologies have been adopted) using more water as shown in Table 7.18: a comparison between water use in each plant.

Table 7.18: Water use in existing and proposed new sodium cromoglycate plants

Stage	Existing plant Mass of water used (kg)	Proposed new plant Mass of water used (kg)
1&2	9.79×10^3	1.14×10^4
3	5.51×10^4	6.41×10^4
4	8.51×10^3	9.90×10^3
5	5.55×10^3	6.74×10^3
6	1.20×10^4	1.44×10^4
7	3.15×10^3	5.29×10^3
8	3.33×10^3	3.61×10^3

However the new process has more emissions being disposed of to land than the existing process. These emission changes are discussed in more detail when evaluated by the EPPT in Chapter 8.

7.3 Associated Octel - Tetra ethyl lead and tetra methyl lead processes

Associated Octel has produced antiknock additives at Ellesmere Port since 1954. The principal components of Motor Fuel Antiknock Compounds (MFAKC) are tetra alkyl leads, specifically tetra ethyl lead and tetra methyl lead. The batch processes used to produce tetraethyl lead (TEL) and tetra methyl lead (TML) are described in this section. The plant has the capacity to produce 100,000 tonnes of MFAKC per year. TEL is produced in one of 26 autoclaves, each of which has its own batch distillation unit and a capacity of 550 kg. There are also 10 dual purpose autoclaves that can produce 600 kg of TEL or TML. The operation of all autoclaves is sequential on a 2 hr 40 min schedule. There is an ethyl chloride recovery plant, a methyl chloride recovery plant and an effluent treatment plant onsite. The following section gives a brief overview of the process (HMIP, 1994a).

7.3.1 Process details

The production of tetra alkyl leads involves reacting a lead/sodium alloy with the respective alkyl chloride and is carried out in a six stage process. TEL and TML are then blended in a seventh stage to form MFAKC. This is shown in Figure 7.6.

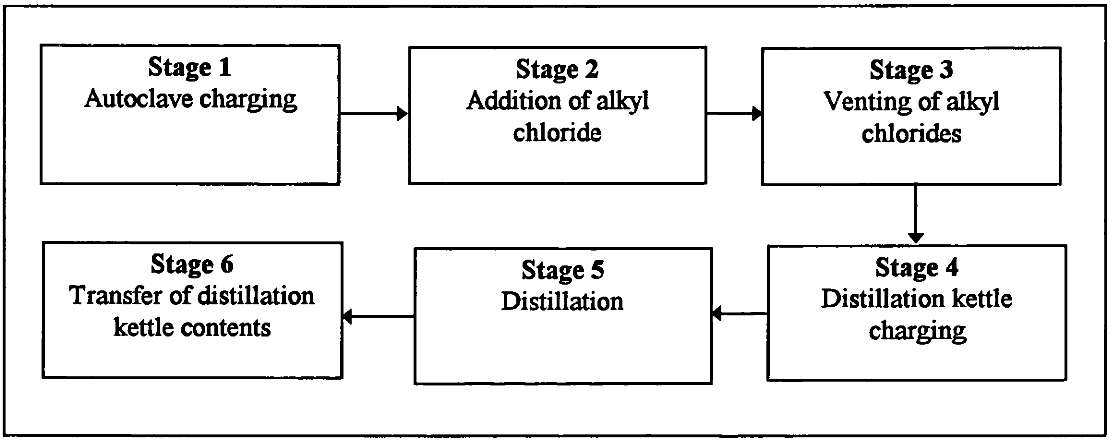


Figure 7.6: Six stages in Associated Octel's tetra alkyl lead processes

The flow diagrams for TEL and TML production are given in Figures 7.7 and 7.8 respectively. The stages in the production of TEL and TML are as follows:

Stage 1: Autoclave charging

The lead/sodium alloy is charged to the autoclave with graphite which acts as a lubricant. In the TEL process this charging displaces vapour from the previous batch containing TEL, butane, volatile organics and nitrogen. The vapours from the TML process are TML, ethane, volatile organics and nitrogen. Aluminium chloride is also added to the TML autoclave as a catalyst to increase the rate of reaction. The autoclave is then sealed.

Stage 2: Addition of alkyl chloride

The relevant alkyl chloride is added in excess to the sealed autoclave to improve the reaction control. The reactions are:

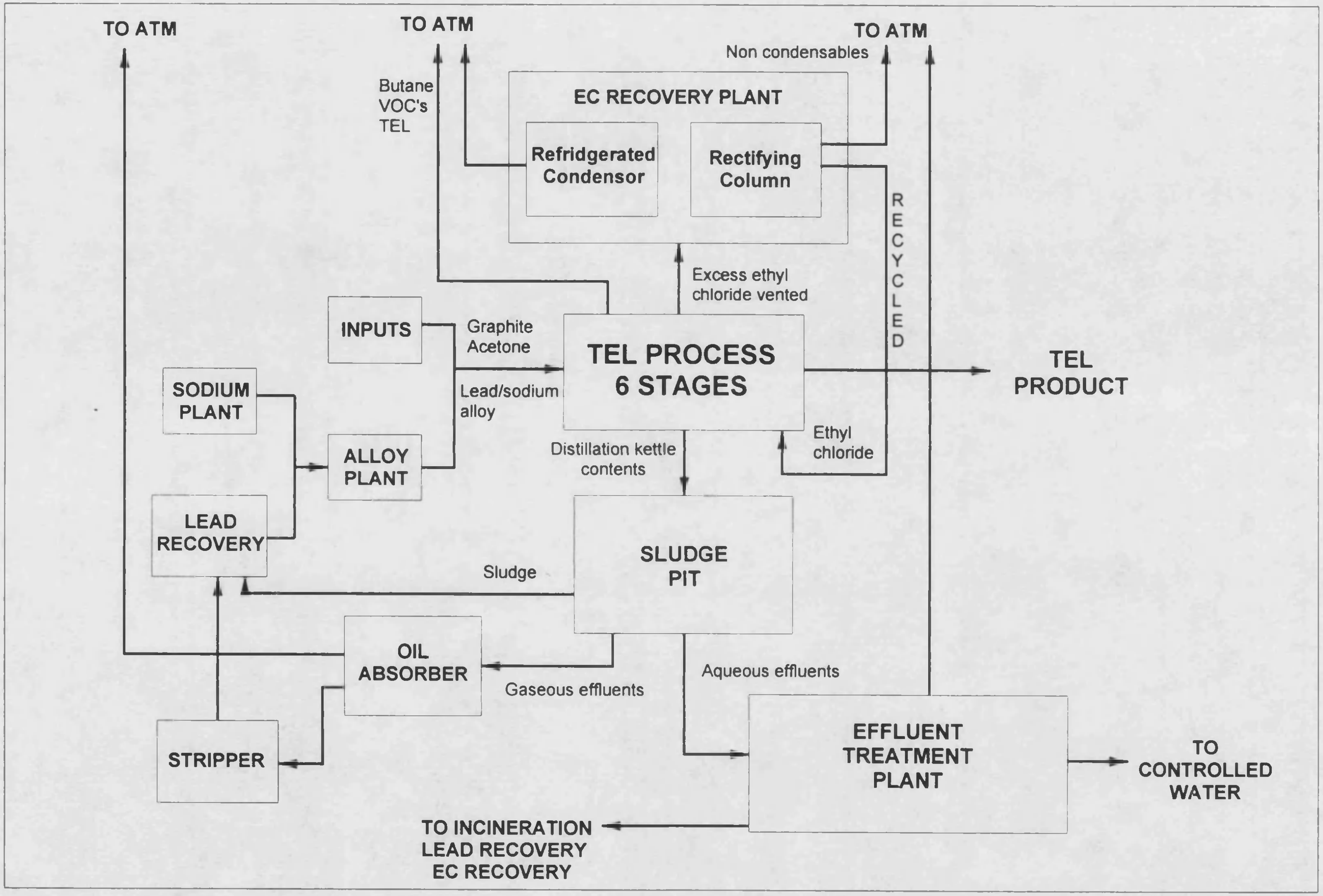


Figure 7.7: Flow diagram of Associated Octel's tetra ethyl lead process

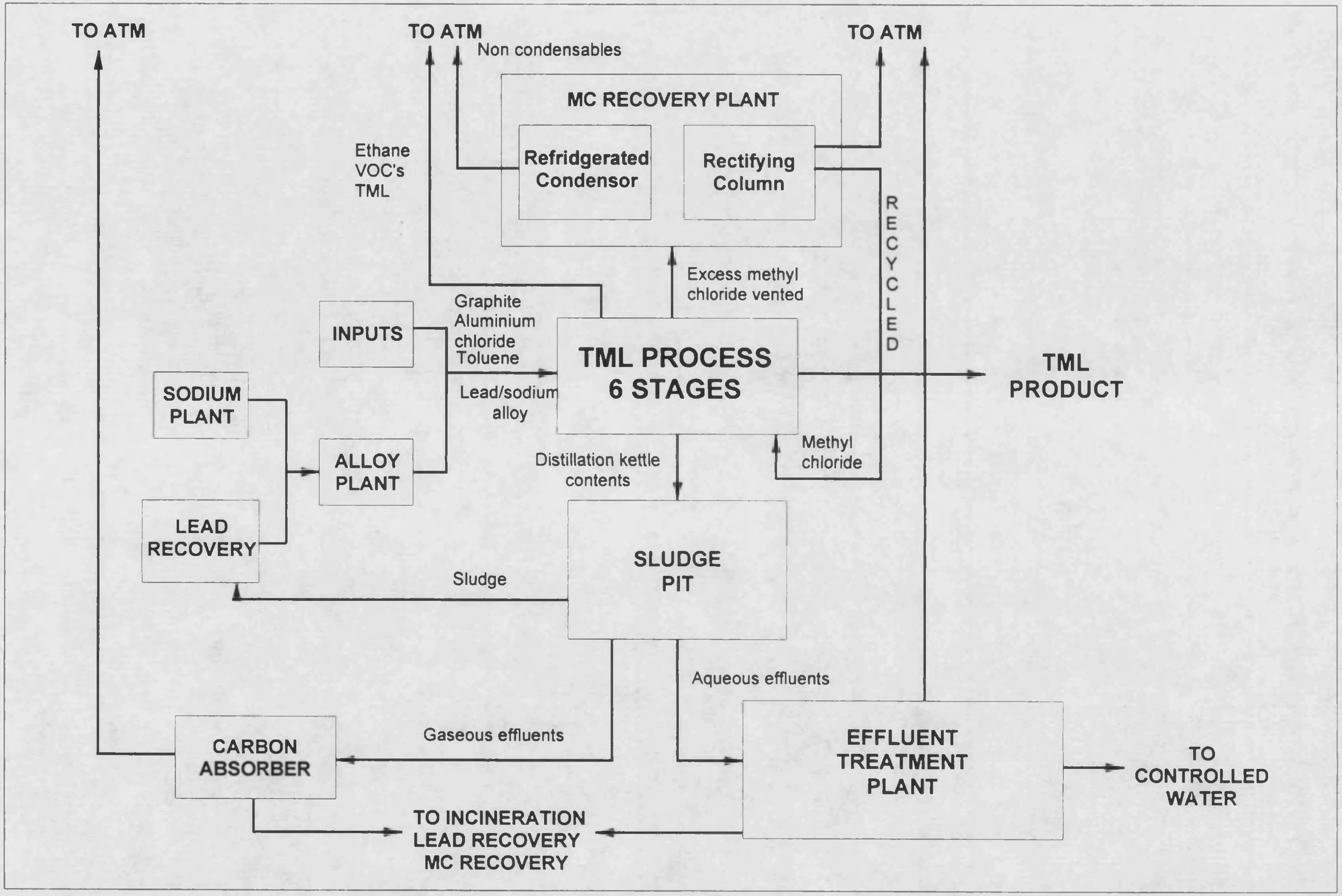


Figure 7.8: Flow diagram of Associated Octel's tetra methyl lead process

TML: $Pb + 4Na + 4CH_3Cl \rightarrow (CH_3)_4Pb + 4NaCl$

TEL: $Pb + 4Na + 4C_2H_5Cl \rightarrow (C_2H_5)_4Pb + 4NaCl$

The following side reactions also occur:

$$2CH_3Cl + 2Na \rightarrow C_2H_6 + 2NaCl$$

$$2C_2H_5Cl + 2Na \rightarrow C_4H_{10} + 2NaCl$$

Acetone is added to the TEL production to promote a stable reaction. Toluene is added to avoid the explosive decomposition of TML in its pure state. The gases produced in these reactions are passed via condensers to the main stack. The reactants are then 'cooked' for 90 minutes.

Stage 3: Venting of alkyl chlorides

After the reaction is complete the excess ethyl and methyl chloride are vented to a recovery plant. The non-condensable components are vented directly to the main stack. The recovered materials are recycled and used in the next batch.

Stage 4: Distillation kettle charging

The contents of the autoclave are transferred to a distillation kettle which is already charged with water, still aids, sodium thiosulphate and ferrous sulphate. Sodium oleate is also added as a wetting agent. The vents from this operation pass into the main stack.

Stage 5: Distillation

The contents of the distillation kettle are initially prevented from condensing to remove residual alkyl chloride which is sent to the recovery unit. Cold water is then fed to the condenser to condense the tetra alkyl lead and water vapours. The condensate is sent to a phase separator.

Stage 6: Transfer of distillation kettle contents

After stage 5 is complete the distillation kettle contents are sent to the sludge pits. The kettle contents include dissolved organic and inorganic lead salts, sodium thiosulphate, sodium hydroxide, sodium chloride, ferrous sulphate, lead alkyl and particulate lead.

Stage 7: Blending

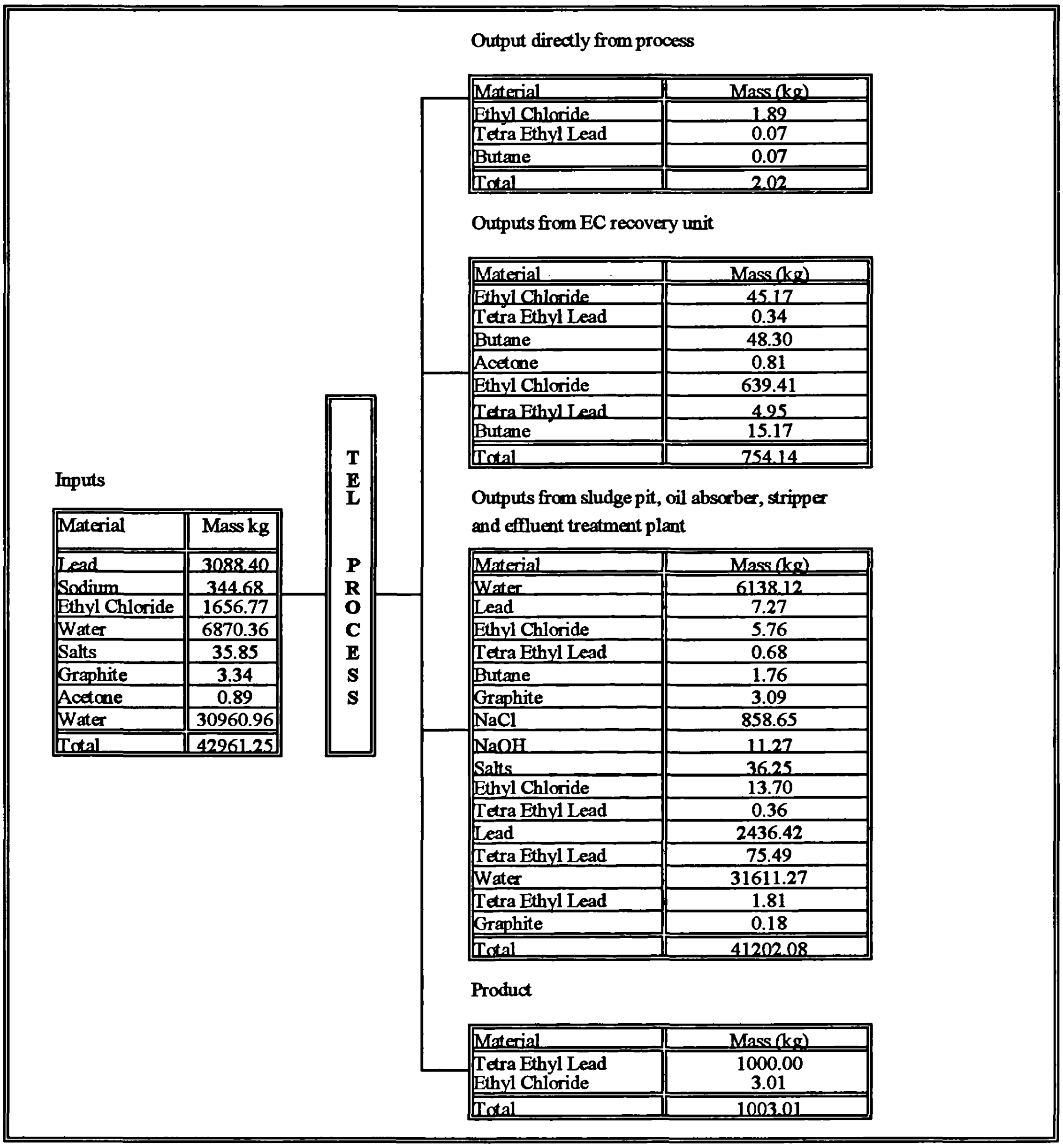
The tetra ethyl lead and tetra methyl lead are blended together with dibromoethane and dichloroethane to give final products.

Effluent treatment

The aqueous effluents from the process are stored in sludge pits and then transferred to the effluent treatment plant. Vapours from the TEL and TML sludge pits pass to the atmosphere via an oil absorber and a carbon adsorber respectively. The carbon from the adsorbers is burnt in the lead recovery furnaces. The liquid effluent is brought into contact with zinc where the trimethyl salts are converted to insoluble TML and inorganic lead which settles out. The sludge from this is burnt in the lead recovery furnaces.

7.3.2 Mass balances

The mass balances for the production of tetra ethyl lead (TEL) and tetra methyl lead (TML) given in the IPC application (HMIP, AK3919) are based on a production rate of 89,000te/yr. The mass balances that have been re-calculated for 1000kg of product are shown in Figures 7.9 and 7.10 for tetra ethyl lead production and tetra methyl lead respectively.



Inputs

Material	Mass kg
Lead	3088.40
Sodium	344.68
Ethyl Chloride	1656.77
Water	6870.36
Salts	35.85
Graphite	3.34
Acetone	0.89
Water	30960.96
Total	42961.25

Output directly from process

Material	Mass (kg)
Ethyl Chloride	1.89
Tetra Ethyl Lead	0.07
Butane	0.07
Total	2.02

Outputs from EC recovery unit

Material	Mass (kg)
Ethyl Chloride	45.17
Tetra Ethyl Lead	0.34
Butane	48.30
Acetone	0.81
Ethyl Chloride	639.41
Tetra Ethyl Lead	4.95
Butane	15.17
Total	754.14

Outputs from sludge pit, oil absorber, stripper and effluent treatment plant

Material	Mass (kg)
Water	6138.12
Lead	7.27
Ethyl Chloride	5.76
Tetra Ethyl Lead	0.68
Butane	1.76
Graphite	3.09
NaCl	858.65
NaOH	11.27
Salts	36.25
Ethyl Chloride	13.70
Tetra Ethyl Lead	0.36
Lead	2436.42
Tetra Ethyl Lead	75.49
Water	31611.27
Tetra Ethyl Lead	1.81
Graphite	0.18
Total	41202.08

Product

Material	Mass (kg)
Tetra Ethyl Lead	1000.00
Ethyl Chloride	3.01
Total	1003.01

Figure 7.9: Tetra ethyl lead mass balance

Inputs

Material	Mass (kg)
Lead	4006.88
Sodium	447.19
Methyl Chloride	2126.00
Water	8528.40
Salts	19.27
Graphite	12.82
Catalyst (AlCl3)	34.38
Toluene	269.17
Water	100268.92
Total	115713.02

TML PROCESS

Output directly from process

Material	Mass (kg)
Methyl Chloride	55.31
Tetra Methyl Lead	1.27
Toluene	0.32
Ethane	29.12
Total	86.00

Outputs from methyl chloride recovery unit

Material	Mass (kg)
Methyl Chloride	154.76
Tetra Methyl Lead	0.71
Ethane	10.40
Toluene	2.37
Methyl Chloride	890.85
Tetra Methyl Lead	62.94
Ethane	0.95
Toluene	13.72
Total	1136.71

Outputs from sludge pit, carbon absorber, and effluent treatment plant

Material	Mass (kg)
Water	107428.95
Lead	960.32
Lead	3125.25
Ethyl Chloride	0.95
Methyl Chloride	3.92
Methyl Chloride	59.34
Tetra Ethyl Lead	1.19
Tetra Methyl Lead	8.70
Tetra Methyl Lead	6.65
Tetra Methyl Lead	13.77
Tetra Methyl Lead	39.56
Toluene	3.05
Toluene	0.63
Toluene	3.44
Toluene	9.89
Ethane	3.32
Tri Alkyl Lead	0.67
DBE (Dibromoethane)	0.20
DCE (1,2 Dichloroethane)	0.40
Catalyst (AlCl3)	34.38
Graphite	48.22
Sodium Chloride	1436.35
Sodium Hydroxide	22.87
Salts	28.25
Flocculant (Acrylamide)	0.79
Total	113241.04

Product

Material	Mass (kg)
Tetra Methyl Lead	1000.00
Toluene	249.27
Total	1249.27

Figure 7.10: Tetra methyl lead mass balance

7.3.3 Emission summary

The main gaseous emissions from the TEL and TML processes are organics arising directly from the process and also from the alkyl chloride recovery units, the sludge pits and the associated operations. These include ethyl and methyl chlorides, tetra ethyl and methyl lead, butane, ethane and toluene.

Large proportions of the ethyl and methyl chloride are recovered together with the tetra ethyl and methyl lead, lead, ethane, butane and toluene. The remaining emissions are treated at the effluent treatment plant and include water, lead, ethyl and methyl chloride, tetra ethyl and methyl lead, ethane, graphite, sodium and aluminium salts and toluene.

7.4 Summary

This chapter has presented the mass balances for four processes. These mass balances are used in Chapters 8 and 9 to assess the environmental impact of each process. Detailed mass balances have been given for the Thomas Swan Pepton process, as these mass balances have been used in Chapter 8 to evaluate the environmental impact of process changes. Detailed stage mass balances are also given for Fisons sodium cromoglycate process. These mass balances have been used in Chapter 8 to demonstrate the use of the EPPT to identify opportunities to minimise environmental impact. Thomas Swan's Pepton process has also been used to demonstrate this aspect of the EPPT. The mass balances for Associated Octel's tetra alkyl lead processes have been used in Chapter 9, together with the mass balances for the Pepton and sodium cromoglycate processes to compare processes and determine their environmental performance.

8. Comparing process options

In previous chapters the EPPT chemical scores, the combination method for mass and chemical score, and the utilities evaluation have been established. In this chapter these aspects of the EPPT are used to evaluate process options developed for the Thomas Swan Pepton process case study. These aspects of the EPPT are also used to compare the changes made to Fisons sodium comoglycate process later in this Chapter.

The process options for Thomas Swan's Pepton process have been derived to provide a comparison between the use of utilities (and additional input chemicals) and the emission of chemicals to the environment. Five process options are considered in this chapter. Options 1 and 2 compare emissions released in the base case with the use of electrical energy. Options 3 and 4 compare the emissions released in the base case with the use of cooling water. The EPPT is then used to identify which part of the process has the highest environmental impact. Option 5 has been generated in order to reduce the environmental impact of the most polluting part of the process. In Option 5 comparison is made between the emissions released in the base case and the emissions arising from the generation of steam.

8.1 Electrical energy based options

Electrical energy can be used to reduce emissions from a chemical process. In Options 1 and 2 electrical energy is used to reduce the amount of gaseous emissions arising during the charging of a reaction vessel. Before discussing process options the base case of the charging operation needs to be described.

During charging, a vessel is filled with the materials which are to be reacted in the next step. In the current operating procedure the vessel is charged with materials at atmospheric pressure with the vessel vent open to relieve pressure. This operation results in gases and vapours being released to the atmosphere. This current operation has been taken as the base case. Two alternative options have been considered. These options are:

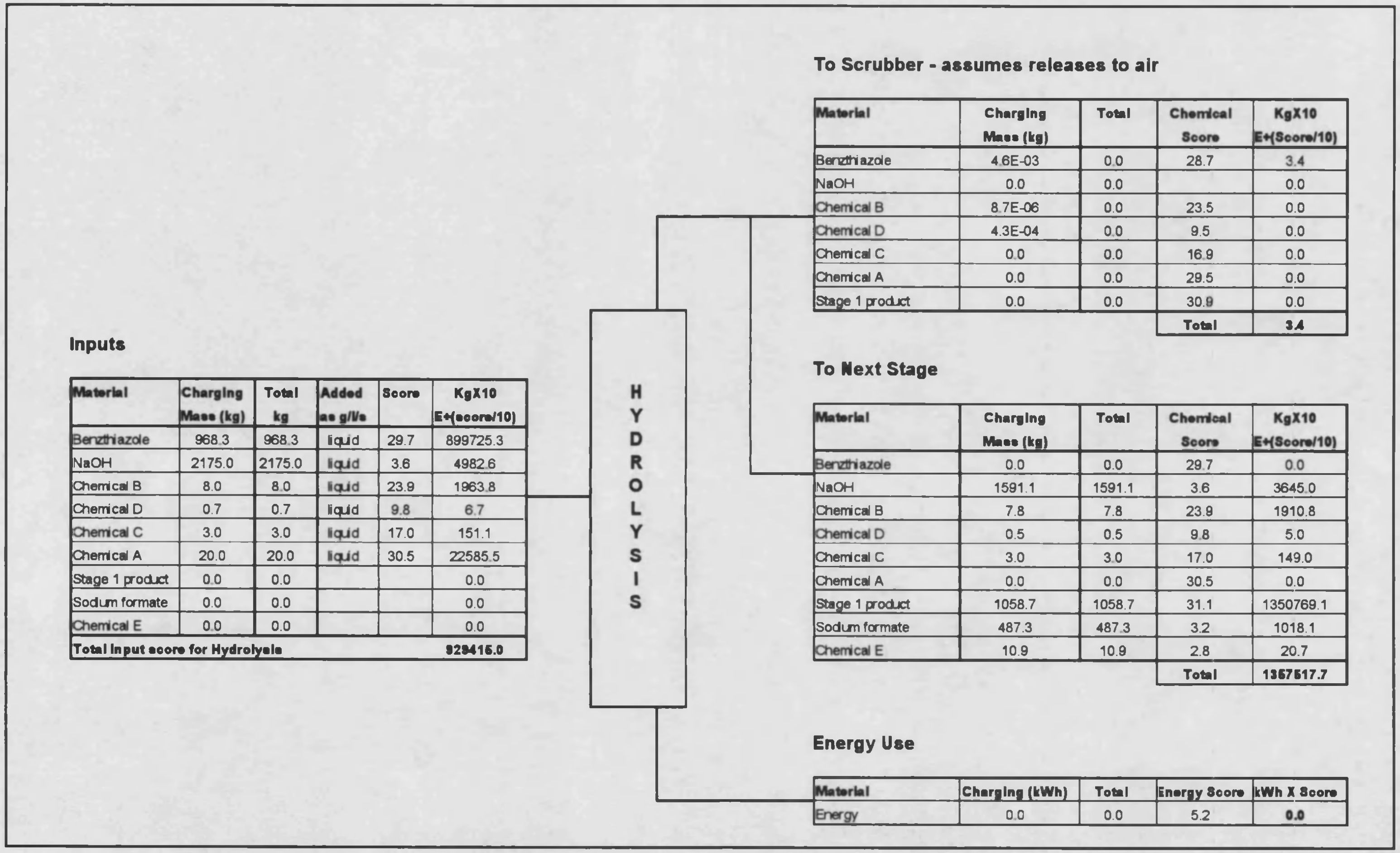
- Option 1: Pressurising the vessel during charging.
- Option 2: Cooling the feed during charging.

In Option 1 electrical energy is used to pump the chemical feed into the vessel. This counteracts the pressure rise which occurs when the vessel vent is closed. In Option 2 electrical energy is used to operate a refrigeration system to cool the feed stream. A cooled feed stream has a reduced amount of organics in the gaseous phase and hence reduces the potential for emission generation.

8.1.1 Option 1: Pressurising during charging

In Option 1 the vessel is charged with the vent closed. As the vessel is closed the pressure inside the vessel increases. This pressure increase requires the feed to be pumped into the vessel. The EPPT has been used to compare the difference between the environmental impact of the gaseous emissions in the base case and the environmental impact of the energy used in Option 1. From this comparison the option with the least environmental impact is identified.

Figures 8.1 and 8.2 show the inputs and outputs and the scores associated with the hydrolysis charging base case and Option 1. Table 8.1 summarises the differences in the EPPT emission scores for the base case and Option 1. The feed to the vessel and the output to the next stage are the same in both cases. Houghton (1998) calculated that 0.1kWh of electrical energy would be required to pump the feed into a closed vessel.



Inputs

Material	Charging Mass (kg)	Total kg	Added as g/l/s	Score	KgX10 E+(score/10)
Benzthiazole	968.3	968.3	liquid	29.7	899725.3
NaOH	2175.0	2175.0	liquid	3.6	4982.6
Chemical B	8.0	8.0	liquid	23.9	1963.8
Chemical D	0.7	0.7	liquid	9.8	6.7
Chemical C	3.0	3.0	liquid	17.0	151.1
Chemical A	20.0	20.0	liquid	30.5	22585.5
Stage 1 product	0.0	0.0			0.0
Sodium formate	0.0	0.0			0.0
Chemical E	0.0	0.0			0.0
Total input score for Hydrolysis					**929415.0**

To Scrubber - assumes releases to air

Material	Charging Mass (kg)	Total	Chemical Score	KgX10 E+(Score/10)
Benzthiazole	4.6E-03	0.0	28.7	3.4
NaOH	0.0	0.0		0.0
Chemical B	8.7E-06	0.0	23.5	0.0
Chemical D	4.3E-04	0.0	9.5	0.0
Chemical C	0.0	0.0	16.9	0.0
Chemical A	0.0	0.0	29.5	0.0
Stage 1 product	0.0	0.0	30.9	0.0
			Total	**3.4**

To Next Stage

Material	Charging Mass (kg)	Total	Chemical Score	KgX10 E+(Score/10)
Benzthiazole	0.0	0.0	29.7	0.0
NaOH	1591.1	1591.1	3.6	3645.0
Chemical B	7.8	7.8	23.9	1910.8
Chemical D	0.5	0.5	9.8	5.0
Chemical C	3.0	3.0	17.0	149.0
Chemical A	0.0	0.0	30.5	0.0
Stage 1 product	1058.7	1058.7	31.1	1350769.1
Sodium formate	487.3	487.3	3.2	1018.1
Chemical E	10.9	10.9	2.8	20.7
			Total	**1357517.7**

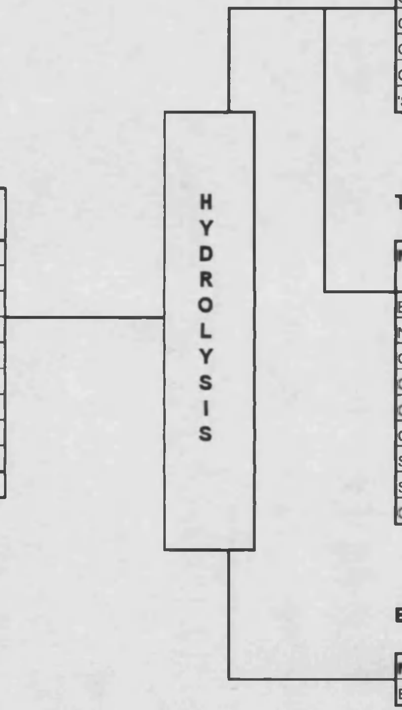
Energy Use

Material	Charging (kWh)	Total	Energy Score	kWh X Score
Energy	0.0	0.0	5.2	**0.0**

Figure 8.1: Thomas Swan Pepton process hydrolysis charging base case

Inputs

Material	Charging Mass (kg)	Total kg	Added as g/l/s	Score	KgX10 E+score/10
Benzthiazole	968.3	968.3	liquid	29.7	899725.3
NaOH	2175.0	2175.0	liquid	3.6	4982.6
Chemical B	8.0	8.0	liquid	23.9	1963.8
Chemical D	0.7	0.7	liquid	9.8	6.7
Chemical C	3.0	3.0	liquid	17.0	151.1
Chemical A	20.0	20.0	liquid	30.5	22585.5
Stage 1 product	0.0	0.0			0.0
Sodium formate	0.0	0.0			0.0
Chemical E	0.0	0.0			0.0
Total input score for Hydrolysis					**929416.0**



To Scrubber - assumes releases to air

Material	Charging Mass (kg)	Total	Chemical Score	KgX10 E+Score/10
Benzthiazole	0.0	0.0	28.7	0.0
NaOH	0.0	0.0		0.0
Chemical B	0.0	0.0	23.5	0.0
Chemical D	0.0	0.0	9.5	0.0
Chemical C	0.0	0.0	16.9	0.0
Chemical A	0.0	0.0	29.5	0.0
'Stage 1 product	0.0	0.0	30.9	0.0
			Total	**0.0**

To Next Stage

Material	Charging Mass (kg)	Total	Chemical Score	KgX10 E+score/10
Benzthiazole	0.0	0.0	29.7	0.0
NaOH	1591.1	1591.1	3.6	3645.0
Chemical B	7.8	7.8	23.9	1910.8
Chemical D	0.5	0.5	9.8	5.0
Chemical C	3.0	3.0	17.0	149.0
Chemical A	0.0	0.0	30.5	0.0
Stage 1 product	1058.7	1058.7	31.1	1350769.1
Sodium formate	487.3	487.3	3.2	1018.1
Chemical E	10.9	10.9	2.8	20.7
			Total	**1357517.7**

Energy Use

Material	Charging (kWh)	Total	Energy Score	kWh X Score
Energy	0.1	0.1	5.2	**0.5**

Figure 8.2: Thomas Swan Pepton process hydrolysis charging Option 1

Table 8.1: Charging base case and Option 1 - pressurising during charging

	EPPT score: release to air	EPPT score: energy use score
Base case	3.4	0.0
Option 1	0.0	0.5

In the Environmental Process Performance Tool the option with the lowest score has the least environmental impact. From the results in Table 8.1 Option 1 would be favourable over the base case.

Closing the vent during charging and pumping materials into the vessel was suggested to Thomas Swan. Thomas Swan's main concern was that the increase in pressure would cause the pressure discs to burst. This eventuality would release emissions and hinder operations. Further calculations by Houghton (1998) demonstrated that the pressure build up would not burst the discs. Thomas Swan therefore are now considering vent closure during charging. It should however be noted that the emissions released during charging are small compared with the releases during other stages and are not an area of great concern. Despite this, the comparison of the charging base case and Option 1 provides an example which demonstrates the application and use of the EPPT.

8.1.2 Option 2: Cooling the feed during charging

The second processing option considered involves cooling the feed in order to reduce the amount of organic material in the vapour phase, thereby reducing gaseous emissions from the vent. Houghton (1998) calculated the energy required for refrigeration (based on a refrigeration plant working to -29°C) to cool the feed at intervals from the existing operating temperature to 0°C. The EPPT has been used to compare the environmental impact of energy used for cooling the feed with the environmental impact of the base case operation. The calculation of the input and output scores for each temperature interval is given in Table 8.2. A summary of the results is given in Table 8.3.

Table 8.2: Thomas Swan Hydrolysis Charging Option 2

	Inputs			Outputs		
Material	**Mass (kg)**	**Chemical score**	**Kgx10$^{(score/10)}$**	**Mass (kg)**	**Chemical score**	**Kgx10$^{(score/10)}$**
At T_r=1						
Benzthiozole	968.0	29.7	899725.3	4.6x10^{-3}	28.7	3.4
Sodium hydroxide	2180.0	3.6	4994.1	0.0	n/a	0.0
Chemical B	8.0	23.9	1963.8	8.7x10^{-5}	23.5	0.0
Chemical D	0.7	9.8	6.7	4.3x10^{-4}	9.5	0.0
Chemical C	3.0	17.0	151.1	0.0	16.9	0.0
Chemical A	20.0	30.5	22585.5	0.0	29.5	0.0
Energy	-	-	-	0.0	5.2	0.0
Total			**929426.5**			**3.4**
At T_r=0.75						
Benzthiozole	968.0	29.7	899725.3	3.0x10^{-3}	28.7	2.2
Sodium hydroxide	2180.0	3.6	4994.1	0.0	n/a	0.0
Chemical B	8.0	23.9	1963.8	8.7x10^{-5}	23.5	0.0
Chemical D	0.7	9.8	6.7	3.5x10^{-4}	9.5	0.0
Chemical C	3.0	17.0	151.1	0.0	16.9	0.0
Chemical A	20.0	30.5	22585.5	0.0	29.5	0.0
Energy	-	-	-	1.93	5.2	10.0
Total			**929426.5**			**12.2**
At T_r=0.5						
Benzthiozole	968.0	29.7	899725.3	2.0x10^{-3}	28.7	1.5
Sodium hydroxide	2180.0	3.6	4994.1	0.0	n/a	0.0
Chemical B	8.0	23.9	1963.8	0.0	23.5	0.0
Chemical D	0.7	9.8	6.7	2.7x10^{-4}	9.5	0.0
Chemical C	3.0	17.0	151.1	0.0	16.9	0.0
Chemical A	20.0	30.5	22585.5	0.0	29.5	0.0
Energy	-	-	-	3.74	5.2	19.4
Total			**929426.5**			**20.9**
At T_r=0.25						
Benzthiozole	968.0	29.7	899725.3	1.3x10^{-3}	28.7	1.0
Sodium hydroxide	2180.0	3.6	4994.1	0.0	n/a	0.0
Chemical B	8.0	23.9	1963.8	0.0	23.5	0.0
Chemical D	0.7	9.8	6.7	2.0x10^{-4}	9.5	0.0
Chemical C	3.0	17.0	151.1	0.0	16.9	0.0
Chemical A	20.0	30.5	22585.5	0.0	29.5	0.0
Energy	-	-	-	5.58	5.2	29.0
Total			**929426.5**			**30.0**
At T_r=0						
Benzthiozole	968.0	29.7	899725.3	8.0x10^{-4}	28.7	0.6
Sodium hydroxide	2180.0	3.6	4994.1	0.0	n/a	0.0
Chemical B	8.0	23.9	1963.8	0.0	23.5	0.0
Chemical D	0.7	9.8	6.7	1.5x10^{-4}	9.5	0.0
Chemical C	3.0	17.0	151.1	0.0	16.9	0.0
Chemical A	20.0	30.5	22585.5	0.0	29.5	0.0
Energy	-	-	-	7.4	5.2	38.5
Total			**929426.5**			**39.1**

where $T_r = \dfrac{T_{feed}\ (^0C)}{T_{normal\ feed\ temperature}\ (^0C)}$

Table 8.3: Cooling the feed during charging

Feed temp T_r	EPPT score: chemical emissions	EPPT score: energy use	EPPT score: total outputs (emissions+energy)
1	3.4	0.0	3.4
0.75	2.2	10.0	12.2
0.5	1.5	19.4	20.9
0.25	1.0	29.0	30.0
0	0.6	38.5	39.1

The data is in Table 8.3 is presented graphically in Figure 8.3. As the feed temperature is reduced the gaseous emissions are reduced but the energy required for cooling increases. In this option the EPPT score for the energy used is much larger than the EPPT score for the gaseous emissions. Combining the emissions score and energy score shows the option with least environmental impact (lowest EPPT score) to be the case at T_r = 1 (base case) where the feed is not cooled. This is currently practised by Thomas Swan.

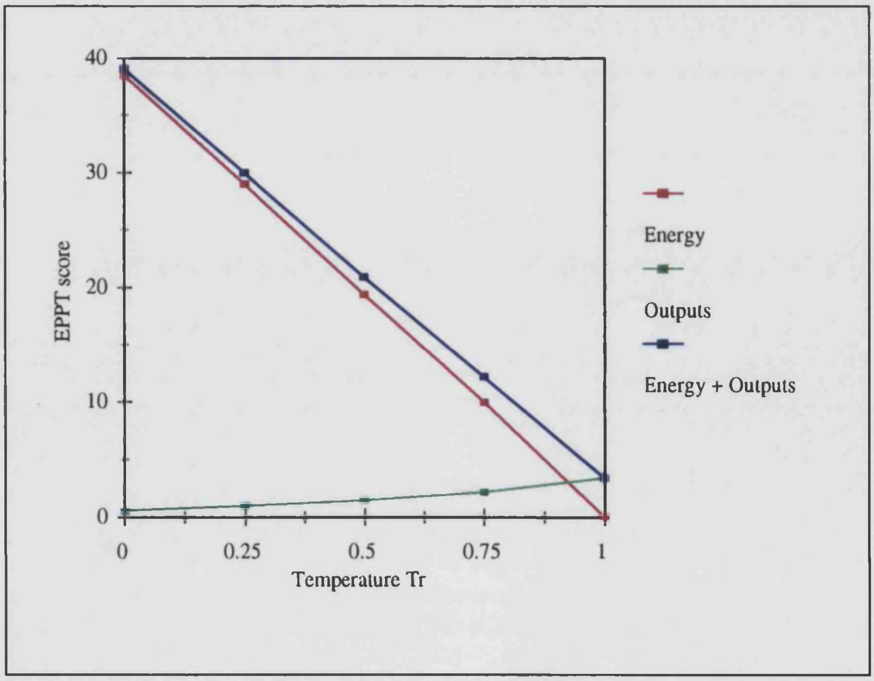


Figure 8.3: Comparison of EPPT emission and EPPT energy scores for Option 2

8.2 Cooling water options

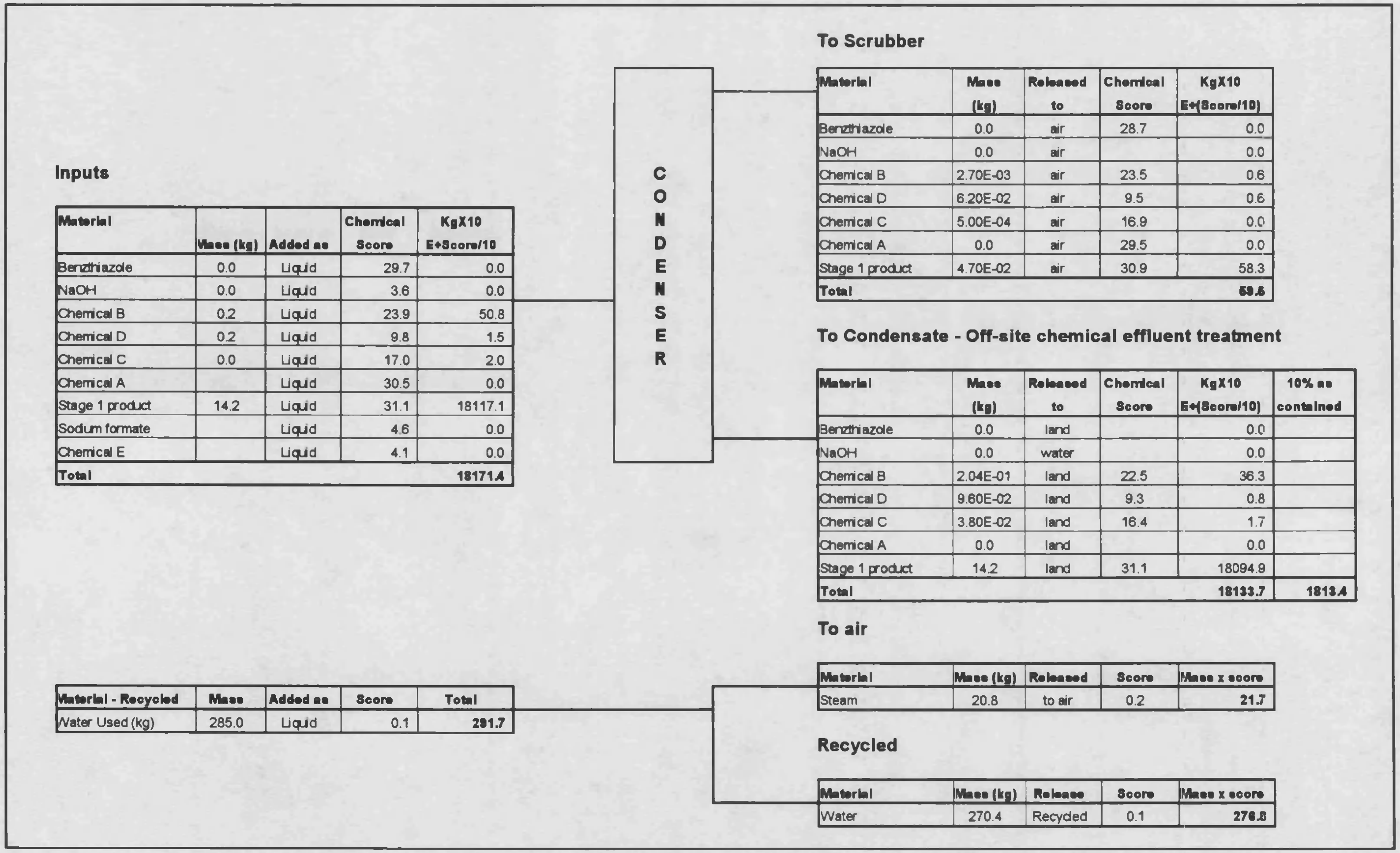
Cooling water is another utility which can be used to reduce emissions from a process. It is used in the following options to reduce the gaseous emissions generated during the venting stage of hydrolysis. The base case is described prior to discussing the options associated with the use of cooling water.

After the vessel has been charged and heated and the reaction has occurred the vessel is vented. In the base case the vented stream is passed through a condenser. The condenser causes the transfer of most of the gaseous emissions to the liquid phase from where the wastes can be treated in an effluent treatment plant. The remaining gaseous emissions that are not condensed are sent to the scrubber. Two venting options in the hydrolysis stage of the Pepton process have been considered and evaluated using the EPPT. The options are:

- Option 3: Reducing the condenser operating temperature.
- Option 4: Cooling the reaction mixture before entering the condenser.

8.2.1 Option 3: Reducing the condenser operating temperature

The first option considered for venting was reducing the operating temperature of the condenser. This option was modelled by Houghton (1998) using 285kg of water to cool the condenser, 7.3% of which was released as steam/water vapour. (Refer to Section 6.2.2 for cooling water calculations). As the emission stream to be condensed was small there was negligible variation in the quantity of cooling water required to cool the stream or in the temperature of the water once cooling was complete. The calculations for the hydrolysis venting Option 3 are shown in Figure 8.4 to 8.6. The results are summarised in Table 8.5.



Inputs

Material	Mass (kg)	Added as	Chemical Score	KgX10 E+Score/10
Benzthiazole	0.0	Liquid	29.7	0.0
NaOH	0.0	Liquid	3.6	0.0
Chemical B	0.2	Liquid	23.9	50.8
Chemical D	0.2	Liquid	9.8	1.5
Chemical C	0.0	Liquid	17.0	2.0
Chemical A		Liquid	30.5	0.0
Stage 1 product	14.2	Liquid	31.1	18117.1
Sodium formate		Liquid	4.6	0.0
Chemical E		Liquid	4.1	0.0
Total				**18171.4**

Material - Recycled	Mass	Added as	Score	Total
Water Used (kg)	285.0	Liquid	0.1	**291.7**

To Scrubber

Material	Mass (kg)	Released to	Chemical Score	KgX10 E+(Score/10)
Benzthiazole	0.0	air	28.7	0.0
NaOH	0.0	air		0.0
Chemical B	2.70E-03	air	23.5	0.6
Chemical D	6.20E-02	air	9.5	0.6
Chemical C	5.00E-04	air	16.9	0.0
Chemical A	0.0	air	29.5	0.0
Stage 1 product	4.70E-02	air	30.9	58.3
Total				**59.5**

To Condensate - Off-site chemical effluent treatment

Material	Mass (kg)	Released to	Chemical Score	KgX10 E+(Score/10)	10% as contained
Benzthiazole	0.0	land		0.0	
NaOH	0.0	water		0.0	
Chemical B	2.04E-01	land	22.5	36.3	
Chemical D	9.60E-02	land	9.3	0.8	
Chemical C	3.80E-02	land	16.4	1.7	
Chemical A	0.0	land		0.0	
Stage 1 product	14.2	land	31.1	18094.9	
Total				**18133.7**	**1813.4**

To air

Material	Mass (kg)	Released	Score	Mass x score
Steam	20.8	to air	0.2	**21.7**

Recycled

Material	Mass (kg)	Release	Score	Mass x score
Water	270.4	Recycled	0.1	**276.8**

Figure 8.4: Thomas Swan Pepton process venting Option 3: Tr = 1

Inputs

Material	Mass (kg)	Added as	Chemical Score	KgX10 E+Score/10
Benzthiazole	0.0	Liquid	29.7	0.0
NaOH	0.0	Liquid	3.6	0.0
Chemical B	0.2	Liquid	23.9	50.8
Chemical D	0.2	Liquid	9.8	1.5
Chemical C	0.0	Liquid	17.0	2.0
Chemical A		Liquid	30.5	0.0
Stage 1 product	14.2	Liquid	31.1	18117.1
Sodium formate		Liquid	4.6	0.0
Chemical E		Liquid	4.1	0.0
Total				**18171.4**

Material - Recycled	Mass	Added as	Score	Total
Water Used (kg)	285.0	Liquid	0.1	**291.7**

CONDENSER

To Scrubber

Material	Mass (kg)	Released to	Chemical Score	KgX10 E+(Score/10)
Benzthiazole	0.0	air	28.7	0.0
NaOH	0.0	air		0.0
Chemical B	1.50E-03	air	23.5	0.3
Chemical D	5.20E-02	air	9.5	0.5
Chemical C	2.80E-04	air	16.9	0.0
Chemical A	0.0	air	29.5	0.0
Stage 1 product	2.40E-02	air	30.9	29.8
Total				**30.6**

To Condensate - Off-site chemical effluent treatment

Material	Mass (kg)	Released to	Chemical Score	KgX10 E+(Score/10)	10% as contained
Benzthiazole	0.0	land		0.0	
NaOH	0.0	water		0.0	
Chemical B	2.06E-01	land	22.5	36.5	
Chemical D	1.06E-01	land	9.3	0.9	
Chemical C	3.87E-02	land	16.4	1.7	
Chemical A		land		0.0	
Stage 1 product	14.2	land	31.1	18128.2	
Total				**18167.3**	**1816.7**

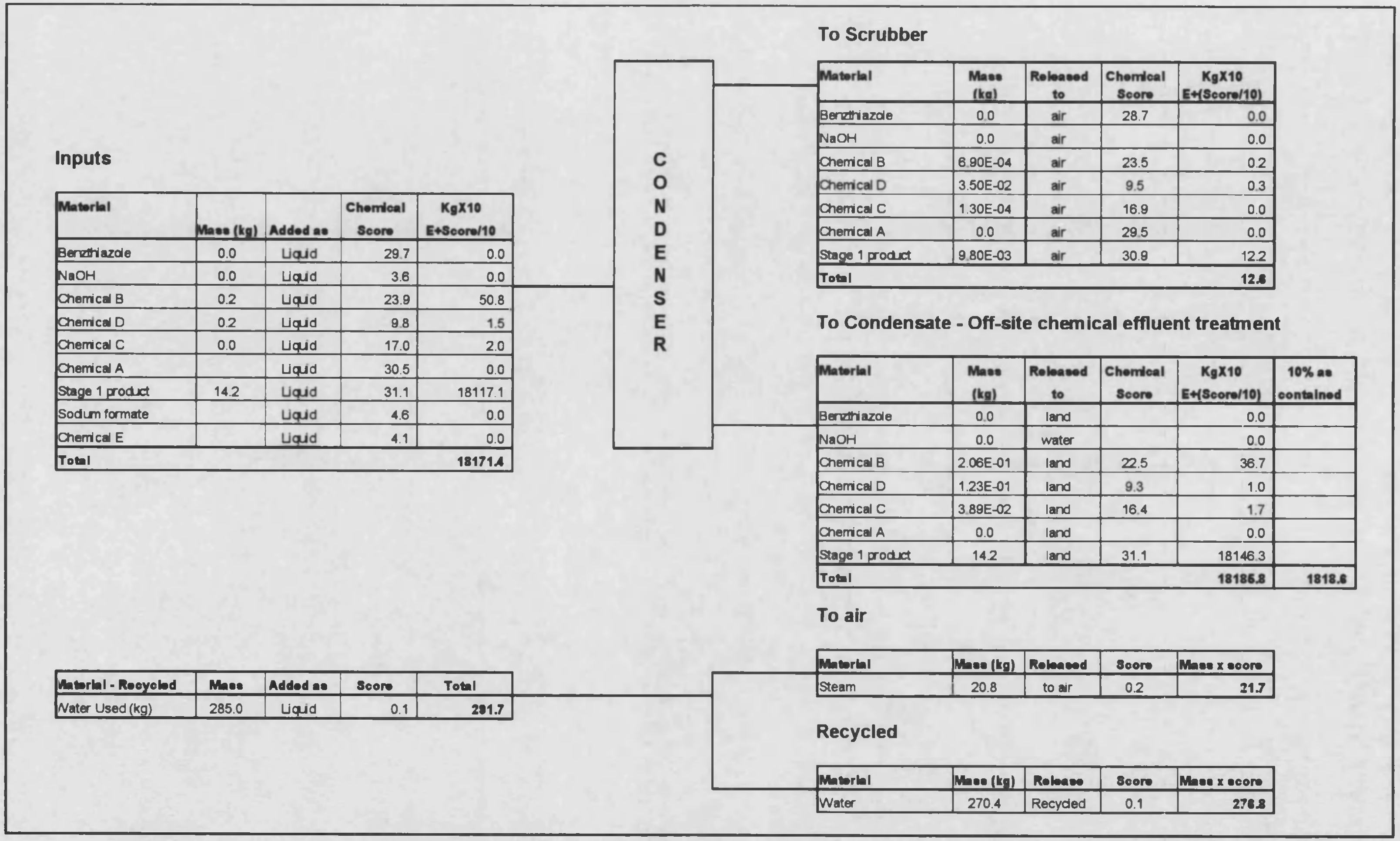
To air

Material	Mass (kg)	Released	Score	Mass x score
Steam	20.8	to air	0.2	**21.7**

Recycled

Material	Mass (kg)	Release	Score	Mass x score
Water	270.4	Recycled	0.1	**276.8**

Figure 8.5: Thomas Swan Pepton process venting Option 3: Tr = 0.67



Inputs

Material	Mass (kg)	Added as	Chemical Score	KgX10 E+Score/10
Benzthiazole	0.0	Liquid	29.7	0.0
NaOH	0.0	Liquid	3.6	0.0
Chemical B	0.2	Liquid	23.9	50.8
Chemical D	0.2	Liquid	9.8	1.5
Chemical C	0.0	Liquid	17.0	2.0
Chemical A		Liquid	30.5	0.0
Stage 1 product	14.2	Liquid	31.1	18117.1
Sodium formate		Liquid	4.6	0.0
Chemical E		Liquid	4.1	0.0
Total				**18171.4**

Material - Recycled	Mass	Added as	Score	Total
Water Used (kg)	285.0	Liquid	0.1	**291.7**

To Scrubber

Material	Mass (kg)	Released to	Chemical Score	KgX10 E+(Score/10)
Benzthiazole	0.0	air	28.7	0.0
NaOH	0.0	air		0.0
Chemical B	6.90E-04	air	23.5	0.2
Chemical D	3.50E-02	air	9.5	0.3
Chemical C	1.30E-04	air	16.9	0.0
Chemical A	0.0	air	29.5	0.0
Stage 1 product	9.80E-03	air	30.9	12.2
Total				**12.6**

To Condensate - Off-site chemical effluent treatment

Material	Mass (kg)	Released to	Chemical Score	KgX10 E+(Score/10)	10% as contained
Benzthiazole	0.0	land		0.0	
NaOH	0.0	water		0.0	
Chemical B	2.06E-01	land	22.5	36.7	
Chemical D	1.23E-01	land	9.3	1.0	
Chemical C	3.89E-02	land	16.4	1.7	
Chemical A	0.0	land		0.0	
Stage 1 product	14.2	land	31.1	18146.3	
Total				**18185.8**	**1818.6**

To air

Material	Mass (kg)	Released	Score	Mass x score
Steam	20.8	to air	0.2	**21.7**

Recycled

Material	Mass (kg)	Release	Score	Mass x score
Water	270.4	Recycled	0.1	**276.8**

Figure 8.6: Thomas Swan Pepton process venting Option 3: Tr = 0.33

Table 8.5: Cooling the condenser during venting

Temp T_r	EPPT score: output from condenser: Gaseous emissions	EPPT score: output from condenser: Condensate	EPPT score: Total output
1.00	59.5	1813.4	1872.9
0.67	30.6	1816.6	1847.2
0.33	12.7	1818.4	1831.1

Cooling the condenser reduces the material in the vapour phase and consequently the gaseous stream sent to the scrubber. The reduction in the gaseous stream score is over 75%. However there is an increase in the condensate score. Combining the gaseous and aqueous output scores for the condenser gives the total EPPT output score from the condenser assuming the scrubber is not in use. The case with cooling to $T_r = 0.33$ has the lowest EPPT output score and therefore the lowest environmental impact. Cooling the condenser more to reduce environmental impact further would require refrigeration with additional equipment and energy requirements. As there is negligible variation in the quantity of cooling water required or in the temperature of the cooling water once cooling was complete the real issue in this option becomes the time required for additional cooling and its influence on the process scheduling.

8.2.2 Option 4: Cooling the reaction mixture before entering condenser

Once the vessel has been charged, heated and the reaction has occurred a liquid/gas mixture exists in the vessel. The base case operation vents the gaseous mixture to a condenser where the vapours are cooled. The condensed vapours are sent to an effluent treatment plant as described in Section 6.3.1. The remaining vapours are sent to the scrubber.

In Option 4 the whole vessel is cooled before releasing the vapour to the condenser. This condenses some of the reaction mixture vapours. Cooling water is required in this option to cool the reaction vessel. Thus Option 4 uses cooling water to provide a reduced vapour stream which is sent to the condenser. The base case has a larger gaseous process stream going to the condenser but no cooling water is used at the reaction vessel. (As with Option 3 it is assumed that the cooling water will be recycled and 7.3% of the water will be lost as water vapour in the cooling tower). The calculation of the EPPT scores for Option 4 are shown in Figure 8.7 and should be compared with hydrolysis venting base case (at $T_r = 1$) shown in Figure 8.4. Table 8.6 summarises the differences between the hydrolysis venting base case and Option 4.

Table 8.6: Venting the vessel at different temperatures

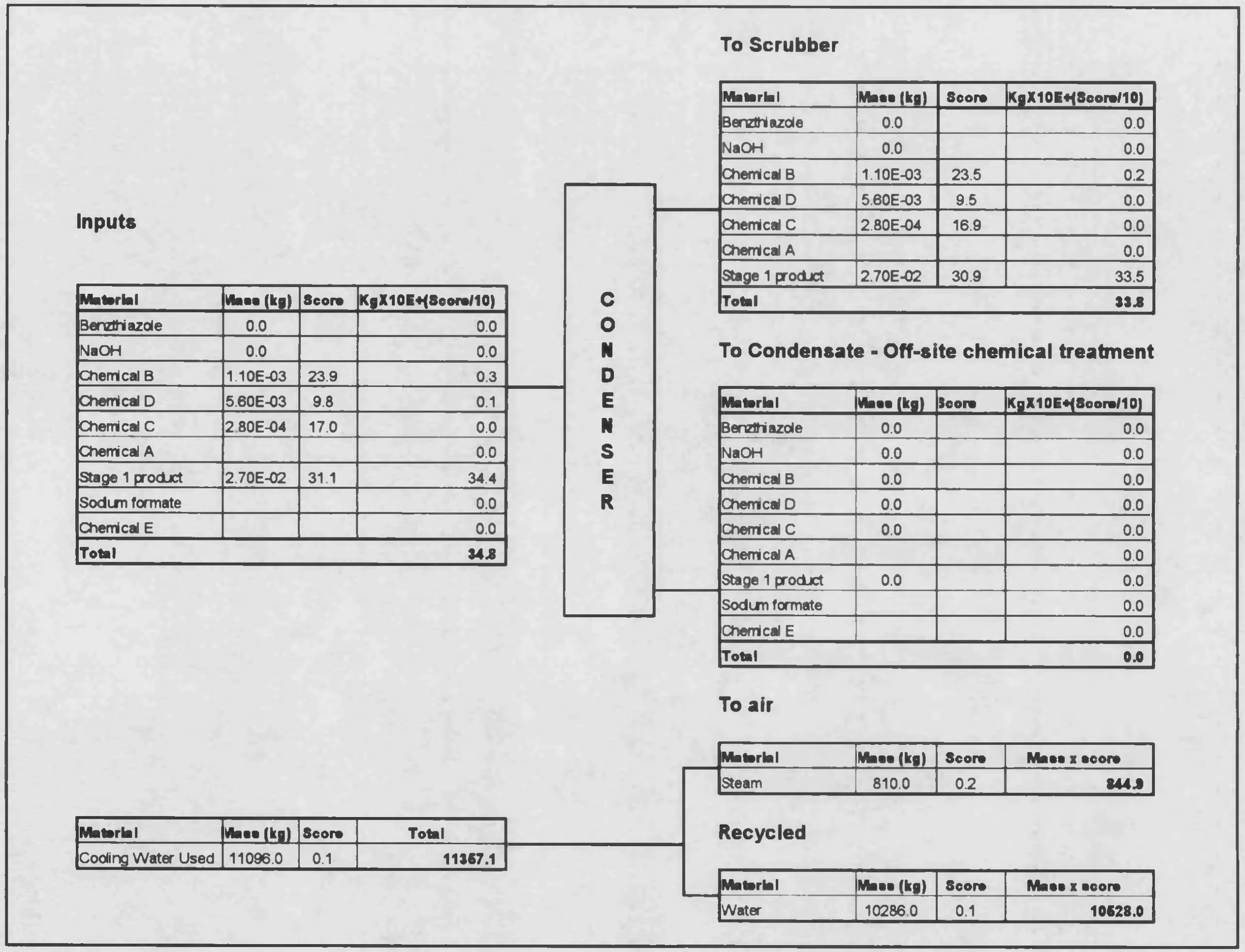
	EPPT score: outputs:			EPPT score: Total outputs
	Gaseous	Water vapour	Aqueous	
Base case	59.5	0.0	1813.4	1872.9
Option 4	33.9	844.9	0.0	878.8

From Table 8.6 it is seen that by cooling the reaction vessel before passing the stream through the condenser (assuming 92.7% of the cooling water is recycled) an EPPT score for outputs of 878.8 is obtained. This is significantly lower than 1873.8 the EPPT output score for the base case, and thus is the option with the lower environmental impact.

After this option was evaluated it was suggested to Thomas Swan as a method of reducing process emissions. However the idea was rejected as they require the organics to be removed from the vessel to produce a pure product. If this option was employed a further operation would be required to remove the organics. An evaluation of this additional operation would be required to determine the Best Environmental Option but it is thought that the base case operation currently used is Best Practicable Environmental Option.

8.3 Using the EPPT to identify pollution problems

The previous sections have shown how the environmental impact of process options can be evaluated and compared to determine the option with the least environmental impact. In the next section the whole Pepton process is evaluated using the EPPT. The EPPT is used here as a tool to identify pollution problems within the process.



Inputs

Material	Mass (kg)	Score	KgX10E+(Score/10)
Benzthiazole	0.0		0.0
NaOH	0.0		0.0
Chemical B	1.10E-03	23.9	0.3
Chemical D	5.60E-03	9.8	0.1
Chemical C	2.80E-04	17.0	0.0
Chemical A			0.0
Stage 1 product	2.70E-02	31.1	34.4
Sodium formate			0.0
Chemical E			0.0
Total			**34.8**

Material	Mass (kg)	Score	Total
Cooling Water Used	11096.0	0.1	**11357.1**

To Scrubber

Material	Mass (kg)	Score	KgX10E+(Score/10)
Benzthiazole	0.0		0.0
NaOH	0.0		0.0
Chemical B	1.10E-03	23.5	0.2
Chemical D	5.60E-03	9.5	0.0
Chemical C	2.80E-04	16.9	0.0
Chemical A			0.0
Stage 1 product	2.70E-02	30.9	33.5
Total			**33.8**

To Condensate - Off-site chemical treatment

Material	Mass (kg)	Score	KgX10E+(Score/10)
Benzthiazole	0.0		0.0
NaOH	0.0		0.0
Chemical B	0.0		0.0
Chemical D	0.0		0.0
Chemical C	0.0		0.0
Chemical A			0.0
Stage 1 product	0.0		0.0
Sodium formate			0.0
Chemical E			0.0
Total			**0.0**

To air

Material	Mass (kg)	Score	Mass x score
Steam	810.0	0.2	**844.9**

Recycled

Material	Mass (kg)	Score	Mass x score
Water	10286.0	0.1	**10528.0**

Figure 8.7: Thomas Swan Pepton process venting Option 4

Having used the EPPT to identify pollution problems, the EPPT is then used to assess process options. Thomas Swan's Pepton process has again been used as an example to demonstrate this use of the EPPT.

A description of Thomas Swan's Pepton process has been given in Chapter 7. The EPPT evaluation of the process is given in Appendix 9. Table 8.7 summarises the EPPT evaluation of the emissions Pepton process.

Table 8.7: EPPT evaluation of Thomas Swan's Pepton process

Inputs

Material	**Mass (kg)**	**Chemical score**	**kg x 10$^{(score/10)}$**
Benzthiazole	592.3	29.7	5.50x10^{5}
Sodium Hydroxide	1330.4	3.6	3.07x10^{3}
Chemical B	4.9	23.9	1.20x10^{3}
Chemical D	3673.5	9.8	3.52x10^{4}
Chemical C	1.8	17.0	9.24x10^{1}
Chemical A	12.2	30.5	1.14x10^{4}
Sodium Bicarbonate	550.5	2.8	1.06x10^{3}
Water	3290.8	0.1	3.36x10^{3}
Hydrogen Peroxide	3621.1	10.4	4.01x10^{4}
Benzoyl Chloride	700.4	10.8	8.36x10^{3}
Total Input	13777.9		**6.54x10^{5}**

Outputs

Material	**Mass**	**Chemical score**	**kg x 10$^{(score/10)}$**
To atmosphere			
Benzthiozole	0.5	28.7	380.5
Chemical B	1.7x10^{-2}	23.5	3.8
Chemical D	2.0	9.5	17.3
Chemical C	2.0x10^{3-}	16.9	0.1
Chemical A	3.9x10^{-3}	28.7	2.9
Stage 1 product	0.2	30.9	301.5
Oxygen	0.1	0.1	0.1
Carbon Dioxide	94.8	7.7	560.9
Total			**1.27x10^{3}**
From effluent treatment to water			
Sodium Formate	291.8	3.2	613.9
Chemical E	6.5	2.8	12.5
Sodium Hydroxide	**951.4**	**3.6**	**2194.7**
Water	**4309.7**	**0.1**	**4400.0**
Sodium Carbonate	231.3	2.8	444.8
Sodium Bicarbonate	171.6	2.8	329.9
Sodium Chloride	255.3	2.5	448.8
Hydrogen Peroxide	9.0	10.4	99.4
Chemical H	23.3	3.2	49.0
Total			**8.59x10^{3}**
From effluent treatment to landfill			
Chemical B	0.6	22.5	105.6
Chemical D	28.3	9.3	242.9
Chemical C	2.0x10^{-2}	16.4	1.17
Stage 1 Product	**8.7**	**31.1**	**11073.2**
Benzoyl Chloride	64.4	10.2	675.5
Pepton	0.5	32.3	801.7
Chemical G	**3.5**	**32.2**	**5826.3**
Chemical F	**9.8**	**32.2**	**16426.0**
Benzthiozole	0.5	29.2	391.7
Total		10% as contained	**3.55x10^{3}**
From drying to atmosphere			
Water	2591.4	0.2	2702.9
Total			**2.70x10^{3}**
TOTAL PROCESS EMISSION SCORE			**1.61x10^{4}**

The highlighted chemicals make large contribution to the overall environmental impact of the process.

8.3.1 Pollutant identification

Water, sodium hydroxide, Stage 1 product, Chemical F and Chemical G are the chemicals with the largest contribution to the environmental impact of the Pepton process. Water and sodium hydroxide have low EPPT chemical scores. Their contribution to the environmental impact is due to the large quantities of these chemicals that are released. Large reductions in the volume of these emissions are required to significantly reduce environmental impact. Recycling and pinch analysis could be used to assess this.

Stage 1 product, Chemical F and Chemical G have high EPPT chemical scores and low volume emissions. Relatively small reductions in emission volumes of these chemicals would cause a significant reduction in environmental impact. These emissions also potentially have the greatest contribution to the environmental impact of the process especially considering the contribution of each chemical to the overall impact has been reduced to 10% to consider disposal to landfill and the assumptions used for disposal to landfill (Chapter 6) are very general.

Having highlighted the most polluting emissions the next step is to identify ways of reducing the volume of these emissions. The recovery of Stage 1 product may be beneficial both financially in terms of increased product, and environmentally in terms of reduced impact and should be considered along with the reduction of Chemical F and Chemical G. As Chemical F has the highest contribution to environmental impact its reduction has been used as an example to demonstrate the capability of the EPPT to identify potential pollution problems. It is presented in the next section.

Initially it was necessary to identify the origin of Chemical F as it is not added directly to the process as a feed or feed contaminant. From the reactions discussed in Chapter 6, Chemical F arises during benzoylation from the reaction of Chemical B with benzoyl chloride. Thus the amount of Chemical F produced could be reduced by removing Chemical B prior to the addition of benzoyl chloride. This is investigated in the following section.

8.4 Options using other chemicals

Process changes for environmental improvement require compromise. Whilst one emission may be reduced others may be increased, or as has been shown in Options 1 to 4 the reduction of emissions may require the additional use of utilities in the form of electricity or cooling water. The prevention of the formation of Chemical F is no exception. Direct steam injection was the method evaluated to remove Chemical B. Combustion of methane is used to generate steam that is used to remove Chemical B from the process. The environmental impact in the use of the additional chemical (methane) was compared with the reduction in environmental impact through Chemical F not being formed.

8.4.1 Option 5: Removal of Chemical B by direct steam injection

Chemical B is a contaminant in the benzthiozole feed in the Pepton process. Chemical B and benzthiozole have boiling points of 185^{0}C and 227^{0}C respectively (Merck, 1993) so distillation should be a viable option. However HYSYS™, the software used by Houghton (1998) to generate process options predicts the boiling point of Benzthiozole to be 187^{0}C therefore distillation couldn't be modelled. The removal of Chemical B was therefore modelled using direct steam injection in the oxidation stage of the process when the benzthiozole had reacted and the boiling points were now sufficiently different. Houghton (1998) modelled this option using the burning of methane as the heat source to generate steam. This option therefore compares the base case which includes Chemical F as an emission with the use of methane to generate steam.

Houghton (1998) modelled the Chemical B removal over fourteen 30 minute time periods. As the time was increased the amount of Chemical B removed was greater but more steam was consequently used. Table 8.8 shows the mass of methane used to produce the steam in the direct steam injection, the mass of Chemical B removed and the consequent reduction in Chemical F formed, and also the carbon dioxide and steam produced from the direct steam injection process.

Table 8.8: Chemical B removal by direct steam injection

Case	Time (hr)	Methane used (kg)	Steam produced (kg)	Carbon dioxide produced (kg)	Chemical B removed (kg)	Chemical F produced (kg)
Base	0	0.0	0.0	0.0	0.0	16.4
1	0.5	16.3	36.6	44.7	0.0	16.4
2	1	33.8	76.0	92.9	0.0	16.4
3	1.5	51.8	116.6	142.5	0.2	15.9
4	2	68.2	153.5	187.6	1.6	13.0
5	2.5	85.8	192.9	235.8	2.8	10.5
6	3	103.3	232.4	284.1	3.8	8.4
7	3.5	120.8	271.9	332.3	4.6	6.7
8	4	138.4	311.4	380.6	5.3	5.2
9	4.5	156.6	352.3	430.5	5.9	3.9
10	5	174.7	393.1	480.5	6.4	2.9
11	5.5	192.9	434.0	530.5	6.8	2.0
12	6	211.0	474.8	580.3	7.2	1.3
13	6.5	229.2	515.7	630.3	7.4	0.7
14	7	246.8	555.2	678.6	7.7	0.2

Table 8.8 shows that increasing the use of methane to produce steam results in an increased amount of Chemical B being removed from the feed. The removal of Chemical B means that Chemical F is not formed. As Chemical F is not formed the environmental impact associated with this part of the process is reduced. However there is an environmental cost associated with the removal of Chemical B to avoid Chemical F formation. This environmental cost is caused by the disposal of Chemical B removed from the feed, and the carbon dioxide and steam produced from the burning of methane. Thus to assess the environmental impact of Option 5 these changes in emissions need to be considered. The environmental impact of each case is evaluated using the EPPT in Table 8.9

Table 8.9: Calculation of the EPPT scores for the outputs for each case.

Emission	Mass (kg)	Score	Mass x $10^{(score/10)}$	Mass (kg)	Score	Mass x $10^{(score/10)}$	Mass (kg)	Score	Mass x $10^{(score/10)}$
	Base case			**Case 1 - 0.5 hours**			**Case 2 - 1 hour**		
Carbon dioxide	0.0	7.7	0.0	44.7	7.7	264.3	92.9	7.7	549.8
Steam	0.0	0.2	0.0	36.6	0.2	38.1	76.0	0.2	79.3
Chemical B	0.0	23.9	0.0	0.0	23.9	0.0	0.0	23.9	0.0
Chemical F	16.4	32.2	27239.2	16.4	32.2	27239.2	16.4	32.2	27239.2
Total			**27239.2**			**27541.6**			**27868.2**
	Case 3 - 1.5 hours			**Case 4 - 2 hours**			**Case 5 - 2.5 hours**		
Carbon dioxide	142.4	7.7	842.7	187.5	7.7	1109.5	235.8	7.7	1394.9
Steam	116.5	0.2	121.5	153.4	0.2	159.9	192.9	0.2	201.1
Chemical B	0.2	23.9	54.3	1.6	23.9	387.5	2.8	23.9	681.0
Chemical F	15.9	32.2	26461.4	13.0	32.2	21692.3	10.5	32.2	17490.6
Total			**27479.9**			**23349.2**			**19767.6**
	Case 6 - 3 hours			**Case 7 - 3.5 hours**			**Case 8 - 3.5 hours**		
Carbon dioxide	284.1	7.7	1680.4	332.3	7.7	1965.8	380.6	7.7	2251.2
Steam	232.4	0.2	242.2	271.9	0.2	283.4	311.4	0.2	324.5
Chemical B	3.8	23.9	926.1	4.6	23.9	1130.7	5.2	23.9	1267.7
Chemical F	8.4	32.2	13982.0	6.6	32.2	11053.6	5.3	32.2	8839.2
Total			**16830.7**			**14433.5**			**12682.7**
	Case 9 - 4.5 hours			**Case 10 - 5 hours**			**Case 11 - 5.5 hours**		
Carbon dioxide	430.5	7.7	2546.9	480.5	7.7	2842.5	530.5	7.7	3138.1
Steam	352.3	0.2	367.2	393.1	0.2	409.8	434.0	0.2	452.4
Chemical B	5.9	23.9	1448.4	6.4	23.9	1570.1	6.8	23.9	1670.9
Chemical F	3.9	32.2	6506.5	2.9	32.2	4763.8	2.0	32.2	3320.7
Total			**10868.9**			**9586.2**			**8582.2**
	Case 12 - 6 hours			**Case 13 - 6.5 hours**			**Case 14 - 7 hours**		
Carbon dioxide	580.3	7.7	3433.1	630.3	7.7	3728.7	678.6	7.7	4014.1
Steam	474.8	0.2	494.9	515.7	0.2	537.5	555.2	0.2	578.7
Chemical B	7.2	23.9	1754.2	7.4	23.9	1823.4	7.7	23.9	1878.8
Chemical F	1.3	32.2	2128.4	0.7	32.2	1138.7	0.2	32.2	345.6
Total			**7810.6**			**7228.3**			**6817.2**

The output scores are graphically represented in Figure 8.8.

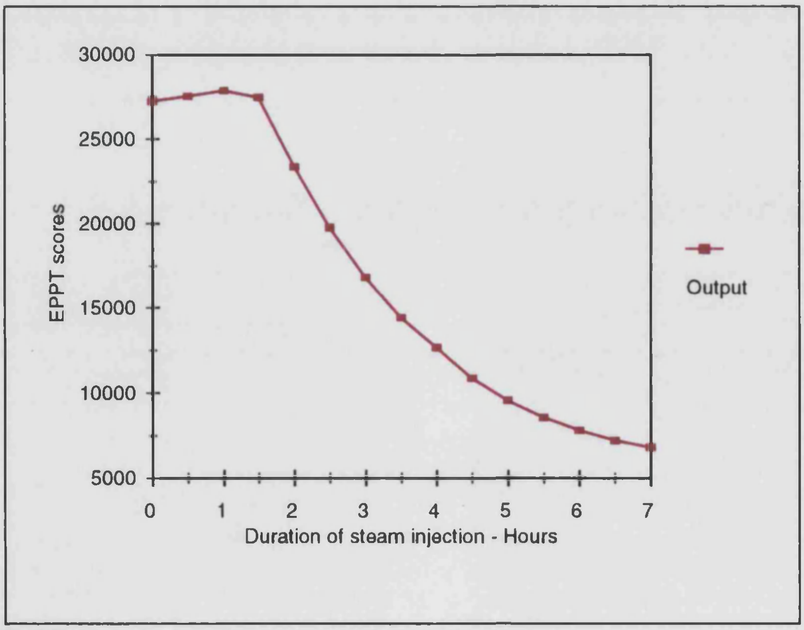


Figure 8.8: EPPT scores for the outputs from Option 5

From Table 8.9 and Figure 8.8 the outputs scores are significantly reduced with increasing use of direct steam injection (after 2 hours) to remove Chemical B. Thus from this option it is apparent that the removal of Chemical B using direct steam injection reduces the environmental impact of this process. However in choosing the Best Practicable Environmental Option (BPEO) the operator must decide on how much to spend in additional methane, equipment and scheduling costs to reduce environmental impact.

8.5 Fison's sodium cromoglycate process environmental improvements

Fison's sodium cromoglycate process has been evaluated using the EPPT. The existing and proposed new plant are compared here to determine whether the improvements adopted by Fison's address (1) the main pollution problems identified using the EPPT and (2) whether the process improvements will improve the environmental performance of the process. The EPPT is also used to identify areas for further imporovements in Fison's sodium cromoglycate process.

As discussed in Section 7.2 Fison's operate a sodium cromoglycate process. Data is available for the existing plant and also a new plant which has been modified to demonstrate 'Best Practicable Environmental Option' (IPC AL 4716). The data for each stage of the old and new processes are shown in Chapter 7 - Tables 7.2 to 7.17. Each stage of the existing and new plants (based on 1000kg production) have been evaluated using the EPPT chemical scoring system. The EPPT calculations for each stage of the existing and new plants are given in Appendix 9.

8.5.1 Identification of pollution problems using the EPPT

The stages of the existing plant have been assessed using the EPPT to highlight the potential for environmental impact reduction. Table 8.10 and the accompanying Figure 8.9 show the mass of emissions released during each stage of the process and the EPPT scores for each stage.

Table 8.10: Mass of emissions released and EPPT scores for the existing plant

Stage	Mass	EPPT score
1&2	10825.0	10905.7
3	41349.5	147959.5
4	12699.0	79581.4
5	5750.1	10220.8
6	16469.1	6879.7
7	3579.0	6414.1
8	5411.6	18625.4

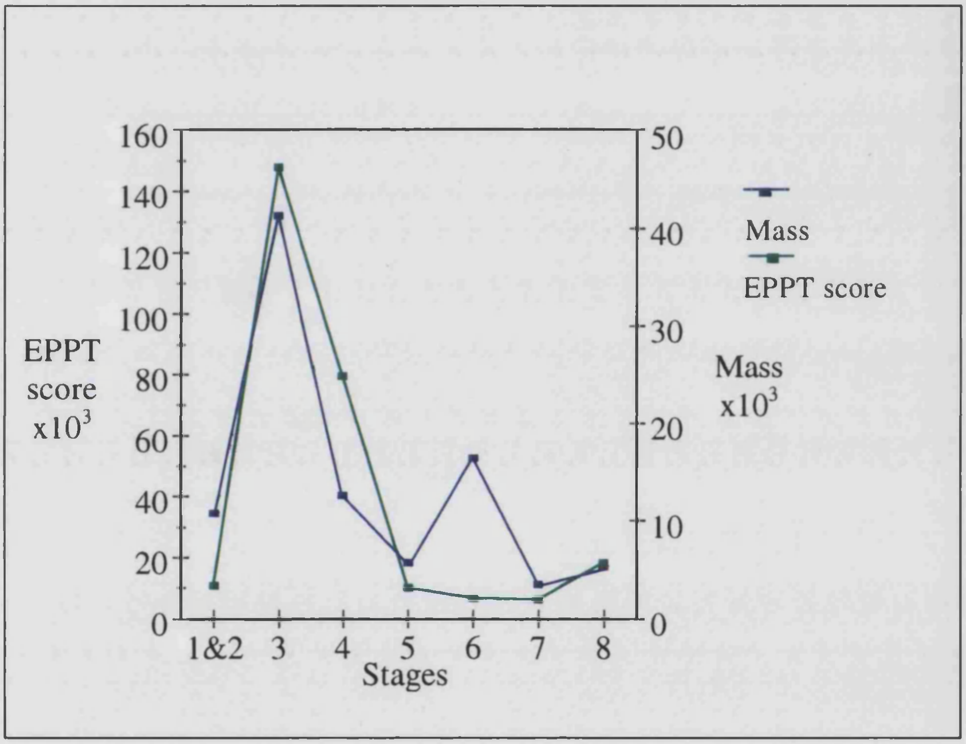


Figure 8.9: Mass and EPPT score of emissions from existing plant

From Figure 8.9 the EPPT score for the emissions from each stage largely follow the pattern of the mass of emissions from each stage with the exception of stage 6 where a large mass of emissions is released which is not reflected in the EPPT score. In this case the rise in mass is mainly from water which has a low score in the EPPT. The main masses of emissions arise in stages 1 to 4 and also in stage 6. The emissions with most environmental impact arise in stages 1 to 4.

From these results this research would suggest that the earlier stages of the process are where the largest reduction in environmental impact could be achieved. Fison's have however focused on the later stages of the process in an effort to achieve 'Best Practicable Environmental Option'. Details of environmental improvement for the first four stages are currently being drawn up.

8.5.2 Fison's plant improvement evaluation

In the new plant the first four stages remain the same but stages 4 to 8 have been modified to increase recycle and reduce emissions. The masses of emissions and EPPT scores for each stage of the new plant are shown in Table 8.11.

Table 8.11: Mass of emissions and EPPT scores for the stages of the new plant

Stage	Mass	EPPT score
1&2	12588.4	12682.3
3	48085.5	172058.4
4	14767.7	92545.4
5	5403.0	10638.2
6	12501.8	3376.9
7	369.6	1050.8
8	18.1	132.9

The masses of emissions from the existing and proposed new plant are shown in Figure 8.10. There are increases in the emissions of the new plant from stages 1 to 4 due to the increased input of stage 4 product into stage 5. However stages 5 to 8 in the new plant have less emissions than the old plant. This is due to the introduction of a nitrogen blanket and a carbon adsorption system that removes the industrial methylated spirits and organics from the gaseous stream.

Figure 8.11 shows a comparison of the EPPT scores calculated for the emissions for stages 5 to 8 of the new and existing plants. The new measures introduced for stages 5 to 8 have caused a decrease in EPPT emission score for these stages. This decrease has also caused a decrease in the EPPT emission score for the whole process despite the increase in the emissions associated with stages 1 to 4.

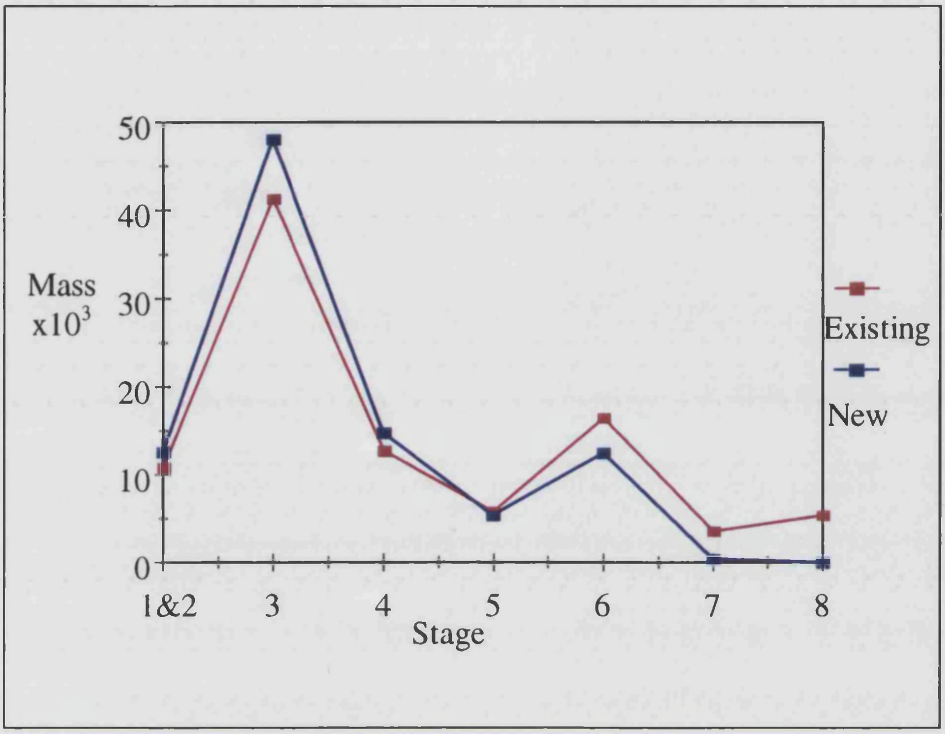


Figure 8.10: Mass of emissions from existing and new plant

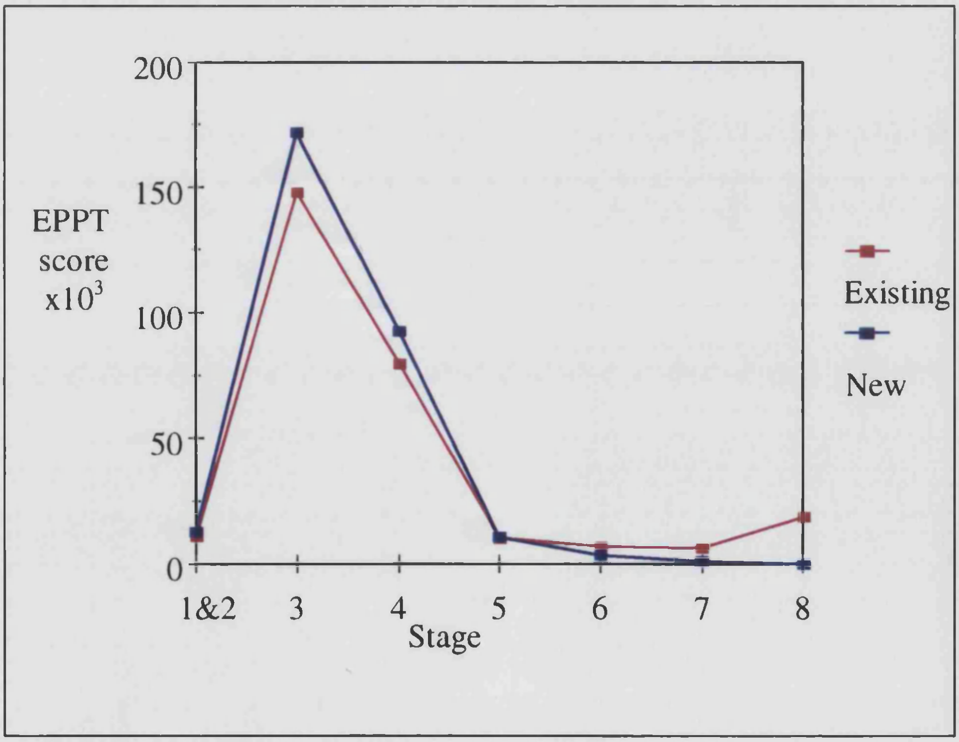


Figure 8.11: EPPT scores for the existing and new plant

It could be suggested that the EPPT was not needed to determine these areas for environmental improvement as they could be derived simply using the mass of emissions. However, the EPPT suggests that improvements to stages 1 to 4 should be prioritised as the actual emissions arising from stage 6 were not as environmentally damaging as those in stages 1 to 4, seen by the lack of a peak in the EPPT score at Stage 6 in Figure 8.11. This is not to suggest the improvements made are not beneficial and have not significantly improved the environmental performance of the plant but simply that they have not addressed the main problem.

8.5.3 Improvements recommended from the EPPT evaluation

Looking in more detail at the main contributors to the EPPT score in stages 2, 3 and 4 (Appendix 9) it is seen that there are three main emissions. The main contributors to the EPPT score for stages 2 to 4 are shown in Table 8.12 (based on existing plant data). The reduction, reuse or recycling of these emissions would have a significant reduction in the environmental impact of the overall process.

Table 8.12: Main chemical contributors to environmental impact for stages 2 to 4

Chemical	Mass released	Score contribution
Stage 1&2		
Water	9776.3	9981.0
Total stage score		**10905.7**
Stage 3		
Aluminium chloride	2685.8	86510.3
Hydrochloric acid	421.8	18158.5
Water	518441.8	42899.0
Total stage score		**147959.5**
Stage 4		
Water	9481.6	9680.2
Hydrochloric acid	1545.9	66553.5
Total stage score		**79581.4**

From Table 8.12 water is shown to have a high score contribution to each stage particularly stage 3. Any measure to reduce water use would be beneficial. This may include recycling with studies made up using pinch analysis. Hydrochloric acid and aluminium chloride are also large contributors to each stage score. Efforts to minimise the release of these chemicals would be beneficial.

8.6 Summary of options

In this Chapter process options generated for the Thomas Swan Pepton process and also the efforts to demonstrate BPEO in the Fisons sodium cromoglycate process have been used to demonstrate the application of the EPPT. These studies have been evaluated using the EPPT to show:

- how the EPPT can be applied to detailed studies to determine the least environmentally damaging process option;
- how the EPPT can be used to identify polluting aspects of the process; and
- how the utilities assessments can be applied to process options to determine environmental impact and to compare process options.

Having determined the environmental impact of various options and improvements, the financial cost of the options and improvements can be determined and these two parameters can be used by the operator to determine the Best Practicable Environmental Option.

9. Process comparison and the EPPT

The comparison of process options has been described and demonstrated in Chapter 8 using the Thomas Swan Pepton case study and the improvements made to Fisons sodium cromoglycate process. The least environmentally damaging options were identified based on the EPPT emission scores for the various options. However, in order to determine the comparative environmental performances of alternative processes it is necessary to obtain the environmental performance profiles (Section 9.4) for each alternative.

In the following sections novel comparison methods are described for the EPPT. These methods are applied to Thomas Swan's Pepton process (TS), Fisons existing (f_{old}) and proposed new (F_{new}) sodium cromoglycate processes, and Associated Octel's tetra ethyl lead (TEL) and tetra methyl lead (TML) processes.

9.1 Basis for process comparisons

In chemical engineering the terms conversion and selectivity are commonly used to describe processes and their associated reactions. These terms have been adopted and modified for use in the EPPT to derive methods for comparing processes. Initially it is necessary to define these terms. Conversion is defined (Coulson and Richardson, 1994) for chemical A in a process as:

$$X_A = \frac{\text{moles of A reacted}}{\text{moles of A fed}} \qquad \text{....... Equation 9.1}$$

There are several definitions for selectivity. For use in the EPPT selectivity is defined as:

$$\text{Selectivity} = \frac{\text{moles of desired product formed}}{\text{moles of undesired product formed}} \qquad \text{....... Equation 9.2}$$

Using this definition, selectivity is infinite if no undesired product is formed.

These terms have been modified for use as process comparisons as will be explained in Sections 9.2.1 to 9.2.4. The modified terms use the EPPT input, emissions and product scores which will be defined in Section 9.1.1.

Applying a conversion approach to the EPPT provides a means of comparing how processes convert inputs into products. It can also be used to compare how processes convert inputs into emissions. These approaches can be then used in the environmental profile of a process to assess overall environmental performance.

The selectivity approach to the EPPT uses the EPPT scores in a similar way to conversion. The selectivity provides a comparison between the product and emissions formed. Each comparison method is described in Section 9.2. The methods are then applied to the five processes in Section 9.3.

9.1.1 Requirements for process comparisons

In order to undertake these novel comparison methods the input score, product score and emission score are required. These scores are defined below:

- the emission score is the EPPT score for all the outputs including utilities but excluding product and recycled material in the production of 1000kg of product.
- the product score is the EPPT score for 1000kg of product and includes other chemicals/contaminants contained in the product.
- the input score is the EPPT score for all the inputs (including recycled material) in the production of 1000kg or product.

9.2 Comparative methods

There are four comparative methods used in conjunction with the EPPT to provide a profile to assess the environmental performance of a process. The comparative methods are:

- The environmental impact comparison
- The environmental selectivity comparison
- The process conversion comparison, and
- The impact conversion comparison.

A value is derived for each comparison method. Each method is described below and applied to five processes (which were described earlier in Chapter 7) in Section 9.3.

9.2.1 The environmental impact comparison

The environmental impact comparison uses the environmental impact value. The environmental impact value is simply the emission score for the process or process option for a unit production rate. In the case of the EPPT 1000kg has been chosen as a 'standard' production rate. Thus,

Environmental impact value = EPPT emission score for 1000kg product

.... Equation 9.3

This approach has been used in Chapter 8 to compare process options and can equally be applied to whole processes. The process or option with the highest EPPT environmental impact score has the greatest environmental impact.

Some chemical processes, however, are inherently more polluting than others as illustrated by Sheldon's analysis of process types described in Section 2.3.1, Table 2.4. These processes have higher environmental impact values than inherently less polluting processes. The inherent polluting nature of a process is usually due to the type of product being manufactured. For example, pharmaceutical processes would be expected to have a higher emission score (and therefore a higher environmental impact value) than a bulk chemical process due to the nature, quantity and quality of the product. Pharmaceutical processes also often have numerous process stages and cleaning schedules which produce a lot of emissions. However, process operation needs to be considered. If an inherently polluting process is operating to minimise environmental impact it should be seen as having better environmental performance than an inherently less polluting process operating where little consideration has been given to the environment. To provide a level playing field on which process comparisons can be made, consideration of the product is required. This is accounted for in the environmental selectivity comparison.

9.2.2 The environmental selectivity comparison

The environmental selectivity comparison uses the environmental selectivity value and is used to compare processes based on the product and emissions produced. It has been defined as:

$$\text{Environmental selectivity value} = \frac{\text{Emission score}}{\text{Product score}} \qquad \text{....... Equation 9.4}$$

A process operating with good environmental selectivity, i.e. one that has a low emission score compared with the product score, would have low environmental selectivity value. A process with poor environmental selectivity would have a high environmental selectivity value as the emission score would be high compared with the product score.

This method is less likely to highlight a producer of a toxic chemical, such as a drug, as a major polluter if that process is being operated with the utmost consideration for the environment. It is more likely to highlight an operator of an inherently low polluting process operating without particularly special consideration of the environment. However, it must be emphasised that the environmental selectivity value has not been used to compare the environmental impact of a process (that is given by the environmental impact value). It just provides some consideration of the nature of the process. It is proposed that this comparison method be combined with an environmental audit based evaluation as discussed in the future work section of Chapter 10.

9.2.3 Product conversion comparison

The product conversion comparison gives an indication of whether a process is converting input score into product score effectively. The product conversion comparison uses the product conversion value. The product conversion value is defined as:

$$\text{Product conversion value} = \frac{\text{Input score}}{\text{Product score}} \quad \text{....... Equation 9.5}$$

A low product conversion value indicates that a large fraction of the input score is converted to product score which is beneficial environmentally as it implies that the inputs are not released as emissions. A high product conversion value indicates that a small fraction of the input score is converted to product score which implies that a large amount of emissions are produced. However, although the product conversion value implies the fraction of input score released as emissions the product conversion value must be used in conjunction with the impact conversion value (Section 9.2.4). This is because the input and output (product and emission) scores do not balance and consequently should be used together as a measure of environmental performance.

9.2.4 The impact conversion comparison

The impact conversion comparison provides a means of assessing how 'ineffective' the process is, that is how the process converts inputs into emissions. The impact conversion comparison uses the impact conversion value which is defined as:

$$\text{Impact conversion value} = \frac{\text{Emission score}}{\text{Input score}} \quad \text{....... Equation 9.6}$$

A high impact conversion value highlights processes which are having a large impact on the environment as large amounts of the process inputs are released to the environment as emissions. A low impact conversion value is good as it emphasises that a very small amount of the inputs are released as emissions. A high impact conversion value indicates that a process might benefit from recycling and/or reusing more chemicals which are presently released as emissions.

9.2.5 Comparison method relationships

Each of the comparison methods described in sections 9.2.2 to 9.2.4 are related.

$$\text{Environmental selectivity value} = \frac{\text{Emission score}}{\text{Product score}} \qquad \text{....... Equation 9.4}$$

$$\text{Product conversion value} = \frac{\text{Input score}}{\text{Product score}} \qquad \text{....... Equation 9.5}$$

$$\text{Impact conversion value} = \frac{\text{Emission score}}{\text{Input score}} \qquad \text{....... Equation 9.6}$$

The relationship is given in Equation 9.7.

$$\text{Impact conversion value} = \frac{\text{Environmental selectivity value}}{\text{Product conversion value}} \qquad \text{....... Equation 9.7}$$

9.3 Application of comparison methods to processes

Having described each process comparison method and outlined the requirements for their use, the following sections derive the appropriate scores and discuss the application of comparison methods to five processes.

9.3.1 Calculation of input, emission and product scores

The EPPT score calculations for each process are shown in Appendix 10. Table 9.1 gives a summary of the data requirements from which comparisons can be made.

Table 9.1: EPPT score summary of the five processes to be compared

Process	Input score	Emission score	Product score
TS	$6.6\text{x}10^5$	$1.6\text{x}10^4$	$1.7\text{x}10^6$
F_{old}	$4.4\text{x}10^7$	$3.5\text{x}10^6$	$1.4\text{x}10^5$
F_{new}	$5.4\text{x}10^7$	$2.3\text{x}10^5$	$1.4\text{x}10^5$
TEL	$4.6\text{x}10^7$	$2.0\text{x}10^4$	$2.8\text{x}10^4$
TML	$6.7\text{x}10^7$	$1.1\text{x}10^6$	$2.3\text{x}10^4$

9.3.2 Environmental impact comparison

As previously discussed the environmental impact score is used to compare the emission score for the process or process option for a unit production rate. Sheldon's (1994) analysis (Section 2.3.4) which is based on the mass of emissions, would suggest that Fisons sodium cromoglycate (a pharmaceutical process) would have a high environmental impact. Thomas Swan's fine chemical Pepton process would have the next highest impact. It is expected that bulk chemical processes such as those operated by Associated Octel would have the least amount of emissions per 1000kg of product. A comparison of processes using the EPPT may rank the processes and process types differently since in the EPPT evaluation the toxicity of the emissions (in terms of score) are considered as well as the masses.

Table 9.2 ranks the processes in terms of environmental impact value. The process with the lowest environmental impact value has the least environmental impact.

Table 9.2: Processes ranked based on their environmental impact

Process	Environmental impact value
TS	$1.6\text{x}10^4$
TEL	$2.0\text{x}10^4$
F_{new}	$2.3\text{x}10^5$
TML	$1.1\text{x}10^6$
F_{old}	$3.5\text{x}10^6$

From this simple analysis Thomas Swan's Pepton process has the lowest environmental impact value and therefore is shown, using the EPPT, to be the least polluting process. Fisons old sodium cromoglycate process with the highest environmental impact value would be the most polluting process with the largest environmental impact. The proposed improvements to Fisons sodium cromoglycate process have reduced the environmental impact of the new process. Thomas Swan's Pepton process was not expected to have the least environmental impact as fine chemical processes are often more polluting than bulk chemical processes in terms of mass of emissions. However this low environmental impact score might suggest that Thomas Swan are operating their Pepton process in an environmentally considerate manner to reduce environmental impact and improve environmental performance.

9.3.3 Environmental selectivity comparison

The environmental selectivity values for the five processes are shown in Table 9.3. A low environmental selectivity value indicates that the process has less effect on the environment than a process with a high environmental selectivity value because the emission score is low compared with the product score.

Table 9.3: Process ranked by environmental selectivity values

Process	Product score	Emission score	Environmental selectivity value Emission score/product score
TS	1.7×10^6	1.6×10^4	9.4×10^{-3}
TEL	2.8×10^4	2.0×10^4	0.71
F_{new}	1.4×10^5	2.3×10^5	1.6
F_{old}	1.4×10^5	3.5×10^6	25.0
TML	2.3×10^4	1.1×10^6	47.8

From Table 9.3 Thomas Swan's Pepton process has by far the lowest environmental selectivity value. This is because the process produces a high scoring product with few emissions. Associated Octel's TEL process and Fisons new process have environmental selectivity values in a similar range. Fisons existing process and Associated Octel's TML process have much higher environmental selectivities.

The rank order of the processes are similar when compared with the rank order of the environmental impact comparison. The only exception being the change in rank order of Associated Octel's tetra methyl lead process and Fisons existing sodium cromoglycate process. This is due to the higher product score of the sodium cromoglycate process compared with the tetra methyl lead process.

Clearly Thomas Swan appear to be operating their process with concern for the environment and attempting to minimise environmental impact. Fisons are operating their process in a environmentally considerate manner. This is also seen in the rise in ranking of the new sodium cromoglycate process compared with the old sodium cromoglycate process. Associated Octel could benefit the environment and improve their environmental performance significantly especially as the EPPT product score is relatively low.

9.3.4 Product conversion comparison

The product conversion value for each of the five processes have been calculated and are ranked in Table 9.4. A low product conversion value is good and shows that many of the inputs are converted to product and consequently are not affecting the environment. A high product conversion value implies that many of the inputs are not converted to product and could potentially be released as emissions which may be detrimental to the environment.

Table 9.4: Product conversion values

Process	Input score	Product score	Product conversion value Input score/Product score
TS	6.6×10^5	1.7×10^6	0.39
F_{old}	4.4×10^7	1.4×10^5	314.3
F_{new}	5.4×10^7	1.4×10^5	385.7
TEL	4.6×10^7	2.8×10^4	1642.8
TML	6.7×10^7	2.3×10^4	2913.0

As is seen from Table 9.4 Thomas Swan's Pepton process is the best at converting inputs into product. This low product conversion value results from the higher product score compared with the input score. Fisons processes have conversion values of approximately 350. These processes are significantly more efficient at converting input score into product score than Associated Octel's tetra alkyl lead processes. However, the new Fisons process appears to be slightly less effective at converting input score into product score than the old Fisons process. This is shown by the decreased product conversion value and has occurred as a result of more inputs being used in the new process to form more stage 4 product which is required for addition to stages 5 to 8.

Whilst the product conversion value highlights those processes which are better at converting inputs into product, the product conversion value should be considered alongside the impact conversion value to give a more complete picture of environmental performance. This aspect is highlighted by the change in the Fisons processes from old to new in an effort to reduce environmental impact. This also suggests that product conversion, which is generally considered to lower the environmental impact, is not necessarily the only way forward to reduce environmental impact.

9.3.5 Impact conversion comparison

The impact conversion comparison is similar to the product conversion comparison with the exception that the inputs released as emissions are considered rather than the product produced. A low impact conversion value is good in environmental terms as it indicates that few of the inputs have been converted to emissions. A high impact conversion value indicates the opposite. The impact conversion value has been calculated for the five processes and results are presented in Table 9.5. The processes have been ranked based on their impact conversion value.

Table 9.5: Impact conversion value

Process	Input score	Emission score	Impact conversion value Emission score/Input score
TEL	$4.6x10^7$	$2.0x10^4$	$4.3x10^{-4}$
F_{new}	$5.4x10^7$	$2.3x10^5$	$4.3x10^{-3}$
TML	$6.7x10^7$	$1.1x10^6$	$1.6x10^{-2}$
TS	$6.6x10^5$	$1.6x10^4$	$2.4x10^{-2}$
F_{old}	$4.4x10^7$	$3.5x10^6$	$8.0x10^{-2}$

Table 9.5 shows that Associated Octel's tetra ethyl lead process has the best (lowest) impact conversion value. This is due to the large amount of recovery and recycling within the process. There is a definite improvement in the new Fisons sodium cromoglycate process after improvements were made to demonstrate BPEO. It is perhaps surprising to see Thomas Swan's Pepton process with a relatively high impact conversion value but this is probably the result of it being a fine chemicals process where opportunities for recovery and recycling are not as easy as in bulk processes such as those operated by Associated Octel.

9.3.6 Product conversion and impact conversion summary

From Tables 9.4 and 9.5 it can be seen that the rank order of the process conversion values and the impact conversion values are quite different. Table 9.6 compares the two.

Table 9.6: Product conversion and impact conversion values and ranking

Product conversion		Impact conversion	
Process	Value	Process	Value
TS	0.39	TEL	$4.3x10^{-4}$
F_{old}	314.3	F_{new}	$4.3x10^{-3}$
F_{new}	385.7	TML	$1.6x10^{-2}$
TEL	1642.8	TS	$2.4x10^{-2}$
TML	2913.0	F_{old}	$8.0x10^{-2}$

The existing sodium cromoglycate process operated by Fisons produces the most emissions from its inputs, shown by the high impact conversion value, but has a comparatively good product conversion value. The new sodium cromoglycate process has dramatically improved the impact conversion value however the process changes have had a slight detrimental effect on the product conversion value. The improved impact conversion is due to the recycling and pollution abatement strategies employed to demonstrate BPEO. The decreased product conversion is due to the increased amount of stage 4 product, and consequently feed, required in the new plant.

The Thomas Swan Pepton process has very good product conversion. However it is ranked rather low with regard to impact conversion. This suggests the process is converting inputs into product well but perhaps recycling or pollution abatement strategies rather than conversion strategies could be studied for further improvements. Both the alkyl lead processes have high product conversion values. However they also have low impact conversion values which is good. This is probably as a result of the large amount of recycling and recovery of lead compounds. The tetra ethyl lead process has a lower impact conversion than the tetra methyl lead process. This is because the alkyl chloride (a main feed of the processes) is gaseous in the tetra methyl lead process and is released to the atmosphere whereas the alkyl chloride in the tetra ethyl lead process is a liquid which is more readily recovered. In these processes strategies to improve conversion could improve environmental performance.

The product conversion and impact conversion values for each process have been plotted in Figure 9.1.

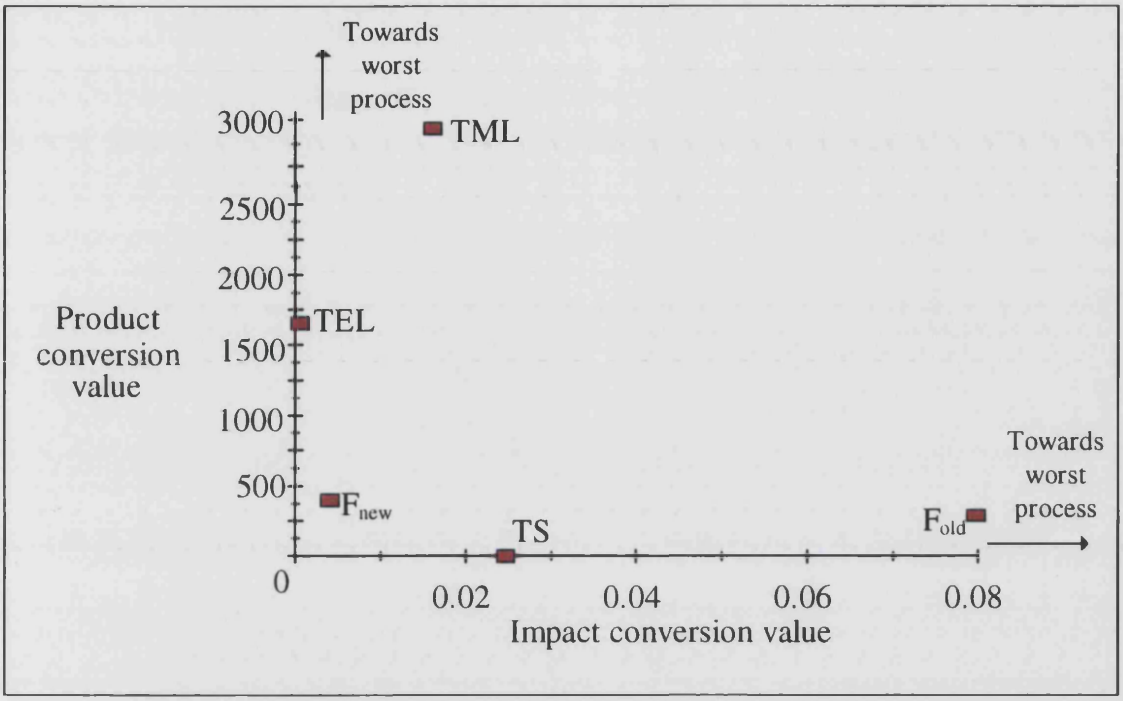


Figure 9.1: Product and impact conversion comparisons for the five processes

The best processes in terms of both product and impact conversion lie in the bottom left of the graph. That is, they should have good product conversion (low product conversion value) and low impact conversion. The worst processes lie at the top right of the graph. These have high product conversion values and high impact conversion values. For those processes located at the top right area of the graph the aim must be initially to move towards the left to reduce the impact conversion value and then look at conversion improvements to move down the product conversion value axis.

9.4 Environmental performance

In the previous sections each process has been studied and compared with the others based on the process comparison methods derived for the EPPT. The values derived from the comparison methods provide the information required to assess the environmental performance of the process. In this section the comparison methods are summarised into an environmental performance profile for each process. This environmental performance profile gives the values for each comparison method and can be used to assess the overall environmental performance of a process. The values environmental performance profile for an ideal process will all have comparison method values of zero.

Environmental performance profile
Ideal process

Environmental impact value	0
Environmental selectivity value	0
Product conversion value	0
Impact conversion value	0

Figure 9.2: Environmental performance profile of an ideal process

The environmental performance profile for the five processes are given in Table 9.7. The processes at the top of the table are those which have the least impact according to the comparison method. Those at the bottom of the table have the most impact.

Table 9.7: Summary process comparison values for each method

Rank	Environmental impact value	Environmental selectivity value	Product conversion value	Impact conversion value
1	TS $1.6\text{x}10^{4}$	TS $9.4\text{x}10^{-3}$	TS 0.39	TEL $4.3\text{x}10^{-4}$
2	TEL $2.0\text{x}10^{4}$	TEL 0.71	F_{old} 314.3	F_{new} $4.3\text{x}10^{-3}$
3	F_{new} $2.3\text{x}10^{5}$	F_{new} 1.6	F_{new} 385.7	TML $1.6\text{x}10^{-2}$
4	TML $1.1\text{x}10^{6}$	F_{old} 25.0	TEL 1642.8	TS $2.4\text{x}10^{-2}$
5	F_{old} $3.5\text{x}10^{6}$	TML 47.8	TML 2913.0	F_{old} $8.0\text{x}10^{-2}$

Assigning a rank to each of the values for each of the processes in the comparison gives an indication of the overall process environmental performance. With an equal weighting assigned to each comparison method the rank order of each comparison method for each process can be summed to provide a means of ranking the process in terms of overall environmental performance. The rank orders have been assigned and summed in Table 9.8. The process with the lowest sum of rank order has the best overall environmental performance and the process with the highest rank order has the worst overall environmental performance according to the EPPT.

Table 9.8: Ranking processes on environmental performance

Process	Environmental impact	Environmental selectivity	Product conversion	Impact conversion	Σ rank order
TS	1	1	1	4	7
TEL	2	2	4	1	9
F_{new}	3	3	3	2	11
F_{old}	5	4	2	5	16
TML	4	5	5	3	17

From Tables 9.7, the comparison method scores, and 9.8, the rank order of the processes, an assessment of the environmental performance of each process using the EPPT can now be determined.

9.4.1 Thomas Swan's Pepton process

Thomas Swan's Pepton process is identified by the EPPT as having the best environmental performance of the five processes under study. However, there is always scope for improvement in environmental performance. Thomas Swan's Pepton process has the lowest environmental impact value of the processes but the company should aim to lower this score towards zero - the ideal process. Process Option 5, the removal of Chemical B to prevent Chemical F formation (as discussed in Chapter 8), would reduce the environmental impact value. Thomas Swan's Pepton process also has the best (lowest) environmental selectivity value but this could still be improved (reduced) through the reduction in emission (environmental impact value) score. Thomas Swan's Pepton process also has a good process conversion value. This is a result of the low input score being converted into a high scoring product. However a high scoring product being created from low scoring inputs may suggest that high scoring emissions are generated. This is shown in the low impact conversion value.

From this assessment Thomas Swan's Pepton process has a fairly good environmental performance but to improve this they should consider reducing emissions as a first priority. Some consideration of improving conversion would also be beneficial to environmental performance. This may be achieved by converting the stage 1 product which is released to effluent treatment (Section 8.3.1) into product, thereby improving product conversion and reducing the emissions score which would also reduce the environmental impact value, improve environmental selectivity and reduce impact conversion. However, the environmental impact of process options to recover the stage 1 product would need to be evaluated using the EPPT to ascertain if the benefits of stage 1 recovery outweigh the additional impacts on the environment.

9.4.2 Associated Octel's tetra ethyl lead process

The TEL process is ranked second in terms of environmental performance. The TEL process has scored fairly well in terms of environmental impact. However improvements can always be made. The large amount of recycling and recovery makes a large contribution to the relatively low environmental impact value. The TEL process has a fairly good ranking in terms of environmental selectivity. This is because the product has a fairly low score. To improve the environmental selectivity value a reduction in the emissions would be necessary. The TEL process has a relatively poor product conversion value indicating that a low percentage of the input score is transformed into product score. Looking at measures to improve product conversion would improve the environmental performance of this process. The TEL process is ranked highest and therefore best out of the five processes in impact conversion score. This is due to the large amount of recycling and recovery in the process.

To improve the overall performance of the TEL process the primary consideration is to improve product conversion. Options to improve product conversion would need to be evaluated by the EPPT to ensure the environmental impact of the process is not increased. Improved product conversion would reduce the potential for emissions and therefore provide a route for improved environmental performance.

9.4.3 Fisons sodium cromoglycate processes

The proposed new sodium cromoglycate process operated by Fisons lies third in the ranking of environmental performance of the five processes under study. This is one place above the old sodium cromoglycate process. The environmental impact value of the proposed new process is significantly improved on the old process due to the pollution abatement and recycling strategies employed to achieve BPEO in the new process. However Fisons should still aim to reduce the environmental impact of the new process. This could be achieved by reducing the emissions from stages 2 to 4 of the process, as identified in Section 9.1 using the EPPT. Reducing the emissions would also improve the product conversion value of the proposed new process, which is already a significant improvement on the existing one. The product conversion in the new process is however slightly reduced than that of the existing one. As explained in Section 9.4.4 this is due to the increased inputs required to provide the increased quantity of the stage 4 product entering the improved latter stages of the process. Ways of improving conversion of inputs into outputs are required to improve environmental performance. It is likely that these will be achieved with the new changes proposed for the initial stages of the process. The impact conversion is significantly reduced from the old to the proposed new process. This is due to the reduction in emissions from the abatement and recycling strategies. The emissions however could still be significantly reduced with the improvements to stages 1 to 4.

Thus the proposed new process will have significantly improved environmental performance compared with the existing one. However, improvements are required to reduce emissions from the initial stages and also improve product conversion.

9.4.4 Associated Octel's tetra methyl lead process

The TML process operated by Associated Octel has the worst environmental performance of the five processes studied. The TML process has a high environmental impact which could be significantly reduced. The impact of this process is more than that of the TEL process as the alkyl chloride used in manufacture is gaseous rather than liquid. Thus the TML process requires alternative recovery equipment and a means of dealing with gaseous emissions. From the IPC application the inclusion of a scrubber to treat gaseous emissions is not detailed and thus it is considered that the methyl chloride that is not recovered is released to the atmosphere. It is the release of the methyl chloride which causes the significant difference between the impact of the TEL and TML processes. The TML process has a relatively poor environmental selectivity due to the high emission (environmental impact) score associated with the production of a relatively low scoring product. Again reduction of emissions would improve the environmental selectivity value and environmental performance. Like the TEL process, the TML process has poor product conversion. The conversion of inputs into outputs is an aspect of this process which should be considered to improve environmental performance. Due to the recycling and recovery associated with this process a moderate ranking in terms of impact conversion resulted. Again the reduction of emissions could improve this.

The TML process has relatively poor environmental performance. The conversion of inputs into product is the main area for concern. Consideration also needs to be given to reducing the gaseous emissions from the TML process whether through recycling/recovery or pollution abatement. There is indication for improvements to VOC control to these processes in the IPC application. However there is no indication of how or when these improvements may be carried out.

9.5 Summary

In this chapter the novel comparison methods derived for the EPPT have been described and applied to the five processes outlined in this thesis. Each method has a specific meaning which provides an insight into the environmental performance of each process. It is envisaged that companies operating processes will use the EPPT and its comparison methods as a means of improving their own environmental performance and as a means of comparing their processes with those of their competitors.

10. Conclusions and further work

The need for a tool to assess the environmental impact of chemical processes has been emphasised by industry, academics and government. Efforts have been made by each of these groups to develop a method to assess environmental impact of chemical processes, however each method has received criticism to some degree. The EPPT has been developed considering the benefits and limitations of existing techniques and has incorporated recommendations for improvements to existing techniques. Thus a tool has been developed which is capable of producing a reproducible and consistent measure of environmental impact. The EPPT provides a novel method to determine the Best Environmental Option. This can be compared with cost analysis to aid in the determination of Best Practicable Environmental Option, a requirement for IPC authorisation.

10.1 Conclusions

This thesis has described the development of the Environmental Process Performance Tool, an environmental assessment tool for batch chemical processes. The aims of the EPPT, as set out in Chapter 3, are to:

1. encompass a wider scope to environmental assessment than current environmental impact index techniques;
2. adopt an integrated approach to environmental assessment;
3. provide a method to determine the Best Environmental Option for a process;
4. provide a means of identifying opportunities for minimising environmental impact;
5. provide a method of comparing processes within and between companies.

Having evaluated existing environmental impact indices and techniques of environmental assessment the scope for the EPPT was defined. The EPPT incorporates aspects of environmental load factors, chemical scoring systems and life cycle assessment. It also considers the recommendations from Elliott (1997) for the inclusion of an energy component. Like EniVal (Elliott, 1997), the EPPT uses mass of chemicals released to assess environmental impact rather than concentration.

With the exception of EniVal (1997) integrated approaches to environmental assessment are rather limited. Of the few multi-media environmental indices that do exist the summation of the impact to each medium to represent the environment is the extent of integration. Elliott's equilibrium fate model for organic chemicals and the inorganic models used in EniVal (1997) have been used to provide an integrated multi-media approach to the EPPT. The fractions derived from these models give the proportion of the chemical in each medium. These model fractions are used in the chemical evaluation.

The environmental impact of each chemical is derived using parameters to represent the toxicity, persistence and effect of each chemical on air, water and soil. To provide a true representation of the environment the impact on the ecosystem needed to be considered. It was the aim of the chemical assessment to represent the toxicity of each chemical on selected micro-organisms, invertebrates and vertebrates from the animal kingdom and algae, monocotyledons and dicotyledons of the plant kingdom. However, sufficient data was not available to represent each of these categories in air, water and soil and therefore the most suitable of the readily available data is used to represent the categories. The persistence of each chemical is represented by degradation and bioconcentration. The effects of the chemicals on each of the media are represented by parameters which are of global, regional and local concern.

To determine the impact of a chemical each of the parameters was evaluated using a scoring system. Each scoring system ranges from 0 to 10 for the toxicity and effect parameters and from 1 to 10 for the persistence parameters. The scoring systems were derived from extensive literature, from existing scoring systems and have been refined by cross-referencing the known effects of chemicals on species and parameters and similar chemicals.

To provide an integrated approach a release score and a long-term score are derived for the emissions of each chemical to each medium. These are combined with a media fraction derived from Elliott's environmental fate models, combined together and normalised giving three chemical scores for each chemical, a chemical score for release to air, a chemical score for release to water and a chemical score for release to soil. All chemical scores lie in the range of 0 and 100.

Assessment factors have been included in the EPPT chemical evaluation to provide a means of determining the accuracy of the score assigned to the chemical. The data used to determine the score for each parameter for each chemical has been evaluated using assessment factors which, like the chemical scores, range from 0 to 100. The chemical assessment factors are not used in the process evaluation but they provide a means of highlighting any weakness in the chemical score due a lack of data. The assessment factors have been incorporated to encourage further toxicity testing which would provide more accurate results in the chemical evaluation and therefore in the EPPT.

The chemical scores are combined with the mass of chemicals to determine the environmental impact of chemicals processes, process options and also to determine the environmental performance of processes. The mass and chemical scores are combined using the inverse logarithm to the base 10 of the chemical score divided by 10. The unit of production is 1000kg. The combination method is a modification of the method used in EniVal which had been analysed for the range and spread of values, errors and sensitivity.

The chemical scores have also been used in the EPPT to derive a comparable score for the use of electricity, cooling water and steam in order for process options to be analysed. Often, processes are changed to decrease the environmental impact of the chemicals released by using more electricity, heating or cooling water. These utility assessments have been used with process options generated for Thomas Swan's

Pepton process to determine the Best Environmental Option. The options which reduced the environmental impact of the process have been suggested to Thomas Swan who are considering their implementation.

The EPPT can also be used to identify opportunities where process improvements could be made. This has been carried out on Thomas Swan's Pepton process and highlighted a major component of the environmental impact arising from a feed contaminant. An option to reduce the impact from the feed contaminant has been evaluated. A way of dealing with this contaminant was also highlighted by the erstwhile HMIP as being an area which would reduce environmental impact. The EPPT was also used to evaluate Fisons sodium cromoglycate process. Fisons have been improving their process to achieve BPEO. The EPPT was used to highlight areas where improvement could be made and where improvements should have perhaps been prioritised over previous improvements.

Combining chemical scores with input, product and emission masses has provided the basis for process comparisons from which environmental performance can be evaluated. Environmental performance is evaluated using four novel comparison techniques: environmental impact comparison, environmental selectivity comparison, product conversion and impact conversion. The environmental impact comparison considers the impact of the emissions per 1000kg of product. The higher the environmental impact value the more polluting the process. The environmental selectivity comparison considers the score of the emissions compared with the score of the product. The product conversion comparison considers how well the process convert input into product and the impact conversion comparison considers how the process converts inputs into emissions. Ideally each of the comparison values should be zero. The values determined for these comparison techniques can then be ranked. The rank order is then summed to determine the process with the best relative environmental performance.

Thus to conclude, unlike the majority of existing techniques the EPPT provides an integrated multimedia approach to environmental impact assessment. It uses the more readily available mass rather than concentration data on which to base its assessment. To address the criticisms of tools such as the Environmental Load Factor (Caughlin, 1993) which are based solely on the mass of emissions and Searle's environmental index (Coates, 1994) which is independent of production, the EPPT combines both mass (in terms of discharge ratio) and impact data of chemicals to provide a realistic contribution of each chemical to overall impact. Unlike existing indices the EPPT also considers the use of utilities and their environmental impact when evaluating process options.

The EPPT provides consistent and reliable results to assess the environmental impact of batch chemical processes. Due to the design of the EPPT it is equally capable of providing consistent and reliable results for continuous chemical processes. Not only does the EPPT assess the environmental impact of chemical processes and process options it can also be used to highlight areas of high environmental impact and hence provide focus for impact minimisation options to be investigated. The EPPT also provides a novel technique to compare chemical processes in terms of environmental performance and hence provide a stimulus for improved environmental performance.

10.2 Further work

Environmental assessment is complicated and subjective. No matter what analysis is carried out there is always an argument to counter the results. The subjectivity is also a major issue, as discussed in Chapter 4, both from an ecotoxicologist's point of view through the use of single organisms to represent groups of species or even ecosystems and also through the combining of unrelated parameters which includes the subjectivity of weighting parameters. This research has attempted to provide a way forward to assessing chemical processes and process options. It is not without potential criticism on a number of issues but it does provide a foundation on which further work can be built and improvements made.

A major consideration when developing the EPPT was the lack of data. Any improvements or initiatives to develop assessment techniques and encourage the environmental assessment of chemicals would be beneficial. This would enable the incorporation of more realistic parameters into the chemical assessment to at least provide the basic representation to the plant and animal kingdom. More detailed physical data would also be beneficial to improve the results of Elliott's environmental fate model and perhaps use the more detailed and accurate dynamic models such as those developed by Wania and Mackay (1995).

The current chemical evaluation assesses chemicals on their individual impact. However, most waste streams contain numerous chemicals often with synergistic, antagonistic or additive effects. The Environment Agency is currently undertaking research into the direct toxicity assessment of waste streams rather than looking at individual chemicals. In the future, perhaps results from direct toxicity assessment could be combined in the EPPT to assess the environmental impact of waste streams more accurately.

Further utilities assessments would also enhance the EPPT and would allow a direct comparison between, for example, the use of gas or nuclear fuel to generate electricity.

The pollution abatement considerations discussed in Chapter 6 have some very gross assumptions. This is an area which could be significantly improved to increase the accuracy of the EPPT evaluation. Further investigation of the emissions arising from landfill are necessary for a more accurate EPPT evaluation. There is also a need to evaluate scrubbers using the EPPT. In the options evaluated in this thesis it was assumed releases were directly to atmosphere. Evaluation of the inputs, in terms of gaseous process stream and additional inputs, and gaseous and aqueous outputs are needed. If specific scrubber data is available for a process this would provide the best environmental impact assessment. However a generalised scrubber model could be developed which, for example, would indicate that 80% of the organics are removed to the aqueous stream, 90% of the acidic gases are removed to the aqueous stream etc.

There is also a need to evaluate effluent treatment plants in a similar way to scrubbers. A specific effluent treatment plant has been evaluated for use in the Associated Octel tetra alkyl lead processes. For other processes it was assumed that there were no additional inputs to the effluent treatment plant. Water and non-metallic inorganic salts were discharged to controlled waters, metallic inorganic salts were sent to landfill, 90% of organics were degraded in the effluent treatment plant, the remaining 10% was sent to landfill, and there were no emissions to air. These general assumptions need to be improved by evaluating effluent treatment plants in more detail using the EPPT. As with scrubbers the most accurate results would be obtained from the evaluation of process specific abatement technology.

The use of the EPPT could be made simpler to use if it were developed into a computer package incorporating the chemical database, environmental fate model, derivation of the chemical score and also linking it to a process simulation package so that the environmental impact of process options could be evaluated automatically. The chemical database developed for the EPPT could be improved by programming the scoring systems for each parameter into the database. This would then allow the chemical scores to be assigned by the computer. The chemical scores could then be linked with the environmental fate models to a spreadsheet in order that the chemical scores for each medium could be calculated by the computer. This would save time and limit the likelihood of human error. The chemical score could then be assigned directly to the emissions arising from the process simulation to determine the environmental impact of that option.

It is also envisaged that an assessment of the environmental performance of the company could be combined with the environmental performance of the process. An environmental audit could be undertaken within the company looking at the environmental performance in terms of energy saving, recycling and waste minimisation strategies and the use of design approaches to minimise waste such as those developed by Houghton (1998). These would be evaluated and used in conjunction with the environmental performance profile to provide an environmental performance profile of the process and the company.

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APPENDIX 1

Bioconcentration factor derivation

Bioconcentration factor derivation

The bioconcentration factor (BCF) is used to evaluate the bioaccumulation tendency of a chemical. The BCF gives an indication of the amount of chemical that is likely to accumulate in organisms. The BCF is expressed as:

$$\text{BCF} = \frac{\text{Concentration of chemical at equilibrium in the organism (wet weight)}}{\text{Mean concentration of the chemical in the water}} \quad \text{....... Equation A1.1}$$

The bioconcentration factor is not always available. However bioconcentration can be calculated using solubilities, octanol-water partition coefficients and soil adsorption coefficients. These parameters are usually available or can be derived from experimentally derived correlations.

The octanol-water partition coefficient, K_{ow}, provides a measure of how a chemical will partition itself between an organic phase and water and consequently an indication of how a chemical will be taken up by an organism. K_{ow} values range from 10^{-3} to 10^{7}. Chemicals with a K_{ow} of less than 10 tend to be hydrophilic with a low bioconcentration factor. The dimensionless octanol-water partition coefficient is defined as:

$$K_{ow} = C_O / C \quad \text{....... Equation A1.2}$$

where C_O = concentration of the chemical in octanol in mg/l or μg/l, and
C = concentration of the chemical in water in mg/l or μg/l

The octanol-water partition coefficient can be derived from correlations using the organic carbon coefficient as shown in Table 4.16. The organic carbon coefficient, K_{oc}, is defined as:

$K_{oc} = C_c/C$ .... Equation A1.3

where C_c = concentration adsorbed (μg adsorbed/kg organic carbon, or ppb)

K_{oc} can also be estimated from K_p, the soil adsorption coefficient:

$K_{oc} = K_p/f_{oc}$ .... Equation A1.4

where f_{oc} = fraction of organic carbon in the soil (dimensionless)

The soil adsorption coefficient measures the tendency of a chemical to be adsorbed by soil or sediment and is defined as:

$K_p = X / C$ .... Equation A1.5

where X = concentration of soil in ppb or μg/kg, and

C = concentration in water in ppb or μg/kg

Table A1.1: Correlations between K_{oc} and chemical properties (LaGrega, 1994)

Class of chemical	Number of chemicals	Equation	Remarks
Pesticides	45	log Koc = 0.544 log Kow +1.377	
Aromatics	10	log Koc = 1.00 log Kow -0.21	
Chlorinated hydrocarbons	15	log Koc = -0.577 log S + 4.277	S in μmol/l
Aromatics	10	log Koc = -0.54 log S + 0.44	S in mole fraction
Pesticides	106	log Koc = -0.55 log S + 3.64	S in mg/l
Not stated	-	log Koc = 0.681 log BCF + 1.963	

APPENDIX 2

Database references

EPPT chemical database data source references

Source number	Reference
1	IRPTC database, UNEP 1990
2	Health and safety executive, 1994, EH40/94 Occupational exposure limits 1994, Her Majesty's Stationary Office, UK
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16	UK Terrestrial Effects Review Group, 1988, The Effects of acid deposition, HMSO , London
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20	CemoS, Computer database from Wagner, J.O. et al, 1996, Guidelines for selection of applications of fate and exposure models, Environmental Science and Pollution Research, 3 (1) pp 47-51
21	World Health Organisation, 1987, Air Quality Guidelines for Europe.
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APPENDIX 3

List of chemicals on the EPPT chemical database

CAS number	Chemical name
10102-44-0	Nitrogen oxides (to represent NOx)
106-42-3	Para-xylene
106-89-8	Epichlorohydrin
106-97-8	Butane
1067-53-4	Tris(3,6 DioxaHeptyl)amine
108-10-1	Isobutyl methyl ketone
108-24-7	Acetic anhydride
108-46-3	Resorcinol
108-88-3	Toluene
109-66-0	Pentane
120-75-2	2-Methyl benzthiazole
124-38-9	Carbon dioxide
127-09-3	Sodium acetate
1305-78-8	Calcium oxide
1310-73-2	Sodium hydroxide (solution)
1327-53-3	Arsenic trioxide
1333-74-0	Hydrogen
135-57-9	2,2 dibenzamido diphenyl disulphide (Pepton)
141-53-7	Sodium formate
141-97-9	Ethyl acetoacetate
1411-88-4	2,2 diamino diphenyl disulphide (Stage 2 Product)
144-55-8	Sodium bicarbonate
15826-37-6	Sodium chromoglycate
21645-51-2	Aluminium hydroxide
497-19-8	Sodium carbonate
50-00-0	Formaldehyde
532-32-1	Sodium benzoate
62-53-3	Aniline
630-08-0	Carbon monoxide
64-17-5	Ethanol
64-19-7	Acetic acid
67-56-1	Methanol
67-64-1	Acetone
67-66-3	Chloroform
71-43-2	Benzene
74-82-8	Methane
74-84-0	Ethane
74-85-1	Ethylene
74-87-3	Methyl chloride
7429-90-5	Aluminium
7439-89-6	Iron
7439-92-1	Lead
7439-95-4	Magnesium
7439-96-5	Manganese
7439-97-6	Mercury

7440-02-0	Nickel
7440-23-5	Sodium
7440-38-2	Arsenic
7440-43-9	Cadmium
7440-44-0	Particulates
7440-47-3	Chromium
7440-50-8	Copper
7440-66-6	Zinc
7440-70-2	Calcium
7446-09-5	Sulphur dioxide
7446-70-0	Aluminium chloride
75-00-3	Ethyl chloride
75-74-1	Tetramethyl lead
7553-56-2	Iodine
7631-86-9	Silica
7631-99-4	Sodium nitrate
7647-01-0	Hydrochloric acid
7647-14-5	Sodium chloride
7664-93-9	Sulphuric acid
7681-52-9	Sodium hypochlorite
7681-57-4	Sodium metabisulphite
7697-37-2	Nitric acid
7720-78-7	Iron sulphate
7722-84-1	Hydrogen peroxide
7726-95-6	Bromine
7727-37-9	Nitrogen
7732-18-5	Water-steam
7732-18-5	Water
7732-18-5	Heated water - Cooling water etc
7757-82-6	Sodium sulphate
7778-18-9	Calcium sulphate
7782-42-5	Graphite
7782-44-7	Oxygen
7782-50-5	Chlorine
78-00-2	Tetraetyl lead
93-98-1	Benzanilide (Benzamide-N-Phenyl)
95-16-9	Benzthiozole
95-53-4	o-toluidine
95-92-1	Diethyl oxalate (partitions & score - oxalic acid)
98-88-4	Benzoyl chloride
98-95-3	Nitrobenzene
No CAS No.	Sodium 2-aminothiophenate (Stage 1 Product)
No definite CAS No	Methyl benzanilide (data as benzanilide)

APPENDIX 4

Elliott's equilibrium fate model equation derivations

Elliott's equilibrium fate model equation derivation

Elliott model is based on a global mass balance where:

$$V_Tc_T = V_Ac_A + V_Wc_W + V_Sc_S \qquad \text{....... Equation A4.1}$$

where:

V_i = the volume of system i in m^3

c_j = concentration of pollutant j in moles/m^3

Subscript A = in air

Subscript W = in water

Subscript S = in soil

Subscript T = in total system

Equation A4.1 is simplified to:

$$V_Tc_T = V_T(ac_A + wc_W + sc_S) \qquad \text{....... Equation A4.2}$$

where:

a = atmosphere volume fraction

w = water volume fraction

s = soil volume fraction

Which gives:

$$c_T = ac_A + wc_W + sc_S \qquad \text{........ Equation A4.3}$$

Expressions also required for this model are the equilibrium equations for the air-water and soil-water subsystems. These are Henry's Law and the linear soil adsorption isotherm respectively.

$$c_W = K_w c_A \qquad \text{....... Equation A4.4}$$

$$c_S = d\, f_{oc}\, K_{oc}\, c_W \qquad \text{....... Equation A4.5}$$

where:

K_w = the inverse of Henry's Law constant

d = the soil density

f_{oc} = the fraction of organic carbon in the soil

K_{oc} = organic carbon coefficient

Equations A4.3 to A4.5 can be solved to give the fraction of a pollutant in each sub-system. Thus:

Fraction of chemical in the air:

$$F_a = \frac{a}{(a + wK_w + sdf_{oc}K_{oc}K_w)} \qquad \text{...... Equation A4.6}$$

Fraction of chemical in the water:

$$F_w = \frac{w}{\left(\frac{a}{K_w} + w + sdf_{oc}K_{oc}\right)} \qquad \text{....... Equation A4.7}$$

Fraction of chemical in the soil:

$$F_s = \frac{sdf_{oc}K_{oc}}{\left(\frac{a}{K_w} + w + sdf_{oc}K_{oc}\right)} \qquad \text{....... Equation A4.8}$$

APPENDIX 5

Comparison of Elliott's and Neely's distribution model volume fractions

Comparison of Elliott's and Neely's volume fractions

Table A5.1 shows a comparison of Elliott's and Neely's volume assessment. Whilst the actual volumes between the approaches are not directly comparable the volume fractions derived in Table A5.2 are.

Table A5.1: Comparison of Elliott's (1997) and Neely's (1981) volume assessments

	Elliott	**Neely**
Basis	Global volumes	Volumes related to area of 7 x $10^5 m^2$.
Air	Calculations are based on the combined height of the Troposphere and the Stratosphere. The Troposphere, in which the Earth's weather is contained, is 8km at the poles, 15 km at the equator and it contains 85% of the total atmospheric mass and almost all of the water vapour. The Stratosphere contains the ozone layer. Thus using a height of 53km for the atmosphere, the volume is calculated to be 2.7 x 10^{19} m^3.	Only the Troposphere is used with an average height of 10km, thus giving a volume of 7 x 10^{15} ml.
Water	The volumes of the oceans and seas (97% of all water), and fresh water (land ice, soil water, lakes and rivers) are combined together. An average depth for the oceans and seas of 3808m is used thus generating a volume of 1.4 x 10^{18} m^3.	A depth of 10m is used for calculating the water compartment. Thus the volume of the water compartment is 7 x 10^{12} ml.
Land	Soil is used for the land volume. An estimated 27% of the earth is covered with soil at an estimated 1m depth giving a volume of 1.4 x 10^{14} m^3.	Sediment is used as the land volume. Bottom sediments are assumed to be 3cm deep, density of 1.5 x 10^6 g/m^3. The weight of sediment is 3.15 x 10^{10}g.

Table A5.2 provides a summary of the volumes and volume fractions derived from each assessment.

Table A5.2: The volume and volume fractions derived by Elliott and Neely.

	Elliott		**Neely**	
	Volumes	Fraction	Volumes	Fractions
Air	2.73×10^{19} m^3	0.95	7×10^{15} ml	0.99
Water	1.35×10^{18} m^3	0.05	7×10^{12} ml	9.99×10^{-4}
Land	9.18×10^{13} m^3	3.2×10^{-6}	3.15×10^{10}g/ 1.5×10^{6} g/m^3 $= 2.1 \times 10^{4}$ m^3 $=2.1 \times 10^{10}$ ml	2.99×10^{-6}

Criticism can be made of the volumes used in both the Neely and Elliott models. Adopting a global overview was somewhat ambitious on Elliott's part due to the dynamic nature of chemical distribution in the environment. Most existing models are based on a smaller unit area, in Neely's case 7×10^5m^2. When considering the size of the study unit used by any model care must be made to ensure that the volumes associated with the study unit are on the same relative scale. Elliott's volumes are more consistent with regard to scale than those of Neely.

When considering the air sub-system, the majority of interactions in the air, with the exception of ozone depletion, take place in the Troposphere. This is where the Earth's weather is contained. The troposphere ranges from 8 to 15 km from the Earth's surface. The Stratosphere considered by Elliott is 53km above the Earth's surface. It could be argued that Elliott's air volume is over-estimated and Neely's estimate considering only the Troposphere is more accurate.

When considering the water volumes Elliott's model, considering the Earth as a whole, accounts for marine water as well as freshwater with a depth of almost 4km. Neely's 10m estimate of water depth is very low especially considering the majority of water on the Earth is in the ocean. Neely's estimate of water depth is not on the same scale as the air.

The majority of soil on the Earth is 15cm deep. Elliott's estimate of 1m depth is rather large and Neely's estimate is low at 3 cm.

To improve the Elliott and Neely volume fractions new model volumes were considered. In the air media, the impact of a chemical on the atmosphere is considered to be 10km above the Earth, thus avoiding the extremities of the Stratosphere. In the water media, Elliott's 4km depth of water was considered appropriate. This is comparable with the impact on the atmosphere without considering the absolute depths of the ocean which would be as extreme as considering the stratosphere in air. In the soil media, the average depth of soil is 15cm. However the influence of chemicals penetrating deeper in to the Earth and reaching aquifers is well-known. Thus, in order to keep the soil sub-system on the same relative level as the air and water sub-systems, Elliott's estimation of 1m depth has been retained. These changes gave rise to the volumes and volume fractions shown in Table A5.3.

Table A5.3: Suggested volumes and volume fractions for consideration

	Volume	Fraction
Air	5.11×10^{18} m^3	0.79
Water	1.35×10^{18} m^3	0.21
Soil	9.18×10^{13} m^3	1.4×10^{-5}
Total		1.00

These fractions were evaluated using chemicals tested by Elliott. They were also compared with a recent source of data (Croner's, 1997) detailing the significant long-term chemical compartments. The significant compartments detailed by Croner's were derived using Mackay's equilibrium model with a theoretical world of 1km x 1km x 6km and expert opinion. The application of Elliott's model using the suggested volume fractions in Table A4.3 were not reflected in the significant compartments detailed in Croner's. Elliott's test chemicals were also evaluated using Elliott's volume fractions against Croner's assessment of significant compartments. In the majority of cases Elliott's model using the Elliott's fractions identified the same significant compartments. Hence, for the purpose of the EPPT the distribution model and volume fractions assigned by Elliott has been used in this study. The results of the model have also been compared with Croner's (1997) assessment to ensure consistency.

APPENDIX 6

Summary of chemical scores and assessment factors

Summary of the chemical scores and assessment factors derived for the chemicals contained in the EPPT database

Chemicals have been ranked according to the mean of the chemical scores. Where blank cells appear in the table a chemical score has not been derived for this medium as there is no long-term impact associated with the chemical to that medium. The chemical is also unlikely to be released to that medium.

CAS number	Chemical name	Air		Water		Soil		Mean score
		Score	AF	Score	AF	Score	AF	
7732-18-5	Water			0.1	96.7			0.1
7782-44-7	Oxygen	0.1	87.6					0.1
1333-74-0	Hydrogen	0.1	73.3					0.1
7732-18-5	Water-steam	0.2	97.2					0.2
7732-18-5	Heated water - Cooling water etc	0.3	93.3	1.1	93.3			0.7
7440-23-5	Sodium			1.3	64.7			1.3
7727-37-9	Nitrogen	2.3	53.3					2.3
7757-82-6	Sodium sulphate			2.5	46.7	2.3	45.0	2.5
7647-14-5	Sodium chloride			2.5	57.7			2.5
497-19-8	Sodium carbonate			2.8	41.7			2.8
127-09-3	Sodium acetate			2.8	53.0			2.8
7631-99-4	Sodium nitrate			2.8	57.3			2.8
144-55-8	Sodium bicarbonate			2.8	44.7			2.8
7782-42-5	Graphite					3.1	48.1	3.1
141-53-7	Sodium formate			3.2	46.0			3.2
532-32-1	Sodium benzoate			3.2	53.0			3.2
7778-18-9	Calcium sulphate			3.6	32.1	3.6	30.8	3.6

CAS number	Chemical name	Air		Water		Soil		Mean score
		Score	AF	Score	AF	Score	AF	
1310-73-2	Sodium hydroxide (solution)			3.6	58.0			3.6
67-56-1	Methanol	4.9	74.0	4.3	65.0	3.7	65.4	4.3
7440-70-2	Calcium			4.3	70.7	4.3	70.8	4.3
7631-86-9	Silica			4.5	73.2	4.5	74.2	4.5
106-97-8	Butane	4.7	70.9					4.7
1305-78-8	Calcium oxide					4.8	45.4	4.8
141-97-9	Ethyl acetoacetate	5.5	47.8	5.4	48.0	5.1	45.1	5.3
67-64-1	Acetone	6.1	65.8	5.9	65.1			6.0
7720-78-7	Iron sulphate					6.9	33.9	6.9
74-84-0	Ethane	7.1	85.7					7.1
64-17-5	Ethanol	7.7	64.3	6.8	61.1			7.2
109-66-0	Pentane	7.4	71.4	7.3	61.6			7.4
124-38-9	Carbon dioxide	7.7	60.0	7.2	55.0			7.5
108-24-7	Acetic anhydride	7.6	60.8	7.4	48.6			7.5
108-46-3	Resorcinol	7.9	46.5	8.1	44.5	8.0	42.7	8.0
7681-57-4	Sodium metabisulphite			8.1	26.7			8.1
74-85-1	Ethylene	9.9	70.9	8.6	62.7			9.2
108-88-3	Toluene	9.5	88.6	9.8	86.6	9.3	85.9	9.5
64-19-7	Acetic acid	10.2	61.4	9.6	62.3			9.9
630-08-0	Carbon monoxide	9.9	80.5					9.9
106-89-8	Epichlorohydrin	10.1	57.6	9.9	63.4	9.7	57.0	9.9
7722-84-1	Hydrogen peroxide	9.8	69.2	10.4	57.7			10.1
108-10-1	Isobutyl methyl ketone	10.4	62.0	9.9	56.1			10.2
98-88-4	Benzoyl chloride	11.1	66.7	10.8	66.7	10.2	65.0	10.7
74-82-8	Methane	11.2	86.3	10.7	73.2	10.8	72.8	10.9
75-74-1	Tetramethyl lead	11.2	65.4	13.1	58.5	12.6	51.4	12.3

CAS number	Chemical name	Air		Water		Soil		Mean score
		Score	AF	Score	AF	Score	AF	
7681-52-9	Sodium hypochlorite			12.7	39.0			12.7
78-00-2	Tetraetyl lead	13.1	64.6	14.3	57.4	13.9	50.7	13.8
95-92-1	Diethyl oxalate (partitions & score - oxalic acid)	12.5	8.4	14.8	20.8	14.1	16.6	13.8
106-42-3	Para-xylene	13.7	83.6	14.2	83.1	13.7	78.9	13.9
7440-44-0	Particulates	14.9	74.4					14.9
7439-95-4	Magnesium			15.7	35.4	15.2	29.6	15.5
7647-01-0	Hydrochloric acid	15.9	58.6	16.3	47.0			16.1
95-53-4	o-toluidine	16.9	64.9	17.0	69.9	16.4	64.2	16.8
21645-51-2	Aluminium hydroxide					17.0	10.8	17.0
7664-93-9	Sulphuric acid			20.2	40.7			20.2
7697-37-2	Nitric acid			20.2	37.0			20.2
7553-56-2	Iodine	21.3	49.1					21.3
15826-37-6	Sodium chromoglycate			21.4	9.3			21.4
7782-50-5	Chlorine	21.9	56.9	21.9	55.7			21.9
75-00-3	Ethyl chloride	22.9	62.4	23.3	51.4	23.7	52.1	23.2
62-53-3	Aniline	23.5	72.7	23.9	65.6	22.5	66.7	23.3
50-00-0	Formaldehyde	24.1	65.3	24.4	60.0	23.2	57.3	23.9
7446-09-5	Sulphur dioxide	24.3	83.1	23.6	72.1			24.0
7446-70-0	Aluminium chloride			24.8	62.7	25.1	49.3	24.9
71-43-2	Benzene	25.3	74.9	25.1	75.0	25.3	71.1	25.2
7439-96-5	Manganese			26.2	43.2	25.5	29.6	25.9
10102-44-0	Nitrogen oxides (to represent NOx)	29.3	82.5	26.9	69.1			28.1
95-16-9	Benzthiozole	28.7	47.4	29.7	42.8	29.2	45.2	29.2
120-75-2	2-Methyl benzthiazole	29.5	46.8	30.5	44.1	30.3	45.8	30.1
7429-90-5	Aluminium			30.2	53.2	30.1	45.8	30.1
98-95-3	Nitrobenzene	30.0	63.0	30.9	57.5	30.3	51.6	30.4

CAS number	Chemical name	Air		Water		Soil		Mean score
		Score	AF	Score	AF	Score	AF	
No CAS No.	Sodium 2-aminothiophenate (Stage 1 Product)	30.9	47.9	31.1	31.6	31.1	34.4	31.0
1067-53-4	Tris(3,6 DioxaHeptyl)amine			31.3	16.0			31.3
1411-88-4	2,2 diamino diphenyl disulphide (Stage 2 Product)	31.8	47.9	32.0	31.6	31.9	34.4	31.9
93-98-1	Benzanilide (Benzamide-N-Phenyl)	31.3	34.1	32.2	19.3	32.2	26.2	31.9
No CAS No	Methyl benzanilide (data as benzanilide)	31.6	34.1	32.2	19.3	32.2	26.2	32.0
135-57-9	2,2 dibenzamido diphenyl disulphide (Pepton)	32.4	47.9	32.9	31.6	32.3	34.4	32.5
7440-38-2	Arsenic			33.7	64.6	33.9	59.6	33.8
7439-89-6	Iron			35.6	51.1	35.1	43.5	35.3
74-87-3	Methyl chloride	35.5	67.1					35.5
1327-53-3	Arsenic trioxide					35.7	72.7	35.7
67-66-3	Chloroform	39.1	59.5	38.7	58.3			38.9
7439-92-1	Lead			41.8	66.1	41.7	65.0	41.8
7439-97-6	Mercury					45.1	79.2	45.1
7440-47-3	Chromium			45.1	53.2	45.1	45.0	45.1
7726-95-6	Bromine	46.3	56.6	46.3	50.1			46.3
7440-66-6	Zinc			46.7	68.2	46.7	69.6	46.7
7440-50-8	Copper			51.5	64.6	51.7	64.2	51.6
7440-43-9	Cadmium					57.5	73.9	57.5
7440-02-0	Nickel			65.7	65.7	66.7	66.2	66.2

APPENDIX 7

Electrical energy calculations

Electrical energy calculations

Steam:

Powergen, 1995:

13×10^6 m^3 of steam produced when generating 13 terawatt hours of electricity

13×10^6 m^3 of steam produced when generating 13×10^9 kWh of electricity

How much steam is produced when generating 1kWh of electricity (in kilograms)?

Assume $1m^3$ of steam weighs 0.59kg at 1 bar (Perry, 1984)

1kWh of electricity generates :

$$\frac{13 \times 10^6 m^3 \text{ X } 0.59 kg/m^3}{13 \times 10^6} = 5.900 \times 10^{-4} \text{kg of steam}$$

Carbon dioxide:

Department of the Environment, 1994:

$51\text{x}10^6$ tonnes of CO_2 is generated when producing 298,469 GWh of electricity

$51\text{x}10^6$ tonnes of CO_2 is generated when producing $298{,}469\text{x}10^6$ kWh of electricity

$\frac{51\text{x}10^6 \text{ tonnes of } CO_2}{298{,}469\text{x}10^6}$ is generated when producing 1kWh of electricity

1.709×10^{-4} tonnes of CO_2 is generated when producing 1kWh of electricity

1.709×10^2 kg of CO_2 is generated when producing 1kWh of electricity

Methane:

Department of the Environment, 1994:

3000 tonnes of CH_4 is generated when producing 298,469 GWh of electricity

3000 tonnes of CH_4 is generated when producing $298{,}469\text{x}10^6$ kWh of electricity

$\frac{3000 \times 10^3 \text{ kg of } CH_4}{298,469\text{x}10^6}$ is generated when producing 1kWh of electricity

1.005×10^{-5} kg of CH_4 is generated when producing 1kWh of electricity

Sulphur dioxide:

Department of the Environment, 1994:

2,427,000 tonnes of SO_2 is generated when producing 298,469 GWh of electricity

2,427,000 tonnes of SO_2 is generated when producing $298,469\text{x}10^6$ kWh of electricity

$\frac{2,\ 427,000 \times 10^3 \text{ kg of } SO_2}{298,469\text{x}10^6}$ is generated when producing 1kWh of electricity

8.131×10^{-3} kg of SO_2 is generated when producing 1kWh of electricity

Particulates:

Department of the Environment, 1994:

25,000 tonnes of particulates is generated when producing $298,469\text{x}10^6$ kWh of electricity

$\frac{25000 \times 10^3 \text{ kg of Particulates}}{298,469\text{x}10^6}$ is generated when producing 1kWh of electricity

8.376×10^{-5} kg of Particulates is generated when producing 1kWh of electricity

Nitrogen oxides:

Department of the Environment, 1994:

694,000 tonnes of NO_x is generated when producing $298,469\text{x}10^6$ kWh of electricity

$\frac{694,000 \times 10^3 \text{ kg of } NO_x}{298,469\text{x}10^6}$ is generated when producing 1kWh of electricity

2.325×10^{-3} kg of Particulates is generated when producing 1kWh of electricity

Volatile organics compounds:

Department of the Environment, 1994:

12,000 tonnes of VOC's are generated when producing 298,469x10^6 kWh of electricity

$\dfrac{12{,}000 \times 10^3 \text{ kg of VOC's}}{298{,}469\text{x}10^6}$ are generated when producing 1kWh of electricity

4.021 x 10^{-5} kg of VOC's are generated when producing 1kWh of electricity

Carbon monoxide:

Department of the Environment, 1994:

45,000 tonnes of CO is generated when producing 298,469x10^6 kWh of electricity

$\dfrac{45{,}000 \times 10^3 \text{ kg of CO}}{298{,}469\text{x}10^6}$ is generated when producing 1kWh of electricity

1.508 x 10^{-4} kg of CO is generated when producing 1kWh of electricity

APPENDIX 8

Cooling water calculations

Cooling water calculations

These cooling water calculations are based on cooling tower data given in Coulson and Richardson, Volume 1 (1994). Figure A8.1 gives a simplistic diagram of water and air inputs and outputs to a cooling tower.

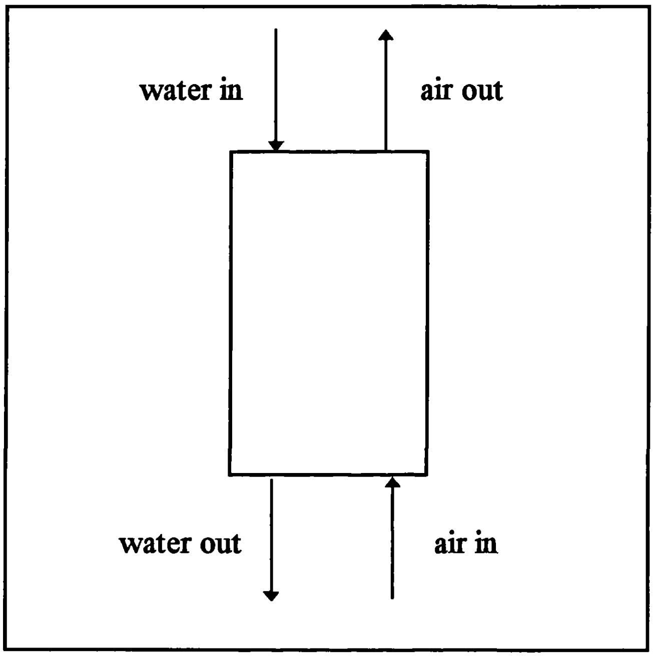

Figure A8.1: Simplistic diagram of a cooling tower

Typical flow rates:

Water in = 0.26 kg/m^{2}s

Air in = 0.897 m^3/m^{2}s x 1.245 kg/m^3 = 1.116 kg/m^{2}s (at temperature 20°C)

$\therefore$ 1 kg/m^{2}s air $\equiv$ 4.292 kg/m^{2}s water

or 0.233 kg/m^{2}s air $\equiv$ 1 kg/m^{2}s water

Assuming:

Water in at 30°C

Water out at 20°C

Average water temperature = 25°C

Air in at 20°C, 20% relative humidity = 0.003kg/kg

Air out at 25°C, 100% relative humidity = 0.02kg/kg

Inc in water, in air = 0.02 - 0.003 = 0.017 kg water/kg air

∴ Cooling 1 kg water from 30°C to 20°C

gives $0.017 \frac{\text{kg water}}{\text{kg air}} \times 4.292 \frac{\text{kg}}{\text{m}^2\text{s}} = 0.073$ kg steam

∴ ≈ 7.3% of water evaporated

APPENDIX 9

EPPT assessments of stages of:

Fisons - Existing sodium cromoglycate process

Fisons - Proposed new sodium cromoglycate process

EPPT stage assessment of Fisons existing sodium cromoglycate process

Inputs - OLD

Stage 1/2	kg/1000kg In	Added As:	Score	Kg X 10 E+(score/10)
Resorcinol	429.7	Solid	8.0	2729.9
Ethyl Acetonacetate	584.4	Liquid	5.4	2003.0
Sulphuric Acid	0.7	Liquid	21.2	98.7
Acetic Anhydride	871.3	Liquid	7.4	4799.4
IMS	4782.6	Liquid	6.7	22113.9
Water	9789.4	Liquid	0.1	9994.4
Ethanol				0.0
Acetic Acid				0.0
Stage 2 Product				0.0
Total	16458.2			41739.3

Outputs - OLD

Stage 1/2	Released to:	Mass released Kg	Score	Kg X 10 E+(score/10)	Impact Score when product and recovery are considered but no additional treatment	Treatment Category	Impact Score when product, recovery and additional treatment are considered
Resorcinol		0.0	8.0	0.0	0.0		
Ethyl Acetonacetate	Water	76.6	5.4	262.4	262.4	' org	26.2
Sulphuric Acid	Water	0.7	20.2	78.4	78.4	' inorg	78.4
Acetic Anhydride	Air	0.0	7.6	0.2	0.2	$	0.2
IMS	Recovered	4781.6	6.7	22109.1			
IMS	Air	1.0	6.7	4.7	4.7	$	4.7
Water	Water	9776.3	0.1	9981.0	9981.0	' inorg	9981.0
Ethanol	Water	179.7	6.8	856.1	856.1	' org	85.6
Acetic Acid	Water	789.6	9.6	7184.8	7184.8	' org	718.5
Acetic Acid	Air	1.1	10.2	11.1	11.1	$	11.1
Stage 2 Product	Product	851.6	12.1	13842.6			
Total				54330.4	18378.7		10905.7

Stage 3	kg/1000kg In	Added As:	Score	Kg X 10 E+(score/10)
Stage 2 Product	851.6	Liquid	12.1	13842.6
AlCl3	2729.4	Solid	25.1	879147.9
NaCl	343.9	Solid	2.5	604.6
Hydrochloric acid	386.5	Liquid	16.3	16638.9
Water	55133.2	Liquid	0.1	56287.7
HCl	0.0			0.0
Al salts	0.0			0.0
Stage 3 Product	0.0			0.0
Total	59444.5			966521.6

Stage 3	Released to:	Mass Released Kg	Score	Kg X 10 E+(score/10)	Impact Score when product and recovery are considered but no additional treatment	Treatment Category	Impact Score when product, recovery and additional treatment are considered
Stage 2 Product							
AlCl3	Offsite	2685.8	25.1	865102.7	865102.7	+	86510.3
NaCl	Offsite	363.9	2.5	639.7	639.7	+	64.0
Hydrochloric acid	Water	386.5	16.3	16638.9	16638.9	' inorg	16638.9
Water	Product	3274.2	0.1	3342.8			0.0
Water	Water	40927.7	0.1	41784.7	41784.7	' inorg	41784.7
Water	Offsite	10914.1	0.1	11142.6	11142.6	+	1114.3
HCl	Water	35.3	16.3	1519.6	1519.6	' inorg	1519.6
HCl	Air	0.0	15.9	1.3	1.3	$	1.3
Al salts	Offsite	25.8	21.0	3264.3	3264.3	+	326.4
Stage 3 Product	Product	851.6	14.0	21243.0			
Total				964679.7	940093.9		147959.5

Stage 4	kg/1000kg In	Added As:	Score	Kg X 10 E+(score/10)
Stage 3 Product	851.6	Liquid	14.0	21243.0
NaOH	1739.4	Liquid	3.6	4012.3
Sodium metabisulphat	1.2	Solid	8.1	7.6
Hydrochloric acid	2339.5	Liquid	16.3	100719.9
Water	8515.6	Liquid	0.1	8693.9
Acetone				0.0
CO2				0.0
NaCl				0.0
Stage 4 Product				0.0
Total	13447.2			134676.8

Stage 4	Released to:	Mass Released Kg	Score	Kg X 10 E+(score/10)	Impact Score when product and recovery are considered but no additional treatment	Treatment Category	Impact Score when product, recovery and additional treatment are considered
Stage 3 Product				0.0	0.0		
NaOH				0.0	0.0		
Sodium metabisulphate	Water	1.2	8.1	7.6	7.6	' inorg	7.6
Hydrochloric acid	Water	1545.9	16.3	66553.5	66553.5	' inorg	66553.5
Water	Product	154.4	0.1	157.7			0.0
Water	Water	9481.6	0.1	9680.2	9680.2	' inorg	9680.2
Acetone	Water	226.5	5.9	873.3	873.3	' org	87.3
Acetone	Air	0.0	6.1	0.1	0.1	$	0.1
CO2	Air	171.9	7.7	1016.7	1016.7	$	1016.7
NaCl	Water	1271.9	2.5	2235.9	2235.9	' inorg	2235.9
Stage 4 Product	Product	593.8	15.8	22730.2			
Total				103255.2	80367.3		79581.4

Stage 5	kg/1000kg In	Added As:	Score	Kg X 10 E+(score/10)
Stage 4 Product	593.8	Liquid	15.8	22730.2
Epichlorohydrin	181.7	Liquid	9.9	1787.5
MIBK	725.5	Liquid	9.9	7139.1
Sodium Carbonate	114.9	Solid	2.8	221.0
CO2	0.0			0.0
TDA-1	3.0	Solid	31.3	3990.1
IMS	7658.8	Liquid	6.7	35412.6
Water	5550.6	Liquid	0.1	5686.9
NaCl				0.0
Stage 5 Product				0.0
Total	14828.2			76947.5

Stage 5	Released to:	Mass released Kg	Score	Kg X 10 E+(score/10)	Impact Score when product and recovery are considered but no additional treatment	Treatment Category	Impact Score when product, recovery and additinal treatment are considered
Stage 4 Product							
Epichlorohydrin	Water	1.0	9.9	9.8	9.8	org	1.0
MIBK	Recovered	725.5	9.9	7139.1			
Sodium Carbonate	Water	11.4	2.8	22.0	22.0	inorg	22.0
CO2	Air	43.0	7.7	254.2	254.2	$	254.2
TDA-1	Water	3.0	31.3	3990.1	3990.1	inorg	3990.1
IMS	Recovered	7649.5	6.7	35369.8			0.0
IMS	Air	9.3	8.7	67.9	67.9	$	67.9
Water	Water	5568.2	0.1	5684.8	5684.8	inorg	5684.8
NaCl	Water	114.3	2.5	200.9	200.9	inorg	200.9
Stage 5 Product	Product	703.1	17.7	41212.8			
Total				93951.3	10229.6		10220.8

Stage 6	kg/1000kg In	Added As:	Score	Kg X 10 E+(score/10)
Stage 5 Product	703.1	Liquid	17.7	41212.8
Sodium metal	222.7	Solid	1.3	298.3
Hydrogen	0.0			0.0
Ethanol	4312.5	Liquid	6.8	20546.1
Diethyl Oxalate	1648.4	Liquid	14.8	49867.5
Chloroform	5768.2	Liquid	38.7	42564007.0
Water	12047.2	Liquid	0.1	12299.5
Hydrochloric acid	381.0	Liquid	16.3	16402.6
NaOH	181.1	Liquid	3.6	417.9
NaCl				0.0
IMS	5208.3	Liquid	6.7	24082.3
Stage 6 Product		Liquid		0.0
Total	30472.7			42728934.1

Stage 6	Released to:	Mass released Kg	Score	Kg X 10 E+(score/10)	Impact Score when product and recovery are considered but no additional treatment	Treatment Category	Impact Score when product, recovery and additinal treatment are considered
Stage 5 Product							
Sodium metal							
Hydrogen	Air	9.7	0.1	9.9	9.9	$	9.9
Ethanol	Recovered	2712.3	6.8	12922.2			
Ethanol	Water	1763.2	6.8	8400.6	8400.6	org	840.1
Ethanol	Air	16.7	7.7	97.9	97.9	$	97.9
Diethyl Oxalate	Product	15.6	12.2	259.9			
Diethyl Oxalate	Water	1062.5	12.2	17673.8	17673.8	org	1767.4
Diethyl Oxalate	Air	0.0	12.2	0.0	0.0	$	0.0
Chloroform	Recovered	5357.4	38.7	39532642.6			0.0
Chloroform	Air	410.8	0.7	486.0	486.0	$	486.0
Water	Water	12131.2	0.1	12385.2	12385.2	org	1238.5
Hydrochloric acid				0.0	0.0		0.0
NaOH	Water	150.9	3.6	348.0	348.0	org	34.8
NaCl	Water	610.6	2.5	1073.4	1073.4	org	107.3
IMS	Recovered	4894.8	6.7	22632.5			
IMS	Air	313.6	8.7	2297.9	2297.9	$	2297.9
Stage 6 Product	Product	1023.4	19.5	91846.3			
Total				39703076.1	42772.6		6879.7

Stage 7	kg/1000kg In	Added As:	Score	Kg X 10 E+(score/10)
Stage 6 Product	1023.4	Liquid	19.5	91846.2
Diethyl oxalate	15.6	Liquid	14.8	470.8
IMS	6904.9	Liquid	6.7	31927.2
Water	3155.7	Liquid	0.1	3221.8
NaOH	164.8	Liquid	3.6	380.2
Carbon	72.4	Solid	3.1	147.8
Ethanol	0.0			0.0
Sodium oxalate	0.0			0.0
Stage 7 product				0.0
Total	11336.9			127993.9

Stage 7	Released to:	Mass released Kg	Score	Kg X 10 E+(score/10)	Impact Score when product and recovery are considered but no additional treatment	Treatment Category	Impact Score when product, recovery and additinal treatment are considered
Stage 6 Product							
Diethyl oxalate							
IMS	Recovered	6506.9	6.7	30086.8			
IMS	Air	398.0	8.7	2916.7	2916.7	$	2916.7
Water	Water	3155.7	0.1	3221.8	3221.8	inorg	3221.8
NaOH					0.0		
Carbon	Land	72.4	3.1	147.8	147.8	&	14.8
Ethanol	Recovered	178.6	6.8	850.9			
Ethanol	Air	10.9	7.7	64.2	64.2	$	64.2
Sodium oxalate	Air	14.3	11.4	196.6	196.6	$	196.6
Stage 7 product	Product	1000.0	21.4	137720.9			
Total				175205.8	6547.1		6414.1

Stage 8	kg/1000kg In	Added As:	Score	Kg X 10 E+(score/10)
Stage 7 Product	1000.0	Liquid	21.4	137720.9
IMS	13845.0	Liquid	6.7	64016.7
Water	3335.0	Liquid	0.1	3404.8
Stage 8 product				0.0
Total	18180.0			205142.4

Stage 8	Released to:	Mass released Kg	Score	Kg X 10 E+(score/10)	mpact Score when product and recovery are considered but no additional treatment	Treatment Category	mpact Score when product, recovery and additinal treatment are considered
Stage 7 Product							
IMS	Recovered	11768.4	6.7	54414.6			
IMS	Air	2076.7	8.7	15218.2	15218.2	$	15218.2
Water	Water	3223.8	0.1	3291.3	3291.3	* Inorg	3291.3
Water	Air	111.2	0.2	115.9	115.9	$	115.9
Stage 8 product	Product	1000.0	21.4	137720.9			
Total				210761.0	18625.4		18625.4

* all liquid effluent with the exception of Al rich go to onsite effluent treatment. Organics are removed by bio-org to a level of 10%. The 10% is sent to landfill.

^ all recovered liquid are reused and not considered an output to the environment

+ Al rich liquid effluents are assumed to go to an offsite effluent treatment plant where removal is to a level of 10% and ultimate disposal is to landfill where they are scored 10% of the land score for that chemical

$ all gaseous emissions are assumed to be released to the atmosphere. In reality the acid emissions are scrubbed but there was insufficient data in the IPC application to enable the scrubber to be modelled

% contained in the product - not added to outputs

& Disposed of to land

EPPT stage assessment of Fisons proposed new sodium cromoglycate process

Inputs - NEW

Stage 1/2	kg/1000kg In	Added As:	Score	Kg X 10 E+(score/10)
Resorcinol	499.7	Solid	8.0	3174.7
Ethyl Acetonacetate	679.6	Liquid	5.4	2329.4
Sulphuric Acid	0.9	Liquid	21.2	114.8
Acetic Anhydride	1013.3	Liquid	7.4	5581.2
IMS	5561.7	Liquid	6.7	25716.3
Water	11384.1	Liquid	0.1	11622.5
Ethanol				0.0
Acetic Acid				0.0
Stage 2 Product				0.0
Total				48538.8

Outputs - NEW

Stage 1/2	Released to:	Mass released Kg	Score	Kg X 10 E+(score/10)	Impact Score when product and recovery are considered but no additional treatment	Treatment Category	Impact Score when product, recovery and additional treatment are considered
Resorcinol			8.0	0.0	0.0		
Ethyl Acetonacetate	Water	89.0	5.4	305.2	305.2	org	30.5
Sulphuric Acid	Water	0.9	20.2	91.2	91.2	inorg	91.2
Acetic Anhydride	Air	0.0	7.6	0.2	0.2		0.2
IMS	Recovered	5560.5	6.7	25710.8			
IMS	Air	1.2	6.7	5.5	5.5		5.5
Water	Water	11368.9	0.1	11606.9	11606.9	inorg	11606.9
Ethanol	Water	209.0	6.8	995.5	995.5	org	99.6
Acetic Acid	Water	918.2	9.6	8355.2	8355.2	org	835.5
Acetic Acid	Air	1.2	10.2	12.9	12.9		12.9
Stage 2 Product	Product	990.3	12.1	16097.6			
Total				63181.0	21372.7		12682.3

Stage 3	kg/1000kg In	Added As:	Score	Kg X 10 E+(score/10)
Stage 2 Product	990.3	Liquid	12.1	16097.6
AlCl3	3174.0	Solid	25.1	1022363.4
NaCl	399.9	Solid	2.5	703.0
Hydrochloric acid	449.4	Liquid	16.3	19349.5
Water	64114.6	Liquid	0.1	65457.1
HCl				0.0
Al salts				0.0
Stage 3 Product				0.0
Total				1123970.5

Stage 3	Released to:	Mass Released Kg	Score	Kg X 10 E+(score/10)	Impact Score when product and recovery are considered but no additional treatment	Treatment Category	Impact Score when product, recovery and additional treatment are considered
Stage 2 Product							
AlCl3	Offsite	3123.3	25.1	1006030.3	1006030.3		100603.0
NaCl	Offsite	399.9	2.5	703.0	703.0		70.3
Hydrochloric acid	Water	449.4	16.3	19349.5	19349.5	inorg	19349.5
Water	Product	3807.6	0.1	3887.3			0.0
Water	Water	47595.0	0.1	48591.6	48591.6	inorg	48591.6
Water	Offsite	12692.0	0.1	12957.8	12957.8		1295.8
HCl	Water	41.0	16.3	1767.1	1767.1	inorg	1767.1
HCl	Air	0.0	15.9	1.5	1.5		1.5
Al salts	Offsite	30.0	21.0	3796.1	3796.1		379.6
Stage 3 Product	Product	990.3	14.0	24703.6			
Total				1121787.8	1093196.9		172058.4

Stage 4	kg/1000kg In	Added As:	Score	Kg X 10 E+(score/10)
Stage 3 Product	990.3	Liquid	14.0	24703.6
NaOH	2022.7	Liquid	3.6	4665.9
Sodium metabisulphate	1.4	Solid	8.1	8.9
Hydrochloric acid	2720.6	Liquid	16.3	117127.4
Water	9902.8	Liquid	0.1	10110.2
Acetone				0.0
CO2				0.0
NaCl				0.0
Stage 4 Product				0.0
Total				156616.0

Stage 4	Released to:	Mass Released Kg	Score	Kg X 10 E+(score/10)	Impact Score when product and recovery are considered but no additional treatment	Treatment Category	Impact Score when product, recovery and additional treatment are considered
Stage 3 Product				0.0			
NaOH				0.0			
Sodium metabisulphate	Water	1.4	8.1	8.9	8.9	inorg	8.9
Hydrochloric acid	Water	1797.7	16.3	77395.3	77395.3	inorg	77395.3
Water	Product	179.6	0.1	183.3			0.0
Water	Water	11026.2	0.1	11257.1	11257.1	inorg	11257.1
Acetone	Water	263.4	5.9	1015.5	1015.5	org	101.6
Acetone	Air	0.0	6.1	0.1	0.1		0.1
CO2	Air	199.9	7.7	1182.4	1182.4		1182.4
NaCl	Water	1479.1	2.5	2600.2	2600.2	inorg	2600.2
Stage 4 Product	Product	690.5	15.8	26433.0			
Total				120075.8	93459.4		92545.5

Stage 5	kg/1000kg In	Added As:	Score	Kg X 10 E+(score/10)
Stage 4 Product	690.5	Liquid	15.8	26433.0
Epichlorohydrin	210.6	Liquid	9.9	2072.6
MIBK	856.6	Liquid	9.9	8429.2
Sodium Carbonate	133.3	Solid	2.8	256.3
CO2	0.0			0.0
TDA-1	3.5	Solid	31.3	4685.5
IMS	5968.7	Liquid	6.7	27598.0
Water	6739.2	Liquid	0.1	6880.3
NaCl				0.0
mpurities	319.5			
Stage 5 Product				0.0
Total				76354.9

Stage 5	Released to:	Mass released Kg	Score	Kg X 10 E+(score/10)	mpact Score when product and recovery are considered but no additional treatment	Treatment Category	mpact Score when product, recovery and additional treatment are considered
Stage 4 Product							
Epichlorohydrin	Water	0.5	9.9	5.2	5.2	org	0.5
MIBK	Recovered	856.6	9.9	8429.2			
Sodium Carbonate	Water	12.9	2.8	24.8	24.8	inorg	24.8
CO2	Air	50.0	7.7	295.6	295.6	$	295.6
TDA-1	Water	3.5	31.3	4685.5	4685.5	inorg	4685.5
IMS	Recovered	5900.2	6.7	27281.3			0.0
IMS	Air	1.4	8.7	10.3	10.3	$	10.3
IMS	Water	67.1	8.7	491.7	491.7	org	491.7
Water	Product	1.1	0.1	1.1	1.1		1.1
Water	Recovered	1931.7	0.1	1972.2			
Water	Air	21.4	0.2	22.3	22.3	$	22.3
Water	Water	4805.5	0.1	4906.1	4906.1	inorg	4906.1
NaCl	Recovered	11.2	2.5	19.6			
NaCl	Water	121.7	2.5	214.0	214.0	inorg	200.9
mpurities							
Stage 5 Product	Product	817.7	17.7	47926.5			
Total				96285.4	10656.6		10638.8

Stage 6	kg/1000kg In	Added As:	Score	Kg X 10 E+(score/10)
Stage 5 Product	817.7	Liquid	17.7	47926.5
Sodium metal	259.0	Solid	1.3	347.0
Hydrogen	0.0			0.0
Ethanol	3701.8	Liquid	6.8	17636.4
Diethyl Oxalate	1916.2	Liquid	14.8	57736.6
Chloroform	7147.5	Liquid	38.7	52741387.5
Water	14458.7	Liquid	0.1	14761.5
Hydrochloric acid	455.4	Liquid	16.3	19608.3
NaOH	49.2	Liquid	3.6	113.4
NaCl				0.0
IMS	4470.7	Liquid	6.7	20671.9
Stage 6 Product		Liquid		0.0
Total				52920189.1

Stage 6	Released to:	Mass released Kg	Score	Kg X 10 E+(score/10)	mpact Score when product and recovery are considered but no additional treatment	Treatment Category	mpact Score when product, recovery and additional treatment are considered
Stage 5 Product							
Sodium metal							
Hydrogen	Air	11.3	0.1	11.5	11.5	$	11.5
Ethanol	Recovered	3857.6	6.8	18378.8			
Ethanol	Product	47.5	6.8	226.3			
Ethanol	Air	5.6	7.7	33.2	33.2	$	33.2
Diethyl Oxalate	Product	0.0	12.2	0.1			
Diethyl Oxalate	Water	1253.0	12.2	20842.9	20842.9	org	2084.3
Chloroform	Recovered	7146.7	38.7	52736002.3			
Chloroform	Air	0.7	0.7	0.9	0.9	$	0.9
Water	Water	10494.3	0.1	10714.0	10714.0	org	1071.4
Water	Product	28.1	0.1	28.7			
Water	Recovered	4040.0	0.1	4124.6			
Hydrochloric acid				0.0			
NaOH	Water	0.5	3.6	1.1	1.1	org	0.1
NaCl	Water	730.0	2.5	1283.2	1283.2	org	128.3
IMS	Recovered	4410.0	6.7	20391.0			
IMS	Air	6.5	8.7	47.3	47.3	$	47.3
IMS	Product	54.3	6.7	251.0			
Stage 6 Product	Product	1190.2	19.5	106808.2			
Total				52919145.2	32934.2		3377.0

Stage 7	kg/1000kg In	Added As:	Score	Kg X 10 E+(score/10)
Stage 6 Product	1190.2	Liquid	19.5	106808.2
Diethyl oxalate	0.6	Liquid	14.8	18.2
IMS	8488.4	Liquid	6.7	39248.7
Water	5297.2	Liquid	0.1	5408.1
NaOH	182.0	Liquid	3.6	419.9
Carbon	135.2	Solid	3.1	276.1
mpurities	13.3			
Ethanol				0.0
Sodium oxalate				0.0
Stage 7 product				0.0
Total				152179.2

Stage 7	Released to:	Mass released Kg	Score	Kg X 10 E+(score/10)	mpact Score when product and recovery are considered but no additional treatment	Treatment Category	mpact Score when product, recovery and additional treatment are considered
Stage 6 Product	Product	65.5	19.5	5874.5			
Stage 6 Product	Recovered	2.8	19.5	254.9			
Diethyl oxalate							
IMS	Recovered	8418.2	6.7	38924.0			
IMS	Air	4.3	8.7	31.8	31.8	S	31.8
IMS	Land	65.9	6.6	304.0	304.0	L	304.0
Water	Water	354.8	0.1	362.2	362.2	' inorg	362.2
Water	Product	42.1	0.1	43.0			
Water	Recovered	4835.6	0.1	4936.8			
Water	Land	64.7	0.1	66.1	66.1	L	66.1
NaOH	Water	10.4	3.6	24.1	24.1	' org	2.4
mpurities	Product	13.3					
Carbon	Land	135.2	3.1	276.1	276.1	L	276.1
Ethanol	Recovered	195.7	6.8	932.4			
Ethanol	Air	0.1	7.7	0.6	0.6	S	0.6
Sodium oxalate	Land	0.6	11.4	7.6	7.6	L	7.6
Stage 7 Product	Recovery	72.7	21.4	10011.9			
Stage 7 Product	Product	1023.5	21.4	140953.4			
Total				196873.9	1072.5		1050.8

Stage 8	kg/1000kg In	Added As:	Score	Kg X 10 E+(score/10)
Stage 7 Product	1023.5	Liquid	21.4	140953.4
IMS	18203.9	Liquid	6.7	84171.3
Water	3608.3	Liquid	0.1	3683.8
Stage 8 product				0.0
Total				228808.5

Stage 8	Released to:	Mass released Kg	Score	Kg X 10 E+(score/10)	mpact Score when product and recovery are considered but no additional treatment	Treatment Category	mpact Score when product, recovery and additional treatment are considered
Stage 7 Product							
IMS	Recovered	18185.7	6.7	84087.4			
IMS	Air	18.1	8.7	132.9	132.9	S	132.9
Water	Recovered	3608.3	0.1	3683.8	3683.8		3683.8
Stage 8 Product	Recovered	23.5	21.4	3232.5	3232.5		3232.5
Stage 8 Product	Product	1000.0	21.4	137720.9			
Total				228857.6	7049.2		7049.2

APPENDIX 10

EPPT assessments of:

Thomas Swan - Pepton process

Fisons - Existing sodium cromoglycate process

Fisons - Proposed new sodium cromoglycate process

Associated Octel - Tetra ethyl lead process

Associated Octel - Tetra methyl lead process

EPPT Assessment of Pepton Process from Mass Balance (per 1000kg)

Inputs

Material	Mass	Chemical Score(Liquid)	KgX10 E+(Score/10)
Benzthiazole	592.3	29.7	5.50E+05
Sodium Hydroxide	1330.4	3.6	3.07E+03
Chemical B	4.9	23.9	1.20E+03
Chemical D	3673.5	9.8	3.52E+04
Chemical C	1.8	17.0	9.24E+01
Chemical A	12.2	30.5	1.37E+04
Sodium Bicarbonate	550.5	2.8	1.06E+03
Water	3290.8	0.1	3.36E+03
Hydrogen Peroxide	3621.1	10.4	4.01E+04
Benzoyl Chloride	700.4	10.8	8.36E+03
Total Input	13777.9		**6.56E+05**

PEPTON PRODUCTION

Gaseous Waste to Air

Material	Mass	Chemical Score (air)	KgX10 E+(Score/10)
Benzthiazole	5.2E-01	28.7	380.5
Chemical B	1.7E-02	23.5	3.8
Chemical D	2.0	9.5	17.3
Chemical C	2.9E-03	16.9	0.1
Chemical A	3.9E-03	28.7	2.9
Stage 1 Product	2.4E-01	30.9	301.5
Oxygen	1.0E-01	0.1	0.1
Stage 2 Product	6.7E-08	31.8	0.0
Carbon Dioxide	94.8	7.7	560.9
Total	97.7		**1.27E+03**

Aqueous Waste to Chemical Effluent Treatment

Material	Mass	Chemical Score (water)	KgX10 E+(Score/10)
Chemical B	0.6	23.9	146.7
Chemical D	28.3	9.8	271.3
Chemical C	2.4E-02	17.0	1.2
Stage 1 Product	8.7	31.1	11042.6
Benzoyl Chloride	64.4	10.8	768.5
Hydrogen Peroxide	9.0	10.4	99.4
Sodium Formate	291.8	3.2	613.9
Chemical E	6.5	2.8	12.5
Sodium Hydroxide	951.4	3.6	2194.7
Water	4309.7	0.1	4400.0
Sodium Carbonate	231.3	2.8	444.8
Sodium Bicarbonate	171.6	2.8	329.9
Sodium Chloride	255.3	2.5	448.8
Pepton	0.5	32.9	914.1
Chemical G	3.5	32.2	5795.5
Chemical F	9.8	32.2	16339.3
Benthiazole	0.5	29.7	437.6
Chemical H	23.3	3.2	49.0
Total	6366.1		**4.43E+04**

See *1

Product to drying

Material	Mass	Chemical Score (liquid)	KgX10 E+(Score/10)
Benzoyl Chloride	9.0	10.8	107.1
Sodium Formate	6.3	3.2	13.2
Chemical E	1.7	2.8	3.2
Hydrogen Peroxide	0.8	10.4	8.6
Sodium Hydroxide	21.8	3.6	50.3
Water	2591.4	0.1	2645.7
Sodium Carbonate	2.2	2.8	4.2
Sodium Bicarbonate	8.9	2.8	17.1
Sodium Chloride	2.4	2.5	4.2
Pepton	1000.0	32.9	1940885.9
Chemical G	0.1	32.2	162.8
Chemical F	0.2	32.2	396.8
Total	3644.7		**1.94E+06**

See *2

Recycle Between Batches

Material	Mass	Chemical Score (liquid)	KgX10 E+(Score/10)
Toluene	3669.4	9.8	35204.3
Total	3669.4		**3.52E+04**

*2 Chemical Effluent Treatment/per 1000kg product

Aqueous Waste to Chemical Effluent Treatment

Material	Mass	Chemical Score (liquid)	KgX10 E+(Score/10)
Chemical B	0.6	23.9	146.7
Chemical D	28.3	9.8	271.3
Chemical C	0.0	17.0	1.2
Stage 1 Product	8.7	31.1	11042.6
Benzoyl Chloride	64.4	10.8	768.5
Hydrogen Peroxide	9.0	10.4	99.4
Sodium Formate	291.8	3.2	613.9
Chemical E	6.5	2.8	12.5
Sodium Hydroxide	951.4	3.6	2194.7
Water	4309.7	0.1	4399.9
Sodium Carbonate	231.3	2.8	444.8
Sodium Bicarbonate	171.6	2.8	329.9
Sodium Chloride	255.3	2.5	448.8
Pepton	0.5	32.9	914.1
Chemical G	3.5	32.2	5795.5
Chemical F	9.8	32.2	16339.3
Benthiazole	0.5	29.7	437.6
Chemical H	23.3	3.2	49.0
Total	6366.1		4.43E+04

EFFLUENT TREATMENT

To Water

Material	Mass	Chemical Score (liquid)	KgX10 E+(Score/10)
Sodium Formate	291.8	3.2	613.9
Chemical E	6.5	2.8	12.5
Sodium Hydroxide	951.4	3.6	2194.7
Water	4309.7	0.1	4400.0
Sodium Carbonate	231.3	2.8	444.8
Sodium Bicarbonate	171.6	2.8	329.9
Sodium Chloride	255.3	2.5	448.8
Hydrogen Peroxide	9.0	10.4	99.4
Chemical H	23.3	3.2	49.0
Total			8.59E+03

To Land

Material	Mass	Chemical Score (soil)	KgX10 E+(Score/10)
Chemical B	0.6	22.5	105.6
Chemical D	28.3	9.3	242.9
Chemical C	0.0	16.4	1.1
Stage 1 Product	8.7	31.1	11073.2
Benzoyl Chloride	64.4	10.2	675.5
Pepton	0.5	32.3	801.7
Chemical G	3.5	32.2	5826.3
Chemical F	9.8	32.2	16426.0
Benzthiozole	0.5	29.2	391.7
Total		10%as contained	3.55E+03

*3 Drying/1000kg Product

Product to drying

Material	Mass	Chemical Score (liquid)	KgX10 E+(Score/10)
Benzoyl Chloride	9.0	10.8	107.1
Sodium Formate	6.3	3.2	13.2
Chemical E	1.7	2.8	3.2
Hydrogen Peroxide	0.8	10.4	8.6
Sodium Hydroxide	21.8	3.6	50.3
Water	2591.4	0.1	2645.7
Sodium Carbonate	2.2	2.8	4.2
Sodium Bicarbonate	8.9	2.8	17.1
Sodium Chloride	2.4	2.5	4.2
Pepton	1000.0	32.9	1940885.9
Chemical G	0.1	32.2	162.8
Chemical F	0.2	32.2	396.8
Total	3644.7		1.94E+06

DRYING

Dry Product

Material	Mass	Chemical Score (land)	KgX10 E+(Score/10)
Benzoyl Chloride	9.0	10.2	94.1
Sodium Formate	6.3	3.2	13.2
Chemical E	1.7	2.8	3.2
Hydrogen Peroxide	0.8	10.4	8.6
Sodium Hydroxide	21.8	3.6	50.3
Sodium Carbonate	2.2	2.8	4.2
Sodium Bicarbonate	8.9	2.8	17.1
Sodium Chloride	2.4	2.5	4.2
Pepton	1000.0	32.3	1702158.5
Chemical G	0.1	32.2	163.5
Chemical F	0.2	32.2	398.6
Total	1053.3		1.70E+06

Water evaporated

Material	Mass	Chemical Score (gas)	KgX10 E+(Score/10)
Water	2591.4	0.2	2702.9
Total	2591.4		2.70E+03

Fisons - Sodium Chromoglycate Existing Process EPPT Assessment

Inputs

MATERIAL	Mass Kg	Added as:	Chemical Score	Kg X 10 E+(Score/10)
Resorcinol	429.7	Solid	8.0	2729.9
Ethyl Acetonacetate	584.4	Liquid	5.4	2003.0
Sulphuric Acid	0.7	Liquid	20.2	78.4
Acetic Anhydride	871.3	Liquid	7.4	4799.4
IMS	38399.6	Liquid	6.7	177552.7
Water	97526.8	Liquid	0.1	99569.0
Ethanol	4312.5	Liquid	6.8	20546.1
Acetic Acid	0.0	Liquid	9.6	0.0
AlCl3	2729.4	Solid	24.8	824255.7
Al(OH)3	0.0		17.0	0.0
NaCl	343.9	Solid	2.5	604.6
Hydrochloric acid	3106.9	Liquid	16.3	133761.4
HCl	0.0	Liquid	16.3	0.0
NaOH (50/50 soln)	2085.3	Liquid	3.6	4810.4
Sodium metabisulphite	1.2	Solid	8.1	7.6
Acetone	0.0	Liquid	5.9	0.0
CO2	0.0	Gas	7.7	0.0
Epichlorohydrin	181.7	Liquid	9.9	1787.5
MIBK	725.5	Liquid	9.9	7139.1
Sodium Carbonate	114.9	Solid	2.8	221.0
TDA-1	3.0	Solid	31.3	3990.1
Sodium metal	222.7	Solid	1.3	298.3
Hydrogen	0.0	Gas	0.1	0.0
Diethyl Oxalate	1648.4	Liquid	14.8	49667.5
Chloroform	5768.2	Liquid	38.7	42564007.0
Carbon	72.4	Solid	3.1	147.8
Sodium oxalate	0.0	Liquid	11.4	0.0
Stage 8 product	0.0	Solid	21.4	0.0
TOTAL	159128.6			4.39E+07

* all liquid effluent with the exception of Al rich go to onsite effluent treatment. Organics are removed by bio-org to a level of 10%. The 10% is sent to landfill

^ all recovered liquid are reused and not considered an output to the environment

+ Al rich liquid effluents are assumed to go to landfill where they are contained and score 10% of the land score

$ all gaseous emissions are assumed to be released to the atmosphere. In reality the acid emissions are scrubbed but there was insufficient data in the IPC application to enable the scrubber to be modelled

% contained in the product - not added to outputs

& Disposed of to land

Outputs

MATERIAL	Released to	Mass kg	Chemical Score	Kg X 10 E+(Score/10)	Impact Score when product and recovery are considered but no additional treatment	Treatment Category	Impact score when product, recovery and additional treatment are considered
Resorcinol		0.0		0.0	0.0		0.0
Ethyl Acetonacetate	Water	76.6	5.4	262.4	262.4	* org	26.2
Sulphuric Acid	Water	0.8	20.2	78.7	78.7	* inorg	78.7
Acetic Anhydride	Air	0.0	7.6	0.2	0.2	$	0.2
IMS	Air	2798.5	8.7	20508.2	20508.2	$	20508.2
IMS	Recovered	35601.1	6.7	164612.9		^	
Water	Product	3428.6	0.1	3500.4		%	
Water	Water	84264.6	0.1	86029.0	86029.0	* inorg	8602.9
Water	Air	111.2	0.2	115.9	115.9	$	115.9
Water	Offsite/Land	10914.1	0.1	11142.6	11142.6	+	1114.3
Ethanol	Water	1942.9	6.8	9256.7	9256.7	* org	925.7
Ethanol	Air	27.6	7.7	162.0	162.0	$	162.0
Ethanol	Recovered	2890.9	6.8	13773.1		^	
Acetic Acid	Water	789.6	9.6	7184.9	7184.9	*org	718.5
Acetic Acid	Air	1.1	10.2	11.1	11.1	$	11.1
AlCl3	Offsite/Land	2685.8	25.1	865101.8	865101.8	+	86510.2
Al(OH)3	Offsite/Land	25.8	17.0	1283.2	1283.2	+	128.3
NaCl	Water	1996.8	2.5	3510.2	3510.2	*inorg	3510.2
NaCl	Offsite/Land	343.9	2.5	604.5	604.5	+	60.5
Hydrochloric acid	Water	1932.3	16.3	83192.4	83192.4	* inorg	83192.4
HCl	Water	35.3	16.3	1519.8	1519.8	* inorg	1519.8
HCl	Air	0.0	15.9	1.2	1.2	$	1.2
NaOH (50/50 soln)	Water	150.9	3.6	348.0	348.0	* inorg	348.0
Sodium metabisulphite	Water	1.2	8.1	7.6	7.6	* inorg	7.6
Acetone	Water	226.5	5.9	873.3	873.3	* org	87.3
Acetone	Air	0.0	6.1	0.1	0.1	$	0.1
CO2	Air	214.8	7.7	1270.9	1270.9	$	1270.9
Epichlorohydrin	Water	1.0	9.9	9.7	9.7	* org	1.0
MIBK	Recovered	725.5	9.9	7139.1		^	
Sodium Carbonate	Water	11.4	2.8	22.0	22.0	* inorg	22.0
TDA-1	Water	3.0	31.3	3988.0	3988.0	* org	398.8
Sodium metal				0.0	0.0		
Hydrogen	Air	9.7	0.1	9.9	9.9	$	9.9
Diethyl Oxalate	Water	1062.5	12.5	18937.8	18937.8	* org	1893.8
Chloroform	Air	410.8	39.1	3323846.9	3323846.9	$	3323846.9
Chloroform	Recovered	5357.4	38.7	39532628.8		^	
Carbon	Land	3.1		3.1	3.1	&	3.1
Sodium oxalate	Air	14.3	11.4	196.6	196.6	$	196.6
Stage 8 product	Product	1000.0	21.4	137720.9		%	
TOTAL		159059.6		4.43E+07	4.44E+06		3.54E+06

Recovery	3.97E+07	Impact Score	
Product	1.41E+05	Reduction	9.04E+05
	4.43E+07		

Fisons - Sodium Chromoglycate Proposed New Process EPPT Assessment

Inputs

MATERIAL	Mass kg	Added as:	Chemical Score	Kg X 10 E+(Score/10)
Resorcinol	499.7	Solid	8.0	3174.6
Ethyl Acetonacetate	679.6	Liquid	5.4	2329.4
Sulphuric Acid	0.9	Liquid	20.2	91.3
Acetic Anhydride	1013.3	Liquid	7.4	5581.2
IMS	42693.4	Liquid	6.7	197406.3
Water	115504.9	Liquid	0.1	117923.5
Ethanol	3701.8	Liquid	6.8	17636.4
Acetic Acid	0.0	Liquid	9.6	0.0
AlCl3	3180.0	Solid	24.8	960341.6
Al(OH)3	0.0		17.0	0.0
NaCl	399.9	Solid	2.5	703.0
Hydrochloric acid	3625.5	Liquid	16.3	156085.3
HCl	0.0	Liquid	15.9	0.0
NaOH (50/50 soln)	2253.9	Liquid	3.6	5199.3
Sodium metabisulphite	1.4	Solid	8.1	8.9
Acetone	0.0	Liquid	5.9	0.0
CO2	0.0	Gas	7.7	0.0
Epichlorohydrin	210.6	Liquid	9.9	2072.6
MIBK	856.6	Liquid	9.9	8429.1
Sodium Carbonate	133.3	Solid	2.8	256.3
TDA-1	3.5	Solid	31.3	4686.2
Sodium metal	259.0	Solid	1.3	347.0
Hydrogen	0.0	Gas	0.1	0.0
Diethyl Oxalate	1916.2	Liquid	14.8	57736.4
Chloroform	7147.5	Liquid	38.7	52741409.7
Carbon	135.3	Solid	3.1	276.1
Sodium oxalate	0.0	Liquid	11.4	0.0
Stage 6 Product	0.0		0.0	0.0
Stage 7 Product	0.0		0.0	0.0
Stage 8 product	0.0	Solid	21.4	0.0
TOTAL	184216.1			5.43E+07

* all liquid effluent with the exception of Al rich go to onsite effluent treatment. Organics are removed by bio-org to a level of 10%. The 10% is sent to landfill

^ all recovered liquid are reused and not considered an output to the environment

+ Al rich liquid effluents are assumed to go to landfill where they are contained and score 10% of the land score

$ all gaseous emissions are assumed to be released to the atmosphere. In reality the acid emissions are scrubbed but there was insufficient data in the IPC application to enable the scrubber to be modelled

% contained in the product - not added to outputs

& Disposed of to land

Outputs

MATERIAL	Released to	Mass Kg	Chemical Score	Kg X 10 E+(Score/10)	Impact Score when product and recovery are considered but no additional treatment	Treatment Category	Impact score when product, recovery and additional treatment are considered
Resorcinol		0.0		0.0	0.0		0.0
Ethyl Acetonacetate	Water	89.0	5.4	305.2	305.2	* org	30.5
Sulphuric Acid	Water	0.9	20.2	91.3	91.3	* inorg	91.3
Acetic Anhydride	Air	0.0	7.6	0.2	0.2	$	0.2
IMS	Air	31.5	8.7	231.1	231.1	$	231.1
IMS	Recovered	42474.6	6.7	196394.4			
IMS	Product	54.3	6.7	251.0		%	
IMS	Water	67.1	6.7	310.3	310.3	* org	31.0
IMS	Land	65.9	6.6	304.0	304.0	+	30.4
Water	Product	4058.5	0.1	4143.5		%	
Water	Water	85644.6	0.1	87438.0	87438.0	* inorg	8743.8
Water	Air	21.4	0.2	22.3	22.3	$	22.3
Water	Offsite	12692.0	0.1	12957.8	12957.8	+	1295.8
Water	Land	64.7	0.1	66.1	66.1	+	6.6
Water	Recovered	14415.5	0.1	14717.4			
Ethanol	Water	209.0	6.8	995.6	995.6	* org	99.6
Ethanol	Air	5.8	7.7	33.8	33.8	$	33.8
Ethanol	Recovered	4053.3	6.8	19311.2			
Ethanol	Product	47.5	6.8	226.3		%	
Ethanol	Land	1.5	6.8	7.3	7.3		
Acetic Acid	Water	918.3	9.6	8355.3	8355.3	*org	835.5
Acetic Acid	Air	1.2	10.2	12.8	12.8	$	12.8
AlCl3	Offsite	3123.3	25.1	1006030.0	1006030.0	+	100603.0
Al(OH)3	Offsite	30.0	17.0	1492.2	1492.2	+	149.2
NaCl	Water	2330.8	2.5	4097.4	4097.4	*inorg	4097.4
NaCl	Offsite	399.9	2.5	703.0	703.0	+	70.3
NaCl	Recovered	11.2	2.5	19.6			
Hydrochloric acid	Water	2247.1	16.3	96744.5	96744.5	* inorg	96744.5
HCl	Water	41.1	16.3	1767.3	1767.3	* inorg	1767.3
HCl	Air	0.0	15.9	1.6	1.6	$	1.6
NaOH (50/50 soln)	Water	10.9	3.6	25.2	25.2	* inorg	25.2
Sodium metabisulphite	Water	1.4	8.1	8.9	8.9	* inorg	8.9
Acetone	Water	263.4	5.9	1015.5	1015.5	* org	101.6
Acetone	Air	0.0	6.1	0.1	0.1	$	0.1
CO2	Air	249.8	7.7	1478.0	1478.0	$	1478.0
Epichlorohydrin	Water	0.5	9.9	5.2	5.2	* org	0.5
MIBK	Recovered	856.6	9.9	8429.1			
Sodium Carbonate	Water	12.9	2.8	24.8	24.8	* inorg	24.8
TDA-1	Water	3.5	31.3	4686.2	4686.2	* org	468.6
Hydrogen	Air	11.3	0.1	11.5	11.5	$	11.5
Diethyl Oxalate	Water	1253.0	12.5	22333.6	22333.6	* org	2233.4
Chloroform	Air	0.7	39.1	5906.4	5906.4	$	5906.4
Chloroform	Recovered	7146.7	38.7	52736023.0			
Carbon	Land	135.3	3.1	276.1	276.1	&	276.1
Sodium oxalate	Land	0.6	11.4	7.5	7.5	$	7.5
Stage 6 Product	Recovered	2.8	21.4	392.0			
Stage 7 Product	Recovered	72.7	21.4	10035.4			
Stage 8 Product	Recovered	23.5	21.4	3232.3			
Stage 8 product	Product	1000.0	21.4	137720.9		%	
TOTAL		184145.6		5.44E+07	1.26E+06		2.25E+05

Recovery 5.30E+07 Impact Score
Product 1.42E+05 Reduction 1.03E+06

5.44E+07

Associated Octel TEL process - EPPT assessment

Mass released per 1000kg of product produced
Based on daily flows averaged over 12 months

Inputs

Material	Mass kg		Chemical Score	Mass X 10 E+(Score/10)
Lead	3088.4	solid	41.7	45997385.6
Sodium	344.7	solid	1.3	461.8
Ethyl Chloride	1656.8	liquid	23.3	356867.4
Water	37831.3	liquid	0.1	38623.5
Salts	35.9			35.9
Graphite	3.3	solid	3.1	6.8
Acetone	0.9	liquid	5.9	3.4
Total	42961.3			4.64E+07

Effluent treatment plant: specific to process
Percentages calculated from effluent treatment data
for tetra alkyl lead processes given in IPC application

Lead	99.5% recovered
Organics	10% to landfill 90% degrade Lead orgs - recovered
Inorganics	All to water except 99.5% lead (recovered)

TEL PROCESS

Output directly from process

Material	Mass kg	Released to:	Chemical score	Mass X 10 E+(Score/10)
Ethyl Chloride	1.9	Atm	22.7	350.6
Tetra Ethyl Lead	0.1	Atm	13.1	1.4
Butane	0.1	Atm	4.7	0.2
Total	2.0			3.52E+02

Outputs From EC Recovery Unit

Material	Mass kg	Released to:	Chemical score	Mass X 10 E+(Score/10)	Excluding recycle
Ethyl Chloride	45.2	Atm	22.7	8391.0	8391.0
Tetra Ethyl Lead	0.3	Atm	13.1	7.0	7.0
Butane	48.3	Atm	4.7	141.9	141.9
Acetone	0.8	Atm	6.1	3.3	3.3
Ethyl Chloride	639.4	Recycled (liquid)	23.3	137651.2	
Tetra Ethyl Lead	4.9	Recycled (liquid)	14.3	133.5	
Butane	15.2	Recycled (gas)	4.7	44.6	
Total	754.1			1.46E+05	8.54E+03

Outputs From Sludge Pit, Oil Absorber & Stripper

Material	Mass kg	Released from:	Released to:	Chemical score	Mass X 10 E+(Score/10)	Excluding Recycle etc	With treatment
Water	6138.1	Sludge Pit	Eff Trtmt - inorg	0.1	6266.6	6266.6	6266.6
Lead	7.3	Sludge Pit	Eff Trtmt - inorg (99.5% rec)	41.8	110618.7	110618.7	553.1
Ethyl Chloride	5.8	Sludge Pit	Eff Trtmt - org	23.3	1239.6	1239.6	124.0
Tetra Ethyl Lead	0.7	Sludge Pit	Eff Trtmt - org (rec)	14.3	18.3	18.3	0.0
Butane	1.8	Sludge Pit	Eff Trtmt - org	4.6	5.1	5.1	0.5
Graphite	3.1	Sludge Pit	Eff Trtmt - inorg	3.1	6.3	6.3	6.3
NaCl	858.6	Sludge Pit	Eff Trtmt - inorg	2.5	1509.4	1509.4	1509.4
NaOH	11.3	Sludge Pit	Eff Trtmt - inorg	3.6	26.0	26.0	26.0
Salts	36.3	Sludge Pit	Eff Trtmt		36.3	36.3	36.3
Ethyl Chloride	13.7	Oil Absorber	Atm	22.7	2545.0	2545.0	2545.0
Tetra Ethyl Lead	0.4	Oil Absorber	Atm	13.1	7.5	7.5	7.5
Lead	2436.4	Stripper	Recovered	41.8	37048922.8		
Tetra Ethyl Lead	77.3	Stripper	Recovered	14.3	2036.6		
Water	31611.3	Stripper	Reuse	0.1	32273.2		
Graphite	0.2	Stripper	In Water	3.1	0.4	0.4	0.4
Total	41202.1				3.72E+07	1.50E+05	1.11E+04

Product

Material	Mass kg	Produced as:	Chemical score	Mass X 10 E+(Score/10)
Tetra Ethyl Lead	1000.0	Liquid	14.3	26977.4
Ethyl Chloride	3.0	Liquid	23.3	647.1
Total	1003.0			2.76E+04

Associated Octel TML process - EPPT assessment

Mass released per 1000kg of product produced
Based on daily flows averaged over 12 months

Inputs

Material	Mass kg		Chemical score	Mass X 10 E+(Score/10)
Lead	4006.9	solid	41.7	59676962.6
Sodium	447.2	solid	1.3	599.1
Methyl Chloride	2126.0	liquid	35.5	7560717.9
Water	108797.3	liquid	0.1	111075.5
Salts	19.3	solid	6.1	77.6
Graphite	12.8	solid	3.1	26.2
Catalyst (AlCl3)	34.4	solid	25.1	11073.3
Toluene	269.2	liquid	9.8	2582.4
Total	115713.0			6.74E+07

TML PROCESS

Effluent treatment plant: specific to process
Percentages calculated from effluent treatment data
for tetra alkyl lead processes given in IPC application

Lead	99.5% recovered
Organics	10% to landfill
	90% degrade
	Lead orgs - recovered
Inorganics	All to water except 99.5% lead (recovered)

Output directly from process

Material	Mass kg	Released to:	Chemical score	Mass X 10 E+(Score/10)
Methyl Chloride	55.3	Atm	35.5	196681.9
Tetra Methyl Lead	1.3	Atm	12.0	19.9
Toluene	0.3	Atm	9.5	2.8
Ethane	29.1	Atm	7.1	148.6
Total	86.0			1.97E+05

Outputs From MC Recovery Unit

Material	Mass kg	Released to:	Chemical score	Mass X 10 E+(Score/10)	Excluding recycle
Methyl Chloride	154.8	Atm	35.5	550371.8	550371.8
Tetra Methyl Lead	0.7	Atm	12.0	11.2	11.2
Ethane	10.4	Atm	7.1	53.1	53.1
Toluene	2.4	Atm	9.5	20.9	20.9
Methyl Chloride	890.9	Recycled	35.5	3168154.8	
Tetra Methyl Lead	62.9	Recycled	13.1	1288.0	
Ethane	0.9	Recycled	7.1	4.8	
Toluene	13.7	Recycled	9.8	131.6	
Total	1136.7			3.72E+06	5.50E+05

Outputs From Sludge Pit, Carbon Absorber & Stripper

Material	Mass kg	Released from:	Released to:	Chemical Score	Mass X 10 E+(Score/10)	Excluding recycle etc	With treatment
Water	21485.8	Sludge Pit	Eff treatment-inorg	0.1	21935.7	21935.7	21935.7
Water	85943.2	Sludge Pit	Reused	0.1	87945.0		
Lead	960.3	Sludge Pit	Eff treatment-inorg (rec)	41.7	14302650.6	14302650.6	71513.3
Lead	3125.2	Sludge Pit	Recovery	41.7	46546216.1		
Ethyl Chloride	0.9	Sludge Pit	Eff treatment-org	23.3	204.4	204.4	20.4
Methyl Chloride	3.9	Sludge Pit	Eff treatment-org	35.5	13928.1	13928.1	1392.8
Methyl Chloride	59.3	Carbon Absorber	Atm	35.5	211032.1	211032.1	211032.1
Tetra Ethyl Lead	1.2	Sludge Pit	Eff treatment-org (rec)	14.3	32.0	32.0	
Tetra Methyl Lead	8.7	Sludge Pit	Eff treatment-org (rec)	13.1	178.1	178.1	
Tetra Methyl Lead	6.6	Carbon Absorber	Atm	12.0	104.6	104.6	104.6
Tetra Methyl Lead	13.8	Carbon Absorber	Recovered	13.1	281.7		
Tetra Methyl Lead	39.6	Sludge Pit	Recovered	13.1	809.6		
Toluene	3.0	Sludge Pit	Eff treatment-org	9.8	29.2	29.2	29.2
Toluene	0.6	Carbon Absorber	Atm	9.5	5.6	5.6	5.6
Toluene	3.4	Carbon Absorber	Recovered	9.8	33.0		
Toluene	9.9	Sludge Pit	Recovered	9.8	94.9		
Ethane	3.3	Sludge Pit	Eff treatment-org	7.1	17.0	17.0	17.0
Tri Alkyl Lead	0.7	Sludge Pit	Eff treatment-org (rec)	13.7	15.8	15.8	
DBE (Dibromoethane)	0.2	Sludge Pit	Eff treatment-org	29.9	193.7	193.7	193.7
DCE (1,2 Dichloroethane)	0.4	Sludge Pit	Eff treatment-org	31.2	515.5	515.5	515.5
Catalyst (AlCl3)	34.4	Sludge Pit	Eff treatment-inorg	24.8	10263.1	10263.1	10263.1
Graphite	48.2	Sludge Pit	Eff treatment-inorg	3.1	98.5	98.5	98.5
Sodium Chloride	1436.3	Sludge Pit	Eff treatment-inorg	2.5	2525.0	2525.0	2525.0
Sodium Hydroxide	22.9	Sludge Pit	Eff treatment-inorg	3.6	52.7	52.7	52.7
Salts	28.2	Sludge Pit	Eff treatment-inorg	6.1	113.8	113.8	113.8
Flocculant (Acrylamide)	0.8	Sludge Pit	Eff treatment-inorg	20.6	90.0	90.0	90.0
Total	113241.0				6.12E+07	1.46E+07	3.20E+05

Product

Material	Mass kg	Produced as:	Chemical score	Mass X 10 E+(Score/10)
Tetra Methyl Lead	1000.0	Liquid	13.1	20464.4
Toluene	249.3	Liquid	9.7	2315.6
Total	1249.3			2.28E+04