THE FUTURE OF THE PETROCHEMICAL INDUSTRY

A MARKAL-MATTER Analysis

B.J. Groenendaal
D.J. Gielen

Acknowledgement

Abstract

This report discusses the MARKAL-MATTER results regarding the impact of greenhouse gas policies on the petrochemical industry in Western Europe from an integrated chain perspective. The MARKAL-MATTER model gives insight in how different technologies might develop in the next decades at different emission permit prices. This report first describes the present situation in the petrochemical industry. Next, techno-economic emissions reduction options are discussed. The results of this modelling study show that up to 75% emission reduction can be achieved in the life cycle of petrochemicals through various emission reduction strategies. However, significantly costs are involved with these strategies and the R&D effort should focus on new and non-traditional research areas.

CONTENTS

GLOSSARY

ABS	Acrylonitrile Butadiene Styrene
AES	Alkyl Ether Sulphate
BTX	Benzene Toluene Xylene
CPW	Clean Plastic Waste
DRP	Deutsche Reifen Produktion
DFE	Design For Environment
DMT	DiMethylTerephthalate
ECN	Netherlands Energy Research Foundation
FCC	Fluid Catalic Cracking
GHG	GreenHouse Gas
IEA	International Energy Agency
LPG	Liquefied Petroleum Gas
MARKAL	MARKet ALlocation
MATTER	MATerials Technologies for greenhouse gas Emission Reduction
MEK	MethylEthylKeton
MPW	Mixed Plastic Waste
MSW	Municipal solid Waste
MTBE	MethylTriButhylEthylene
MTO	Methanol to Olefins
NEU-CO_2	Non Energy Use- CO_2
NOP-MLK	Dutch national research programme on global air pollution and climate change
OECD	Organisation for Economic Co-operation and Development
O-Xylene	Ortho Xylene
P-Xylene	Para Xylene
PA	PolyAmide
PBD	PolyButhylene Diethylene
PE	PolyEthylene
PET	PolyEthylene Terephthalate
PFC	PerFluoroCarbons
PO	PolyOlefins
PP	PolyPropylene
PS	PolyStyrene
PUR	PolyURethane
PVC	PolyVinylChloride
SAN	Styrene AcryloNitrile
SBR	Styrene Butadiene Rubber
TPA	TerePhthalic Acid
UF	Urea Formaldehyde
UNFCCC	United Nations Framework Convention on Climate Change
VCM	VinylChloride Monomer

Definitions

Refineries: large industries that convert crude oil into oil products. Only the oil products that are used in the petrochemical industry are mentioned in this study.

Petrochemical industry: large industries that convert oil products into petrochemicals. In this study fossil-based transportation fuels are considered to be non-petrochemicals. Transportation fuels produced in the petrochemical industry based on biomass are considered to be petrochemicals.

Carbon leakage is the relocation of industrial activities from countries with strong GHG emission reduction policies to countries with no or weak GHG emission reduction policies, thus off-setting the emission reduction.

SUMMARY

This report is a product of the MATTER project (MATerials Technologies for greenhouse gas Emission Reduction). MATTER is a joint project of the Netherlands Energy Research foundation ECN and 4 other Dutch institutes. The MARKAL model calculations that are presented in this study are part of the ECN contribution in this project. This model covers all energy flows and material flows in the Western European economy 'from the cradle to the grave' for the period 1990-2050. The results in this report are based on model version 5.0.

Goals
The goal of the MATTER project is the analysis of the potential contribution of materials policies for greenhouse gas (GHG) emission reduction. The emphasis is on techno-economic optimisation. Energy and materials systems must be analysed together because they interact.

The emphasis in this study is on long-term solutions. The reason for this broad time horizon is that only significant GHG emission reduction will have a significant impact on the systems configuration. However, such a goal can only be achieved within a time frame of several decades because of the long life of the existing capital equipment. Moreover, new technology is required to achieve a significant GHG emission reduction. The development rate of this technology is another limiting factor. Especially this R&D perspective may be relevant for industries.

The goal of this report is the presentation of modelling results to an industry audience. The emphasis is on the model results and on the development of industry strategies, based on these results. The development of industry strategies is made on the basis of an integrated chain management perspective 'from cradle to grave'.

Focus
This report focuses on the petrochemical industry. It covers the production of plastics, solvents and detergents. The production of fertilisers, lubricants and asphalt are excluded from this category. There is a strong link between the petrochemical industry and the refining sector. The petrochemical industry nowadays gets its feedstocks from the refineries. Beside feedstocks refineries produce intermediates used by the petrochemical industry.

This report focuses on the effect of increasing greenhouse gas emission permit prices on petrochemical industries. The effect of five cases, a base case, a 20• /t case, a 50• /t case, a 100• /t case and a 200• /t CO_2 case will be discussed. It is assumed that the permit prices gradually grow from no penalty in 1990 to the penalty set in 2020. Although the highest two permit prices seem rather unrealistic, permit prices could be an instrument to fulfil the goals set in the Kyoto protocol.

The following questions will be answered in this report:
1. What are the relevant energy and material flows in Western Europe in the life cycle of petrochemical products from a GHG perspective?
2. What is the relation between these flows and GHG emissions? (Chapter 2)
3. Which options exist to reduce these emissions in the next 3 decades? (Chapter 2)
4. Does it make sense from a Western European cost-effectiveness perspective to reduce these emissions? (Chapter 3)
5. How far can these emissions be reduced at acceptable costs? (Chapter 5)
6. Which problems must be solved in order to achieve this emission reduction? (Chapter 6)
7. Which recommendations can be formulated for R&D and investment decisions? (Chapter 6)

Chapter 2 describes the present situation of Western Europe petrochemical industry. In Chapter 3 the different techno-economic emission reduction options for the petrochemical industry to reduce its greenhouse gas (GHG) emissions are discussed. A number of strategies (groups of options with similar characteristics) have been suggested in order to mitigate CO_2 emissions. Chapter 4 describes how the energy and materials system of the petrochemical industry is modelled. Therefore the MARKAL (MARKet ALlocation) linear programming model is discussed. With the MARKAL linear programming model the impact of carbon emission penalties is studied in this MATTER (MATerials Technologies for greenhouse gas Emission Reduction) project. The results of the MATTER calculations are presented in Chapter 5. The conclusions can be found in Chapter 6. The main conclusions are presented underneath.

Results

The current petrochemical complex is based on oil and gas derived feedstocks (naphtha, gas oil, LPG, ethane, aromatic fractions). The steam cracking of these feedstocks is the basis for the petrochemical industry. Increasing quantities of intermediates are recovered from refineries. After fractionation, different components are converted into plastics, fibers, solvents, resins, detergents and other products. Total production amounted in 1994 to 42.4 Mt products (excluding lubricants and energy products such as pyrolysis gasoline). Plastics and resins constitute 67% of this total production. The petrochemical industry consumes approximately 3 EJ final energy, 8% of the total Western European final energy use. This energy use is forecast to increase in the future, both in a situation without GHG policy and (even more) in a situation with GHG policies. The strong growth due to GHG policies can be attributed to an increased production of methanol and ethanol (as fuels for the transportation sector). The production of other petrochemical products is only to a limited extent affected by GHG policies.

The potential GHG emissions increase from approximately 250 Mt in 1990 to 370 Mt in 2030 (an increase by 48%). However, the actual emissions amount only 320 Mt in 2030, of which approximately 60 Mt can be attributed to the waste incineration, so the actual emission allocated to the petrochemical industry is approximately 260 Mt. 60 Mt is related to the production of adipic acid. The remaining 200 Mt is related to the energy use in the industry and the production of short life petrochemical production. The petrochemical industry contributes approximately 4% to the total Western European emission of 5100 Mt in 2030.

Until 2010, Western European industry will not be affected significantly by the GHG emission reductions. However, beyond 2010, further emission reductions will affect the petrochemical industry and iron and other industries like steel, aluminium, paper and wood etc. As a consequence, the emissions will be reduced significantly for most materials. Therefore, the emission reduction that can be achieved through materials substitution is limited.

The changing structure of the energy supply system must also be considered. For example the changing electricity production affects the potential for GHG emission reduction through energy recovery from plastic waste. The market for transportation fuels will be affected by a change towards biofuels and electricity in the transportation sector. This will affect the availability of naphtha, currently a by-product of oil refining.

Nowadays the Western European petrochemical industry contributes to GHG-emission reduction through N_2O mitigation technologies. These technologies are introduced in the production process of Adipic acid. The total contribution is approximately 60 Mt CO_2 equivalents in 2030 (compared to the base case). Basically two main strategies can be discerned for the petrochemical industry with regard to CO_2 emissions related to feedstock use:
- renewable feedstocks,
- recycling of waste plastics.

The industry will be significantly affected by any GHG penalty. Actual emissions will decline from 320 Mt in the base case to 250 Mt in case of a 50 • /t CO_2 penalty. This is a decline of 22%, compared to a decline of 50% for the whole economy. At a penalty of 200 • /t CO_2 emissions decline with 125 Mt, this is a decline of 61%, compared to a decline of 75% for the whole economy. The 50 • /t CO_2 penalty scenario should be considered as an scenario causing some pain without extreme impacts on the economical structure, while the 200 • /t penalty represents an extreme scenario. At GHG penalties of 100 • /t and more, the energy and carbon feedstock input changes from fossil fuels to biomass.

The main GHG emission reduction strategy is feedstock substitution (65% of the GHG emission reduction), followed by N_2O emission mitigation (15%), recycling/energy recovery (10%) and increased materials efficiency (10%). The development of such strategies will require significant R&D efforts, but can simultaneously enhance the sustainability of this industry sector.

The integration of the refinery sector and the petrochemical industry is currently one of the strong competitive advantages compared with steel and paper/board industry. Significant changes can be expected in the transportation fuels market from GHG-emission of 100• /t and higher. This will affect the availability of naphtha, gas and gas oil. It is an important incentive to develop alternative carbon sources, materials, products and product applications.

Implications
The threat for industry is that these new production processes are not dependent upon the existing petrochemical structure. Agricultural processing industries and pulp and paper industries are examples of non-petrochemical sectors that make inroads into this market. Especially the pulp production has a significant resource base of 20-30 Mt ligning per year, which is an attractive source of cheap biomass feedstocks. The agricultural overproduction in Western Europe and the imminent expansion towards the east will result in a strong drive to find new applications for this agricultural land. It is recommended for the petrochemical industry to participate in this trend through the development of new production routes.

The industry has developed many new plastic waste recycling technologies during the last decade. GHG emission permit prices can increase the cost-effectiveness of these recycling strategies significantly. However, the waste plastic market has a decidedly different structure than the naphtha market. It is recommended to develop a reliable supply structure before any activities in this field are developed.

Given the international character of many materials producing industries, carbon leakage[1] is a serious threat. Policy makers are sensitive to such problems. Three scenarios can be drawn: first, industries outside Western Europe are subjected to similar emission reduction policies, second, petrochemical industry is exempted from GHG emission reduction policies, third, a system of tradable emission permits in Western Europe is developed. In the third case, industries can even benefit from such GHG policies, if their initial emissions are high. When the industries can achieve emission reductions at lower costs than elsewhere, they can sell permits at a profit. Looking at likely competitors, emission reductions in the United States are even more difficult to achieve than emission reductions in Western Europe. The situation for producers in the Middle East is not clear because it is uncertain whether these countries will participate in GHG emission reduction schemes.

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[1]   Carbon leakage is the replacement of industrial activities to countries with strong GHG emission reduction policies to counties with no or weak GHG emission reduction policies.

Within Europe, the market potential in Eastern Europe and the imminent participation of these countries in the European Union will pose an important incentive for new production capacity in the east. An additional advantage is that this region has sufficient land for a future agrification strategy.

Biomass is a renewable carbon source with a neutral CO_2 balance. Basically, four routes can be considered how biomass can be integrated into the petrochemical complex:
1. Feedstock substitution: biomass for oil and natural gas feedstocks for the production of intermediates such as ethylene, butadiene, etc.
2. Fermentation of biomass to ethanol and methanol.
3. New bioplastics, bio-solvents etc. based on naturally occurring molecules.
4. Substitution of plastics by wood products such as sawn wood, wood panels or paper.

The model calculations indicate that the first two routes seem the most attractive. A mix of pyrolysis processes and fermentation must be applied in order to achieve maximum substitution of existing petrochemicals. Some of these processes have been proven on a commercial scale. For other technologies still major research is required in order to introduce them.

Recycling is the other important strategy to reduce the feedstock consumption. Current waste policies aim for increased incineration with energy recovery as a substitute for waste disposal. This will result in increased GHG emissions. A number of different recycling technologies are available and suitable for different waste qualities to produce different materials. An optimal mix from a GHG emission point of view consists of a mix of back-to-polymer, back-to-monomer and back-to-feedstock technologies at the expense of energy recovery technologies such as waste incineration. Most of these technologies have already been developed on a commercial scale. The introduction of a collection system seems merely a matter of process economics, which can be influenced by emission permit prices.

The current IPCC emission accounting guidelines are not clear with regard to the CO_2 emission accounting for the petrochemical industry. Different countries apply different accounting methods. Such differences can give future problems because they can affect the competitive position of national industries in a Europe-wide operating industry. International co-ordination of emission accounting guidelines with regard to petrochemicals is currently proceeding in the framework of the NEU-CO_2 project that is funded by the Environment and Climate programme of the European Union (http://www.eu.fhg.de, 1999). It is recommended that the industry participate in this project.

MATTER model calculations show that the petrochemical industry is one of the few industries that may actually improve its export position if GHG permit prices would be introduced. The export of carbon containing petrochemical products is accounted for as carbon export. The industry can negotiate an exemption from GHG permit prices for the non-energy use of fossil fuels. If biomass is used as a feedstock, this should be considered as a net carbon storage that deserves a subsidy equal to the penalty on emissions.

1. INTRODUCTION

This report is a product of the MATTER project (MATerials Technologies for greenhouse gas Emission Reduction). This project is part of the Dutch national research programme on global air pollution and climate change (NOP-MLK). MATTER is a joint project of the Netherlands Energy Research foundation ECN and 4 other Dutch institutes. The MARKAL model calculations that are presented in this study are part of the ECN contribution to this project.

The goal of the MATTER project is the analysis of the potential contribution of materials policies for greenhouse gas (GHG) emission reduction. The emphasis is on techno-economic optimisation. While energy systems engineering for GHG emission reduction has received a lot of attention, little attention has been paid up till now to the potential for materials systems engineering (covering the life cycle of all materials in the economy).

Energy and materials systems must be analysed together because they interact. For example energy is used for the industrial production of materials, the materials selection of transportation equipment influences the energy efficiency, waste materials can be used for energy recovery.

ECN has developed an integrated energy and materials systems engineering model for Western Europe, called the MATTER model. This model covers all energy flows and material flows in the Western European economy 'from cradle to grave' for the period 1990-2050. The results in this report are based on model version 5.0, documented on the MATTER Internet site (http://www.ecn.nl/unit_bs/etsap/markal/matter/, 1999).

The emphasis in this study is on long-term solutions. The reason for this broad time horizon is that only significant GHG emission reduction will prevent climate change and such a goal can only be achieved within a time frame of several decades because of the long life of the existing capital equipment. Moreover, new technology is required to achieve a significant GHG emission reduction. The development rate of this technology is another limiting factor. Especially this R&D perspective may be relevant for industries.

The goal of this report is the presentation of modelling results to an industry audience. This is a difference with earlier work, which focused on the government/academic audience. The emphasis is on the model results and on the development of industry strategies, based on these results. The development of industry strategies is made on the basis of an integrated chain management perspective (Dutch Chemical Industry, 1991). The documentation of the model structure, input data etc. in this report is limited. More extensive documentation can be found in a large number of publications and on the Internet (http://www.ecn.nl/unit_bs/etsap/markal/ matter/, 1999).

This report focuses on the petrochemical industry. It covers the production of plastics, solvents and detergents. There is a strong link between the petrochemical industry and the refining sector. The petrochemical industry nowadays gets its feedstocks from the refineries; the feedstocks consist of standard refinery products. Beside feedstocks refineries produce intermediates which are used in the petrochemical industry. The petrochemical industry produces pyrolyse gas oil, which are used in the refineries. The production of fertilisers, lubricants and asphalt are excluded from this study, this interaction is accounted for in the results.

The method in this study to analyse and optimise GHG emission reduction is to use increasing greenhouse gas emission penalties on petrochemical industries. This is done for analytical purpose, not to advocate taxation policies. The permit prices are only used to find least cost solutions

for various policy targets. The results of five cases in the MARKAL-MATTER model have been analysed. There is a base case that represents the business as usual situation with no penalties on CO_2 emissions. The other four cases describe the impact of increasing emission permit prices (20, 50, 100 and 200• /t CO_2) on the systems configuration of the petrochemical industry. Although the high penalties may seem rather unrealistic at the moment, they are in line with 50-75% emission reduction in the next 30 years. It is assumed that the permit prices gradually grow from no penalty in 1990 to the full penalty set in 2020 (see also Box 1).

Box 1: Interpretation of results

The analyses in this report are based on the results of the MARKAL MATTER model. They represent an approach where the whole energy and materials system 'from cradle to grave' is optimised at once. As a consequence, the results represent the outcome of general policy approaches that choose the optimal set of options from a Western European regional perspective. The results do not represent the results of separate sectional policies, which can be applied independently. Note that the emission penalties, which are shown in this report, do not represent the emission reduction costs for individual sectors. In many cases, it is more cost-effective to reduce emissions through technological change instead of paying the penalties. Earlier analyses have shown that for the economy as a whole, the average costs represent approximately one fifth of the marginal costs (Gielen, 1999). If industries get tradable emission permits and they can reduce their emissions at costs lower than the value of the permit (i.e. below the marginal costs of the whole economy), they may even make a profit out of GHG emission policies.

MARKAL is a linear programming model, that minimises an objective function (i.c. total discounted costs) under constraints (e.g. the attainment of certain production levels, the availability of certain technologies, certain environmental policy constraints etc.). The economy is modelled as a system of interdependent technical processes. These process descriptions implicitly yield a very detailed input-output structure linking several hundreds of processes that are included in the model in a dynamic perspective, covering the total life cycle for both energy and materials. Many products and services can be generated through a number of alternative (sets of) processes that feature different costs and different GHG emissions. Process routes are selected on the bases of costs (a simulation of the market situation).

A discussion if emission permit prices are the most likely instrument to reduce the greenhouse gas emissions is beyond the scope of this study. In this study it is assumed that in the coming decades actions have to be taken to reduce the GHG emissions. Whether these actions are driven through regulation or pricing makes no difference for the energy and materials system configuration found in this study. It merely shows what these configurations look like under serious emission reduction requirements. With this information, industries can prepare themselves for possible far reaching GHG emission targets.

The following questions will be answered in this report:
1. What are the relevant energy and material flows in Western Europe in the life cycle of petrochemical products from a GHG perspective? (Chapter 2)
2. What is the relation between these flows and GHG emissions? (Chapter 2)
3. Which techno-economic options exist to reduce these emissions in the next 3 decades? (Chapter 3)
4. Does it make sense from a Western European cost-effectiveness perspective to reduce these emissions? (Chapter 5)
5. How far can these emissions be reduced at acceptable costs? (Chapter 5)
6. Which problems must be solved in order to achieve this emission reduction? (Chapter 6)

7. Which recommendations can be formulated for R&D and for investment decisions? (Chapter 6).

2. PRESENT SITUATION

The petrochemical industry converts oil products and natural gas into petrochemicals. In this chapter an introduction of the petrochemical industry is given. The analysis includes both the feedstock and the waste side of the life cycle of petrochemical products. In this study plastic waste handling processes are seen as petrochemical activities. Crude oil is the feedstock for refineries of which the petrochemical industry feedstocks are made of. Refineries deliver oil products like naphtha as feedstock to the petrochemical industry.
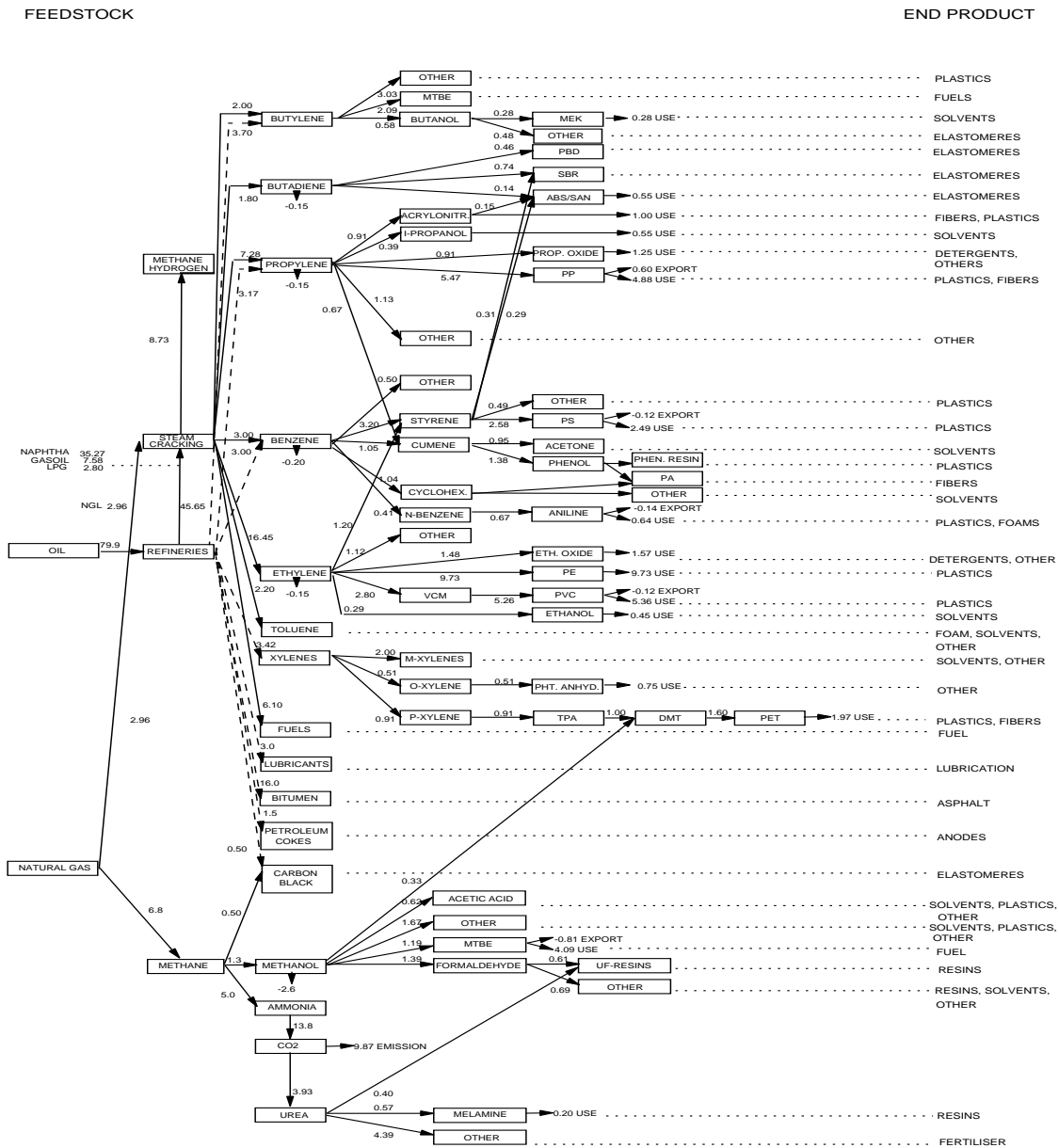

Figure 2.1 *Structure of the Western European petrochemical industry (material and energy flows in tons; exports and one-end arrows refer to exports-imports; acronyms see the glossary)*

Figure 2.1 shows the energy and material flows of the supply side for the petrochemical industry. The oil input in the refineries in Figure 2.1 is the part of refinery input, which is refined to petro-chemical feedstocks or petrochemical products. The oil input for transportation fuels is excluded from this figure. The left side of the Figure 2.1 reports the feedstocks and the right side the end products. Some end products are out of the scope of this study like fuels, asphalt, anodes and fer-tilisers. These products are imputed to other economic sectors like transportation, steel industry or agriculture. Refineries and some basic petrochemical technologies convert feedstocks into in-intermediates.

2.1 Feedstocks

Refineries convert crude oil into oil products part of which is used for petrochemical processing. Refineries can use different qualities of feedstock oil. Lighter crude oil types are preferred be-cause of high value end products. Returns from the petrochemical industry are also used by the refining industry. Naphtha is the main feedstock in the West-European petrochemical industry. It is used in the basic petrochemical steam cracking process. It amounts to 35 Mt (see Figure 2.1). Naphtha consists of refinery products in the 30°C to 210°C distillation range. Gas oil is the sec-ond most important feedstock for the petrochemical steam cracking process. It amounts to 8 Mt (see Figure 2.1). Gas oil is primarily a medium distillate, distilling between 180°C and 380°C. Gas oil used as petrochemical feedstock includes also heavy gas oils that distil between 380°C and 540°C. Liquefied Petroleum Gas (LPG) is the third most important feedstock, it amounts to 3 Mt (see Figure 2.1). LPG consists of light saturated paraffinic hydrocarbons that are derived from the refinery processes, crude oil stabilisation and natural gas processing plants. They consist mainly of propane (C_3H_8) and butane (C_4H_{10}) or a combination of the two. Ethane from natural gas is the fourth input for the steam cracking processes. With 3 Mt its share is of the same mag-nitude as the LPG share.

2.2 Petrochemical intermediate products

Steam cracking is the key process in the petrochemical industry, producing ethylene, propylene, butylene and benzene. The bulk of the intermediates are gaseous or liquid. These intermediates are converted into a whole range of polymers (plastics), solvents, resins, fibres, detergents, am-monia and other synthetic organic compounds. The petrochemical energy and material balances in this study excludes urea, lubricants, bitumen, petroleum cokes and fuel products. These products are generally not accounted for in petrochemical energy and material statistics.

2.3 Petrochemical product applications

Plastics constitute the single most important category of petrochemical products. The plastics are used in several sectors. The most important application on a mass base is packaging, followed by building/construction (see Figure 2.2). These two applications and rest category together con-sume almost 60% of the total Western-European plastic use.

A considerable discrepancy exists between materials consumption and the release of waste mate-rials for plastics and elastomeres (see Figure 2.3). This is due to the increasing stock of materials in products. A total of 4 Mt of plastics are stored per year in the product group 'buildings and constructions' alone.

In 1994 18 Mt of the plastic waste was disposed of in landfill sites (see Figure 2.3). Some energy is recovered in waste incineration installations. 5 million tonnes of plastic waste were incinerated. Disposal results in considerable amounts of fossil carbon being stored in landfill sites.

The term 'loss' in Figure 2.3 includes the actual losses of material during use (for example, detergents flushed away with the washing water). It also includes limited net exports of products, waste products and waste materials. For example: in the case of plastics, 0.2 Mt of waste plastics is exported to other regions. The net exports of product packaging can also be substantial, but no figures have been encountered. The total of storage and loss is calculated from the data on materials consumption and waste release, and on the basis of the dissipative use of certain materials. The gap between consumption and waste release is 19.1 Mt.
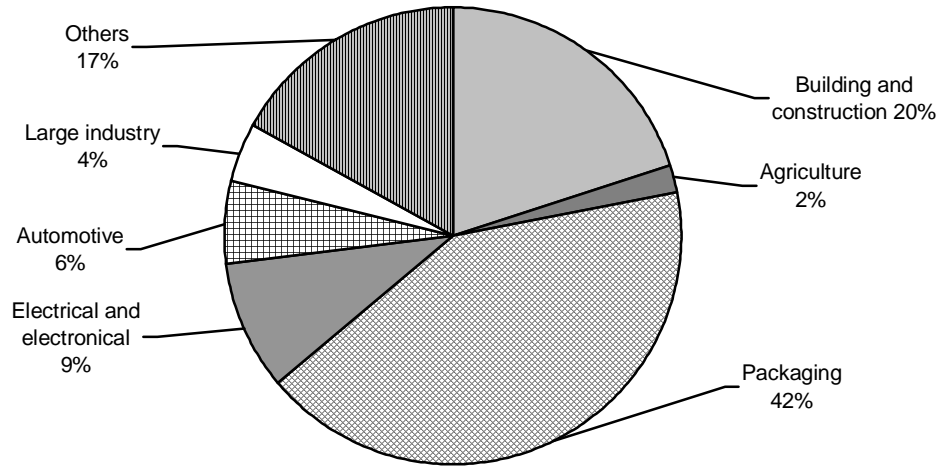

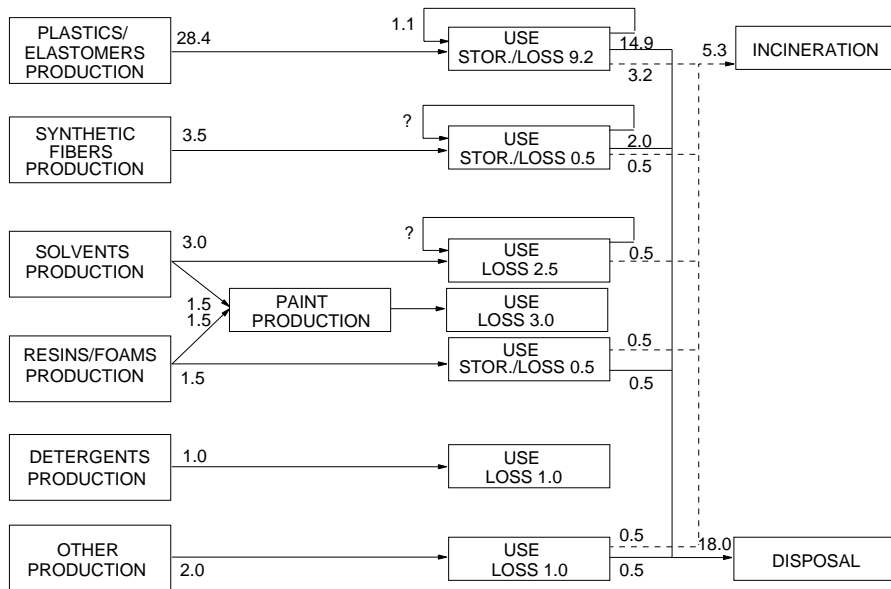Figure 2.2 *Plastics consumption by industry sector, Western Europe 1997 (AMPE, 1999)*

Figure 2.3 *Petrochemical product balance, Western Europe, 1994. Figures indicate material flows in million tonnes per year (Biggin, 1994; Hentefricke, 1994; Kunststoffe, 1993; AMPE, 1996)*

2.4 Energy balances of the petrochemical industry

The total Western European final energy consumption in 1990 was about 40 EJ. From this total consumption approximately 10%, 4.0 EJ, was consumed by the chemical industry, see Table 2.1. The figures in the column IEA represent the whole chemical industry while the MARKAL-MATTER model represents only the petrochemical industry. The IEA-correction column in Table 2.1 does not include the ammonia, chlorine and some other fine chemicals. The figures for ammonia are estimated to be (410 PJ gas, 35 PJ electricity and 25 PJ heat[2]) and for chlorine (80 PJ electricity and 10 PJ heat (Gielen, 1997)). The figures for electricity and gas have been lowered with 100 PJ each for the fine chemical industry. MARKAL-MATTER underestimates the electricity used for lighting and transportation at the production sites. Transportation means the pumping of products and intermediates between different places at the production site. Finally in this report the figure for electricity of IEA is lowered with 100 PJ for lighting and transportation at the production sites. In Chapter 5 the MARKAL-MATTER results will be compared with the IEA-correction figures in Table 2.1.

Table 2.1 *Western European OECD[3] energy consumption in the chemical industry in 1990 (Energy Balances, 1993-1994)*

	Chemical and Petrochemical [PJ/year]		*Of which feedstocks [PJ/year]*	
	IEA	IEA-correction	*IEA*	*IEA-correction*
Coal	252	252		
Crude oil	1	1		
Petroleum products	2044	2044	*1699*	*1699*
Natural gas	1060	550	*408*	*200*
Combust Renew. & Waste	28	28		
Electricity	599	284		
Heat	45	10		
Total	4029	3169	*2107*	*1899*

2.5 Conclusions

From Table 2.1 it is obvious that oil and gas are the main energy sources used in the Western European chemical and petrochemical industry (77%). More than half of the energy used comes from oil (51%). Oil and gas are the only two feedstocks for the chemical and petrochemical industry. With a share of 81% oil is by far the most important feedstock.

Figure 2.3 shows that oil and gas are mainly used to produce plastics. This is also the most interesting product group for GHG emission reduction. In several cases plastics can be replaced by renewable materials, biomass can replace oil and gas as a carbon source and plastic waste can be reused to produce new plastics (see Chapter 3).

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[2] The figures for the ammonia production are calculated with the MARKAL-MATTER model.

[3] Western-Europe OECD countries; Austria, Belgium, Denmark, Finland, France, Germany, Greece, Ireland, Luxembourg, Netherlands, Norway, Portugal, Spain, Sweden, Switzerland and United Kingdom.

3. TECHNO-ECONOMIC EMISSION REDUCTION OPTIONS

This chapter discusses possible routes for the petrochemical industry to reduce its greenhouse gas (GHG) emissions. A number of strategies (groups of options with similar characteristics) have been suggested in order to mitigate CO_2 emissions (Bruce, Lee, Haites, 1996; Watson, Zinyowera, Moss, 1996). For reducing other greenhouse gases the emphasis is on end-of-pipe technology and on substitution (Beeldman et al., 1998). Each reduction option has its own point of impact in the petrochemical industry. The following analysis is split into 4 sections:
1. energy related strategies,
2. feedstock substitution strategies,
3. material strategies,
4. reduction of N_2O emissions.

3.1 Energy related GHG reduction strategies

A number of GHG emission reduction options exist in relation to CO_2 emissions from energy use:
1. increased energy efficiency,
2. fuel substitution,
3. end of pipe strategies: CO_2 removal and underground storage.

The energy strategies and materials strategies are closely linked in the case of the petrochemical industry because most fossil fuels are used both as energy carrier and as feedstock within the same process.

The bulk of the fossil fuels are used for feedstock purposes (see Table 2.1). As a consequence, the potential for energy related GHG emission reduction is limited. Moreover, the efficiency of most petrochemical processes is already comparatively high. This is especially the case for the key steam cracking process.

Increased energy efficiency
Current trends in the petrochemical industry are aiming for increased efficiency based on a number of different approaches:
- Pinch technology.
- Process integration, e.g. CHP (co-production of electricity and process steam).
- New process routes based on new catalysts (e.g. gas phase polymerisation instead of high-pressure polymerisation).
- New process routes based on new technologies for material production (e.g. high temperature steam cracking).
- New separation technology (e.g. membranes, freeze/melt crystallisation).

The potential for increased energy efficiency is limited. Estimates indicate a potential of 10-20% (based on: EU DGXVII, 1997; Patel et al., 1999; Little, 1998). The data that are applied in this study are based on Joosten (1998).

Fuel substitution

The petrochemical industry applies mainly oil products and natural gas for its heating purposes. These could be substituted by renewable energy carriers or by electricity based on CO_2-free energy sources. These options have been considered. The most important processes are modelled separately (e.g. production of ethylene on the basis of biomass, including biomass heating) see section 3.4. Other energy demand is modelled as a single category (e.g. 'low temperature heat'), where different energy carriers can be applied.

CO_2 removal and underground storage

Because of the use of the carbon fraction of the oil input as a feedstock for plastics and other petrochemicals, the potential for CO_2 removal from off-gases is limited. According to one source, CO_2 could be recovered from steam crackers at a cost price of approximately 50 • per tonne CO_2 (excluding transportation and storage, additionally 10• per tonne CO_2) (Farla, Hendriks, Blok, 1992). The potential is in the range of 25 Mt CO_2. However, no more recent source has been found for this option. For this reason, it is not analysed in more detail. An interesting option exists with regard to CO_2 removal from ethylene oxide production. Per tonne of ethylene oxide, 0.88 tonne of CO_2 is produced as by-product. Only de-hydration and compression are necessary. The total Western European ethylene oxide production amounted to 1.6 Mt in 1992, so the potential for CO_2 removal and storage is only 1.2 Mt CO_2. This is of secondary importance for the industry as a whole. As a consequence, it is not considered in more detail. In conclusion, the potential for end-of-pipe technology with regard to CO_2 is limited for the petrochemical industry. More attractive is the application of end-of-pipe technology for N_2O emissions in the adipic acid production (see Section 3.4).

3.2 Feedstock substitution strategies

Because the bulk of the fossil fuels are used as feedstock, feedstock substitution is an important GHG emission reduction strategy. This because of the feedstock part of the fossil fuels is used to produce products. A part of the products is incinerated after it has been used (see Figure 2.3).

Steam cracking

Naphtha is the main feedstock for Western Europe steam crackers. Beside naphtha, gas oil, ethane and LPG are important fossil feedstocks. The steam crackers produce valuable products such as ethylene and propylene and a C4 fraction containing buthene and butadiene. Besides valuable products, methane, hydrogen and fuel oil are produced which, are used as fuels for the process. Furthermore, ethane and propane are produced, which are recycled to the reactor to increase the ethylene and propylene yields. Recycle streams are 67%, 14%, 5% and 4% compared to feedstock input for ethane, LPG, naphtha and gas oil cracking respectively (Straton, Hemming, Teper, 1983). Cracking efficiency on mass base is 85%, 65%, 56% and 48% compared to feedstock input for ethane, LPG, naphtha and gas (Straton, Hemming, Teper, 1983; Chauvel, LeFebre, 1989). Therefore, from GHG emission point of view ethane cracking is preferred.

A part of the crackers in Europe have the possibility to switch between fossil feedstocks. The majority of these flexible crackers can either use naphtha or gas oils. Some of them can also use LPG but, due to limited LPG storage facilities, opportunities are limited (Zehnder, 1998). Flexible crackers demand larger investments but have the possibility to use the feedstock which is cheapest at the moment, or which produces the current most valuable output products. This can also be an advantage in a situation when the industry is confronted with emission restrictions.

The shares of the output products depend on the feedstock type. Hitherto, ethylene has been the most valuable product followed by propylene and C4. In Table 3.1 the yields of the valuable products are presented (Phyllipsen, Worrell, Blok, 1995).

Table 3.1 *Output of valuable products from 4 different steam crackers*

[t output/t input]	Ethane	LPG	Naphtha	Gas oil
Ethylene	0.81	0.51	0.30	0.23
Propylene	0.02	0.17	0.16	0.14
C4	0.03	0.07	0.10	0.11

Oxidative coupling of natural gas

Oxidative coupling of natural gas converts methane into valuable products, of which ethylene is the most important. The methane conversion process takes place at relatively low pressures. Important features of the methane conversion step are the conversion percentage and the C_{2+} selectivity. Multiplied they describe the yield of hydrocarbons in a single pass through. The process has the peculiarity that increasing the methane conversion percentage is associated with a decrease of the C_{2+} selectivity. Although model calculations predict that with membrane reactors a C_2 yield of about 50% should be possible, C_2 yields in experiments have not yet exceeded 20% (Miguel et al., 1996). From different publications it can be derived that a combination of a methane conversion rate of 80% and a C_{2+} selectivity of 30% is a feasible target for the nearby future (Geem, 1992; Albright, Crynes, Nowak, 1992).

Because of the relatively low conversion rates the process involves extensive recycling streams. This affects both the investments and energy use for product separation. Membrane separation could be an option in future. However, much research has still to be done. So up to about 2020 membranes can not be used. It is even doubtful if membrane separation will ever be able to replace conventional separation (Gielen, Vos, Van Dril, 1996).

Flash pyrolysis of biomass

With the flash pyrolysis process biomass is cracked at high temperatures and short residence time into ethylene, BTX, CO and CO_2. The type of wood used influences the product distribution of the process. The ethylene yield varies between 20.7% for fir wood and 27.4% for pinewood, respectively (Steinberg, Fallon, Sundaram, 1992). One must emphasise that flash pyrolysis of biomass has only been tested on a laboratory scale. At the moment a pilot plant is operating in Canada, therefore it has been estimated that the process becomes commercially available in 2010 (Joosten, 1998). Theoretical the flash pyrolysis process can use a wide range of biomass sources, only wood chips are considered in this study.

The process has much in common with the naphtha cracking process. Therefore the missing information is adapted from the naphtha cracking process, which is scaled according to feedstock input (8.3 ton biomass per ton ethylene versus 3.3 ton naphtha per ton ethylene). It is assumed that the process delivers enough high pressure steam (hps) to drive the compressors so that the electricity demand is relatively low, like it is for naphtha cracking. The costs for the flash pyrolysis process were derived from the naphtha cracking process and scaled according to feedstock input. Additionally, the costs have been increased with 25%, which accounts for the relatively expensive methane recycle streams of the biomass flash pyrolysis process (Joosten, 1998). Because the energy as well the feedstock for this process is renewable the net GHG emissions are very low. Only the electricity used in the process emit some greenhouse gasses when generated with fossil fuels.

Methanol and/or ethanol to olefins

Methanol to olefins produces ethylene and propylene via catalytic dehydration of methanol. The methanol can be produced from fossil fuels or from biomass. Experiments show that the product composition of the process is highly dependent on the catalyst used (Geem, 1992; Redwan, 1997; Schönfelder et al., 1994). To a lesser degree the product output can be influenced by changing the reaction temperature which influences the reaction severity (HCP). Processes with high propylene co-production are most feasible (Geem, 1992). Although a commercially MTO process, that is ready to be implemented, is available, no plants have been build yet (HCP). Dehydrogenation of ethanol is basically the same process as methanol to olefins. Dehydrogenation of ethanol was historically widely applied but abandoned because of high feedstock costs. Methanol as well ethanol, when produced from, are feedstock substitution options, which can reduce GHG emissions to a large extend. With biomass feedstocks only the GHG emissions for the electricity and heat if produced with fossil fuels must be accounted to this process.

Pyrolysis DRP process for mixed plastic waste

Pyrolysis is the process where mixed plastic waste is heated in an oxygen-free atmosphere. At a temperature of several hundred degrees, the hydrocarbons decompose to yield a mixture of solid, liquid, and gaseous products. Product composition depends on temperature and pressure (Kaminsky, 1992). The higher the temperature, the more gaseous products are formed (Ehrig, 1992). An important fraction of this gaseous product is ethylene if plastics are used as feedstock. Pure ethylene is the most valuable product that can be used for plastic production. The ethylene yield results vary considerably. References state a yield of up to 40%. Such a high value is not yet proven on a large scale. In this study, a lower ethylene yield value was used. It is estimated that 25% of the lower heating value (LHV) of the plastic waste is used for process heating purposes. Plastic pyrolysis technology is tested on pilot plant scale. Coke and oil by-products had problems of quality in the past; the present status is unclear (Kaminsky, 1993).

The Pyrolysis process has a direct CO_2 emission of about 3.2 ton CO_2 per ton ethylene. This is caused by the 25 of the lower heating value of the plastic waste input used as processing energy. This emission is significant higher as the steam cracking direct emissions, which are between 0.25 t/t and 1.15 ton CO_2 per ton ethylene. However, the indirect emission of the pyrolysis process is 0 t/t and the indirect emissions of the steam cracking processes are between 3.4 and 13.5 t/t so that he total CO_2 balance is in favour of the pyrolysis process (Joosten, 1998; Gielen, Okken, 1993).

3.3 Changing materials use

Energy use (and GHG) emissions in the materials life cycle are generally concentrated in the materials production and waste handling stages[4]. There are two strategies that can be followed: either reduce the emissions per unit of material, or reduce the materials use. This section focuses on the latter type.

Generally speaking there are three different strategies to reduce the GHG emissions through changes in material use. Firstly materials could be used more efficiently so less material is needed. Secondly other materials such as metals, paper, wood, etc can substitute petrochemical products. Especially substitution by renewable materials such as wood and paper can reduce the GHG emissions significantly. The third option is recycling of petrochemical products.

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[4]   Exceptions exist e.g. in the transportation sector (fuel efficiency depends on vehicle weight).

However, caution must be exercised when following this generic guideline. Higher GHG emissions during primary materials production may also be offset by GHG emission reductions in the waste stage, e.g. because of recycling. If a certain option affects several of the product life cycle stages by increasing emissions in one part of the life cycle and decreasing emissions in the other part, a life cycle analysis approach is required for proper assessment. If flows of energy and materials are exchanged between the life cycle of the individual material/product and the other parts of the energy and materials system, a systems approach is required for proper assessment.

As a consequence of this complexity, design rules can only be used to develop ideas. There is no initial preference for specific design strategies. Design for Environment (DFE) emphasises the importance of an increased product life. Options such as increased reliability/durability, easier maintenance/repair, modular structures, classic design or a strong product/user relation are mentioned. The assessment of these options requires extensive design knowledge and this is only available at the very detailed product level. Moreover, classic design and a strong product/user relation are considered to be options that influence the production performance. Consequently, the assessment of their potential requires a social sciences approach, beyond the scope of this techno-economic optimisation.

Strategies that affect product service mix or welfare level cannot be evaluated simply on the basis of cost-effectiveness. Apart from the modelling constraints, policies focusing on changing lifestyles are unpopular with the public and most policy-makers (Uitdenbogerd, Brouwer, Groot-Marcus, 1998). For these reasons, they will not be considered in the analysis. The eight strategies are set out in more detail in Table 3.1. In this table, DFE rules of thumb are grouped into improvement strategy categories.

Product design is a balancing act between materials requirements on one hand, and complexity (and costs) on the other. In this study it is assumed that there is still a certain potentials for increased materials efficiency. The balance between materials and costs may shift in favour of increased materials efficiency if the environmental impacts are included in the costs.

Table 3.2 *Improvements within the strategy categories*

Strategy	Approach
1. Increased resource efficiency	Reduced losses during materials production
2. Increased materials efficiency	Improvement of the chemical or physical materials quality
	Reduced variation in materials quality
	More diverse materials standardisation
	Reduced materials losses during product manufacturing
	Less materials intensive product design
3. Increased product efficiency	Increased product life
	More efficient product use, e.g. shared car ownership
	Development of multi-functional products
4. Recycling/energy recovery from waste materials	Increased waste recovery
	Increased waste recycling (including cascading)
	Increased energy recovery
5. Reuse of waste products	Increased product recovery
	Increased product reuse
6. Substitution of natural resources	Renewable organic feedstocks
7. Substitution of materials	Renewable materials (e.g. wood products)
	Less CO_2 intensive materials
	Materials with superior physical characteristics
	Recyclable materials
8. Substitution of products	Less materials intensive products
	Products that require less maintenance
	Products with longer life, or multifunctional products

The minimum amount of material for a design is not only determined by the materials properties, but also by the processing equipment: what size can be processed, which shapes can be manufactured. These limitations are especially relevant for the short-term improvement potential, but less relevant on the long term, because equipment must be replaced anyway.

Many products, especially those manufactured in small series, are not engineered for minimum materials consumption. Rules of thumb, or trial and error procedures, are in such cases used to determine the minimum amount of material. Examples show that significant savings can still be achieved. Input data for products are discussed in (McKeever, Anderson, 1988; Brezet, Van Hemel, 1997; Philips, 1992).

Three strategies (1, 2 and 3) from Table 3.2 will not be discussed in this report. These efficiency strategies are complex issues that require a detailed discussion, and such a discussion is beyond the scope of this study. For more information about the MARKAL-MATTER model see Annex A, or the MARKAL-MATTER Internet site (http://www.ecn.nl/ unit_bs/etsap/ markal/matter/, 1999). Strategy 6 is already been discussed. Strategies 4 and 5 have partly been discussed in paragraph 3.2 but get more attention in this paragraph. The strategies 7 and 8 are the strategies on which the MARKAL-MATTER models focuses. Strategy 7 includes switch from plastics to wood or to plastics from renewable feedstock. Also plastics which are recyclable belong to this group. Strategy 8 includes options like thinner materials with the same strength or materials that fulfil the needs of the traditional material with less maintenance. If some kind of carbon emission penalty is set the strategies 7 and 8 can become important for the petrochemical industry.

This paragraph focuses further on a number of recycling techniques because a number of new plastic waste recycling technologies have been developed in the last decade, especially in Germany because of the packaging legislation that specifies certain recycling rates. Eight types of plastic waste management options are modelled, each capable of handling a certain waste quality. The eight types are; re-extrusion, solvent separation, pyrolysis DRP process (see Paragraph 3.2), Hydrogenation VEBA process, plastic waste injection in blast furnaces, plastic waste incineration in cement kilns, grate firing and disposal. Also a separation in three different plastic waste types is made, clean plastic waste (CPW), mixed plastic waste (MPW) and plastics in municipal solid waste (MSW). Clean plastic waste can be processed with technologies that require low quality waste inputs (e.g. incineration), but the other way around is impossible without an upgrading effort. Every upgrading technology has energy input so that the overall recycling efficiency declines. Only re-extrusion is suitable for CPW, a large group of solvent separation, pyrolysis, hydrogenation, blast furnaces and cement kilns are capable of MPW processing. Grate firing and disposal are suitable for plastics in MSW. Clean Plastic waste is called High Quality Waste in Figure 3.1, which shows the different plastic waste management strategies.
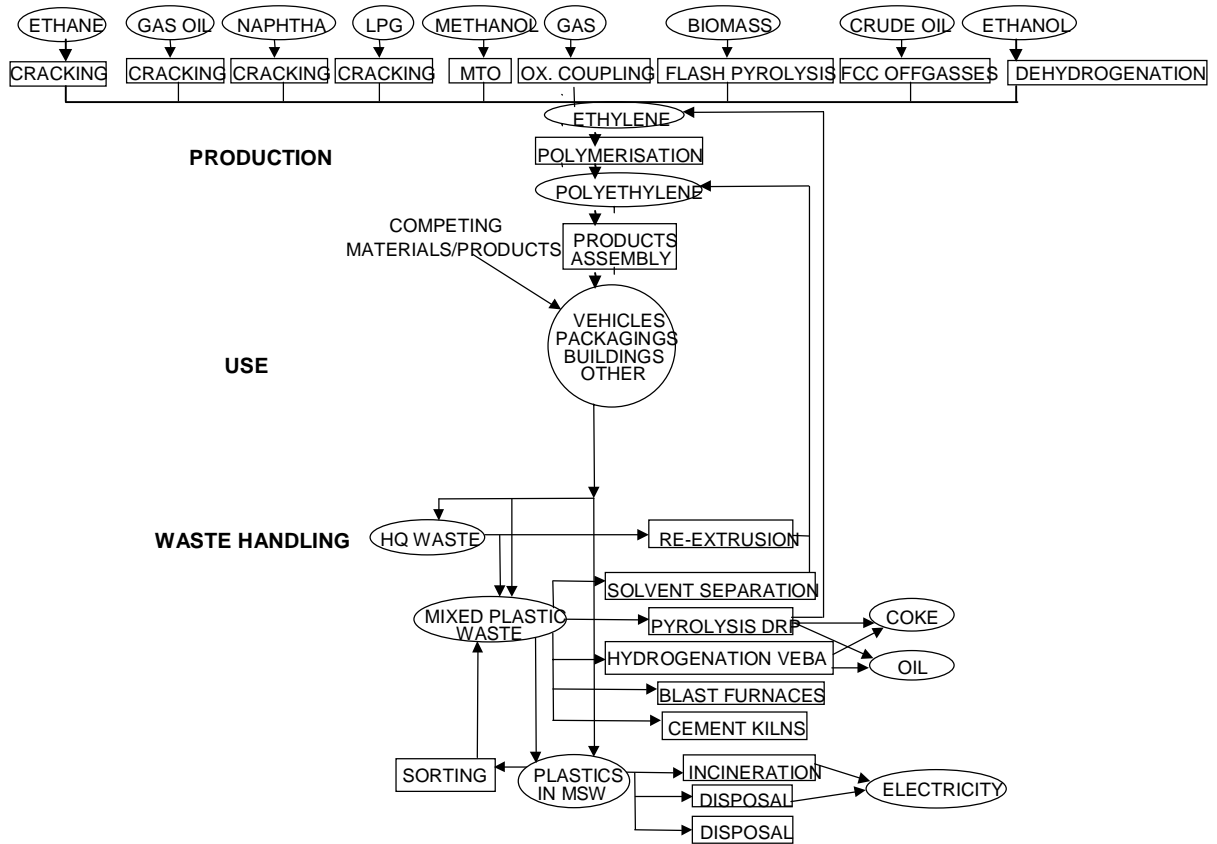
ETHANE GAS OIL NAPHTHA LPG METHANOL GAS BIOMASS CRUDE OIL ETHANOL

CRACKING CRACKING CRACKING CRACKING MTO OX. COUPLING FLASH PYROLYSIS FCC OFFGASSES DEHYDROGENATION

ETHYLENE

PRODUCTION

POLYMERISATION

POLYETHYLENE

COMPETING
MATERIALS/PRODUCTS

PRODUCTS
ASSEMBLY

VEHICLES
PACKAGINGS
BUILDINGS
OTHER

USE

WASTE HANDLING   HQ WASTE   RE-EXTRUSION

SOLVENT SEPARATION

MIXED PLASTIC
WASTE

PYROLYSIS DRP   COKE

HYDROGENATION VEBA   OIL

BLAST FURNACES

CEMENT KILNS

SORTING   PLASTICS
IN MSW   INCINERATION   ELECTRICITY

DISPOSAL

DISPOSAL

Figure 3.1 *Model structure for polyethylene, the most important plastic type*

Figure 3.1 shows a waste cascade for plastics. Three types of plastic waste are modelled. The first one is clean plastic waste, representing pure plastics that can be re-extruded to yield polymers. The second type is mixed plastic waste. Mixed plastics, e.g. shredder residues, can only be recycled to high-grade polymers after separation. The third type is plastic in municipal solid waste, e.g. food packaging. Grate incineration and disposal are options for treatment of this waste stream. The upgrading process is modelled by 'dummy' processes, which convert clean plastic waste into mixed plastic waste and mixed plastic waste into plastics in municipal solid waste. Upgrading is modelled as a sorting process that converts plastics in municipal solid waste into 'mixed plastic waste'. The cost for this sorting process is based on the German DSD (Duales System Deutschland).

Re-extrusion
Re-extrusion technology is only applicable for clean plastic waste types. The plastic is ground and extruded. The material output quality depends to a large extent on the waste input quality, additives can improve the output quality (Menges, Michaeli, Bittner, 1992; Ehrig, 1992). If mixed plastics are used as input, the resulting material will only be suitable for a limited number of applications. Re-extrusion recycles the plastics to the production process. In the production process new plastic products are made from a mixture of new and recycled plastic. The net GHG emissions are lower for the re-extrusion process. This is caused by the emission effect of the saved fossil feedstocks, which are larger than the extra GHG emissions due to the extra energy needed for this process.

Solvent separation

This process is based on the difference in solvability of plastics in organic solvents. The process uses selective dissolution at increasing temperatures and flash devolatilisation to separate mixed plastics into component polymers with pigments and fillers predominantly removed. The process has been developed on a pilot plant scale, it is uncertain what results will be achieved on industrial plant scale (Visalli, 1992; Schurr, Schneider, 1998).

Hydrogenation VEBA process

Mixed plastic waste can be treated with hydrogen to produce feedstock such as a naphtha-like product and a hydrogenation residue that can be used in coke production. A pilot plant has been set up in Germany and the construction of a large-scale plant is scheduled. The technology can be characterised as a thermal hydrocracking/hydrogenation process. The reactions take place in a liquid phase reactor and a gas phase reactor at temperatures of 400-450°C and a pressure of up to 250 bar. The main problem at present is the feeding of plastics into the reactor. Data for hydrogen consumption are still uncertain, but they would seem to be significantly higher (as might be expected on the basis of the plastics chemical structure) (Niemann, Wenzel, 1993).

Blast furnaces

Plastic waste is injected in blast furnaces to serve as reduction agent for absorbing oxygen from ironoxide. Normally, heavy oil is used for this purpose. By injection of plastic waste, a part of the heavy oil is saved (Patel, 1996). It is disputable whether the process has to be regarded as material substitution or not. Heavy oil or plastic waste injection does not primarily aim at combustion for heat production, but at obtaining a chemical reaction in which the reduction agent is materially involved. Therefore, in this study this process is considered as material recycling. Mixed plastic waste injection into blast furnaces is currently practised on pilot plant scale in Germany (Janz, 1996; Lindenberg et al., 1996). Cost data have not been encountered. Because the additional equipment is similar to the equipment for incineration in cement kilns, the same cost data have been used.

Plastic waste incineration in cement kilns

Incineration of waste types in cement kilns is widely spread over the whole of Europe. Mixed plastic waste incineration in cement kilns was developed in Italy. The application of plastic waste requires special waste injection equipment due to its low weight. Investment costs for storage, transportation, and injection equipment is approximately 40• /t plastic waste capacity. Cost of labour, etc., is an additional 10• /t (Knopf, 1995).

Grate firing (municipal solid waste)

Current grate firing systems achieve an efficiency of 20-22%. Higher efficiencies are possible if the incineration plant is coupled to combined cycle power plants. Low temperature steam from the incineration plant is further heated in the power plant and subsequently used in a steam turbine. Such combined plants can achieve an efficiency of 28% for the incineration part. One such plant has been built in the Netherlands and is currently operating (Van der Knijff, 1995).

Disposal (municipal solid waste)

Disposal costs are largely determined by government intervention. There are large differences from one country to another. It is expected that disposal in landfills will become increasingly difficult. This study assumes that disposal costs will increase from 50• /t in 1990 to 150• /t in 2010. After 2010 the disposal costs will subsequently increase to 200• /t in 2040. Products can also be seen as a way of disposal. This is because the carbon in the products is fixed and won't be emitted to the atmosphere in short or long time. Therefore the carbon in plastic products can be seen as being disposed.

The advantage of recycling technologies from a GHG emission point of view depends on the reference technology (incineration or disposal) (Gielen, Okken, 1993; 1994). The main saving is the feedstock energy of the plastics, which constitutes two thirds of the energy input into primary plastics production. If only renewable feedstocks are used in plastic production, the GHG emission reduction effect from recycling becomes negligible.

3.4   Reduction of industrial N_2O emissions

Western-European adipic acid production amounted in 1992 to 650 kt (Weissermel, 1994). Adipic acid is produced in 10-20 industrial plants. Adipic acid is an intermediate in the production of nylon 6.6. Its chemical structure is $COOH(CH_2)_4COOH$. It is produced from cyclohexane that is converted into a mixture of cyclohexanol and cyclohexenone by catalytic oxidation. The mixture is catalytically converted into adipic acid. Two catalyst systems are applied. One uses HNO_3, the other one uses oxygen. In the system that uses HNO_3, significant amounts of N_2O are generated as by-product. The N_2O- concentration in the off-gases is 20 volume % (Weissermel, 1994; Ayres, 1996). In 1998 ca. 2 million tons of adipic acid is produced. The manufacture of adipic acid also results in the production of offgases containing ca. 0.3 ton of nitrous oxide per ton of adipic acid (equivalent to 90 t CO_2/t) (Chemical Week, 1999; Castellan et al., 1991). From 1991 the major producers of adipic acid start to develop and implement technologies to reduce N_2O emissions. In 1990 the emissions for Western Europe equals 40 - 60 Mtons CO_2 equivalents. If oxygen is used, no N_2O is produced. However, this new process is not yet widely applied. Other new process routes start from butadiene. In conclusion, alternative process routes can on the long term easily reduce the N_2O emissions in adipic acid production.

In conclusion, removal of N_2O in exhaust gases poses the most attractive alternative. In 1999 N_2O abatement facilities are now operating at nearly all sites of the major adipic acid producers[5]. The industry is using three different technologies; advanced thermal destruction, catalytic destruction and conversion of N_2O to nitric acid, see Table 3.3. All technologies have demonstrated the capability to very efficiently abate N_2O emissions, 90 - 98% emission reductions. Technology choice is a matter determined by individual sit economics. Based on Table 3.3 emission reduction costs are below 1• /t CO_2 equivalents (Gielen et al., 1998).

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[5]   Although in 1999 nearly all adipic acid producing sites are operating N_2O abatement facilities, the Base Case in 2030 still emits 50 Mt CO_2 equivalent/year N_2O. In reality the N_2O emissions will probably decline sharp from 2000 onwards. The newest N_2O abatement technologies are not modelled in the MARKAL-MATTER cause lack of data in the period constructing the model.

Table 3.3 *Abatement of N_2O by major adipic acid manufacturers (Reimer et al., 1999)*

Site or Manufacturer	1990 emissions [1000 metric tons]	Technology Implemented	Investment [million US$]	Start-up completed	Estimated abatement in 2000 [%]	Est. 2000 Emissions [1000 metric tons]	Estimated reduction in 2000 [1000 metric tons]	Reduction costs [US$/metric tons]
Singapore (Du Pont)	--	Thermal	10	1994	98	0.4	--	--
Orange, TX (Du Pont)	44.1	Catalytic	7.3	1996	90	5.5	38.6	189
Maitland, Ont (Du Pont)	34.6	Catalytic	10.6	1997	90	3.8	30.8	344
Victoria, TX (Du Pont)	4.4	Switch thermal/ Catalytic	12	1997	95	5.1	-0.7	--
Wilton, UK (Du Pont)	81.3	Thermal	17	1998	94	3.8	77.5	219
Ashai	20	Thermal	5.0	1999	98	0.6	19.4	258
BASF[1]	58	Catalytic	7.3	1997	95	3.2	54.8	133
Bayer	15.5	Thermal	4.0	1993	96	0.8	14.7	272
Rhodia (Chalampe)[1]	55	Conversion to HNO_3	16.8	1998	98	1.7	53.3	315
Solutia[2]	1.6	Switch thermal/ benzene oxidant	--	>2002	98	2.1	-0.5	--
Total major producers	314.5					27		
Est. Total (all prod.)	370.5					140		

[1] Based on Scott (Chemical Week, 1998).
[2] Based on Tullo (1999).

4.   MODELING THE ENERGY AND MATERIALS SYSTEM

4.1   The MARKAL model

The MARKAL linear programming model is a representation of (part of) the economy of a region. The economy is modelled as a system, represented by processes and physical and monetary flows between these processes. These processes represent all activities that are necessary to provide products and services. Many products and services can be generated through a number of alternative (chains of) processes. The model contains a database of several hundred processes, covering the whole life cycle for both energy and materials. The model calculates the least-cost system configuration that meets certain energy, materials and product demand. This system configuration is characterised by process capacities, activities and flows.

Processes and model constraints are input data that must be provided by the model user. Constraints are determined by the maximum introduction rate of new processes, the availability of resources, environmental policy goals, etceteras (Gielen, 1998).

Processes are characterised by their physical inputs and outputs of energy and materials, by their costs, and by their environmental impacts. From the GHG emission, carbon dioxide, methane, nitrous oxide and perfluorcarbons are considered. Waste volumes and land requirements are other environmental impacts that are considered. Emissions are accounted for in physical units. Emissions are valued in financial terms on the basis of a CO_2-equivalent penalty level, which is set by the model user. Upstream emissions are in the MARKAL methodology transferred in the process chain through the increased prices (or marginal costs) of energy, materials and products. Annex A gives a more detailed description of the MARKAL model.

4.2   MATTER: Western European MARKAL

Approximately one third of all greenhouse gases emissions can be attributed to the materials system. Changes in material flows can influence the GHG emissions significantly. The Western European MARKAL-MATTER model[6] has been developed within the MATTER project (Materials Technologies for GHG Emission Reduction) in order to study these strategies in more detail. The model covers more than 25 energy carriers and 125 materials. More than 50 products represent the applications of these materials and 30 categories of waste materials are modelled.

This study focuses on the petrochemical industry in Western European because this sector can be seen as a closed system. The import and export flows are small compared to the total amount of petrochemical products used in Western Europe. Policy by governments or the industry its self are relatively unaffected by developments in other parts of the world.

Improvement options in the energy system are considered simultaneously with the material system solutions. Integrated assessment of improvements in the energy system and the materials system is important because different reduction strategies influence each other's efficiency. For example if the reference electricity production becomes less CO_2 intensive, electricity production in waste incineration plants becomes a less attractive option. As a consequence of such interactions, the assessment of the potential and the cost-effectiveness of reduction strategies require an integrated

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[6]   Western-Europe are the OECD countries; Austria, Belgium, Denmark, Finland, France, Germany, Greece, Ireland, Luxembourg, Netherlands, Norway, Portugal, Spain, Sweden, Switzerland and United Kingdom.

system approach. Apart from the slow capital replacement rate, a dynamic approach is required because of the time lag between materials consumption and waste release beyond the product life. For example, changing materials consumption in one year can influence the recycling potential in future years. Moreover, GHG emission reduction will take decades because the remaining life of standing capital equipment must be considered. Changing technology, changing consumption patterns, changing resource prices and changing environmental policy goals are other issues that must be considered in a dynamic analysis. Annex A gives more information about the MATTER models that have been developed and the MARKAL-MATTER model which, is used for this study.

4.3   Materials and waste materials selection

The selection of materials is based on the analysis in (van Duin, 1997; Gielen, 1998). The selection covers all key groups of materials from a GHG emission point of view: ceramic materials, inorganic materials, metals, natural organic materials, plastics and other synthetic organic materials. These groups of materials are further disaggregated in this analysis. A list of materials that are separately modelled is shown in Table B.9 in Annex B. Also a list of all waste materials is provided in Table B.8 in Annex B.

The level of detail for materials and products is to a large extent determined by their relevance from a GHG-emission point of view. The general rule that has been applied is that all material flows with an upstream GHG emission that equals at least 0.1% of the total Western European GHG emission are separately modelled (which corresponds to approximately 5 Mt CO_2 equivalents per year). A material flow or product group is further based on the uniformity of the production processes, the uniformity of the applications and the availability of statistical data regarding material flows.

From a CO_2 emission point of view, the energy intensity has been used as an important indicator for the selection process. From a CH_4 emission point of view, the natural organic materials (paper and board, wood products, other natural fibres) deserve special attention because of CH_4 formation during their decomposition in landfill sites. Regarding N_2O, industrial production processes of nitric acid, Adipic acid and Caprolactam have been modelled separately. Finally PFC emissions related to primary aluminium smelting have been considered.

In Table B.9 in Annex B a list of all waste materials that are separately modelled in MARKAL-MATTER is shown. Three types of materials from Annex B have no waste material equivalent. First, intermediates have no waste equivalent (see Table B.6 in Annex B). Second, some materials are consumed or dissipated during their use phase. Examples of such materials are fertilisers. A third group consists of waste materials that are irrelevant from a GHG emission point of view, because they can neither be recycled (with significant GHG benefits) or be used for energy recovery. For example, used concrete is not separately modelled. Its recycling as concrete filler is not relevant from a GHG emission point of view. Its disposal has been accounted for through a disposal fee.

Several waste material qualities have been modelled if the quality of the waste material limits the recycling potential. The waste quality depends on the product category for which the material is applied. For example the bulk of plastic packaging ends up in Municipal Solid Waste (MSW). The technological potential and the economics of plastic waste recycling are highly dependent on the quality of the waste flow.

The modelled waste materials are characterised by their fixed chemical composition, Clean poly-styrene waste, clean polythene waste etceteras. Instead of modelling aggregated waste streams such as household waste, shedder waste, demolition waste etceteras. This approach provides some insight into the changing waste flow composition. Especially over a period of decades the composition will change significantly. As a consequence, its potential for energy recovery and for recycling will change also. The waste material approach with different waste qualities allows modelling of waste cascades. An example of a cascade within the model is shown in Figure 3.1 in the previous chapter.

5.   RESULTS: THE IMPACT OF GHG POLICIES

5.1   Refineries

The total amount of refinery products in the base case scenario increases in the modelling period 1990-2050 with approximately 40%, see Figure 5.1. All the petrochemical products do not change significantly in production volume except for gasoline and gas oil. The growth in gasoline volume is the result of a growing fuel demand in the transport sector. Gas oil is one of the cheapest feedstocks to produce ethylene and propylene, see Table 5.1.
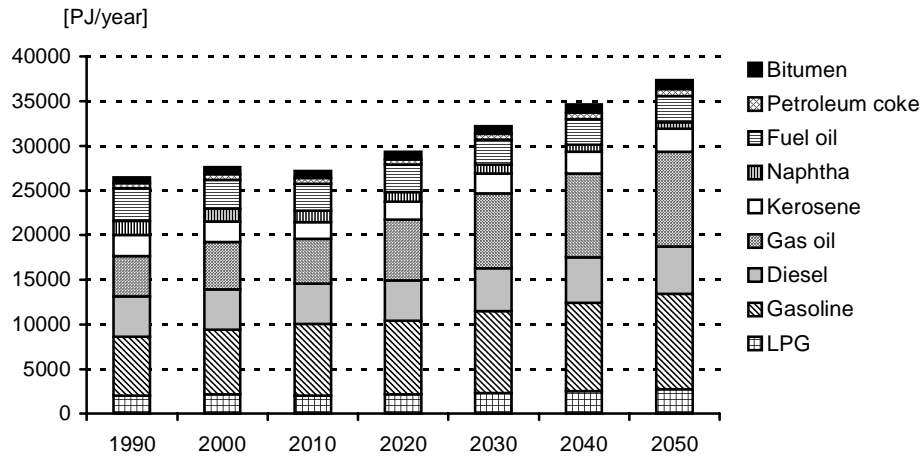

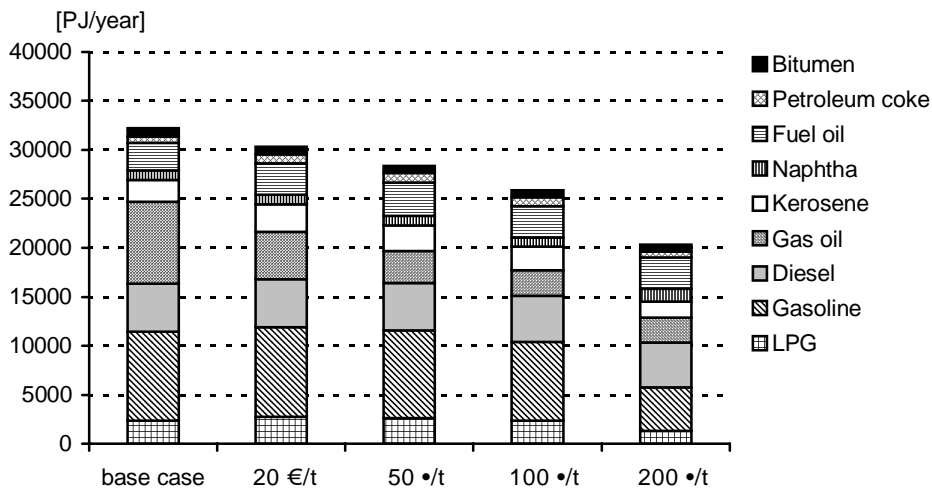Figure 5.1 *Refinery products in the base case in the period 1990-2050*

Figure 5.2 *Refinery products in 2030 with increasing permit prices*

Figure 5.2 represents total production of the refineries with increasing emission permit prices. A higher emission penalty results in a 35% decrease in total production volume. Gasoline and gas oil are the products with a significant decline, LPG and kerosene show also a slight decline in production. The decline of refinery products is caused by replacement of fossil-based feedstocks by renewable based feedstocks like biomass and waste. However, the production of biofuels is allocated to the petrochemical industry.

5.2   Petrochemical industry

Figure 5.3 shows a 40% increase in ethylene production in the base case for the period 1990-2050. The production switches from naphtha cracking in 1990 to gas oil cracking in 2050. In 2050 gas oil has a share of 80% in total ethylene production. LPG cracking quadruples its amount of production in 2010 after witch the amount declines to its original contribution in 2050. The ethane cracking process is in 2050 almost completely gone because of declining ethane availability. In 2040 and 2050 less than 0.5 Mt ethane is produced with the waste pyrolysis process.
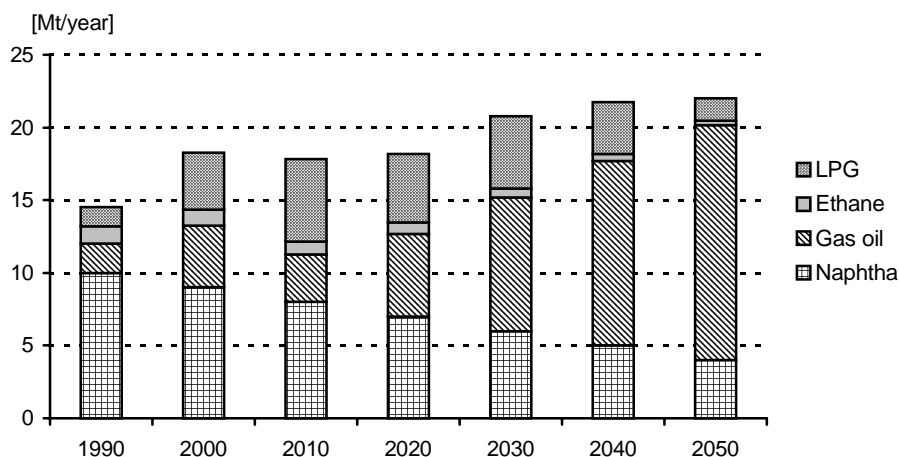
[Mt/year]

Figure 5.3 *Ethylene production in the base case in the period 1990-2050*

The rise in total production in Figure 5.3 is the result of a growing demand for plastics. The replacement of naphtha by gas oil is a feedstock switch. The availability of gas oil increases while naphtha is more expensive. However, LPG and ethane are cheaper than gas oil until around 2030 gas oil rapidly increases its share in feedstocks. The available LPG is then mainly applied as transportation fuel. There is not enough ethane available for a larger share in feedstock.

In Figure 5.4 ethylene production switches from fossil-based feedstock to renewable feedstocks. Up to a penalty of 50 • /t the production switches from gas oil to LPG cracking and the total production is not affected. In the 100 and 200 • /t cases the total ethylene production is about 15% lower than in the other cases. At 100 • /t the use of gas oil is about 60% less than in the previous case. Ethylene production from Fluid Catalytic Cracking off-gases (a-refining activity) emerges in the market. In the 200 • /t case the use of LPG is reduced by 75% compared to the 100 • /t case. Waste pyrolysis, wood pyrolysis and the MTO process have gained a substantial share in the ethylene production. The amount of naphtha and ethane used for the production of ethylene remains constant because of a lower bound in the model. It is assumed that always a certain amount of naphtha and ethane will be produced where no other application can be found for.
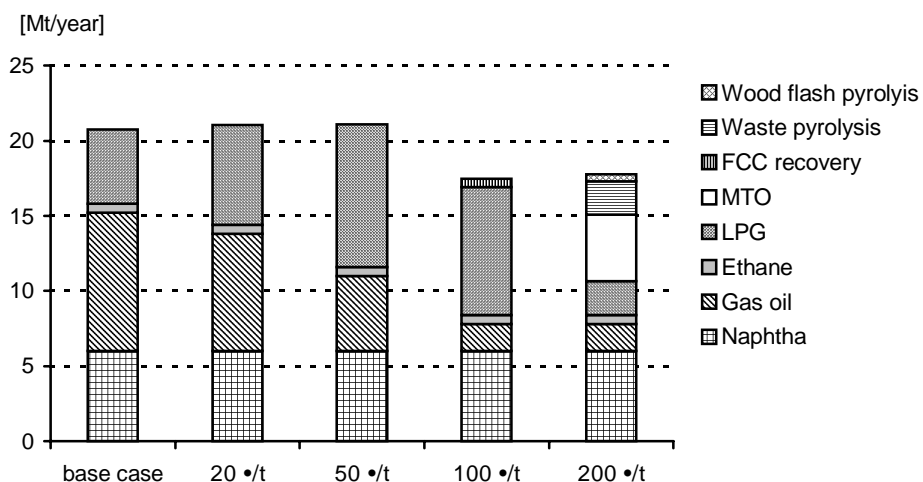
[Mt/year]

Figure 5.4 *Ethylene production in 2030 with increasing permit prices*

The total production of propylene is lower than the total production in the statistics. This is probably caused by incompleteness of the model. The rise in total propylene production is the result of a growing demand for plastics, see Figure 5.5. The total production almost doubles from 1990 to 2050. The decline of naphtha is limited through a minimum bound in the model because it is assumed that a certain amount of naphtha will be produced wherefore no other application can be found for. The growth of gas oil is caused by its relative low price, see Table 5.1. The market for refinery products is limited therefore refinery residues are more and more used to produce propylene. The amount of LPG quadruples in the period 2010-2030 but declines in 2050.
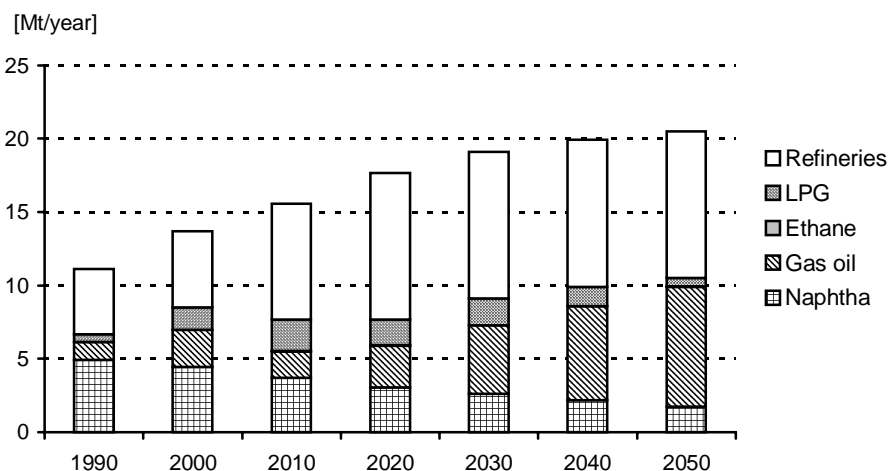
[Mt/year]

Figure 5.5 *Propylene production in the base case in the period 1990-2050*

The propylene production decreases by 10% with a higher emission penalty, see Figure 5.6. The naphtha cracker and the recovery from refineries stay at the same level. Gas oil cracking declines from 5 Mt to 1 Mt. The LPG cracker grows first from 1.5 Mt to 5 Mt however, declines sharply to 0.5 Mt in the 200 • /t case. In the 200 • /t case all the LPG is use in the transportation sector. The MTO processes compensate the propylene production decline. In 2050 the MTO process has a share of 25% in total propylene production. The amount of propylene produced with the ethane cracking process is very small, 0.01 Mt/year in the base case till the 100 • /t case. In the 200 • /t case the production of propylene with the ethane cracking process has increased till 0.03 Mt/year. Although ethane cracking is shown in the legend of Figure 5.3 ethane cracking is not shown in the figure itself because of its insignificance.
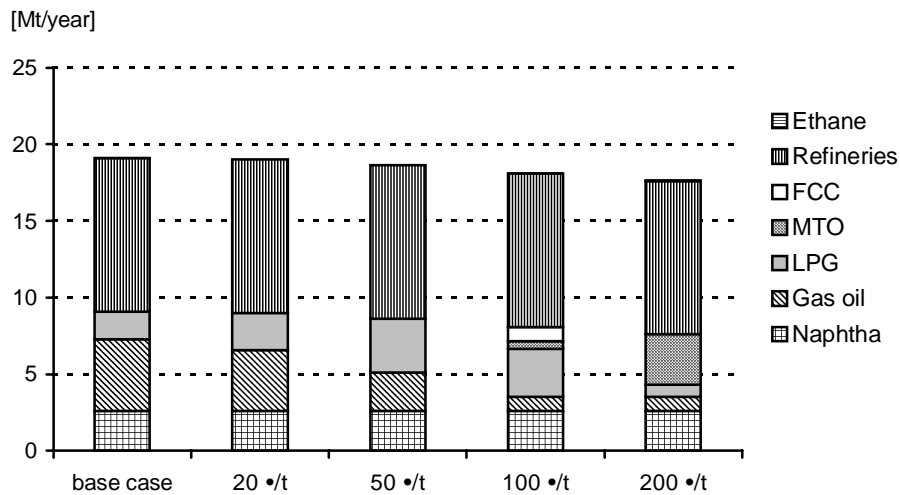
Figure 5.6 *Propylene production in 2030 with increasing permit prices*

The majority of the produced ethylene is used to produce polyethylene, see Figure 5.7. However, the total quantity of ethylene used for polyethylene production does not change. The growth of 50% comes from ethylene oxide (+35%), styrene (+62%), VCM (+125%) and others (+180%).
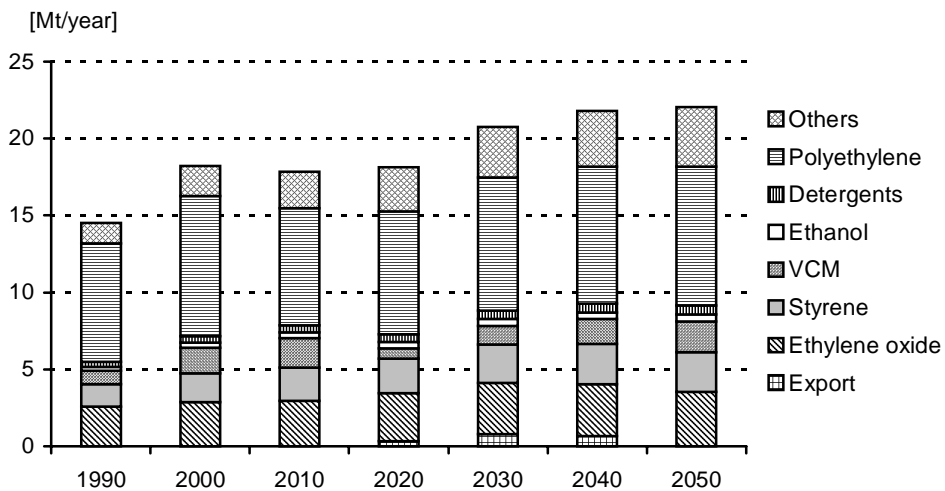
Figure 5.7 *Ethylene use in the base case in the period 1990-2050*

Up until 50 • /t the total ethylene use is not affected, see Figure 5.8. A decline of 20% in the 100 and 200 • /t cases is the most important impact of increased permit prices. This is caused by a decrease of ethylene export and a 50% reduction in the production of other products. Also no ethylene is used to produce ethanol and detergents in the 100 and 200 • /t cases. The production of ethylene oxide, styrene, VCM and polyethylene require in all the cases the same amount of ethylene.
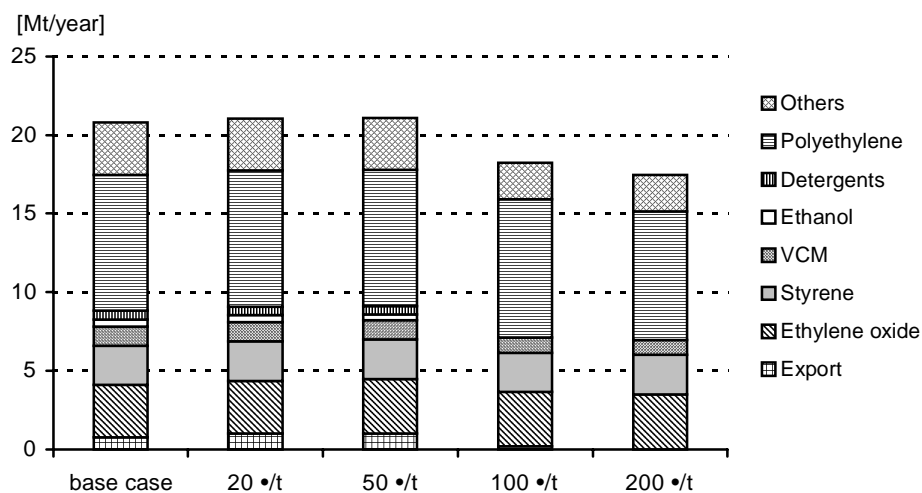
Figure 5.8 *Ethylene use in 2030 with increasing permit prices*

When the propylene production Figure 5.5 is compared to propylene use in Figure 5.9 small differences in the totals appear. Losses in the production processes are responsible for these differences. All the categories in Figure 5.9 increase. The residual use and the production of acrylonitrile double in the period 1990-2050 while the others change less.
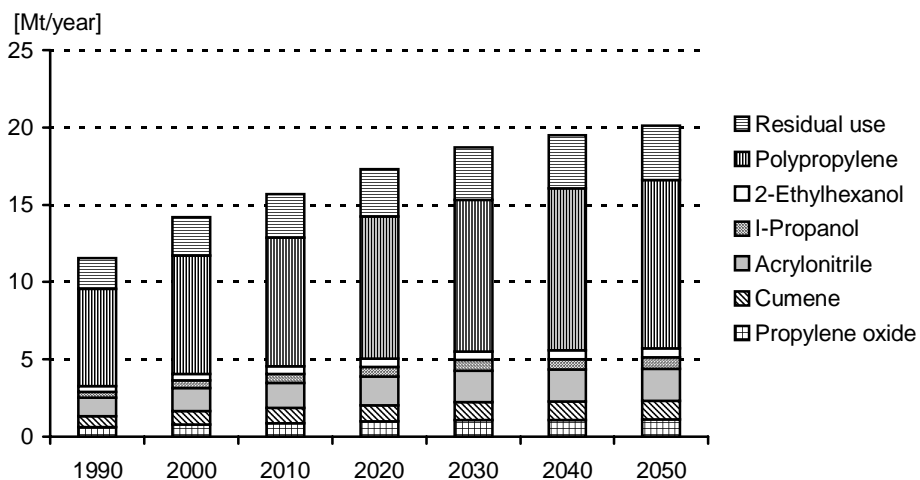
Figure 5.9 *Propylene use in the base case in the period 1990-2050*

The influence of emission permit prices on the use of propylene is limited. A decrease of 5% in use occurs in the 100 and 200 • /t cases, see Figure 5.10. This reduction is caused by a slight decline in propylene oxide production and the ending of I-propanol production. The polypropylene production is in all the cases the main user of propylene.

[Mt/year]
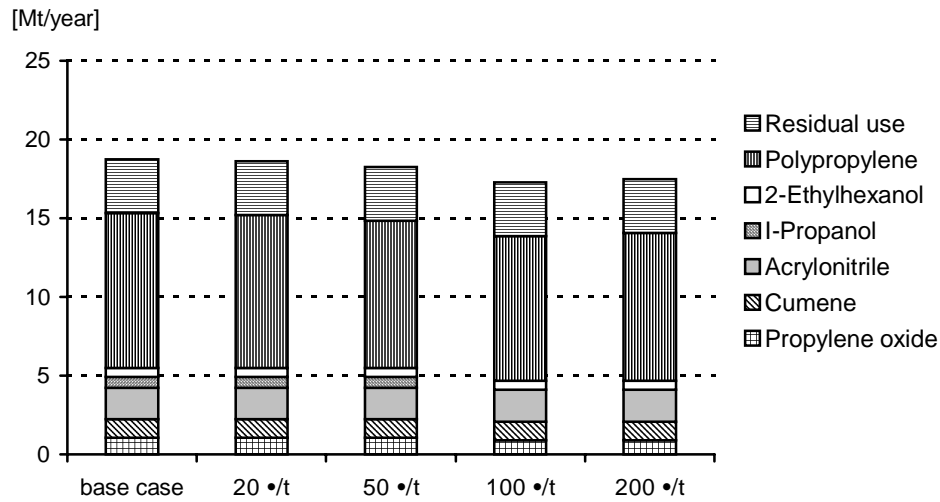
Figure 5.10 *Propylene use in 2030 with increasing permit prices*
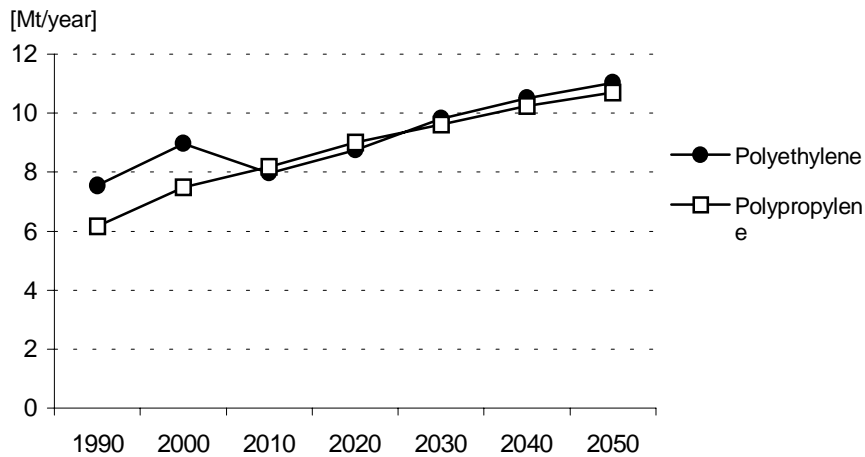
[Mt/year]

Figure 5.11 *Polyethylene and polypropylene production in the base case*

In Figure 5.11 the total production of polyethylene and polypropylene is shown. Polypropylene grows much more than polyethylene. The production goes from 6 Mt/year to 11 Mt/year whereas Polyethylene grows from 7.5 Mt/year to 10.5 Mt/year. Polypropylene becomes more wanted resulting in a small decline in price, from 793 • /t to 725 • /t. The price of polyethylene declines from 906 • /t to 259 • /t, see Table 5.3. In 2010 the price of polyethylene is for the first time lower than the price of polypropylene, which explains the kink in the polyethylene line.

Figure 5.12 shows that the polyethylene and polypropylene production are hardly affected by increasing emission permit prices. This is probably caused by the elastic demand, which is not in the version of the MARKAL_MATER model used for this study. Overproduction of materials or intermediates has no effect on the market price. Up till 100 • /t polyethylene is little more favoured than polypropylene. However, in the 200 • /t case polyethylene decreases a little and polypropylene increase a little.
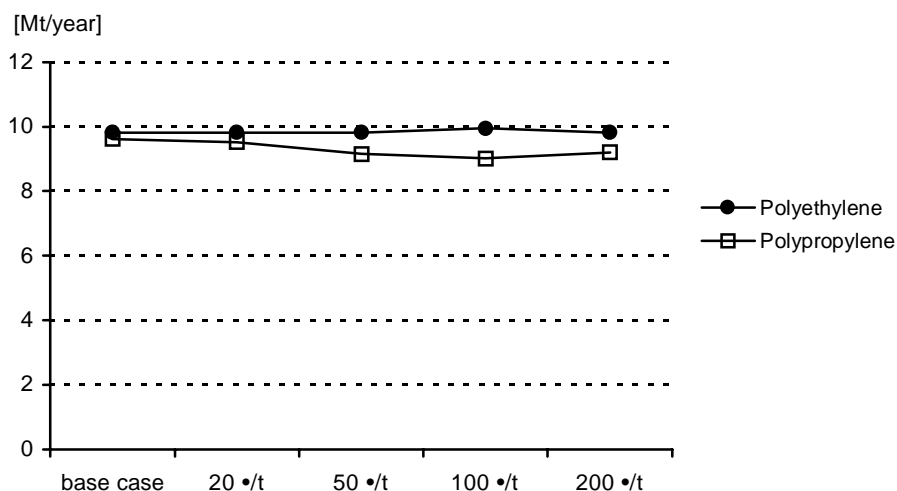
Figure 5.12 *Polyethylene and polypropylene production in 2030*

All the petrochemical products grow in volume so that the total production more than doubles in the period 1990-2050, see Figure 5.13. The main increase comes from MBTE. In 1990 no MTBE was produced in 2050 about 30 Mt MTBE is produced. The rise in MTBE comes from a substitution from lead additives to oxygenates based on the use of MTBE.
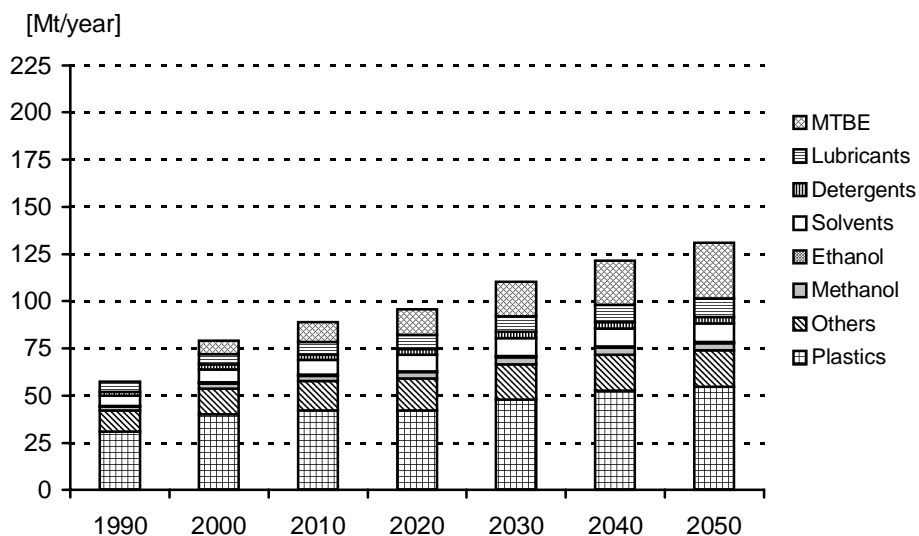
Figure 5.13 *Petrochemical products in the base case in the period 1990-2050*

When emission permit prices are introduced, the amount and the composition of petrochemical production change significantly, see Figure 5.14. There are hardly any differences between the base, 20 • /t and 50 • /t cases only methanol decreases in the 50 • /t case. In the 100 • /t case the total amount of products grows with 35% due to an extra production of 41 Mt ethanol used for the transportation sector. In the 200 • /t case the production grows with another 65 Mt. Ethanol production grows with another 55 Mt and methanol growths with 25 Mt. The MTBE production declines simultaneously with 15 Mt.

A growing demand for transport fuels with no or low carbon emissions results in a shift from MBTE to methanol and ethanol. The production of plastics is hardly affected.
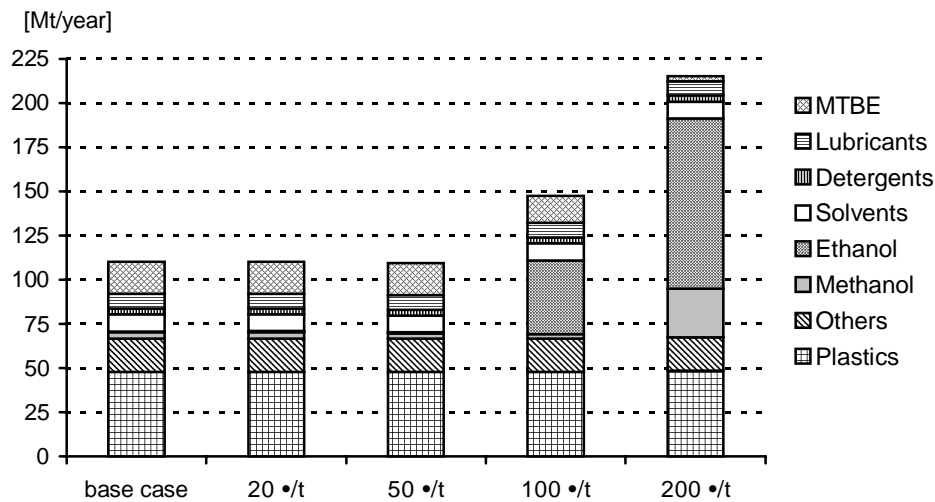
Figure 5.14 *Petrochemical products in 2030 with increasing permit prices*

5.3 Waste handling

The total waste production in the period 1990-2050 increases from 20 Mt to 45 Mt, Figure 5.16. In this period plastic waste processing shifts from 90% disposal to 30% disposal, 42% incineration and blast furnaces and 28% recycling techniques. This shows that recycling, incineration and blast furnaces become more attractive than disposal. Increasing disposal penalties make disposal an unattractive option.
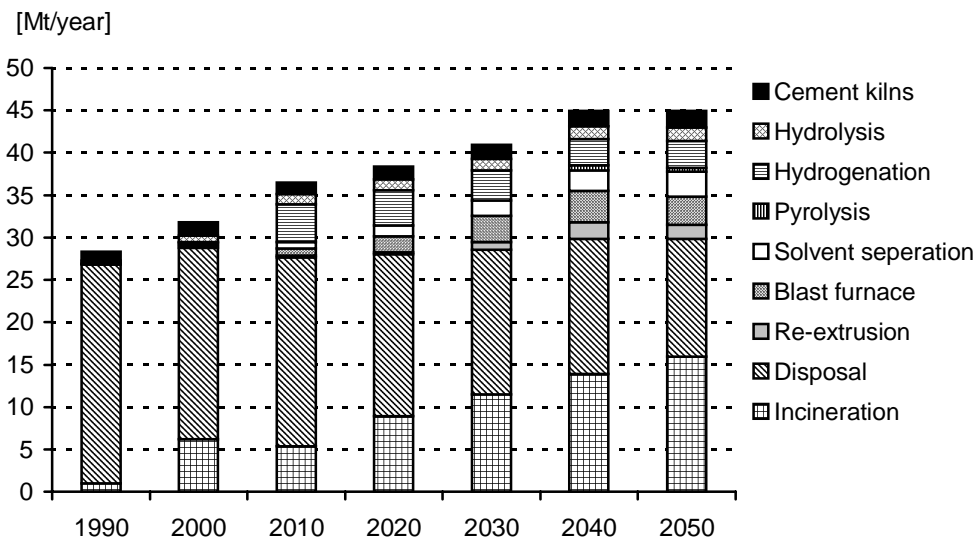
Figure 5.15 *Plastic waste handling in the base case in the period 1990-2050*

At emission permit prices of 100 and 200 • the amount of plastic waste declines with 5%, see Figure 5.16. The way of plastic waste processing does not chance up to penalties of 50 • /t. In the 100 • /t case blast furnace declines from 3 Mt to 0 Mt and incineration decreases with 2.5 Mt the re-extrusion process increases from 1 Mt to 2 Mt. In the 200 • /t case incineration decreases to 0.5 Mt and hydrogenation decreases from 3.5 Mt to 2.5 Mt, re-extrusion increases with 1 Mt and the pyrolysis process is the new processing technique with a share of 9 Mt. These figures indicate that recycling becomes more attractive with increasing emission permit prices. Incineration techniques are unfavourable at penalties of 100 and 200 • /t. Disposal is hardly affected by emission permit prices an increase from 17 Mt to 18.5 Mt.

In general with increasing penalties storage and recycling replace the incineration techniques. Although the decline in amount is rather small it is significant in perspective of the emissions due to the shift in processing techniques.
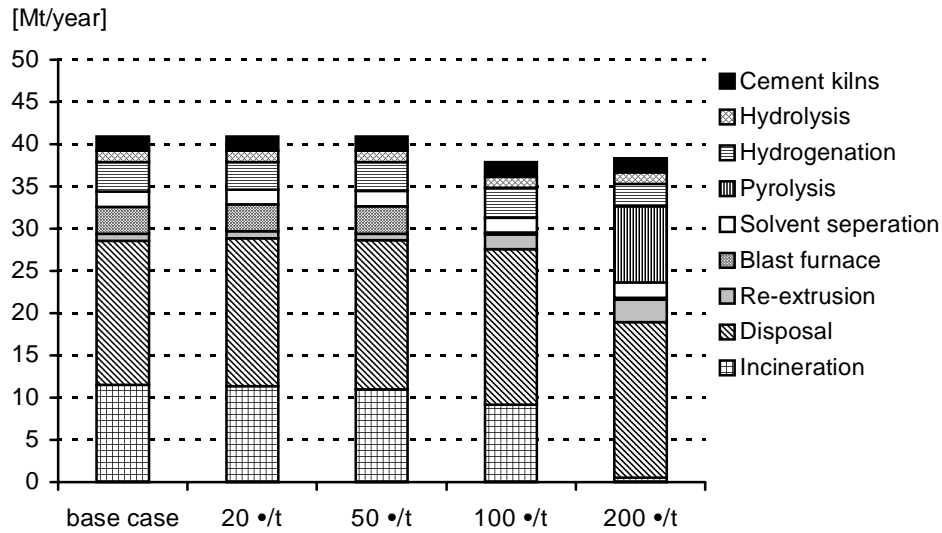
Figure 5.16 *Plastic waste handling in 2030 with increasing permit prices*

The total energy recovery from waste in the base case in the period 1990-2050 increases from 250 PJ to 1050 PJ, see Figure 5.17. From the four selected waste materials only the amount of wood declines from75 Mt to 50 Mt. Kitchen waste increases with 150% and paper waste increases with 300%. But plastic waste increases the most with a factor 13. The increase for plastic waste is caused by a combination of increasing waste quantities and a shift from disposal to incineration. The decline of wood incineration is caused by an increasing demand for wood in the power generating sector and the use of wood as feedstock, for example the petrochemical industry.
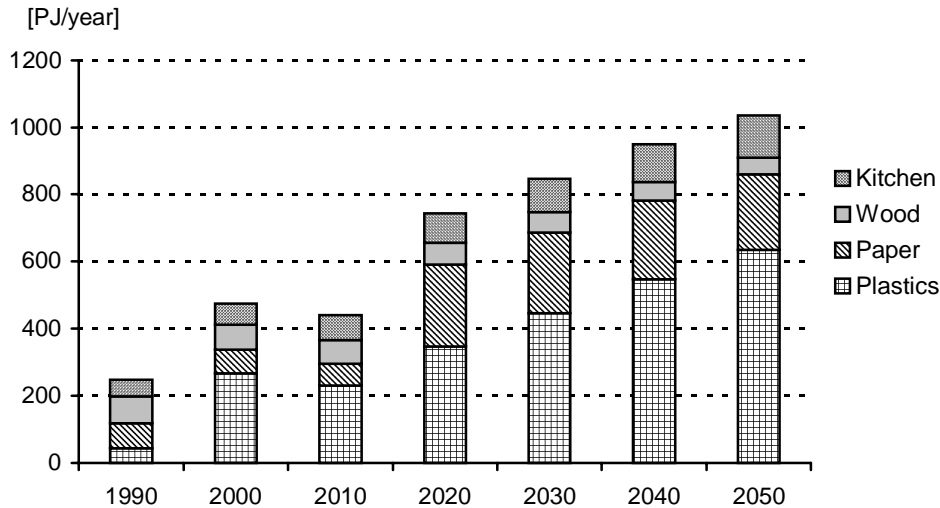
Figure 5.17 *Waste incineration in the base case in the period 1990-2050*

Emission permit prices affect the waste incineration from 50 • /t and onwards, see Figure 5.18. At 50 • /t the amount of plastic incinerated declines with 25 PJ and paper waste increases with 170 PJ. At a penalty of 100 • /t plastics decline some more and paper is still growing. At 200 • /t only 20 PJ plastic is incinerated, paper with 480 PJ and kitchen waste with 570 PJ are the main incinerated waste types. The decline of plastic waste incineration comes from an increase in recycling of plastic waste. The high GHG emission permits make it profitable to recycle instead of

incinerating the plastic waste. The increase of paper and kitchen waste comes from a prohibition on disposal of waste. This reduction in plastic waste incineration corresponds with the plastic waste-handling shift in Figure 5.16; higher emission permit prices increase recycling processes and decrease incineration processes. Although recycling of plastics is a better way of reducing GHG emissions, it is a more expensive way.
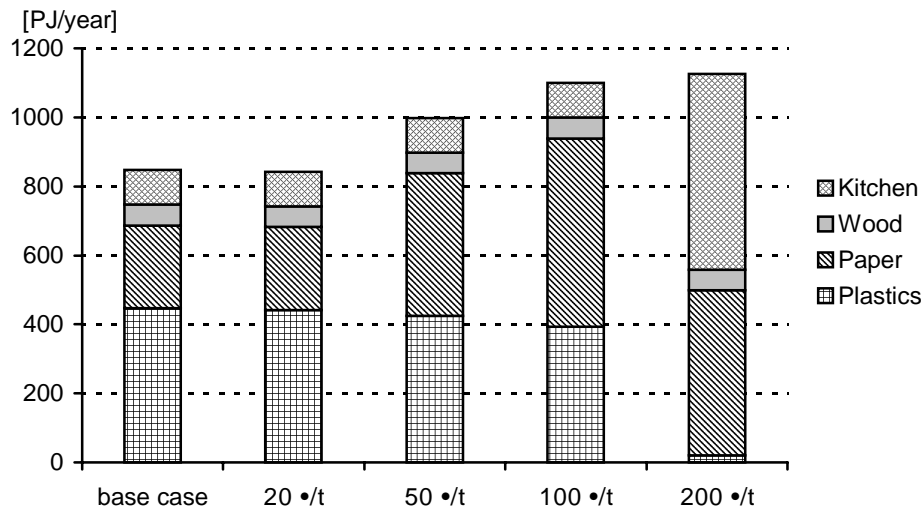
Figure 5.18 *Waste incineration in 2030 with increasing permit prices*

5.4   Price impacts

The shadow prices in the Table 5.1 to Table 5.6 come from MARKAL-MATTER calculations. The model prices for 1990 (market price) in Table 5.1, Table 5.3 and Table 5.5 come from literature. The comparison of these prices and the shadow prices show for the feedstocks the reality content of the model. The comparison of these prices and the shadow prices show for ethylene and propylene lack of reality content of the model (Gielen, Vos, Van Dril, 1996; CBS, 1989-1992; European Chemical News, 1995; Chemical Week, 1995).

Table 5.1 *Shadow prices of the main petrochemical feedstock for plastic production in the base case*

		Market price	2010	2030	2050
Ethylene	[• /t]	469	157	100	128
Propylene	[• /t]	339	177	494	523
Wood	[• /GJ]	3.80	3.87	5.02	5.02
Naphtha	[• /GJ]	5.73	4.14	4.74	5.20
LPG	[• /GJ]	3.29	2.81	3.52	4.25
Gas oil	[• /GJ]	3.08	3.40	3.87	4.29
Ethane	[• /GJ]	1.35[7]	3.29	4.12	4.60

Table 5.1 shows the change in prices for five petrochemical feedstocks and two plastic intermediates. All the feedstocks increase in price in time, except naphtha. There is a significant gap between the market price and the shadow price for ethylene. This has several reasons, profits are not included in the model, the market is not ideal (MATTER assumes an ideal market) and some data in the model is probably not correct. The low prices for propylene in 2010 comes from the

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[7]   The market price for ethane is actually the market price for natural gas. One should keep in mind that the market price of natural gas is lower than the ethane market price. In reference (CBS, 1989-1992) no data for ethane was found.

rapid grow in propylene demand. The low prices for ethylene in 2010, 2030 and 2050 are probably not correct. Ethylene as a by-product from certain petrochemical processes can overfeed the ethylene market resulting in low ethylene prices. The MARKAL-MATTER model requires one iteration round before all the model outputs correspond with each other. In 2010 the rapid growing demand has not been translated in a corresponding increase in shadow price.

Table 5.2 shows the effect of increasing emission permit prices on the prices of feedstocks and intermediates in the petrochemical industry. All the products increase in price. However, wood only increases with 85% where the other products increase at least 325%. Ethylene increases with a factor 10.

Table 5.2 *Shadow prices of the main petrochemical feedstock for plastic production 2030 [• /t]*

	Base case	20• /t case	50• /t case	100• /t case	200• /t case
Ethylene	100	123	210	500	1023
Propylene	494	734	983	1373	1603
Wood	5.02	5.02	5.67	6.80	9.33
Naphtha	4.74	6.21	8.61	12.28	19.03
LPG	3.52	4.79	6.73	11.47	18.00
Gas oil	3.87	5.47	7.74	11.58	19.03
Ethane	4.12	5.36	7.23	10.35	16.58

The abbreviations used in the tables 5.3 to 5.6 can be found in the glossary.

Table 5.3 shows the change in prices for eight different plastics in the base case in the period 1990-2050. Most plastics increase in price except PUR and PET. Again there is a significant gap between market prices and shadow prices, especially for polyethylene and PUR. This has several reasons, profits are not included in the model, the market is not ideal (MATTER assumes an ideal market) and some data in the model is probably not correct. The low prices for polypropylene in 2010 come from the rapid growth in polypropylene demand, an increase with 50% see Figure 5.9. The MARKAL-MATTER model requires one iteration round before all the model outputs correspond with each other. In 2010 the rapid growing demand has probably not been translated in a corresponding increase in shadow price.

Table 5.3 *Shadow prices of the main plastics in the base case [• /t]*

	Market price	2010	2030	2050
PE	906	293	228	259
PP	793	368	693	725
PS	1036	452	451	571
PVC	714	524	438	516
PUR	2776	418	414	427
PET	1223	846	860	906
ABS	1313	543	630	702
SBR	898	538	603	637

Table 5.4 shows the changing prices for eight different plastics with increasing emission permit prices. All the plastics increase in price by approximately 50%. Polyethylene and PVC first decline but become at high emission penalties (200 • /t) more expensive than in the base case.

Table 5.4 *Shadow prices of the main plastics in 2030 [• /t]*

	Base case	20• /t case	50• /t case	100• /t case	200• /t case
PE	228	195	198	334	386
PP	693	882	1054	1044	1057
PS	451	471	511	604	652
PVC	438	431	436	481	495
PUR	414	440	480	473	691
PET	860	967	1094	1164	1191
ABS	630	660	707	777	917
SBR	603	523	468	521	823

In Table 5.5 four different plastic waste types prices are shown. Each plastic waste type is separated in two qualities, mixed plastic waste and plastic waste as a part of municipal solid waste. All the plastic waste types, as a part of municipal solid waste becomes more costly to get rid off. While the waste handling of plastics in MSW is costly, mixed plastic waste generates revenues.

Table 5.5 *Shadow prices of the main plastic waste materials in the base case [• /t]*

	Market price[8]	2010	2030	2050
PO mixed	-150	-198	-145	-137
PO MSW	-150	-457	-382	-371
PS mixed	-150	1118	1331	1104
PS MSW	-150	-425	-355	-345
PVC mixed	-150	350	83	195
PVC MSW	-150	-150	-142	-138
PET mixed	-150	-196	-180	89
PET MSW	-150	146	156	198

With increasing emission permit prices it becomes less attractive to produce polyolefins waste, see Table 5.6. The reason is the net CO_2 emission for waste handling. For PET waste the situation is opposite to that of polyolefins waste (because recycling decreases CO_2 emissions). Polystyrene and PVC in mixed waste increase also in price.

The different plastic types in mixed waste increase in value because they can relatively easy be recycled. The production of plastics from recycled materials generates less CO_2 emissions than the production of plastics from primary fossil feedstocks.

Table 5.6 *Shadow prices of the main plastic waste materials in 2030 [• /t]*

	Base case	20• /t case	50• /t case	100• /t case	200• /t case
PO mixed	-145	-151	-173	-201	-221
PO MSW	-382	-419	-471	-615	-638
PS mixed	1331	1647	2074	1953	2325
PS MSW	-355	-398	-460	-615	-786
PVC mixed	83	65	102	233	233
PVC MSW	-142	-159	-182	-183	-183
PET mixed	-180	-183	-230	-295	917
PET MSW	156	253	367	428	375

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8   The -150 • /t price in the second column of Table 5.5 is the price currently paid for plastic waste handling. No difference is made in different waste qualities or different plastic types. The MARKAL_MATTER model does make difference in quality and type therefore different prices are calculated, which are presented in Table 5.5.

The polyolefins in municipal solid waste become much more expensive because the separation technologies are not cost effective. Electricity generation with the incineration of MSW increases CO_2 emissions compared to the reference situation because competing reference electricity production becomes more efficient and emissions per GJ generated decline rapidly in time with increasing penalties.

The positive GHG balance for mixed plastics waste and the negative GHG balance for plastics in municipal solid waste explains the widening price gap in Table 5.5 and Table 5.6.

5.5   Final energy use and GHG emissions

The rise in total energy consumption is the result of a growing demand for petrochemical products whether produced with fossil or renewable energy sources. Oil and gas remain the dominant feedstocks.

The total energy uses for the petrochemical industry doubles in the period 1990-2050, see Figure 5.19. This effect is caused by the rapidly rising product demand and the limited efficiency improvement potential.

The energy use for 1990 in Figure 5.19 calculated with MARKAL-MATTER is lower than the energy use in Western Europe OECD reported by IEA, see Table 2.1.

The major part of the difference is caused by the different electricity figures. It is assumed that the difference can be explained because the electricity needed for pumping half fabricates through pipes and lighting of buildings, which are not modelled separately in the MATTER model.

[PJ/year]
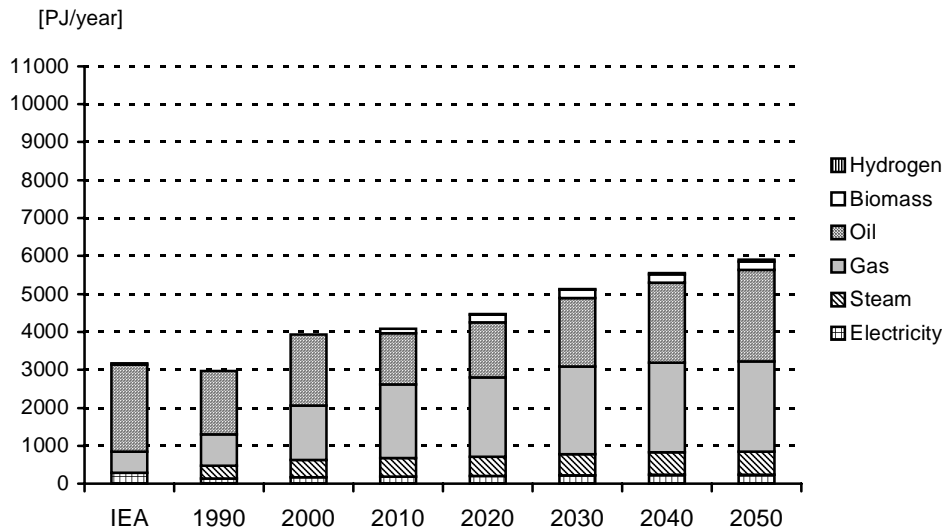
Figure 5.19 *Final petrochemical energy use in the base case in the period 1990-2050*

In Figure 5.20 it is obvious that the emission permit prices influence the composition of the fuel supply. Biomass, methanol and ethanol replace oil and gas from 50 • /t upward. The penalties replace up to 40% of fossil energy use. The totals direct energy and feedstock demand remains almost constant till a GHG emission permit of 50 • /t. At an emission permit of 50 • /t the share of biomass is growing. At an emission permit of 100 • /t biomass has become the largest contributor to the total energy use. The share of biomass in final petrochemical energy use is in the 200 • /t case more significant than the other five energy carriers together.

Figure 5.20 *Final petrochemical energy use in 2030 with increasing permit prices*

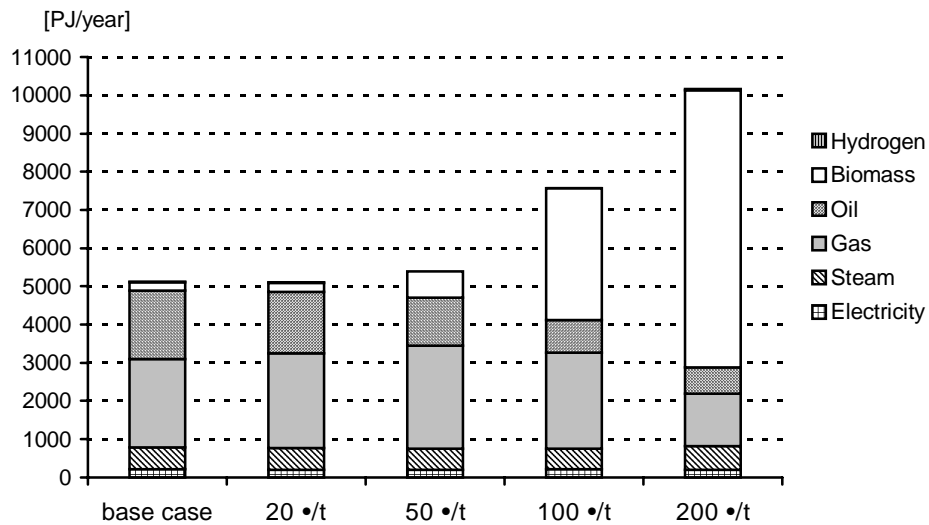Figure 5.21 shows a schematic overview of the carbon accounting for petrochemicals. All flows are numbered 1-9. The problems exist with regard to the feedstock use (Gielen, 1997). The potential emissions are the fossil fuels (flow 1), and the carbon in biomass. However, the net CO_2 emission of biomass is zero because of the CO_2 uptake (flow 8). The net potential emissions consist thus of the fossil fuels (flow 1).

However, some carbon is stored in products, flow 5 and in disposal sites, flow 6. Corrections are required for this net storage. The actual emissions (the guiding principle in the IPCC GHG accounting guidelines) are short life materials (flow 4) + CO_2 emissions from materials production (flow 9) + CO_2 emissions from materials incineration (flow 7) - renewable carbon uptake (flow 8).

However, this is difficult from an accounting point of view. As a consequence, a different method is applied. The actual net emission is the potential net emission (flow 1) – the storage of carbon in long life materials (flow 5+6+7) - carbon release from incineration (flow 7).

Two corrections have to be applied for the actual net emissions, the net exports must be added and the actual net emissions have to be cut down with the petrochemical N_2O emissions. However, It is yet unclear how export must be treated in the carbon accounting balance. The actual emissions are the fossil fuels (flow 1) + the petrochemical N_2O emissions - storage in long life materials (flow 5) - storage in disposal sites (flow 6) – (exports + imports). This categorisation is shown in Figure 5.24 and 5.25, where disposal is split into the disposal of plastics in disposal sites and the underground storage of CO_2.
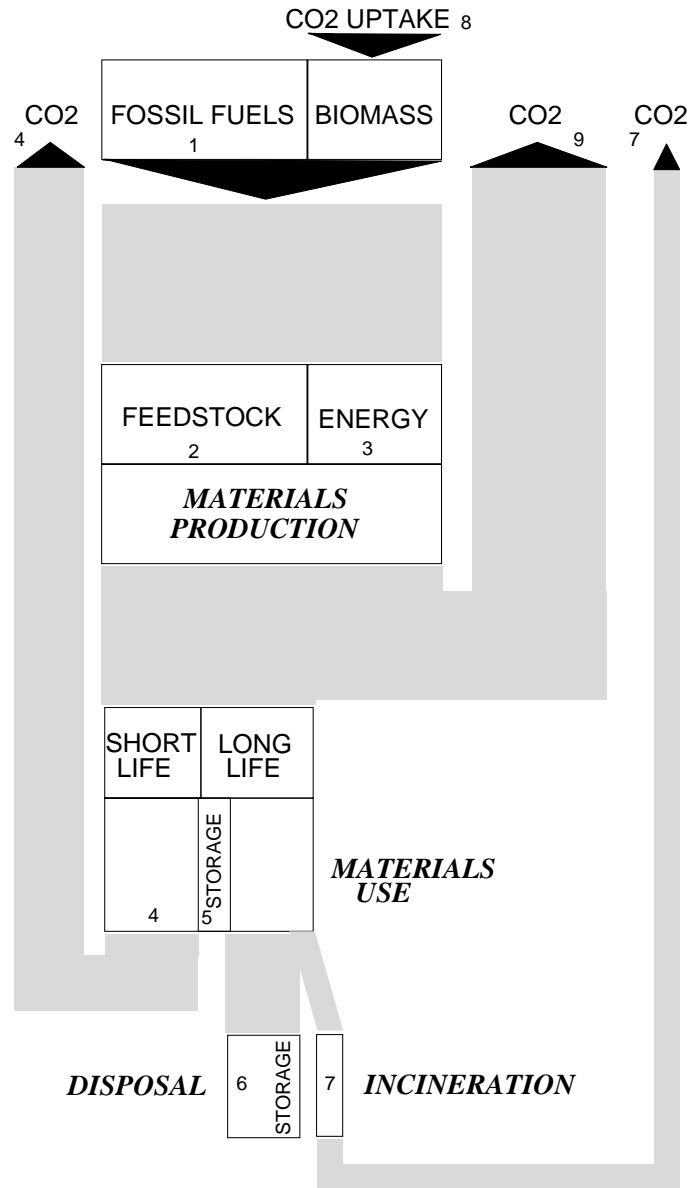
Figure 5.21 *Schematic overview of the carbon accounting for petrochemicals*

The total emission for the petrochemical industry of CO_2 equivalents almost doubles in the base case, see Figure 5.22. The increase comes mainly from gas that grows with 300%. The emissions belonging to electricity, steam and N_2O double where emission from oil remains almost constant. A growing demand for plastics and no GHG reduction policy causes the growth in the base case.
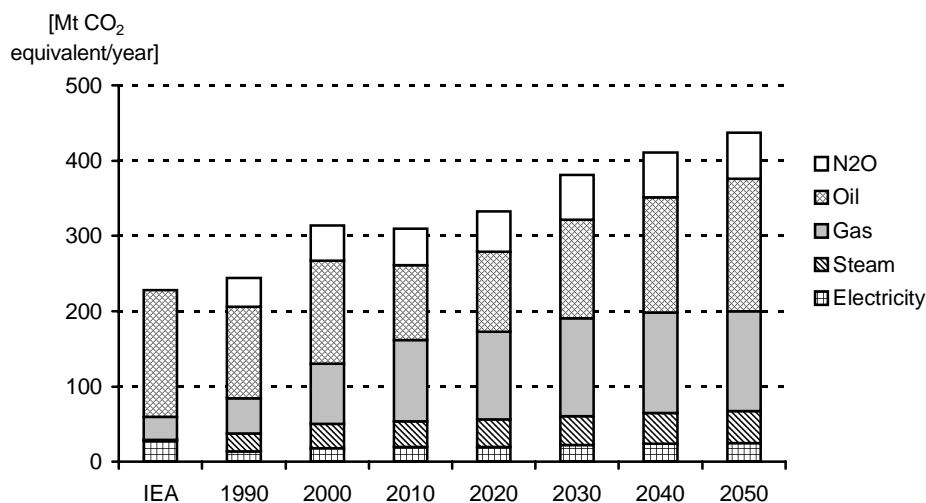
Figure 5.22 *Total potential GHG emissions in the base case in the period 1990-2050*

When emission permit prices are introduced the total emission of CO_2 equivalents declines from 380 Mt to 195 Mt for the petrochemical industry, see Figure 5.23. At an emission permit price of 20 • /t the N_2O emission is gone, which alone is a decrease of 60 MT CO_2 equivalent. Oil decreases from 130 Mt to 50 Mt CO_2 equivalent. Gas first slightly increases from 130 Mt to 150 Mt at 50 • /t, but declines from 140 Mt in the 100 • /t case to 80 Mt in the 200 • /t case. Steam and electricity remain almost constant at 40 and 20Mt CO_2 equivalent respectively. From the base case till the emission permit price of 100 • /t oil is replaced by gas. This is caused by the demand for fossil feedstocks with lower CO_2 emission per ton carbon used to produce petrochemicals. At emission permit prices of 100 • /t and more the non-fossil feedstocks and energy carriers become cost competitive. The decline in CO_2 equivalent emissions proves that these non-fossil feedstocks are being used.

The bars in Figure 5.24 have the same totals as the bars in Figure 5.23. However, in Figure 5.24 the CO_2 emission is allocated to output sectors[9] instead of input energy carriers[10]. The N_2O emissions are gone at an emission penalty of 20 • /t CO_2 equivalent. Three sectors increase in CO_2 emissions, export (from 10 Mt to 20 Mt), CO_2 storage (from 0 Mt to 10 Mt in the 100 and 200 • /t cases) and disposal (from 50 Mt to 55 Mt). CO_2 storage in products decreases from 5 Mt to 1 Mt but, the main decrease comes from energy & short life products from 190 Mt to 60 Mt. Beside carbon storage in products and energy & short life products, emissions from incineration and recycling decline with 10 Mt.

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[9]   Output sectors are the sectors where the emissions take place or where the carbon flows leave the system (e.g. disposal, exports).

[10] Input energy carriers are the direct and indirect fossil and non-fossil energy carriers that are used in the petro-chemical industry to produce petrochemicals.
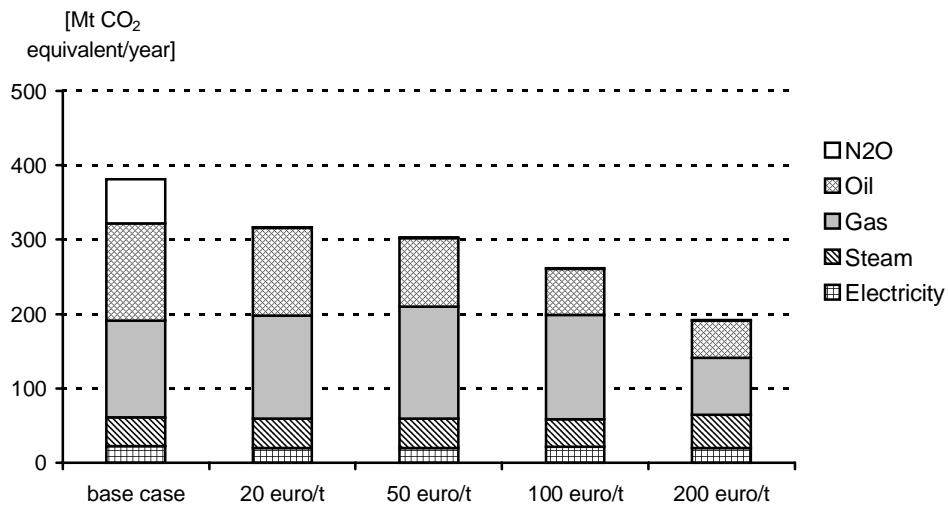
Figure 5.23 *Total potential GHG emissions in 2030 with increasing permit prices[11]*
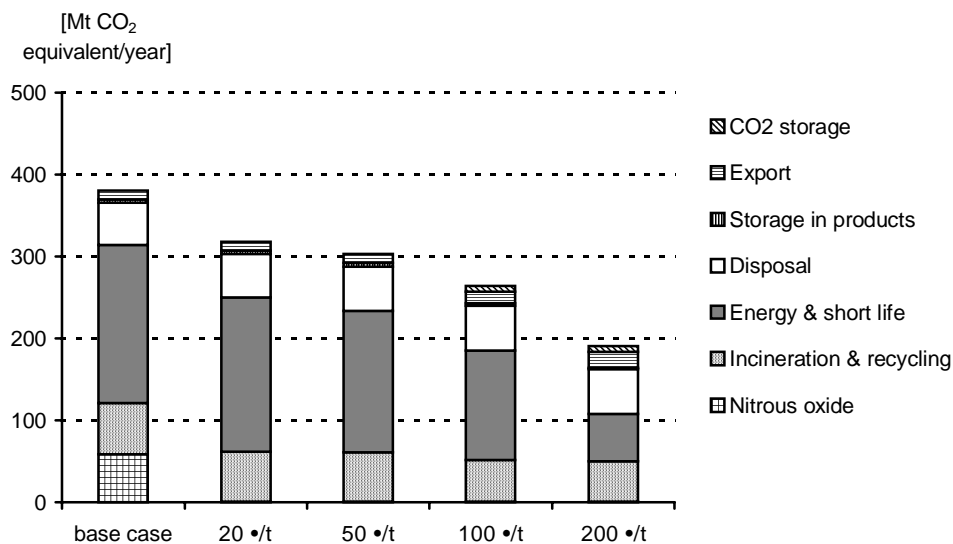
Figure 5.24 *GHG balance in 2030 per sector in CO_2 equivalent/year with increasing permit prices*

The carbon and nitrous oxide emissions from 'energy and short life', 'incineration and recycling' and 'nitrous oxide' together is the total emission of CO_2 equivalents/year for the petrochemical industry. The amount of CO_2 being stored slightly increases with increasing emission permit prices, 56 Mt in the base case and 63 Mt in the 200 • /t case. The CO_2 emission decreases from 315 Mt in the base case to 110 Mt in the 200 • /t case.

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[11] See footnote 5 on page 23.

6.   CONCLUSIONS

The following questions have been raised in Chapter 1:
1. What are the relevant energy and material flows in Western Europe in the life cycle of petrochemical products from a GHG perspective? (Chapter 2)
2. What is the relation between these flows and GHG emissions? (Chapter 2)
3. Which techno-economic options exist to reduce these emissions in the next 3 decades? (Chapter 3)
4. Does it make sense from a Western European cost-effectiveness perspective to reduce these emissions? (Chapter 5)
5. How far can these emissions be reduced at acceptable costs? (Chapter 5)
6. Which problems must be solved in order to achieve this emission reduction? (Chapter 6)
7. Which recommendations can be formulated for R&D and for investment decisions? (Chapter 6)

6.1   Relevant energy and material flows

The current petrochemical complex is based on oil and gas derived feedstocks (naphtha, gas oil, LPG, ethane, aromatic fractions). The steam cracking of these feedstocks is the basis for the petrochemical industry. Increasing quantities of intermediates are recovered from refineries. After fractionation, different components are converted into plastics, fibers, solvents, resins, detergents and other products. Total production in 1994 amounted to 42.4 Mt products (excluding lubricants and energy products such as pyrolysis gasoline). Plastics and resins constitute 67% of this total production. The petrochemical industry consumes approximately 3 EJ final energy, 8% of the total Western European final energy use. This energy use is forecast to increase in the future, both in a situation without GHG policy and (even more) in a situation with GHG policies. This growing energy use is a product of significantly increasing production and moderately increasing energy efficiency and a change in product mix to more energy intensive products. The strong growth due to GHG policies can be attributed to an increased production of methanol and ethanol (as fuels for the transportation sector). One can argue whether this production should be considered as part of the petrochemical industry or as part of the refining sector. The production of other petrochemical products is only to a limited extent affected by GHG policies (see below).

6.2   The relation between energy and material flows and GHG emissions

From a GHG emission point of view the industry has a unique position because a significant part of this energy is used as feedstock, which does not result in CO_2 emissions in the production stage. Only in the use stage (for dissipative applications) and in the waste handling stage (e.g. plastics incineration) do these processes contribute to GHG emissions. The potential GHG emissions increase from approximately 250 Mt in 1990 to 370 Mt in 2030 (an increase by 48%). However, the actual emissions amount only 320 Mt in 2030, of which approximately 60 Mt can be attributed to the waste incineration, so the actual emission allocated to the petrochemical industry is approximately 260 Mt. 60 Mt is related to the production of adipic acid. The remaining 200 Mt is related to the energy use in the industry (including the upstream emissions in electricity production) and the production of short life petrochemical production (of which emissions are allocated to the petrochemical industry). The petrochemical industry contributes approximately 4% to the total Western European emission of 5100 Mt in 2030.

6.3   Technologically feasible strategies

Greenhouse gas emission reduction will have significant impact on the selection of feedstocks, the selection of process technologies and the waste management strategies for petrochemical products. The industry should consider such impacts in the formulation of strategies. Until 2010, Western European industry will not be affected significantly by the GHG emission reductions that have been agreed within the framework of UNFCCC in Kyoto December 1997. However, beyond 2010, further emission reductions can be expected. These reductions will affect the petrochemical industry and iron and steel, aluminium, paper and wood etc. As a consequence, the competition between these materials will be affected by these strategies. However, the emissions can be reduced significantly for most materials. As a consequence, the emission reduction that can be achieved through materials substitution is limited.

Not only the emission reduction for competing materials must be considered. The changing structure of the energy supply system must also be considered. For example the changing electricity production affects the potential for GHG emission reduction through energy recovery from plastic waste. The market for transportation fuels will be affected by a change towards biofuels and electricity in the transportation sector. This will affect the availability of naphtha, currently a by-product of oil refining.

6.4   Cost-effective strategies

Nowadays the Western European petrochemical industry contributes to GHG-emission reduction through N_2O mitigation technologies. These technologies are introduced in the production process of Adipic acid. The total contribution is approximately 60 Mt CO_2 equivalents in 2030 (compared to the base case).

Basically two main strategies can be discerned for the petrochemical industry with regard to CO_2 emissions related to feedstock use:
* renewable feedstocks,
* recycling of waste plastics.

Both strategies are to some extending already part of the current industrial practice. A significant part of the oleochemistry is based on natural resources, which are applied for the production of detergents etc. Natural solvents and natural lubricants make inroads into the market that used to be a petrochemical market. These trends will be accelerated by GHG emission reduction policies.

The industry will be significantly affected by any GHG penalty. Actual emissions will decline from 320 Mt in the base case to 250 Mt in case of a 50 • /t CO_2 penalty. This is a decline of 22%, compared to a decline of 50% for the whole economy. At a 200 • /t CO_2 penalty emissions decline with 125 Mt, this is a decline of 61%, compared to a decline of 75% for the whole economy. The 50 • /t CO_2 penalty should be considered a realistic scenario, while the 200 • /t penalty represents an extreme scenario.

The main GHG emission reduction strategy is feedstock substitution (65% of the GHG emission reduction), followed by N_2O emission mitigation (15%), recycling/energy recovery (10%) and increased materials efficiency (10%).

At GHG penalties of 100• /t and more, the energy and carbon feedstock input changes from fossil fuels to biomass. Part of this biomass is directly used in fermentation and pyrolysis processes. Another part is first converted into methanol and ethanol and subsequently applied. The development of such strategies will require significant R&D efforts, but can simultaneously enhance the sustainability of this industry sector.

6.5   The integrated production complex problem

The integration of the refinery sector and the petrochemical industry is currently one of the strong competitive advantages compared with steel and paper/board industry. Significant changes can be expected in the transportation fuels market from GHG-emission of 100 • /t and higher. This will affect the availability of naphtha, gas and gas oil. It is an important incentive to develop alternative carbon sources, materials, products and product applications.

The threat for industry is that these new production processes are not dependent upon the existing petrochemical structure. Agricultural processing industries and pulp and paper industries are examples of non-petrochemical sectors that make inroads into this market. Especially the pulp production has a significant resource base of 20-30 Mt lignin per year which is currently incinerated, but which poses an attractive source of cheap biomass feedstocks. The agricultural overproduction in Western Europe and the imminent expansion of the European Union towards the east will result in a strong drive to find new applications for this agricultural land. The materials market may pose such a market. It is recommended for the petrochemical industry to participate in this trend through the development of new production routes.

The industry has developed much new plastic waste recycling technologies during the last decade. However, most of these technologies are not cost-effective in the current market conditions. GHG emission permit prices can increase the cost-effectiveness of these strategies significantly. As a consequence, recycling strategies will benefit from serious GHG emission reduction beyond 2010. However, the waste plastic market has a decidedly different structure than the naphtha market. It is recommended to develop a reliable supply structure before any activities in this field are developed.

6.6   Selection of production locations: the carbon leakage issue

Given the international character of many materials producing industries, carbon leakage (relocation of industries to regions with less stringent emission reduction policies) is a serious threat. Policy makers are sensitive to such problems. Three scenarios can be drawn: first, industries outside Western Europe are subjected to similar emission reduction policies, second, petrochemical industry is exempted from GHG emission reduction policies, third, a system of tradable emission permits in Western Europe is developed. In the third case, it is important which initial distribution of permits is applied. Industries can even benefit from such GHG policies, if their initial emissions are high but they can achieve emission reductions at lower costs than elsewhere, so they can sell permits at a profit. Looking at likely competitors, emission reductions in the United States are even more difficult to achieve than emission reductions in Western Europe. The situation for producers in the Middle East is not clear because it is uncertain whether these countries will participate in GHG emission reduction schemes.

Within Europe, the market potential in Eastern Europe and the imminent participation of these countries in the European Union will pose an important incentive for new production capacity in the east. An additional advantage is that this region has sufficient land for a future agrification strategy.

6.7 R&D planning for the period beyond 2010

Biomass is a renewable carbon source with a neutral CO_2 balance. Carbon derived directly from the atmosphere seems a less attractive carbon source. Basically, four routes can be considered how biomass can be integrated into the petrochemical complex:

1. Feedstock substitution: biomass for oil and natural gas feedstocks for the production of intermediates such as ethylene, butadiene, etc.
2. Fermentation of biomass to ethanol and methanol.
3. New bioplastics, bio-solvents etc. based on naturally occurring molecules.
4. Substitution of plastics by wood products such as sawn wood, wood panels or paper.

The model calculations indicate that the first two routes seem the most attractive. A mix of pyrolysis processes and fermentation must be applied in order to achieve maximum substitution of existing petrochemicals. Some of these processes have been proven on a commercial scale. Their introduction seems merely a matter of process economics, which can be influenced by permit prices. For other technologies such as flash pyrolysis, the technological feasibility is still uncertain and major research is required in order to introduce such technologies.

Recycling is the other important strategy that can be applied in order to reduce the feedstock consumption. Current recycling rates are rather low. Current waste policies aim for increased incineration with energy recovery as a substitute for waste disposal. This will result in increased GHG emissions. A number of different recycling technologies are available and suitable for different waste qualities to produce different materials. For different waste quality types, different waste management technologies must be applied to achieve optimal conversion rates. An optimal mix from a GHG emission point of view consists of a mix of back-to-polymer, back-to-monomer and back-to-feedstock technologies at the expense of energy recovery technologies such as waste incineration. Most of these technologies have already been developed on a commercial scale. The introduction of a collection system seems merely a matter of process economics, which can be influenced by emission permit prices.

6.8 Accounting issues

The current IPCC emission accounting guidelines are not clear with regard to the CO_2 emission accounting for the petrochemical industry. Different countries apply different accounting methods. Especially the treatment of exports and the allocation of emissions for short life materials to economic sectors is not clear. Such differences can give future problems because they can affect the competitive position of national industries in a Europe-wide operating industry. International co-ordination of emission accounting guidelines with regard to petrochemicals is currently proceeding in the framework of the NEU-CO_2 project that is funded by the Environment and Climate programme of the European Union (http://www.eu.fhg.de./nenergy/). It is recommended that the industry participate in this project.

Matter model calculations show that the petrochemical industry is one of the few industries that may actually improve its export position if GHG permit prices would be introduced. The export of carbon containing petrochemical products is accounted for as carbon export. The industry can negotiate an exemption from GHG permit prices for the non-energy use of fossil fuels. If biomass is used as a feedstock, this should be considered as a net carbon storage that deserves a subsidy equal to the penalty on emissions.

ANNEX A THE MATTER MARKAL MODEL

The Essentials of a MARKAL model

At present MARKAL is one of the most widely applied models for analysing the impacts of GHG emission reduction policies, although its results often have to be completed using top down models (like General Equilibrium models) in addition. A MARKAL model[12] is a representation of (part of) the economy of a particular region. The economy is modelled as a system of interdependent technical processes. These processes are characterised by their physical and economic properties which determine the physical and monetary flows between these processes within that (part of the) economy of a region. It is a linear programming model, that maximises an objective function (e.g. costs) under constraints (e.g. the attainment of certain production levels, the availability of certain technologies, certain environmental policy constraints etc.). In the following paragraphs the processes and the optimisation procedure are briefly described.

Processes

Processes or technical options are the building blocks of a MARKAL model. They are characterised by, their *physical inputs and outputs* of energy and materials, their *costs*, and by other characteristics (in this study their *GHG emissions and waste volumes*). Beside the building blocks the model does calculations for a certain time period, the modelling period. The modelling period is split into a number of periods generally covering 5 or 10 years.

These process descriptions implicitly yield a very detailed input-output structure linking several hundreds of processes that are included in the model in a dynamic perspective, covering the total life cycle for both energy and materials. Of course not all substance flows in the entire economy are analysed. First, not all processes in the economy are included in the model. Secondly not all emissions are included in the description of the processes. This study for example is confined to GHG emissions. Other applications of a MARKAL model concentrate on other aspects of the same processes.

Processes represent all activities that are necessary to provide certain products and services, in this study: the provision of energy and materials. These processes are listed in Volume 3 of this study. Many products and services can be generated through a number of alternative (sets of) processes that feature different costs and different GHG emissions.

Process descriptions follow a standard format, consisting of two data sheets. One sheet describes the physical inputs and outputs (of energy and materials). The other characterises the economic data and the other process data. The input data structure depends to some extent on the process that is characterised. Data for different types of power plants, conversion processes, and end-use technologies are characterised in different ways. A schematic example of the input for conversion processes is shown in Table A.1. The data input is divided into nine time periods (column heading 1 to 9). The length of the time period is set by the user of the model and is usually 5 or 10 years (10 years in this model version). One column is reserved for time-independent variables (TID). The physical data do not represent the total mass and energy balance where input equals output (because of flows that are not accounted for). The cost characteristics of the processes are divided into investment costs (which are proportional to the installed capacity), fixed annual costs

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[12] The MARKAL linear programming model was developed 20 years ago within the international IEA/ETSAP framework (International Energy Agency/Energy Technology Systems Analysis Programme). More than 50 institutes in 27 countries use nowadays MARKAL. MARKAL is an acronym for MARKet ALlocation. At present it is the most widely used model for analysing the impacts of GHG emission reduction policies, although its results often have to be completed using top down models (like General Equilibrium models) in addition.

(proportional to the installed capacity) and variable costs (proportional to production volume). The user of the model can impose restrictions on the deployment of certain processes (technical options). Such restrictions may include political preferences, intentions expressed in policy papers, or long term physical constraints such as land availability.

Increasing process efficiency is modelled by decreasing inputs per unit of output (such as for energy carrier A and material A in Table A.1). Decreasing costs or changing restrictions can be modelled in a similar way. This is illustrated for the investment costs in Table A.1, which decrease in time. This is a way to account for so-called 'learning curves', accounting for decreasing costs as the installed capacity increases.

Table A.1 *MARKAL model data structure for a conversion process*

Sheets	Period	Unit	TID	1	2	3	4	5	6	7	8	9
Sheet 1: Physical flows												
Inputs	Energy carrier A	[GJ/unit]		2.0	1.9	1.8	1.7	1.7	1.7	1.7	1.7	1.7
	Energy carrier B	[GJ/unit]		1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0
	Material A	[t/unit]		5.0	4.5	4.2	4.0	4.0	4.0	4.0	4.0	4.0
Outputs	Energy carrier C	[GJ/unit]		0.1	0.1	0.1	0.1	0.1	0.1	0.1	0.1	0.1
	Product A	[unit]		1	1	1	1	1	1	1	1	1
Sheet 2: Other data												
	Investments	[• /unit cap.]		100	80	70	60	60	60	60	60	60
	Fixed annual costs	[• /unit cap./yr.]		5	5	5	5	5	5	5	5	5
	Variable costs	[• /unit]		2	2	2	2	2	2	2	2	2
	Delivery costs	[• /t A]		1	1	1	1	1	1	1	1	1
	Availability factor	[unit/unit cap.]		0.9	0.9	0.9	0.9	0.9	0.9	0.9	0.9	0.9
	Life	[periods]	2									
	Start	[period]	1									
	N_2O emissions	[t/unit activity]		0.1	0.9	0.8	0.8	0.8	0.8	0.8	0.8	0.8
	Residual capacity	[unit cap.]		2	0	0	0	0	0	0	0	0
	Maximum capacity	[unit cap.]		5	10	50	50	50	50	50	50	50
	Minimum capacity	[unit cap.]		0	0	0	0	0	0	0	0	0

Bounds
- The data sheets also allow for certain restrictions on the application of certain processes. These application restrictions are called 'bounds.' In this study the following bounds play a role: bounds on maximum penetration of certain technologies, reflecting e.g. social and strategic considerations (e.g. a maximum bound on nuclear and hydropower, a maximum import of natural gas from Russia).
- Bounds on the maximum investment rate in certain new technologies.
- Bounds reflecting the standing capacity from earlier periods (e.g. for the existing building stock).
- Bounds on the availability of natural resources (e.g. disposal capacity, land availability).

Time span
The time span to be modelled is divided into nine periods of equal length, generally covering a period of decades. The model is used to calculate the least-cost system configuration for the whole time period, meeting product and service demands and meeting emission reduction targets. This optimisation is based on a so-called 'perfect foresight' approach, where all time periods are simultaneously optimised. Future constraints are taken into account in current investment decisions.

In summary
The user of the model determines the processes from the database that will enter the calculations; he or she also determines the constraints for the individual processes, as well as constraints for the whole region. Constraints are determined by the demand for products and services, the maximum introduction rate of new processes, the availability of resources, environmental policy goals for energy use and for emissions etc. Processes are characterised by their physical inputs and outputs of energy and material, by their costs, and by their environmental impacts. Environmental impacts are endogenised in the process costs and the costs of energy and material flows between processes. The time scale is chosen according to the questions analysed. Since most of the processes take a long time to reach their maximum penetration (often at the expense of others), such time horizons tend to cover several decades, in this study until 2030.

The calculation of least cost combinations (LCCs) of processes /technical options
MARKAL requires as input projections of energy service demands - for example room space to be heated or vehicle-miles to be travelled, for example - and projected resource costs. In the model used (MARKAL MATTER), also the materials demand for these services are included.

Then, a reference case is defined in which; for example, no measures are required to reduce carbon dioxide emissions. This is the base case scenario. A series of runs is then made with successive emission permit prices. These penalties affect the selection of least-cost processes (see below). Because of the underlying detailed input output relations (imputed by means of the data sheets), interdependencies between the various processes or technical options are taken into account. The model thus automatically calculates the combined effects of these interdependent options. Moreover, the integrated dynamic systems approach ensures also that interactions between technical options in one period and interactions between periods are reflected.

In each case, the model will find the least expensive combination (least cost combinations, LCCs) of technologies that meet that requirement - up to the limits of feasibility -. But with each further restriction the total energy (energy materials) system cost will increase[13]. Thus, the total future cost of emission reductions is calculated according to how severe such restrictions may become. These can be plotted as continuous abatement cost curves. In addition, the marginal cost of emission reduction in each time period[14] is determined. These curves can also be read as the reductions that can be achieved at various levels of costs (GHG permit prices). This is of special interest in establishing abatement policy because it can be interpreted as the minimum amount of carbon tax, or the minimum price of GHG permits that would be needed to achieve this level of abatement.

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[13]   In the linear programming approach all processes are characterised as black boxes with a linear relation between inputs and outputs of energy and materials, costs and emissions. Economies of scale are not taken into account for any given process type.

[14]   More precisely, the costs of the most expensive technology that must be applied in order to meet the predetermined level of emissions is calculated. So, actually the model calculations give us the cost of the marginal technology. All other technologies that are part of the least cost combination (LCC) cost less per unit of emission reduction. Those who can apply these more cost effective technologies will, when they are confronted with a tax or with a price of tradable permits, apply that technology, to avoid paying the tax or to free permits they can sell on the market. As a consequence more expensive technologies will not be deployed.

Some uses of MARKAL are:
- to identify least-cost energy systems,
- to identify cost-effective responses to restrictions on emissions,
- to perform prospective analysis of long-term energy balances under different scenarios,
- to evaluate new technologies and priorities for R&D,
- to evaluate the effects of regulations or prices (taxes, tradable permits, subsidies), or both,
- to project inventories of greenhouse gas emissions,
- to estimate the value of regional co-operation.

The inclusion of materials life cycles
A distinction is made between an energy and a materials system in the most recent MARKAL versions. MARKAL has originally been used as an energy systems analysis tool. Conventional energy system models cover the conversion of primary energy into final energy and the subsequent final energy use in economic sectors. Of course they include industrial use of energy e.g. to produce materials, and will therefore include for example energy efficiency gains in the production of a material. But conventional energy system studies do *not* analyse the effects of changes in materials life cycles such as materials substitution, increased materials efficiency and recycling.

In MATTER-MARKAL (the model used in this study), however, all bulk material flows are included. They include all substances without relevant physical shape (not being consumer or investment goods) that are not defined as energy carriers[15]. The model covers more than 50 types of energy carriers and 150 materials, which means a substantial enlargement of more traditional MARKAL models. More than 100 products represent the applications of these materials. 30 categories of waste materials are modelled. These materials are characterised by their physical characteristics and by their quality. This means that a large number of technical options (processes) are added to the database of energy options. Identifying these options requires for each bulk material a rather detailed analysis of the flow of that particular substance through the economy 'from cradle to grave'.

The inclusion of materials technical options is important for a number of reasons
- By adding materials flows, the model chooses from a more comprehensive set of technological improvement options when calculating the least cost combinations. As a result a typical MATTER-MARKAL estimate of the least costs for attaining a certain GHG emission target tend to be lower than a typical MARKAL estimate. In fact the differences in the obtained least cost combinations are quite substantial.
- Because the energy and materials systems are intricately interwoven, technical improvements influence each other strongly. Ignoring technical improvement options in materials life cycles may lead to an overestimation of the effects of energy options[16] and misguided policy choices.
- It is extremely difficult, if possible at all, to foresee the effects of these interdependencies if one does not apply a formalised model that is based on rather detailed information concerning the interrelationships between the various technical options.
- It requires a comprehensive analysis of energy and materials flows to identify the appropriate points of impact for policy measures (in particular regulatory approaches) and to identify unexpected responses to policy actions.

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[15] With the exception of consumer food products.
[16] For example, a technical change that reduces the emissions of electricity generation, will make the substitution from steel to aluminium (which primary production uses much electricity) more attractive. At the same time, it will reduce the environmental improvements that would result from using secondary aluminium instead of primary aluminium; (Secondary aluminium requires only 5% of the energy needed for primary material). Another example: If spaces are well insulated, an improvement of the efficiency of the heating system will have a less pronounced effect on overall emissions than in the case of poorly insulated buildings.

Figure A.1 shows the energy and materials system model structure on an aggregated sector level and Figure A.2 depicts the intersecoral flows of materials that result from changes in a life cycle of a material. The actual model input data are on the level of individual processes in the product life cycle. Subsequently, these data are aggregated to produce results for economic sectors (see Figure A.1) and for the economy as a whole.
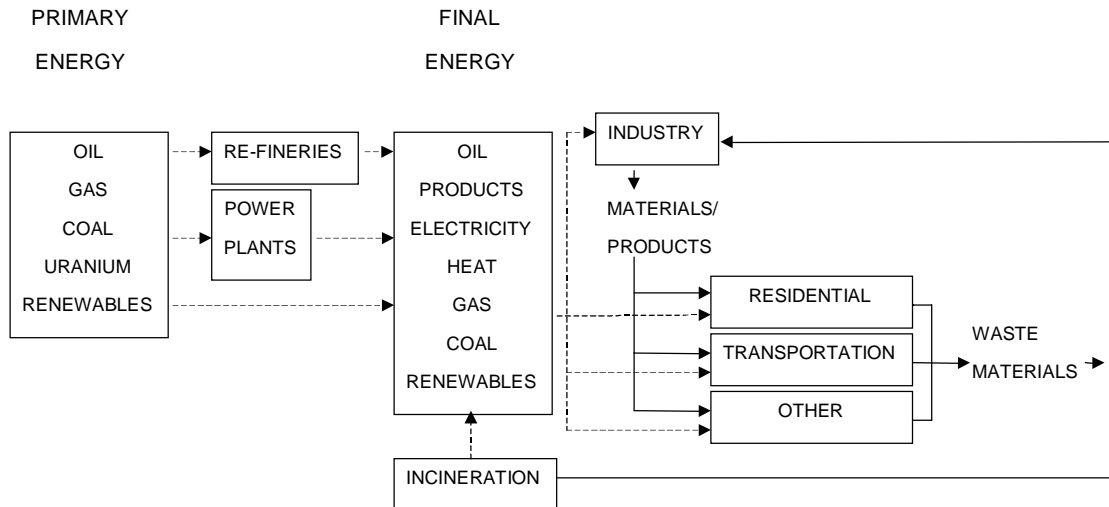

Figure A.1 *Generic MATTER energy and materials system model structure, showing the close interactions of energy and material flows in the economy. Dotted lines indicate energy flows, drawn lines indicate material flows (Gielen, Bos, Gerlagh, 1998)*
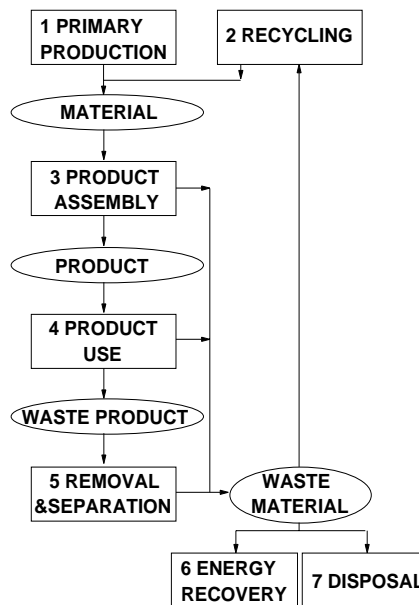

Figure A.2 *Materials system model structure*

Figure A.3 shows the definitions of the energy as well as the materials system. Conceptually it is difficult to separate energy from materials systems. After all, from a physics point of view, all environmentally relevant economic activities are just transformations of matter, using energy, and any distinction between the energy and materials system is arbitrary. In this study, all *energy used for materials production* (e.g. the production of iron, steel, aluminium, building materials etc.) is considered to be *part of the materials system*. This, because this study investigates the GHG effects of changes in materials life cycles. We want to know, for example, what changes in GHG emissions would result from changes in the inputs for of cement production. The effects of such a choice on GHG emissions are obviously strongly influenced by the energy requirements (quantity and quality) of the alternative inputs. Likewise, we want to know the effects on GHG emissions of building a car from aluminium or plastic, instead of from steel, or building a house from wood, instead of from concrete, steel and bricks. In both these cases the energy that goes into these *production* processes are part of the materials system. Ideally, also the energy required for space heating and driving the cars should be linked to the choice between alternative materials and therefore should be part of the materials system. Available energy statistics, however, do not permit this. Therefore, the energy that is needed for the *use* of the house (space heating) or the *use* of the car (fuels to drive it) is part of the energy system.
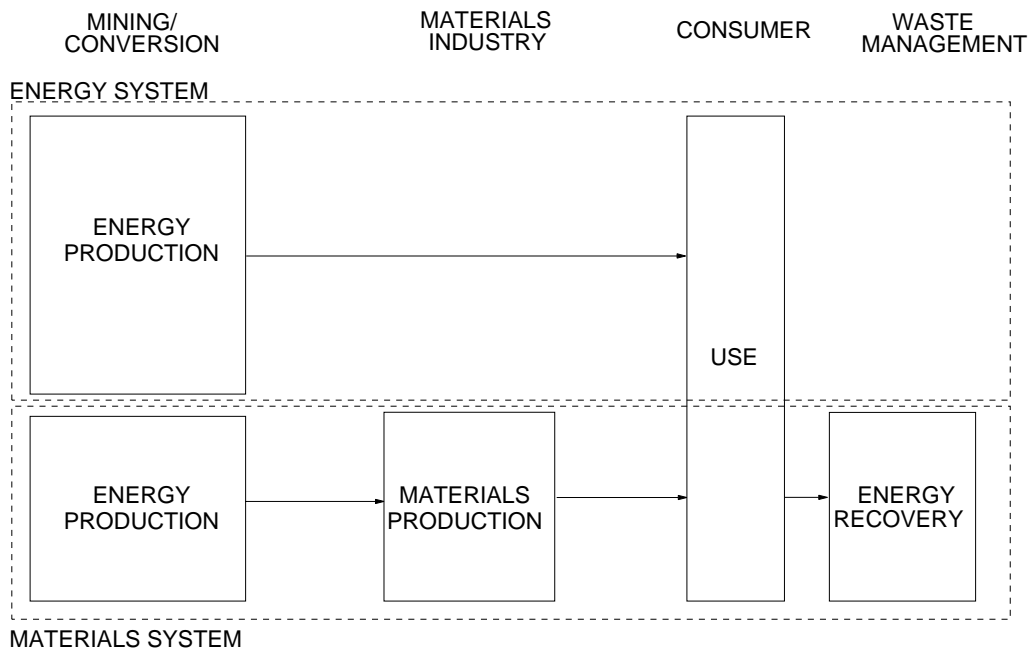

Figure A.3 *Definition of the energy system and the materials system*

MARKAL models are 'bottom up' models, meaning that they start from detailed technical options 'at the work floor' so to speak. The optimisation procedure (calculating least cost combinations) is firmly based on the standard micro-economic tenet that welfare is maximised if the sum of consumers and producers surpluses is maximised (marginal costs equals marginal revenues). These models make maximum use of the available knowledge about technology (For example, at what oil prices, energy from renewable sources becomes profitable, and how much time it is likely to take to install these renewable energy sources). On the other hand these models are based on rather heroic assumptions, like perfect markets, perfect knowledge and foresight and assumptions regarding technological developments over a long period of time. Moreover most MARKAL based models lack the feed back of price changes on the economy and poorly describe trade.

Empirical economic models are top down models. They contain much more economic detail, notably on money and trade flows. Being empirical, the sensitivity of for example investments in renewable energy sources to changes in oil prices is derived from statistical data concerning the past, but such elasticity's can change drastically due to for example technical change. Moreover profound technical changes may occur to slowly to clearly show up in statistical data. On the other hand these models implicitly take non-price factors that influence technical change into account. The lack of technical detail allows for rather general conclusions only.

Figure A.4 shows the (simplified) equilibrium that is achieved in 'common MARKAL' (such as applied in this study).

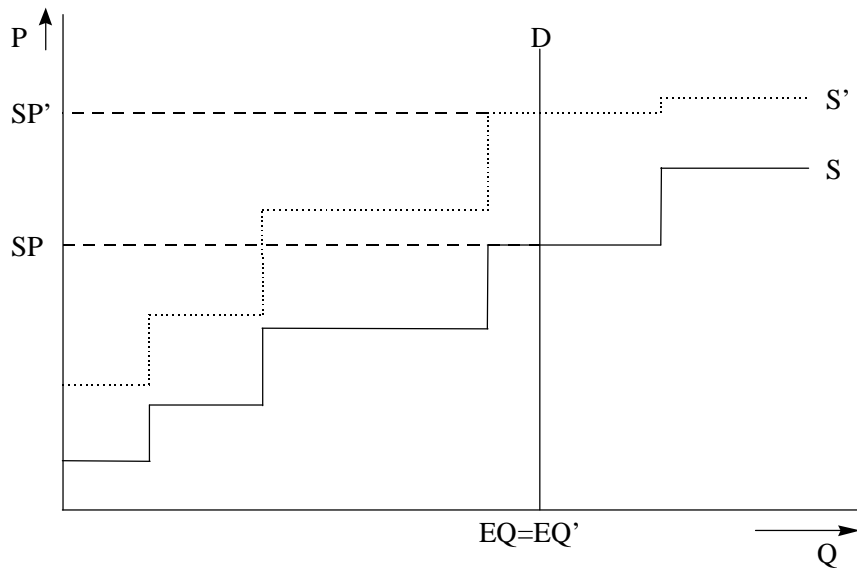

Figure A.4 *Supply and demand equilibrium in common MARKAL. P = Price; SP = shadow price; Q = quantity; EQ = equilibrium; D = demand; S = Supply; S'= supply curve including GHG penalty*

ANNEX B REFINERY AND PETROCHEMICAL TECHNOLOGIES AND MATERIALS USED IN THE MARKAL-MATTER MODEL

The code for the materials and waste materials in Table B.8 and in Table B.9 represents the materials group. The code starts with an M (for materials) or with a W (for waste materials). The second character represents the materials group:

C = ceramic materials
I = inorganic materials
M = metals
N = natural organic materials
P = plastics
S/T = other synthetic organic materials

All material flows are modelled in megatons (Mt). Not all materials are actually included in products; some are intermediates in the production of other materials (e.g. many synthetic organic materials).

Table B.1 *Refineries, current concepts (Van Oostvoorn, 1989)*

OCR	Catalytic reformer
OFC	Fluid catalytic cracker
OFX	Flexi cooker
OH1	Refinery heavy crude
OHC	Hydrocracker
OHF	Hydrocracker for fuel oil
OHY	Hycon
OL1	Refinery light crude
OME	Methanol from natural gas
OVS	Visbreaker
INW	MethylTertiaryButylEther (MTBE) production
IWA	Asphalt production
IJB	Lubricants from refinery

Table B.2 *Refineries, recovery of petrochemical feedstocks*

IOZ	Butylene recovery from refineries
SRT	Propylene recovery from refineries
SRU	Benzene recovery from refineries
SRV	Xylene recovery from refineries

Table B.3 *Refineries, addition of biofuels*

SBA	Ethanol addition to gasoline
SBB	Methanol addition to gasoline

Table B.4 *Refineries, production of hydrogen*

SXA	Hydrogen production from natural gas
SXB	Hydrogen production from fuel oil
SXC	Hydrogen production from petrocokes
SXD	Hydrogen production from electricity

Table B.5 *Petrochemical olefin production*

INA	Petrochemical. Naphtha cracker
INB	Petrochemical. Gas oil cracker
INC	Petrochemical. Ethane cracker
IND	Petrochemical. Oxidative coupling
INE	Petrochemical. Methanol To Olefins (MTO)
INF	Petrochemical. LPG cracker
ING	Ethanol dehydrogenation
INH	Flash pyrolysis wood
INI	Butane dehydrogenation to i-butylene

Table B.6 *Petrochemical intermediates production*
          (Joosten, 1998; Chauvel, LeFebre, 1989)

INK	Ethylene oxide production
INL	Propylene oxide production
INM	Cumene production
INN	Cumene oxidation
INO	Cyclohexane production
INP	Caprolactam production
INQ	Phthalic anhydride
INR	TerePhthalic Acid (TPA) production
INS	Ethylene glycol production
INT	Acrylonitrile production
INU	Styrene production
INV	VinylChloride Monomer (VCM) production
INX	BTX separation
INY	Xylenes separation
INZ	Xylene residue isomerisation
IO0	Caprolactam production incl. N_2O mitigation
IO1	Adipic acid production incl. N_2O mitigation
IO2	Urea Formaldehyde (UF) resin production
IO3	Viscose production
IO4	Cellophane production
IOA	Formaldehyde production
IOB	Urea production
IOC	Aniline production
IOD	Acetic acid production
IOE	Caprolactam production
IOF	Nitro-benzene production
IOG	MethylEtulKeton (MEK) production
IOH	Adipic acid production
IOI	I-propanol production
IOJ	TolueneDiIsocyanate (TDI) production
IOK	Ethanol production from ethylene
IOL	2-ethylhexanol production
IOM	Carbon black production
ION	Acetic anhydride production
IOO	Detergent production synthetic, Alkyl Ether Sulphates (AES)
IOP	Acetic acid production from biomass
IOQ	Butanol/acetone prod. From biomass
IOR	I-propanol from biomass
IOS	Butadiene through flash pyrolysis
IOT	Phenol through lignin hydrotreatment
IOU	Carbon black production from biomass
IOV	Detergent prod. (AES) from palm oil
IOW	Paint production conventional
IOX	Paint production from Marigold oil

Table B.7 *Petrochemical production polymerisation (Joosten, 1998)*

IP1	PolyPropylene production (PP)
IP2	PolyEthylene production (PE)
IP3	PolyVinylChloride production (PVC)
IP4	PlolyStyrene production (PS)
IP5	PolyEthyleneTerephthalate production (PET)
IP6	Acrylonitrile Butadiene Styrene production (ABS)
IP7	Styrene Butadiene Rubber production (SBR)
IP8	PolyUrethane production (PUR)
IP9	Nylon 6 production
IPA	Nylon 6.6 production
IPB	Butadiene Rubber production (BR)
IPC	PUR production from lignin
ISX	PVC production
IOY	PolyHydroxyButyrate/Valerate production (PHB/PHV)

The italic abbreviations and materials in Table B.8 are the petrochemical waste materials, which play a role in the petrochemical industry's strategies. In the glossary the abbreviations are fully written.

Table B.8 *Waste materials in the Western European MARKAL model*

Code	Waste material
WCC	Blast furnace slag [t]
WCF	Fly ash [t]
WCT	Waste glass [t]
WMA	Aluminium scrap [t]
WMB	Copper scrap [t]
WMF	Steel scrap [t]
WMM	Steel scrap in MSW [t]
WMN	Aluminium scrap in MSW [t]
WND	Demolition wood [t]
WNF	Waste natural textile fiber [t]
WNK	Kitchen waste (30% H_2O) [t]
WNP	Waste paper, separately collected [t]
WNQ	Waste paper, wrappings etc. in MSW [t]
WNR	Mixed wood waste (15% H_2O [t]
WNS	Wood process waste (15% H_2O)[t]
WP1	*PolyOlefine waste clean [t]*
WP2	*PolyOlefine waste mixed [t]*
WP3	*PolyOlefine waste MSW [t]*
WP5	*PolyStyrene waste clean [t]*
WP6	*PolyStyrene waste mixed [t]*
WP7	*PolyStyrene waste MSW [t]*
WPA	*PVC waste clean [t]*
WPB	*PVC waste mixed [t]*
WPC	*PVC waste MSW [t]*
WPF	*PET waste clean [t]*
WPG	*PET mixed [t]*
WPH	*PET waste MSW [t]*
WPJ	*Nylon waste mixed [t]*
WPX	*Bioplastics waste [t]*
WSA	Asphalt waste [t]
WSL	Waste lubricants [t]
WSR	*Elastomeres waste [t]*

The italic abbreviations in Table B.9 and materials are the petrochemical materials, which play a role in the strategies of the petrochemical industry. In the glossary the abbreviations are fully written.

Table B.9 *Materials in the Western European MARKAL model*

Code	Material	Code	material
MCA	Concrete building blocks [t]	*MPA*	*Cellophane [t]*
MCB	Bricks [t]	*MPB*	*PHB/PHV (biopol) [t]*
MCC	Cement [t]	*MPC*	*Butadiene Rubber (BR) [t]*
MCD	Ready mix concrete [t concr. equiv.]	*MPE*	*PolyEthylene [t]*
MCE	Prefab concrete [t concr. equiv.]	*MPF*	*Acrylonitrile Butadiene Styrene [t]*
MCH	High strength cement [t conv. cem. equi]	*MPG*	*Styrene Butadiene Rubber [t]*
MCK	Portland cement clinker [t]	*MPM*	*Nylon 6.6 [t]*
MCL	Sand-lime bricks [t]	*MPN*	*Nylon 6 [t]*
MCM	Marble and granite stones [t]	*MPP*	*PolyPropylene [t]*
MCQ	Quicklime (CaO) [t]	*MPR*	*UF Resins [t]*
MCS	Floor tiles + stoneware [t]	*MPS*	*PolyStyrene [t]*
MCT	Glass [t]	*MPT*	*PolyEthylene Terephthalate [t]*
MCY	Gypsum [t]	*MPU*	*PVC [t excl. Additives]*
MCZ	Kaolin [t]	*MPV*	*PVC [t incl. additives]*
MIA	Nitric acid [t]	*MPW*	*PUR [t]*
MIC	Chlorine [t]	*MSA*	*Asphalt [t]*
MIF	Ammonia [t NH_3 equiv.]	*MSB*	*Benzene [t]*
MIK	Potash [t K_2O equiv.]	*MSC*	*Caprolactam [t]*
MIN	NaOH [t]	*MSD*	*Detergents [t]*
MIP	Phosphoric acid [t P_2O_5 equiv.]	*MSE*	*Ethylene [t]*
MIS	Soda [t]	*MSF*	*Propylene [t]*
MIZ	Sodium chloride [t]	*MSG*	*C4-fraction [t]*
MMA	Aluminium [t]	*MSH*	*Butadiene [t]*
MMB	Copper cathode [t]	*MSI*	*Butylene [t]*
MMC	Cast iron [t]	*MSJ*	*BTX [t]*
MMD	Dri quality steel [t]	*MSK*	*Toluene [t]*
MMF	Direct reduced iron [t]	*MSL*	*Lubricants [t]*
MMH	High quality crude steel [t]	*MSM*	*Cyclohexane [t]*
MMI	Iron [t]	*MSN*	*Cumene [t]*
MML	Low quality crude steel [t]	*MSO*	*DiEthylene glycol [t]*
MMM	Medium quality crude steel [t]	*MSP*	*Paint [t paint equivalents]*
MMN	Reinforcement steel [t]	*MSQ*	*Xylenes (mixed) [t]*
MMO	Hot rolled section steel [t]	*MSR*	*Natural elastomeres (rubber) [t]*
MMP	Hot rolled coil steel [t]	*MST*	*Ethylene oxide [t]*
MMQ	Cold rolled coil steel [t]	*MSU*	*Ethylene glycol [t]*
MMR	Cold rolled coil AT&F steel [t]	*MSV*	*Propylene oxide [t]*
MMS	Cold rolled coil F&P steel [t]	*MSW*	*Acrylonitrile [t]*
MMT	Heavy plate steel [t]	*MSX*	*P-Xylene [t]*
MMU	Wire rod steel [t]	*MSY*	*O-Xylene [t]*
MMV	Alloy steel [t]	*MSZ*	*Xylene residue [t]*
MMW	Galvanized/tinplate steel [t]	*MTA*	*TerePhthalic Acid [t]*
MMX	Copper concentrate [t]	*MTB*	*Butanol [t]*
MMY	Semi-finished copper [t]	*MTC*	*Acetone [t]*
MNA	Compost (15% H_2O) [t]	*MTD*	*Phenol [t]*
MNB	Roundwood (15% H_2O) [t]	*MTE*	*Phthalic Anhydride [t]*
MNC	Chipboard [t]	*MTF*	*Styrene [t]*
MNF	Fiber board [t]	*MTG*	*Vinyl Chloride Monomer (VCM) [t]*
MNG	Gravel and sand [t]	*MTH*	*Formaldehyde [t]*
MNK	Palm kernel oil [t]	*MTI*	*Urea [t]*
MNL	*Marigold flower oil [t]*	*MTJ*	*Aniline [t]*
MNM	High quality waste paper pulp [t]	*MTK*	*Acetic acid [t]*
MNN	Low quality waste paper pulp [t]	*MTL*	*HexaMethyleneDiAmine [t]*
MNO	Mechanical pulp [t]	*MTM*	*Nitro-Benzene [t]*
MNP	Packaging paper and sanitary paper [t]	*MTN*	*Methyl Ethyl Keton (MEK) [t]*
MNQ	Graphic paper [t]	*MTO*	*Adipic acid [t]*
MNR	Newsprint [t]	*MTP*	*I-Propanol [t]*
MNS	Wool [t]	*MTP*	*Toluenediisocyanate [t]*
MNT	Sawn tropical hardwood (15% H_2O) [t]	*MTQ*	*2-Ethylhexanol [t]*
MNU	Chemical pulp [t]	*MTS*	*Carbon black [t]*
MNV	*Viscose/rayon [t]*	*MTU*	*Surfactant (AES) [t]*

MNW	Other sawn wood/plywood (15% H_2O) [t]	*MTV*	*acetic anhydride [t]*
SIN	Sinter [t iron equiv.]	ORE	Iron ore [t]
PEL	Pellets [t iron equiv.]	OXY	Oxygen [t]

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