Process Data Descriptions for the production of synthetic organic materials

Input data for the MATTER study

L.A.J. Joosten

98028

Department of Science, Technology and Society
(Natuurwetenschap en Samenleving)
Utrecht University
Padualaan 14
NL-3584 CH Utrecht
The Netherlands

Report No. 98028

ISBN 90-73958-42-3

June 1998

CONTENTS

1. INTRODUCTION

This report describes technologies for the production of synthetic organic materials. It is a result of the MATTER study (MATerials Technologies for CO_2 Emission Reduction). The MATTER study focuses on reduction of CO_2 emissions caused by the use of energy and materials. This report aims at providing input data for the MARKAL model at ECN.

Technologies that are discussed in this report are:

The production of monomers:
- Steamcracking of ethane, LPG, naphtha and gas oil
- Fluid Catalytic Cracking (FCC)
- Oxidative coupling of natural gas
- The Methanol to Olefins (MTO) process
- Biomass (flash) pyrolysis

Polymerisation processes:
- Polymerisation of Polyethylene (PE)
- Polymerisation of Polypropylene (PP)
- Polymerisation of Polystyrene (PS)
- Polymerisation of Polyvinyl Chloride (PVC)
- Production of Polyethylene Therephtalate (PET)
- Production of other thermoplastics (ABS)
- Production of thermosets (PUR)
- Production of synthetic rubbers (SBR)

Plastic processing processes:
- Film extrusion
- Extrusion coating
- Sheets extrusion
- Thermoforming
- Blow moulding
- Injection moulding
- Foaming
- Tubes extrusion
- Profiles extrusion
- Cables extrusion
- Other processes

Plastic waste management processes:
- Disposal
- Incineration without heat recovery
- Incineration with heat recovery
- Plastic waste injection in blast furnaces
- Pyrolysis of mixed plastic waste
- Gasification of mixed plastic waste
- Hydrogenation of mixed plastic waste
- Selective dissolution

- Mechanical recycling
- Chemical recycling

Other processes:
- Crude oil distillation
- Deasphalting of vacuum residue
- Asphalt blowing
- Synthetic lubricants production

1.1 Methodological aspects

For each process the data to be used in MATTER is collected in a datasheet. This datasheet subsequently specifies the process inputs of materials and energy carriers, the process output materials (products) and energy carriers, the process costs and the residual capacity in the year 2000.

Costs, specified for a specific year are calculated into costs for 1994 using the price indices for machinery, as published by Statistics Netherlands (CBS, 1990/1992/1996). Price developments in The Netherlands are assumed to be exemplary for Western European price developments. Subsequently, prices were converted into ECU_{1994} using exchange rates: 1 $\$_{1994}$ = 0.80 ECU_{1994}; 1 Dfl_{1994} = 0.46 ECU_{1994}.

In literature, data on process costs are scarce and often not available in the form that is required for MATTER (ECU or $ per ton). In some cases they could be derived from similar processes. If this was not possible we used some general rules to calculate cost data to be used in MATTER. Investment data in literature do not always refer to total investments (battery limits PLUS offsite costs). If offsite costs are not included, they were estimated at 40% of battery limits investments. If no fixed cost data are available, we calculated them at 4% of investments, including 2% (maintenance) labour.

Operation labour costs are often specified as operators per shift (for example Chauvel *et al.*, 1989). If only data in this form are available we used the following procedure. From several publications that specify labour costs both as [$ per ton] and as [operators per shift] we constructed the relation between [$ per ton] and 1 [operator per shift], depending on the plant capacity. This relation is shown in Figure 1 and can be approached by the formula:

$$X = 146 * Y^{-0.86}$$

With: X = Labour costs per ton per operator
Y = Plant capacity

We calculated labour costs per ton by multiplying this factor X (applied to the specified plant capacity) by the number of operators per shift.

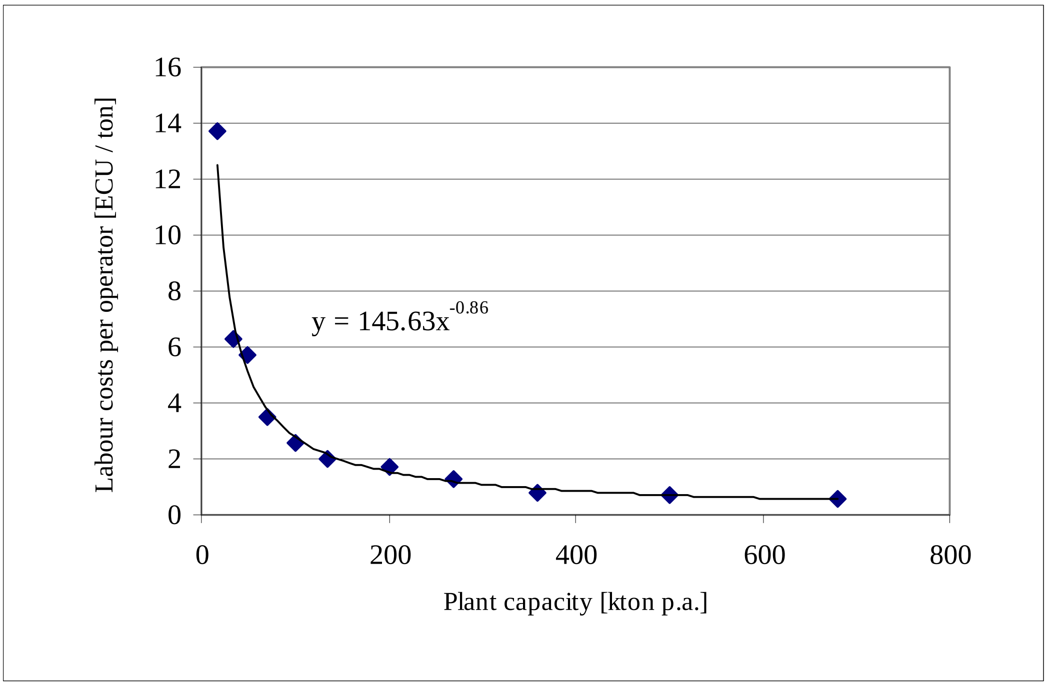


Figure 1 Labour costs per operator as a function of plant capacity

Other general remarks:

- All percentages in this report refer to weight.
- In the tables, parts do not necessarily add to totals due to rounding.
- Energy contents are calculated based on lower heating values (LHV). A list of heating values can be found in Appendix A (Table 58).

2 TECHNOLOGY CHARACTERISATION FOR MATERIALS PRODUCTION

2.1 Olefins production

Olefins (ethylene and propylene) are the main building stones for plastics. They can be produced using several processes and feedstocks. All processes have in common that they produce a range of products and by-products. The shares of the different output products depend on the process and feedstock used and on a minor scale on the process adjustments.

Up to now, ethylene has been the most valuable olefin. For most processes, ethylene is the main output product, followed at a distance by propylene. Other valuable products, produced in minor quantities are butenes (C4) and BTX (Benzene, Toluene, Xylene). The remaining products are considered as fuels: methane, hydrogen and pyrolysis fuel oil. During the last decade, the demand for propylene has grown rapidly, as an effect of the growing demand for polypropylene.

Currently, in Europe, steamcracking is the process mostly used to produce olefins. For steam cracking the ratio between propylene and ethylene yields is virtually fixed for each feedstock. Therefore the growing demand for propylene asks for another process that delivers mainly propylene: Fluid Catalytic Cracking (FCC). According to Patel (1996), 88% of propylene is produced by steamcracking, the remainder (12%) originates from FCC. According to Zehnder (1998), the latter part will grow to about 25% in 2000. The share of a thirth process to produce propylene, dehydration of propane, is expected to remain very limited during the next decades (Patel, 1996), (Zehnder, 1998). In 2000, about 60% of ethylene is used for polyethylene production, about 50% of propylene for polypropylene production (Zehnder, 1998). Other uses for ethylene are: vinyl chloride, ethylene oxide, ethanol, ethylbenzene and others. Other uses for propylene are: isopropanol, acrylnitril, propylene oxide and others.

In the future, other processes, which are presently under development, may become commercial. Investigated in this study are the oxidative coupling of natural gas, the Methanol-to-olefins (MTO) process and the pyrolysis of biomass.

2.1.1 Steamcracking

Virtually all ethylene produced in Europe is obtained by steamcracking. In this process a feedstock (naphtha, gas oil, ethane or LPG) is heated to 800 to 900°C in the presence of steam, by which procedure long molecules fall apart into shorter ones. This results in a mixture of shorter molecules. This mixture is quenched to stop the reaction, compressed, dried and further chilled for distillation. This way the mixture is split into a number of valuable products: ethylene, propylene, a C4 fraction containing butenes and butadiene and pyrolysis gasoline from which benzene, toluene and xylenes can be produced. The process also produces some by-products with limited market value: a mixture of gasses (methane and hydrogen), which is used as fuel for the process, and a mixture of higher carbons, which can also be used as fuel for the process, or sold as pyrolysis fuel oil. Furthermore, ethane and propane are produced, which are recycled to the reactor. Recycle streams are 67%, 14%, 5% and 4% compared to feedstock input for ethane, LPG, naphtha and gas oil cracking respectively (Stratton *et al.*, 1983). This corresponds to conversion percentages of 60%, 88%, 95% and 96% respectively.

In Western Europe, naphtha is the main feedstock, in contrast to the US, where ethane is mostly used. A breakdown of feedstocks used in Europe to produce ethylene is shown in Table 1 (Chauvel and Lefebvre, 1989), as well as a forecast for 2000 (Zehnder, 1998). Total ethylene capacity in EU + EFTA amounted to 15530 kton in 1991 (Chemfacts, 1991) and is forecasted at 20000 kton in 2000 (Zehnder, 1998). A part of the crackers in Europe have the possibility to switch between 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 currently most valuable output products. In the MATTER study, however, flexible crackers are not discerned, for avoiding modelling difficulties.

Table 1 Breakdown of feedstocks for ethylene production in Europe (Chauvel and Lefebvre, 1989), (Chemfacts, 1991) and forecast for 2000 (Zehnder, 1998)

	1989 [%]	2000 [%]
Ethane	8	9
LPG	11	13
Naphtha	69	63
Gas oils	12	15

The shares of the output products highly depend on the feedstock used. Hitherto, ethylene has been the most valuable product. Ethylene yield increases in the direction gas oil, naphtha, LPG, ethane. Yields of the second valuable product, propylene, are about 0.6. 0.5 and 0.4 in proportion to ethylene yields for gas oil naphtha and LPG cracking respectively, whereas ethane cracking hardly delivers any propylene. Exact yields vary somewhat with the composition of the feedstocks and the process adjustments, especially with cracking temperature and reactor residence time. These process adjustments affect the ‘severity’ of the cracking process. ‘High severity cracking’, at higher temperatures and shorter residence times, needs more energy, but brings higher ethylene yields than ‘low severity cracking’, and lower propylene yields. Furthermore, the share of valuable products is higher. During the last decades, new crackers have shifted to higher severity, although the currently increasing demand for propylene may be an incentive for lower severity cracking (Phylipsen *et al.*, 1995).

Because of the influence of severity and exact feedstock compositions on the exact output yields, in literature many different specifications are circulating. From those specifications it gets clear that not all of Europe's steamcrackers operate at high severity. Patel (1996) for example, who describes the German situation, mentions an average ethylene yield for naphtha cracking of about 23%, whereas Stratton *et al.*(1983) mention 30.3% and Chauvel *et al.*(1989) 33.6%. Newly build plants show ethylene yields of about 35% (HCP, 1997). However, it is clear that not all of the European steamcrackers operate at high severity. Therefore we choose the yields specified by Stratton *et al.* (1983), which show modest severity, as representative average for Western Europe in 2000. In 2020. however, it may be assumed that the specification of output products of a plant newly built around 2000 has become an average specification. Therefore we took the specification of a KTI[1] plant (HCP, 1997) as a representative for 2020. For the MATTER study, we modelled steamcracking of gas oil, naphtha, LPG and ethane. Yields, as modelled, are stated in Table 2.

Table 2 Yields of steamcrackers as modelled for MATTER.

	2000[1]				**2020[2]**			
	Ethane	**LPG[3.4]**	**Naphtha**	**Gas oil**	**Ethane**	**LPG[4]**	**Naphtha**	**Gas oil**
	[wt.%]	**[wt.%]**	**[wt.%]**	**[wt.%]**	**[wt.%]**	**[wt.%]**	**[wt.%]**	**[wt.%]**
Ethylene	80	41	30	23	82	44	35	27
Propylene	2	17	16	14	2	15	14	13
C4	3	7	10	11	2	9	8	8
Pyrolysis gasoline	1	7	23	20	2	8	20	20
Methane	7	25	15	8	7	22	16	10
Hydrogen	6	2	1	1	5	2	2	1
Pyrolysis fuel oil	0	1	4	22	0	0	5	20

[1](Stratton *et al.*, 1983); [2](HCP, 1997) KTI plant; [3](Chauvel *et al.*, 1989); [4]Calculated as mean between propane and butane cracking yields.

Ethylene, propylene, C4 and pyrolysis gasoline are regarded as valuable products, methane, hydrogen and pyrolysis fuel oil as fuels. These fuels are used internally for firing the cracking process. Remaining fuels can be used elsewhere and are thus considered as process outputs. We assume that the gaseous fuels (methane / hydrogen) are burned first, followed by the liquid fuels (pyrolysis fuel oil) if the process requires more energy.

Energy consumption for steamcrackers is needed for heating the feedstock, compression after reaction and product separation, with an approximate distribution of 65%, 15% and 20% (Heijningen *et al.* 1992a). In the process much high pressure steam is formed, which can be used for compression and pumping. The alternative, compression and pumping with electrical compressors and pumps is less efficient. Although in 2000 there may still be some crackers which do not use steam compressors and pumps, we assume that the average situation can be described by crackers which do. Because of this, electricity use is relatively low, 30 kWh, 40 kWh, 80 kWh and 100 kWh per ton ethylene for ethane, LPG, naphtha and gas oil cracking respectively (Patel (1996) gives a mean value of 56 kWh for all feedstocks). According to Patel (1996) naphtha and gas oil cracking show net (hp-) steam productions of 0.9 GJ and 1.6 GJ per ton ethylene respectively.

---

[1] Yields of newly built plants by other manufacturers (for example Lummus, Stone & Webster and Linde) do not differ considerably from the yields of this KTI plant.

Energy requirement for steam cracking has shown a considerable decrease during the past decades. According to Steinmeyer (1997), energy consumption for ethane cracking has decreased steadily from 35 MJ/ton ethylene in 1955 to 12 MJ/ton ethylene in 1990. For naphtha, gas oil and LPG cracking, similar declines of energy use may be supposed. However, an energy use of 12 MJ/ton ethylene for ethane cracking seems to be too optimistic as a European average for 2000. According to Patel (1996) the average energy use for ethane cracking in Germany in 1989 amounted to 16.5 GJ/ton ethylene (Naphtha: 25.1 GJ/ton ethylene, Gas oil: 30.3 GJ/ton ethylene). New ethane cracking plants in 1997 show energy consumptions of 12.6 GJ/ton (Stone & Webster, Linde), 13.0 GJ/ton (KTI) and 13.8 GJ/ton (Lummus) (HCP, 1997). Because of the existence of relatively old plants in 2000, we take the plant with the highest energy consumption as representative for 2000. According to Patel (1996), there are a number of possibilities to reduce energy consumption: for example improved isolation, optimised, highly integrated energy streams and on-line monitoring, resulting in a reduction potential of about 20%. Considering the difference in energy consumption between the average German cracker and newly built crackers, it becomes obvious that with the latter at least a part of these improvement options have already been implemented. We assume that in 2020 the best commercial available cracker (in 1997) has become the average European cracker.

Energy data concern the plant including product separation, excluding, however, BTX-separation into benzene, xylene and toluene. Propane and ethane are recycled.

Material and energy balances for ethane, LPG, naphtha and gas oil steamcracking are shown in Table 4 to Table 7. They show that all processes, except ethane cracking, are self-supporting: they produce enough fuels to fulfil the energy demand of the process. For ethane cracking some extra fuel is needed. CO_2 emissions caused by combustion of all fuels needed for the process are included in the datasheets (excluding extra fuel for ethane cracking). They were calculated using the CO_2 production factors as shown in Table 3.

Table 3 CO_2 production factors for fuels combustion

	CO_2 production [kg/kg]
methane	2.74
hydrogen	0
pyrolysis fuel oil	3.35

Table 4 Material and energy balances for ethane steamcracking

	2000 [t/t ethylene]	**2020** [t/t ethylene]	**2000** [GJ/t ethylene]	**2020** [GJ/t ethylene]
Input:				
Ethane	1.24	1.23	59.1	58.2
Output:				
Products				
Ethylene	1	1	47.2	47.2
Propylene	0.03	0.02	1.2	1.0
C4	0.04	0.03	1.8	1.3
Pyrolysis gasoline (BTX)	0.01	0.02	0.6	1.0
Fuels				
Methane	0.09	0.09	4.6	4.6
Hydrogen	0.07	0.06	8.7	7.3
Pyrolysis fuel oil	0.00	0.00	0.0	0.0
Products:	1.08	1.07	50.7	50.4
Fuels:	0.16	0.15	13.3	11.9
Total output:	1.24	1.23	64.0	62.3
Energy requirement:			13.8	13.0
Fuels remaining:				
Methane	0	0	0	0
Hydrogen	0	0	0	0
Pyrolysis fuel oil	0	0	0	0
Total	0	0	-0.6	-1.1

Table 5 Material and energy balances for LPG steamcracking

	2000 [t/t ethylene]	**2020** [t/t ethylene]	**2000** [GJ/t ethylene]	**2020** [GJ/t ethylene]
Input:				
LPG	2.44	2.29	112.1	105.2
Output:				
Products				
Ethylene	1	1	47.2	47.2
Propylene	0.42	0.35	19.0	16.0
C_4	0.18	0.21	8.1	9.3
BTX	0.17	0.18	6.8	7.5
Fuels				
Methane	0.60	0.50	30.2	25.1
Hydrogen	0.05	0.04	5.7	4.8
Pyrolysis fuel oil	0.03	0.01	1.1	0.4
Products:	1.76	1.74	81.1	80.0
Fuels:	0.68	0.55	37.0	30.3
Total output:	2.44	2.29	118.2	110.3
Energy requirement:			17.4	16.7
Fuels remaining:				
Methane	0.26	0.17	12.8	8.4
Hydrogen	0.05	0.04	5.7	4.8
Pyrolysis fuel oil	0.03	0.01	1.1	0.4
Total	0.33	0.22	19.6	13.6

Table 6 Material and energy balances for naphtha steamcracking

	2000 [t/t ethylene]	**2020** [t/t ethylene]	**2000** [GJ/t ethylene]	**2020** [GJ/t ethylene]
Input:				
Naphtha	3.30	2.90	145.2	127.5
Output:				
Products				
Ethylene	1	1	47.2	47.2
Propylene	0.53	0.41	24.5	18.9
C4	0.33	0.24	15.2	10.8
BTX	0.77	0.57	31.3	23.5
Fuels				
Methane	0.50	0.48	25.1	23.9
Hydrogen	0.03	0.05	4.0	6.4
Pyrolysis fuel oil	0.13	0.14	5.6	6.1
Products:	2.63	2.23	118.1	100.4
Fuels:	0.67	0.67	34.7	36.3
Total output:	3.30	2.90	152.8	136.7
Energy requirement:			20.9	19.7
Fuels remaining:				
Methane	0.08	0.08	4.2	4.2
Hydrogen	0.03	0.05	4.0	6.4
Pyrolysis fuel oil	0.13	0.14	5.6	6.1
Total	0.25	0.28	13.7	16.6

Table 7 Material and energy balances for gas oil steamcracking

	2000 [t/t ethylene]	**2020** [t/t ethylene]	**2000** [GJ/t ethylene]	**2020** [GJ/t ethylene]
Input:				
Gas oil	4.31	3.70	183.9	158.2
Output:				
Products				
Ethylene	1	1	47.2	47.2
Propylene	0.61	0.49	27.8	22.2
C_4	0.48	0.31	21.8	14.2
BTX	0.87	0.75	35.6	30.8
Fuels				
Methane	0.35	0.37	17.5	18.6
Hydrogen	0.04	0.05	5.2	6.4
Pyrolysis fuel oil	0.96	0.73	40.9	31.1
Products:	2.96	2.55	132.4	114.4
Fuels:	1.35	1.15	63.5	56.1
Total output:	4.31	3.70	195.9	170.5
Energy requirement:			25.1	23.0
Fuels remaining:				
Methane	0	0	0	0
Hydrogen	0	0	0	0
Pyrolysis fuel oil	0.90	0.77	38.4	33.1
Total	0.90	0.77	38.4	33.1

Costs data were derived from Stratton *et al.*(1983). Investments were calculated into equivalent values for 1994 using indexes from (CBS, 1990, 1992, 1996). This way the following investments were obtained for ethane, LPG, naphtha and gas oil cracking respectively: 438. 501. 691 and 802 ECU_{1994}/t ethylene capacity. These investments include battery limits costs, off-site costs and 15% contingency. If all valuable products are accounted for (ethylene, propylene, C4 and pyrolysis gasoline), these investments correspond to 270-300 ECU_{1994}/t products capacity for gas oil, naphtha and LPG cracking. For ethane cracking higher investments of about 400 ECU_{1994}/t products capacity are required, due to much larger recycle streams and hence much larger separation unit. Fixed costs consist of maintenance labour costs and maintenance materials costs. Variable costs consist of operating labour costs and the costs of water, chemicals (excluding feedstocks) and catalysts. Insurance, taxes and overheads are excluded. Residual capacity data is derived from (Chauvel *et al.*, 1989) and (Chemfacts, 1991).

Energy efficiency can be further improved by gas turbine integration. In that case offgasses of the gas turbine, with a temperature of 500°C and an oxygen concentration of 15-17%, are used in the burners instead of combustion air. This way, energy consumption is decreased by 1.8 GJ/ton ethylene for ethane cracking, 2.9 GJ/ton ethylene for naphtha cracking and 3.3 GJ/ton ethylene for gas oil cracking. Furthermore, more steam is produced. Electricity production amounts to about 50 W per ton ethylene capacity for gas oil cracking. Gas turbine integration leads to extra investments of about 40 ECU_{1994}/t ethylene capacity (Patel 1994). This option is not included in the datasheets for MATTER.

All data needed for input into MATTER is summarised in Table 8 to Table 11.

Table 8 Datasheet for MATTER: ethane steamcracking

MATTER Datasheet				
Process: **Ethane steamcracking**				
			Year:	
		unit	**2000**	**2020**
Input:				
Ethane		[GJ]	59.1	58.2
Electricity		[GJ_e]	0.1	0.1
Fuel		[GJ]	0.6	1.1
Output:				
Products		**[t]**	**1.08**	**1.07**
	Ethylene	[t]	1	1
	Propylene	[t]	0.03	0.02
	C_4	[t]	0.04	0.03
	Pyrolysis gasoline (BTX)	[t]	0.01	0.02
	CO_2	[t]	0.25	0.25
Costs:				
Investments		[ECU_{1994}/t ethylene cap.]	438	432
Fixed		[ECU_{1994}/t ethylene cap. year]	13	13
including labour		[ECU_{1994}/t ethylene cap. year]	*7*	*6*
Variable		[ECU_{1994}/t ethylene]	5	5
including labour		[ECU_{1994}/t ethylene]	*3*	*2*
Lifetime		[year]	25	25
Availability factor		[-]	0.95	0.95
Residual capacity		[kton ethylene / year]	1242	

Table 9 Datasheet for MATTER: LPG steamcracking

MATTER Datasheet			
Process: **LPG steamcracking**			
		Year:	
	unit	**2000**	**2020**
Input:			
LPG	[GJ]	112.1	105.2
Electricity	[GJ$_e$]	0.29	0.29
Output:			
Products	**[t]**	**1.76**	**1.74**
Ethylene	[t]	1	1
Propylene	[t]	0.42	0.35
C_4	[t]	0.18	0.21
Pyrolysis gasoline (BTX)	[t]	0.17	0.18
CO_2	[t]	0.95	0.92
Methane	[GJ]	12.8	8.4
Hydrogen	[GJ]	5.7	4.8
Fuel oil	[GJ]	1.1	0.4
Costs:			
Investments	[ECU$_{1994}$/t ethylene cap.]	501	494
Fixed	[ECU$_{1994}$/t ethylene cap. year]	15	14
including labour	[ECU$_{1994}$/t ethylene cap. year]	*8*	*7*
Variable	[ECU$_{1994}$/t ethylene]	5	5
including labour	[ECU$_{1994}$/t ethylene]	*2*	*2*
Lifetime	[year]	25	25
Availability factor	[-]	0.95	0.95
Residual capacity	[kton ethylene / year]	1708	

Table 10 Datasheet for MATTER: Naphtha steamcracking

MATTER Datasheet

Process: **Naphtha steamcracking**

		Year:	
	unit	**2000**	**2020**
Input:			
Naphta	[GJ]	145.2	127.5
Electricity	[GJ$_e$]	0.29	0.29
Output:			
Products	**[t]**	**2.63**	**2.23**
Ethylene	[t]	1	1
Propylene	[t]	0.53	0.41
C_4	[t]	0.33	0.24
Pyrolysis gasoline (BTX)	[t]	0.77	0.57
CO_2	[t]	1.15	1.08
Methane	[GJ]	4.2	4.2
Hydrogen	[GJ]	4.0	6.4
Fuel oil	[GJ]	5.6	6.1
hp-steam	[GJ]	0.9	0.9
Costs:			
Investments	[ECU$_{1994}$/t ethylene cap.]	691	607
Fixed	[ECU$_{1994}$/t ethylene cap. year]	20	18
including labour	[ECU$_{1994}$/t ethylene cap. year]	*10*	*9*
Variable	[ECU$_{1994}$/t ethylene]	7	6
including labour	[ECU$_{1994}$/t ethylene]	*3*	*3*
Lifetime	[year]	25	25
Availability factor	[-]	0.95	0.95
Residual capacity	[kton ethylene / year]	10716	

Table 11 Datasheet for MATTER: gas oil steamcracking

MATTER Datasheet

Process: **Gas oil steamcracking**

		Year:	
	unit	**2000**	**2020**
Input:			
Gasoil	[GJ]	183.9	158.2
Electricity	[GJ$_e$]	0.36	0.36
Output:			
Products	**[t]**	**2.96**	**2.55**
Ethylene	[t]	1	1
Propylene	[t]	0.61	0.49
C_4	[t]	0.48	0.31
Pyrolysis gasoline (BTX)	[t]	0.87	0.75
CO_2	[t]	1.15	1.02
Fuel oil	[GJ]	38.4	31.1
Hydrogen	[GJ]	0	2.0
hp-steam	[GJ]	1.6	1.6
Costs:			
Investments	[ECU$_{1994}$/t ethylene cap.]	802	689
Fixed	[ECU$_{1994}$/t ethylene cap. year]	23	20
including labour	[ECU$_{1994}$/t ethylene cap. year]	*14*	*12*
Variable	[ECU$_{1994}$/t ethylene]	7	6
including labour	[ECU$_{1994}$/t ethylene]	*4*	*4*
Lifetime	[year]	25	25
Availability factor	[-]	0.95	0.95
Residual capacity	[kton ethylene / year]	1864	

2.1.2 Olefins recovery from FCC offgasses

According to Zehnder (1998), 28% (about 3500 kton) of propylene use in Western Europe in 2000 originates from refinery offgasses. According to Aubrey (1996) refinery offgasses from Fluid Catalytic Cracking (FCC) even contribute about half of propylene use in the US.

In Fluid Catalytic Cracking, heavy (vacuum) gas oils from refineries are cracked into lighter fractions. Table 12 gives an indication of FCC output products and yields. The most important product is gasoline. Lighter fractions can be regarded as by-products.

Table 12 Typical FCC yields (Avidan *et al.*, 1990)

Fraction	Yield [weight %]
Fuel gas (C_{2-} fraction)	4%
C_3 fraction[a]	6%
C_4 fraction[a]	10%
Gasoline	52%
Light gas oil	15%
Heavy fuel oil	7%
Coke	6%

[a] LPG fraction is formed by the C_3 and C_4 fractions together

Fluid Catalytic Cracking can be optimised for maximum production of middle distillates (Chauvel, 1989). In that case C_2 and C_3 yields could be used for olefins production, so as to yield about 0.02 ton propylene and 0.01 ton ethylene per ton feedstock. In practice, however, the C_3 fraction is sold as LPG, together with the C_4 fraction. Therefore only the C_{2-} fraction (offgasses) can be used for olefins production. The composition of this fraction is shown in Table 13. Usually this fraction is considered as fuel gas.

Table 13 FCC offgass composition calculated from (Netzer, 1997)

	[weight %]
Ethylene	18%
Propylene	13%
Hydrogen	1%
Methane	30%
Ethane	21%
Propane	4%
C4	3%
Nitrogen	9%
Carbon Monoxide	0.7%
Carbon Dioxide	0.4%

Table 12 and Table 13 show that per ton FCC feedstock only a small amount of olefins can be obtained (ethylene ~0.7%, propylene ~0.5%). Because of the relatively high throughput of catalytic crackers (1000-3000 kton p.a.), reasonably olefin yields can be obtained.

Netzer (1997) describes a process to recover olefins from FCC offgasses. In this process both propylene and ethylene are recovered. All data from the datasheet (Table 14) are based on this description. For each ton ethylene, 5.6 ton offgasses are needed, with an energy content of 245 GJ. Only ethylene and propylene are considered as products, the rest is valued as fuel gas. After ethylene and propylene extraction 165 GJ fuel gas (3.8 ton) remains.

Maintenance costs were calculated at 4% of investments; labour costs were calculated based on 2 operators per shift and an ethylene plant capacity of 82 kton p.a. (Netzer, 1997)

In Table 14 the data for MATTER are summarised.

Table 14 Datasheet for MATTER: Olefins recovery from FCC offgasses

MATTER Datasheet			
Process: **Olefins from FCC offgasses**			
		Year:	
	unit	**2000**	**2020**
Input:			
FCC offgas	[t]	5.6	5.6
Steam	[GJ]	5.8	5.8
Electricity	[GJ_e]	5.7	5.7
Output:			
Products	**[t]**	**1.72**	**1.72**
Ethylene	[t]	1	1
Propylene	[t]	0.72	0.72
Fuel gas	[GJ]	165.2	165.2
Costs:			
Investments	[ECU_{1994}/t ethylene cap.]	753	753
Fixed	[ECU_{1994}/t ethylene cap. year]	30	30
including labour	[ECU_{1994}/t ethylene cap. year]	*15*	*15*
Variable	[ECU_{1994}/t ethylene]	8	8
including labour	[ECU_{1994}/t ethylene]	*8*	*8*
Lifetime	[year]	25	25
Availability factor	[-]	0.95	0.95
Residual capacity	[kton ethylene / year]		

2.1.3 Oxidative coupling of natural gas

This process converts methane into valuable products, of which ethylene and propylene are the most important. The process consists of two steps: First methane reacts, with the aid of a catalyst, with pure oxygen into ethylene, ethane, propylene and propane. Furthermore, CO and CO_2 are formed as by-products. The methane conversion process takes place at relatively low pressures (atmospheric to about 5 atm.) and a temperature of 750-900 °C. In the second step, a conventional ethane cracker, ethane is cracked into ethylene and small amounts of propane, propylene, C4. pyrolysis gasoline and hydrogen (see paragraph 2.1.1). In the separation section, non-reacted methane and ethane are separated and recycled to the first and second reactors respectively.

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 trough the reactor. The process has the peculiarity that increasing the methane conversion percentage is associated with a decrease of the C_{2+} selectivity. Therefore, the single pass C_{2+} yield is limited (and the C_2 yield still more so). Before the introduction of membrane reactors, many catalysts have been investigated without, however, reaching single pass C_2 yields far above 10% (for example (Kaddouri *et al.*, 1989)). With membrane reactors, in which oxygen can be distributed very evenly, methane conversion rates of 20-30% have been achieved so far, with C_{2+} selectivity selectivities of up to 80% (mol%). With a methane conversion rate of 20%, this corresponds to a C_{2+} yield of 16% (Cordi *et al.*, 1997). Membrane reactors show higher selectivities than conventional fixed bed reactors (Miguel *et al.*, 1996). Although model calculations predict that with membrane reactors a C_2 yield of about 50% should be possible (Lu *et al.*, 1997), C_2 yields in experiments have not yet exceeded 20% (Miguel *et al.*, 1996). An upper bound (of the C_{2+} yield) of about 30% has been argued based on the reaction mechanism considerations (Parkyns *et al.*, 1993). 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 assumption to be reached in the nearby future (v. Geem, 1992), (Geerts *et al.*, 1992), (Amenomiya *et al.*, 1990). This corresponds to a C_{2+} yield of 24%.

Because of the relatively low conversion rates achieved, the process involves extensive recycling streams. 30% conversion corresponds to a recycling stream of 2.3 times, 20% corresponds to 4 times the feedstock input. This affects both investments and energy use for product separation. Membrane separation could be a solution in the future. However, much research has still to be done in the field of membrane separation. So in the nearby future (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 *et al.*, 1996). Therefore, membrane separation is not modelled in MATTER.

For the construction of the MATTER datasheet (Table 17), we base ourselves mainly on studies by Van Geem (1992) and Geerts *et al.* (1992). Both start from a methane conversion rate of 30% and a C_{2+} selectivity of 80-85%. Table 15 shows the product composition of the methane conversion step (v. Geem, 1992). A similar specification by Ferstl *et al.* (1994) is less suitable, because this starts from a C_{2+} selectivity of only 50%.

Table 15 Product composition of methane conversion (v. Geem, 1992)

	Product composition [mol%]
Ethylene	50
Ethane	30
Propylene	1.7
Propane	3.7
CO	5
CO_2	10

There is a lot of discussion going on about the reaction mechanism methane conversion. However, for the construction of a mass balance, the following simplified reactions can be used (Ferstl *et al*, 1994):

Ethylene: $2\ CH_4 + O_2 \rightarrow C_2H_4 + 2\ H_2O$
Ethane: $4\ CH_4 + O_2 \rightarrow 2\ C_2H_6 + 2\ H_2O$
Propylene: $6\ CH_4 + 3\ O_2 \rightarrow 2\ C_3H_6 + 6\ H_2O$
Propane: $3\ CH_4 + O_2 \rightarrow C_3H_8 + 2\ H_2O$
Carbon monoxide: $2\ CH_4 + 3\ O_2 \rightarrow 2\ CO + 4\ H_2O$
Carbon dioxide: $CH_4 + 2\ O_2 \rightarrow CO + 2\ H_2O$

These reactions can be used to calculate the amounts of methane and oxygen needed and the amount of steam formed. After conversion into weight % and taking into account the ethane cracking step (mass and energy balances for ethane cracking are given in paragraph 2.1.1) the total mass and energy balances of the oxidative coupling of methane can be calculated. These are shown in Table 16. Ethylene, propylene, C_4 and pyrolysis gasoline are regarded as valuable products, carbon monoxide, propane, methane and hydrogen as fuels.

Table 16 Mass and energy balance of oxidative coupling of methane

	Input [ton]	**Output [ton]**	**Input [GJ]**	**Fuels output [GJ]**	**Products output [GJ]**	**Total output [GJ]**
Methane	1.43		71.6			
Oxygen	1.48					
Ethylene		1.00			47.2	
CO		0.07		0.7		
CO_2		0.21				
Propane		0.07		3.2		
Propylene		0.04			1.9	
H_2O		1.46				
C_4		0.01			0.6	
Pyrolysis gasoline		0.01			0.2	
Methane		0.03		1.6		
Hydrogen		0.02		2.9		
Total	2.91	2.91	71.6	8.3	50.0	58.3

From Table 16 it can be seen that the process is exothermic. The net reaction energy surplus of both processes together is 13.3 GJ per ton ethylene. It is the combined result of the reaction energy surplus of the methane conversion step of 15.0 GJ per ton ethylene and the reaction energy demand of the ethane cracker of 1.7 GJ per ton ethylene (based on total ethylene production of both processes together). According to Geerts *et al.* (1992), the process produces 8.76 GJ of hp-steam, which can be used for electricity production. This figure is lower than the 13.3 GJ from the energy balance. This is because the process itself needs some energy for compression, which is supposed to be done with steam compressors, and the probable existence of some losses.

According to Geerts *et al.* (1992), the net deliverance of fuel gas amounts to 5.47 GJ. per ton ethylene. Process energy requirement amounts to 2.85 GJ per ton ethylene[2] (v. Geem, 1992). Together, these figures are in keeping with the gross fuels output of 8.3 GJ. per ton ethylene from the process from the energy balance (Table 16). Furthermore, the process needs 55 kWh of electricity per ton ethylene produced (v. Geem, 1992).

Labour costs amount to 37 ECU_{1994} / ton ethylene according to Geerts *et al.* (1992). Other variable costs amount to 51 ECU_{1994} / ton ethylene, whereas the fixed costs amount to 47 ECU_{1994} / ton ethylene capacity. Predictions of investment costs in literature differ somewhat. According to Van Geem (1992) they amount to 1087 ECU_{1994} / ton ethylene capacity. Geerts *et al.* (1992) give depreciation costs of 32.5 ECU_{1994} / ton ethylene capacity per year. With a lifetime of 25 years this corresponds to 813 ECU_{1994} / ton ethylene capacity. We assume investment costs of 900 ECU_{1994} / ton ethylene capacity.

In 2000, no production capacity using this process will be available. It may be introduced from 2010 onwards.

---

[2] CO_2 emissions from combustion of these fuels produced in the process are included in the CO_2 emissions indicated in the datasheet, together with the CO_2 emissions from the process itself

Table 17 Datasheet for MATTER: Oxidative coupling of natural gas

MATTER Datasheet

Process: **Oxidative Coupling of Natural Gas**

	unit	Year:	
		2000	**2010**
Input:			
Natural gas	[GJ]	71.6	71.6
Electricity	[GJ_e]	0.20	0.20
Oxygen	[t]	1.48	1.48
Output:			
Products	**[t]**	**1.06**	**1.06**
Ethylene	[t]	1.0	1.0
Propylene	[t]	0.04	0.04
C_4	[t]	0.01	0.01
Pyrolysis gasoline (BTX)	[t]	0.01	0.01
CO_2	[t]	0.37	0.37
H_2O	[t]	1.46	1.46
Hydrogen	[GJ]	2.4	2.4
Propane	[GJ]	3.2	3.2
hp-steam	[GJ]	8.8	8.8
Costs:			
Investments	[ECU_{1994}/t ethylene cap.]	900	900
Fixed	[ECU_{1994}/t ethylene cap. year]	47	47
Variable	[ECU_{1994}/t ethylene]	88	88
including labour	[ECU_{1994}/t ethylene]	*37*	37
Lifetime	[year]	25	25
Availability factor	[-]	0.95	0.95
Residual capacity	[kton ethylene/year]	0	

2.1.4 Methanol to olefins (MTO)

The MTO process runs via catalytic dehydration of methanol. The reaction takes place at temperatures between 350 and 500°C (Schönfelder *et al.*, 1994b) and a variety of catalysts can be used. Experiments show that the product composition of the process is highly dependent on the catalyst used (v. Geem, 1992), (Redwan, 1997), (Schönfelder *et al.*, 1994a). Most MTO processes are designed to maximise ethylene yield. It is, however, possible to reach very high propylene yields instead (Schoenfelder *et al.*, 1994a), (Chen *et al.*, 1994).

To a lesser degree, the product output can be influenced by changing the reaction temperature, which influences the reaction severity. For example (HCP, 1997) describes a MTO plant of which the ethylene to propylene ratio van be varied between 1.2 and 1.5 by altering the reaction temperature. Current catalysts show a methanol conversion rate of 100%.

According to v. Geem (1992) processes with high propylene co-production are most feasible. Therefore we take the MTO process of IFP as a representative. The material and energy balances of this process are given in Table 18. Ethylene, propylene, C_4 and aromatics are considered as commercial products, the rest as fuels. The fuels are used for the process itself.

Table 18 Material and energy balances for the methanol to olefin (IFP) process

	[t/t ethylene]	[GJ/t ethylene]
Input:		
Methanol	5.98	126.2
Output		
Products		
Ethylene	1	47.2
Propylene	1.11	50.8
C_4	0.36	16.3
Fuels		
Methane	0.07	3.6
Ethane	0.01	0.3
Propane	0.09	4.3
C_{5+}	0.03	1.3
Products:	2.47	114.2
Fuels:	0.20	9.5
Water:	3.31	
Total output:	5.98	123.7
Energy requirement:		12.3
Extra fuel needed:		2.8

According to Stratton *et al.* (1983), the energy consumption of the Mobil MTO process amounts to 11.6 GJ per ton ethylene produced. The Mobil process, however, has a different product distribution. It uses 4.52 ton methanol feedstock per ton ethylene produced, whereas the IFP process uses 5.98 ton methanol feedstock. This is due to the larger propylene production of the IFP process. The higher feedstock throughput of the IFP process affects its energy consumption. We scaled the energy requirement using the ratio of the feedstock inputs required. This way, the energy consumption of the IFP process is calculated at 12.3 GJ per ton ethylene produced. In this figure we included an estimated energy efficiency improvement of 20% between the year of publication (1983) and the starting point of the MATTER model (2000). The process produces 9.5 GJ of fuels per ton ethylene, so 2.8 GJ of extra fuels have to be added to run the process.

According to Stratton *et al.* (1983), the Mobil process needs 2.7 GJ of energy for compression per ton ethylene produced. If scaled this means for the IFP process an energy consumption for compression of 3.6 GJ. The process is exothermic (see Table 18). From the energy balance it can be seen that it produces 2.5 GJ of steam, which can be used for compression. However, 1.1 GJ of steam have to be added to fulfil the energy demand for compression. According to v. Geem (1992), the Union Carbide MTO process needs 55 kWh electricity per ton ethylene produced (feedstock input 4.3 ton methanol per ton ethylene). Scaled to 5.98 ton methanol input, we calculate for the IFP process an electricity input of 75 kWh per ton ethylene.

CO_2 emissions were calculated from the combustion of the process output fuels. CO_2 emissions caused by the combustion of the extra fuel needed are excluded.

Investments for the IFP process are given by v. Geem (1992). His figure of 720 ECU_{1940} per ton ethylene capacity comes close to the figure of 758 ECU_{1940} per ton ethylene capacity, as given by Stratton *et al.* (1983). Fixed costs were derived from Stratton *et al.* (1983) and consist of maintenance materials and maintenance labour. Variable costs were also derived from Stratton *et al.* (1983). They consist of operating labour, catalysts and auxiliary chemicals.

The MTO process is currently ready to be implemented. In HCP (1997) a MTO process is presented, which is commercially available. However, no plants have yet been built. So the MATTER model is free to choose the process from 2005 onwards.

Data for input into MATTER are summarised in the datasheet (Table 19).

Table 19 Datasheet for MATTER: MTO process

MATTER Datasheet Process: **Methanol to olefins**			
		Year:	
	unit	**2000**	**2020**
Input:			
Methanol	[GJ]	126.2	126.2
Electricity	[GJ_e]	0.3	0.3
Fuel	[GJ]	2.8	2.8
hp-Steam	[GJ]	1.1	1.1
Output:			
Products	**[t]**	**2.47**	**2.47**
Ethylene	[t]	1.00	1.00
Propylene	[t]	1.11	1.11
C_4	[t]	0.36	0.36
CO_2	[t]	0.59	0.59
Costs:			
Investments	[ECU_{1994}/t ethylene cap.]	720	720
Fixed	[ECU_{1994}/t ethylene cap. year]	22	22
including labour	[ECU_{1994}/t ethylene cap. year]	*11*	*11*
Variable	[ECU_{1994}/t ethylene]	16	16
including labour	[ECU_{1994}/t ethylene]	*3*	*3*
Lifetime	[year]	25	25
Availability factor	[-]	0.95	0.95
Residual capacity	[kton ethylene / year]	0	

2.1.5 Biomass (flash) pyrolysis

There are several approaches to convert biomass into valuable hydrocarbons including olefins. With the so-called flash pyrolysis process biomass is cracked at high temperatures (about 1000°C), into ethylene, BTX (mainly benzene), carbon monoxide and carbon dioxide (Steinberg *et al.*, 1992). Paushkin *et al.* (1994) propose another route, consisting of three steps: Firstly steam gasification at 1000-1200°C, resulting in a mixture of carbon monoxide, carbon dioxide and hydrogen. Secondly synthesis of hydrocarbons from this mixture over a Co catalyst and thirdly catalytic pyrolysis at 790°C into olefins. This way, 1.5 ton olefins could be obtained from 10 ton of biomass. However, little information on this process is available. Because more processing steps are needed than with the flash pyrolysis process, which probably leads to higher energy demand and investment costs, we did not consider this process as a valuable option for MATTER, but analysed the flash pyrolysis process instead.

For the flash pyrolysis process an entrained down flow reactor is used. It is necessary to keep the reactor residence time short (1 second) in order to prevent unwanted secondary reactions leading to unwanted products (hence the name *flash* pyrolysis). Therefore a high heat-up rate and a rapid cool-down rate are used. Steinberg *et al.* (1992) found that pyrolysis in the presence of methane considerably increases hydrocarbon yields. Methane plays a role in the pyrolysis process, but it is not cracked and is recovered from the product stream and recycled. The type of wood used influences the product distribution of the process. Steinberg *et al.* (1992) found that the ethylene yield varies between 20.7% and 27.4% for fir and pine wood pyrolysis respectively, both with methane. For MATTER we calculated the product distribution as the mean between fir and pine wood pyrolysis, based on data from Steinberg *et al.* (1992). The result is shown in Table 20. Ethylene, benzene (BTX) and carbon monoxide (for methanol production) are regarded as valuable products, ethane as fuel. The process also produces some char and ashes.

Table 20 Product distribution of biomass (flash) pyrolysis with methane at 1000°C (Steinberg *et al.*, 1992). Figures refer to carbon content conversion.

	Fir [%]	**Pine** [%]	**Mean** [%]
Ethylene	20.7	27.4	24.1
BTX	12.7	24.6	18.7
CO	48.1	38.7	43.4
CO_2	3.3	2.7	3.0
Ethane	2.0	0	1.0

Assuming a carbon content of wood of 50% (Gielen *et al.*, 1996) it can be calculated that for each ton of ethylene produced 8.3 ton of biomass is needed. Gielen *et al.* (1996) estimate that, for delivering the process energy use, another 3.5 ton (52.5 GJ) of biomass is needed. So in total 11.8 ton of biomass is needed to produce one ton of ethylene.

The process has much in common with the naphtha cracking process. Therefore we adapted missing information from the naphtha cracking process described in paragraph 2.1.1., which we scaled according to feedstock input (8.3 ton biomass per ton ethylene versus 3.3 ton naphtha per ton ethylene).

We assume that the process delivers enough hp-steam to drive the compressors (which is also the case with naphtha cracking). Therefore the electricity demand is relatively low, like it is also for naphtha steamcracking.

All costs (investments, fixed and variable) were derived from naphtha cracking and scaled according to feedstock input, with an additional increase of 25%, which accounts for the relatively extensive methane recycle streams of the biomass pyrolysis process.

CO_2 emissions in the datasheet (Table 21) only consist of emissions from the process itself. Emissions rising from biomass combustion for firing the process are excluded.

A pilot plant is currently in operation in Canada. Therefore we estimate that the process becomes commercially available in about 2010.

Table 21 Datasheet for MATTER: (flash) Pyrolysis of biomass

MATTER Datasheet

Process: **(Flash) Pyrolysis of Biomass**

		Year:	
	Unit	**2000**	**2020**
Input:			
Biomass feedstock	[GJ]	124.7	124.7
Biomass fuel	[GJ]	52.5	52.5
Electricity	[GJ_e]	0.7	0.7
Output:			
Products	**[t]**	**3.58**	**3.58**
Ethylene	[t]	1	1
Benzene	[t]	0.78	0.78
CO	[t]	1.80	1.80
CO_2	[t]	0.12	0.12
Ethane	[GJ]	2.0	2.0
Costs:			
Investments	[ECU_{1994}/t ethylene cap.]	2176	2176
Fixed	[ECU_{1994}/t ethylene cap. year]	63	63
including labour	[ECU_{1994}/t ethylene cap. year]	*33*	*33*
Variable	[ECU_{1994}/t ethylene]	20	20
including labour	[ECU_{1994}/t ethylene]	*10*	*10*
Lifetime	[year]	25	25
Availability factor	[-]	0.95	0.95
Residual capacity	[kton ethylene / year]	0	

2.2 Polymerisation

The majority of olefins are used for polymerisation into polymers. In Europe a lot of different polymer types and sub-types are produced. The most common types are Polyethylene (PE), Polypropylene (PP), PolyVinyl Chloride (PVC), Polystyrene (PS) and Polyethylene terphtalate (PET). These so-called bulk plastics have a wide field of application in packaging materials, consumer goods and buildings. Apart from these bulk plastics, there are a lot of speciality plastics, generally more expensive but with higher material properties. In our study the latter are collected into the category ‘other thermoplastics’. The chief polymers of this group are Acrylonitrile-Butadiene-Styrene (ABS) and polyamide (the latter is much used as fibre) (APME, 1996). We take ABS as a representative for this group. Of the group of thermosets, PUR is the most widely applied species (APME, 1996) and therefore we take it as a representative for the whole group of thermosets. Furthermore, synthetic rubbers are discerned, for which Styrene Butadiene Rubber is chosen as a representative.

Van Duin (1997) made a forecast for plastic use in Western Europe in 2000. His results are summarised in Table 22. Regarding Western Europe as a whole, import and export streams play no major role. Therefore, plastic production is treated as equivalent to plastic use (Van Duin, 1997). In Table 22, production figures are divided into production from ‘virgin’ feedstocks (primary production) and production from recycled materials (secondary production). Figures for secondary production were derived from (APME, 1996), which states the recycling of the different plastics in 1994 (total: 1057 kton), to which a growth of about 10% was added in order to get a forecast for 2000.

Table 22 Forecast of plastics production in Western Europe (Van Duin, 1997), (APME, 1996) [kton]

Plastic type	Primary production	Secondary production	Total production
PE	9700	800	10500
PP	6800	200	7000
PS	2800	100	2900
PVC	5450	50	5500
PET	2950	50	3000
Other thermoplastics	2800	negligible	2800
Thermosets	5100	negligible	5100
Synthetic rubbers	2200	negligible	2200
	37800	**1200**	**39000**

In the following paragraphs we will successively discuss the polymerisation of PE, PP, PS, PVC, PET, ABS, PUR and SBR. Input materials are limited to the main building stones of the plastics. Additives like plasticisers, stabilisers, fillers and lubricants generally cover a relatively small part of material inputs. General purpose PE and PP have additive contents beneath 3%, PS and PET beneath 5%. Only for PVC, additives can make up a considerable part of material inputs: up to 15% (BUWAL, 1996). In our study, however, additives are not taken into account.

There are five types of polymerisation processes: liquid phase, gas phase, solution, suspension and polycondensation. With the liquid phase process (also referred to as bulk polymerisation or high-pressure polymerisation) the process takes place in liquid phase, at high pressure (LDPE: 1400-3500 bar) or low pressure (PP: 20-40 bar) and a temperature below 100°C.. The gas phase process (also called low-pressure polymerisation) is employed at low pressures (7-20 bar) and a temperature between 70 and 100°C.. Both the liquid phase and the gas phase process run without the aid of a solvent. The solution polymerisation process uses a solvent (for example hexane) and runs at a pressure between 30 and 100 bar and a temperature between 150 and 250°C.. The suspension process is the oldest process. Like the solution process, it uses a solvent. It differs from the solution process in that the produced polymer is not soluble in the solvent which leads to a suspension, from which the polymer prepitates. The process needs a relatively extensive separation unit. The process takes place at a temperature beneath 110°C and a pressure beneath 40 bar. The suspension process is often used as batch process. The emulsion process is comparable tot the suspension process, but is uses water as solvent, with emulsifiers and other additives to suspend the monomer and polymer. The polycondensation process is applied to PET, PUR and nylons. It takes place at higher temperatures (230-285°C). Unlike the polymerisation processes, which are exothermic, the polycondensation process is endothermic.

Energy requirement differs between the processes used. Because no solvent is used in the liquid phase and gas phase processes, only a simplified separation unit is needed, which requires less energy than the more extensive separation units of the solution and suspension processes (EPA, 1997). Furthermore, for polyethylene production, the gas phase process uses considerably less energy than the liquid phase process, because of the lower pressure needed.

It is not possible to apply each process to the production of each polymer. Table 23 gives an overview of processes currently used to produce the different polymers. Processes that are most often applied are indicated with a capital X.

Table 23 Typical polymerisation methods for the polymers discerned in this report (EPA, 1997), (Patel, 1996), (Heijningen *et al.*, 1992a, 1992b)

Plastic type	**Polymerisation method**				
	Liquid phase	**Gas phase**	**Solution**	**Suspension / Emulsion**[a]	**Polycondensation**
PE					
HDPE		x	x	**X**	
LDPE	**X**			x	
LLDPE	x	**X**	x	x	
PP	**X**	**X**	x	**X**	
PS	**X**		x	**X**	
PVC				**X**	
PET	x				**X**
ABS	x			**X**	
PUR					**X**
SBR			**X**	**X**	

[a] Alternative process for PVC, PS, SBR and ABS polymerisation

2.2.1 Polyethylene (PE)

In 1995, 9750 kton of PE were produced, divided between LDPE (4500 kton), LLDPE (1450 kton) and HDPE (3800 kton). Currently, especially LLDPE production is growing rapidly (6-7% p.a.), followed by HDPE (~3% p.a.), while LDPE production is hardly growing (0.5-1% p.a.) (Harzmann *et al.*, 1996), (Kaps *et al.*, 1996). Van Duin (1997) forecasts a PE production in Western Europe in 2000 of 10500 kton. Taking into account the respective growth percentages, we forecast that PE production in 2000 is divided between LDPE (4600 kton), LLDPE (1750 kton) and HDPE (4150 kton).

In 1995 the consumption of HDPE and LDPE (including LLDPE) were divided between the different products / processing processes of the plastic processing industry as can be seen in Table 24.

Table 24 Consumption of LDPE (incl. LLDPE) (Hartzmann *et al.*, 1996) and of HDPE (Kaps *et al.*, 1996), Western Europe, 1995, division between products / plastic processing processes

HDPE		LDPE / LLDPE	
blow moulding	32%	blow moulding	1%
injection moulding	24%	injection moulding	5%
films	19%	films	76%
tubes and plates	15%	tubes	3%
monofilament, band	4%	extrusion coating	7%
others	6%	cable isolation	3%
		others	5%

LDPE can be produced using the liquid phase process or the suspension process (Table 23). Both in The Netherlands (v. Heijningen *et al.*, 1992a) and in Germany (Patel, 1996) the liquid phase process is the only one applied. LDPE can not be produced using the gas phase process. LLDPE can be produced using the gas phase process, the solution process, the suspension process, or a modified form of the liquid phase process. In Germany, in 1989 the division was 60% / 20% / 20% / ~0% for these processes respectively. Though it is technically possible to use the liquid phase process for LLDPE production, it is not feasible (Patel, 1996). HDPE can be produced using either the gas phase process, the solution process, or the suspension process. In Germany, in 1989 the division was 10% / 15% / 75% respectively (Patel, 1996). For lack of a better estimate, we extrapolated these German mixes of polymerisation processes to the mixes for Western Europe.

For the MATTER we do not model all possible processes separately. Because of a relatively similarity between the solution and the suspension process, we model a combined solution / suspension process, the data of which can be seen as mean values for both processes. Because of the relatively low energy consumption and low investment costs for the gas phase process, we modelled it separately. Thus, we discern five PE polymerisation options:

- LDPE liquid phase
- LLDPE gas phase
- LLDPE solution / suspension
- HDPE gas phase
- HDPE solution / suspension

Currently, there is a shift going on in the direction of the production of metallocene polyethylene, using metallocene catalysts instead of conventional Ziegler-Natta catalysts. Metallocene catalysts allow better polymerisation control, leading to improved material quality. Patel (1996) expects that metallocene catalysts will replace about 30% of Ziegler-Natta catalysts during the next ten years. Optimism concerning the introduction of metallocene catalysts is widely shared (for example (v. Stijn, 1996), (EPN, 1996), (ECN, 1997)). Because metallocene catalysts can be used with the same polymerisation processes as the conventional Ziegler-Natta catalysts, there is no need to model them separately. Possible minor changes in energy use (due to changed process adjustments) and costs are neglected (although the price of metallocene catalysts is at present much higher than the price of conventional catalysts, it is expected to drop when they are widely used).

Patel (1996) has carried out an extensive study on energy use and costs involved in the different polymerisation processes. Our input data for MATTER is mainly based on this study. The polymerisation processes need electricity for compression and for processing the polymers into granulate, while steam is needed in the reactor and in the separation unit. The energy requirement for the production of granulate from the raw polymers requires an electricity use of 0.7-1.1 GJ_e per ton PE. The polymerisation processes deliver low pressure and middle pressure steam, which can be used for other processes. However, benefit from this is limited, because of the relatively low temperature and pressure. Steam figures represent net input (LLDPE / HDPE) or net output (LDPE). Because investment data from Patel (1996) concern plants of different capacity (between 100 kton p.a. and 225 kton p.a.) and because larger plants require relatively lower investments (economy of scale), we used the formula:

$$I_1/I_2 = (C_1/C_2)^m$$

to calculate the analogous investments for a 100 kton capacity plant (I = total investments, C = capacity, m = exponent of regression = 0.82 (Patel, 1996)).

The main possibilities to reduce energy use in polymerisation are in shifting between polymerisation processes rather than in improvements of the individual processes. Also substitution of LDPE by LLDPE (produced by the gas phase process) is expected to contribute to the energy savings in this sector (Patel, 1996).

The input data for MATTER can be read from the datasheets, (Table 25, Table 26, Table 27). Fixed costs represent maintenance costs and overhead costs. Variable costs represent catalyst and auxiliary chemical costs and labour costs.

Table 25 Datasheet for MATTER: LDPE polymerisation

MATTER Datasheet

Process: **LDPE polymerisation, liquid phase**

	unit	Year: 2000	2020
Input:			
Ethylene	[t]	1.02	1.02
Electricity	[GJ_e]	3.1	3.1
Output:			
Polyethylene LDPE	**[t]**	**1**	**1**
lp-steam	[GJ]	0.4	0.4
Costs:			
Investments	[ECU_{1994}/t PE cap.]	668	668
Fixed	[ECU_{1994}/t PE cap. year]	42	42
Variable	[ECU_{1994}/t PE]	40	40
including labour	[ECU_{1994}/t PE]	*13*	*13*
Miscellaneous:			
Lifetime	[year]	25	25
Availability factor	[-]	0.95	0.95
Residual capacity	[kton PE / year]	4600	

Table 26 Datasheet for MATTER: LLDPE polymerisation

MATTER Datasheet Process: **LLDPE polymerisation**					
		Gas phase		**Suspension / Solution**	
	unit	**2000**	**2020**	**2000**	**2020**
Input:					
Ethylene	[t]	1.02	1.02	1.02	1.02
Electricity	[GJ_e]	2.0	2.0	1.7	1.7
Steam	[GJ]	0.3	0.3	1.6	1.6
Output:					
Polyethylene LLDPE	**[t]**	**1**	**1**	**1**	**1**
Costs:					
Investments	[ECU_{1994}/t PE cap.]	337	337	618	618
Fixed	[ECU_{1994}/t PE cap. year]	16	16	39	39
Variable	[ECU_{1994}/t PE]	34	34	33	33
including labour	[ECU_{1994}/t PE]	*5*	*5*	*10*	*10*
Miscellaneous:					
Lifetime	[year]	25	25	25	25
Availability factor	[-]	0.95	0.95	0.95	0.95
Residual capacity	[kton PE / year]	1050		700	

Table 27 Datasheet for MATTER: HDPE polymerisation

MATTER Datasheet					
Process: **HDPE polymerisation**					
		Gas phase		**Suspension / Solution**	
	unit	**2000**	**2020**	**2000**	**2020**
Input:					
Ethylene	[t]	1.02	1.02	1.02	1.02
Electricity	[GJ_e]	2.0	2.0	1.7	1.7
Steam	[GJ]	0.3	0.3	2.0	2.0
Output:					
Polyethylene HDPE	**[t]**	**1**	**1**	**1**	**1**
Costs:					
Investments	[ECU_{1994}/t PE cap.]	337	337	740	740
Fixed	[ECU_{1994}/t PE cap. year]	14	14	42	42
Variable	[ECU_{1994}/t PE]	34	34	43	43
including labour	[ECU_{1994}/t PE]	*6*	*6*	*14*	*14*
Miscellaneous:					
Lifetime	[year]	25	25	25	25
Availability factor	[-]	0.95	0.95	0.95	0.95
Residual capacity	[kton PE / year]	400		3750	

2.2.2 Polypropylene (PP)

Polypropylene production in Western Europe in 2000 is forecasted at 7000 kton (v. Duin, 1997). This is the result of a very rapid growth of ~6% p.a. (Beer, 1996). The consumption of PP to produce plastic products is shown in Table 28.

Table 28 Consumption of PP, Western Europe, 1995, division between products / plastic processing processes (Beer, 1996)

Packaging:	36%	
films		*21%*
injection moulding		*13%*
other packaging		*2%*
Textiles, fibres	25%	
Automotive	12.5%	
Electronics	4%	
Components	4%	
Consumer products and others	18.5%	

Polypropylene can be produced with the liquid phase process, the gas phase process and the suspension process (v. Heijningen *et al.*, 1992a), (Patel, 1996). In the Netherlands the division between these processes is 35% / 25% / 40% (v. Heijningen *et al.*, 1992a), in Germany 20% / 40% / 20% (Patel, 1996). For Western Europe we assume that all three processes make up an equal share of polypropylene polymerisation.

The trend towards metallocene catalysts also applies to polypropylene (v. Stijn, 1997). It is possible that in about 10 years metallocene catalysts make up the major part of catalysts for polypropylene polymerisation (Seiler, 1995). Because metallocene catalysts can be used with the same polymerisation processes as the conventional Ziegler-Natta catalysts (Beer, 1996), there is no need to model them separately for MATTER. Possible minor differences in energy use and costs are neglected.

Energy data were derived from Patel (1996), who did an extensive survey into the energy use for PP polymerisation with the three processes mentioned above. From Table 29 it can be seen that the gas phase process needs considerably less steam than the suspension process, whereas the steam requirement for the bulk process (liquid phase) lies in between. The main possibilities to reduce energy use in polymerisation are in shifting between polymerisation processes rather than in improvements of the individual processes.

Patel (1996) does not give specific cost data on the different PP polymerisation processes. He only calculates general investment costs of 913 ECU$_{1994}$ per ton PP capacity for a 100 kton p.a. PP polymerisation plant. This figure comes very close to the result of our own calculations, based on 16 PP polymerisation plants (average capacity 100 kton p.a.) built all over the world between 1990 and 1996 (HCP, 1990-1996), for which we calculated average investment costs of 951 ECU$_{1994}$ per ton. For lack of specific investment data on the specific processes, we use this value for all processes. Fixed and variable costs were derived from equivalent processes for LDPE and HDPE polymerisation. Fixed costs represent maintenance costs and overhead costs. Variable costs represent catalyst and auxiliary chemical costs and labour costs.

The input data for MATTER can be read from Table 29.

Table 29 Datasheet for MATTER: PP polymerisation

MATTER Datasheet							
Process: **PP polymerisation**							
		Liquid phase		**Gas phase**		**Suspension**	
	unit	**2000**	**2020**	**2000**	**2020**	**2000**	**2020**
Input:							
Propylene	[t]	1.02	1.02	1.02	1.02	1.02	1.02
Electricity	[GJ_e]	2.1	2.1	2.1	2.1	2.1	2.1
Steam	[GJ]	1.2	1.2	0.8	0.8	1.8	1.8
Output:							
Polypropylene PP	**[t]**	**1**	**1**	**1**	**1**	**1**	**1**
Costs:							
Investments	[ECU_{1994}/t PP cap.]	951	951	951	951	951	951
Fixed	[ECU_{1994}/t PP cap. year]	42	42	14	14	42	42
Variable	[ECU_{1994}/t PP]	40	40	34	34	43	43
including labour	[ECU_{1994}/t PP]	*13*	*13*	*6*	*6*	*14*	*14*
Miscellaneous:							
Lifetime	[year]	25	25	25	25	25	25
Availability factor	[-]	0.95	0.95	0.95	0.95	0.95	0.95
Residual capacity	[kton PP / year]	2333		2333		2333	

2.2.3 Polystyrene (PS)

PS consumption in Western Europe in 2000 is estimated at 2900 kton (v. Duin, 1996). We assume that total production (primary plus secondary) equals total consumption (no net exports/imports streams of PS for Western Europe as a whole). So production of PS is also estimated at 2900 kton. There are three types of PS: general purpose PS (GPPS), high impact or rubber modified PS (HIPS) and expanded PS (EPS). General purpose PS is crystalline and brittle. HIPS has a rubber (polybutylene) content of about 11%, whereas EPS is foamed with the aid of a blowing agent (pentane, ~8%).

The division of the PS consumption between the plastic products to be produced and the plastic processing processes to be used can be read from Table 30. This is a rough estimate (mind that shares do not add to 100%), in which EPS is not included. EPS is mainly used for home isolation, road construction and packaging purposes.

Table 30 Consumption of PS (excluding EPS), Western Europe, 1995, division between products / plastic processing processes (Wagner, 1996)

	Share	**Product example**
Food packaging	40%	milk products, desserts
Consumer goods housing	25%	TV, audio, computers
Cooling equipment components	5%	inside of refrigerators
Other injection moulding	36%	CD-packaging, video / audio tapes, micro floppy disks
Injection moulding	60%	
Extrusion / thermoforming	40%	

The production of PS is divided into three steps:

- The production of benzene
- The production of styrene from ethylene and benzene
- Polymerisation of styrene to polystyrene (PS).

Benzene production

Benzene consumption in Western Europe is forecasted at 7500 kton in 2000 (Zehnder, 1998). About half of the benzene production is used for styrene production (Patel, 1996), (Zehnder, 1998). Benzene can either be produced from the pyrolysis gasoline (BTX) fraction of steamcrackers or via catalytic reforming of naphtha, which also runs via a BTX fraction (which has, however, a different composition). According to Boustead (1993), about half of the benzene production runs via each route. In this report we consider the benzene production starting from the BTX fraction.

There are several processes to extract benzene from a BTX fraction. In Germany the major process is extractive distillation (70%) (Patel, 1996). We assume that this is the major process for Western Europe as a whole also. Before the BTX fraction is suitable for extractive distillation, prefractionation via distillation is required. Boustead (1993) gives energy requirement figures that are valid for the average of Western European benzene production. If his data on steam consumption are translated from [kg] to [MJ] using an energy content of 2.67 MJ per kg steam, his energy requirement figures correspond to 3.0 GJ per ton benzene, including prefractionation. Patel (1996) mentions 1.2-2 GJ per ton benzene (with and without prefractionation respectively), v. Heijningen *et al.* (1992) mention 10GJ, Chauvel *et al.* (1989) mention 0.5-2.3 GJ per ton benzene, depending on the exact process and BTX fraction used and whether prefractionation is required or not. The value given by v. Heijningen *et al.*

is certainly to high, because it is based on a very old source. Taking into account the fact that in 2000 a part of the plants will be relatively old, and that for the major part of benzene production prefractionation is needed, we use a value of 2.7 GJ per ton benzene for the net energy requirement. For 2020, when most of the old plants will be replaced by newer ones using more up to date technology, we take the average of the values given by Chauvel as representative: 1.4 GJ per ton benzene.

Investment data were taken from Chauvel (1989). 40% of offsite costs were added. They are the average between two processes: the IFP process and the Lurgi Distapex process, each with a benzene capacity of 100 kton p.a. Investments for prefractionation are included. Fixed costs were calculated as 4% of investments (2% labour and 2% materials). Variable costs refer to solvents and operation labour.

Data for MATTER can be read from Table 31.

Table 31 Datasheet for MATTER: Benzene production

MATTER Datasheet			
Process: **Benzene extractive distillation**			
		Year:	
	unit	**2000**	**2020**
Input:			
BTX[a]	[GJ]	43.2	43.2
Electricity	[GJ_e]	0.06	0.03
Steam	[GJ]	1.6	1.4
Fuel	[GJ]	1.0	
Output:			
Products	**[t]**	**1.0**	**1.0**
Benzene	[t]	1.0	1.0
Costs:			
Investments	[ECU_{1994}/t benzene cap.]	25	25
Fixed	[ECU_{1994}/t benzene cap. year]	0.7	0.7
including labour	[ECU_{1994}/t benzene cap. year]	*0.4*	*0.4*
Variable	[ECU_{1994}/t benzene]	1.7	1.7
including labour	[ECU_{1994}/t benzene]	*1.6*	*1.6*
Lifetime	[year]	25	25
Availability factor	[-]	0.95	0.95
Residual capacity	[kton benzene / year]	7500	

[a] Only the part of the BTX that is converted to benzene is indicated. After benzene extraction a mixture of toluene and xylenes remains, which can be further processed to produce toluene and xylenes. Also energy data in this report only concerns energy for benzene extraction, *excluding* energy required for further processing of the BTX fraction.

Styrene production

Nearly all styrene is manufactured by direct dehydrogenation of ethylbenzene, nearly all of which is produced from ethylene and benzene via alkylation (in gas or liquid phase) of benzene (Chauvel, 1989). A negligible part of styrene is produced as co-product from ethylene oxide production. Because 99% of ethylbenzene is used for the production of styrene, we discuss both processes together. Styrene is used for the production of PS (65%, of which EPS: 14%), SBR (14%), ABS (7%) and other polymers (14%) (Chauvel, 1989). Western European styrene production amounted to 3000 kton in 1984. Because PS production has been growing since then by about 3% p.a. in Europe, styrene production has grown also. With a growth percentage of 3% p.a., styrene production in 2000 is calculated at about 5000 kton.

Input-output data were derived from Chauvel *et al.* (1989). For the alkylation step, 0.27 tons of ethylene and 0.75 tons of benzene are required per ton ethylbenzene. Per ton styrene, however, between 1.10 and 1.16 tons of ethylbenzene are required (depending on the reactor type), whereas 30 to 50 kg toluene and 10 to 30 kg. benzene are formed as by-products, of which benzene is recycled to the alkylation step. For the combined process steps 0.31 tons of ethylene and 0.83 tons of benzene are required to produce 1 ton of styrene. The process produces also a small amount of fuels, which is combusted to deliver a part of the process energy. Because these fuels consist mainly of hydrogen, CO_2 emissions from these fuels can be neglected.

We took the energy data given by Boustead (1993), which are the average of 20 Western European styrene plants, as a representative. His data refers to net process energy requirement: the combusted fuels from the process itself are excluded. The ethylbenzene production step produces also a considerable amount of lp- and hp-steam, the usefulness of which is doubtful. According to Chauvel *et al.* (1989), steam production is 0.6 – 2.25 ton per ton ethylbenzene, depending on the process used. From (HCP, 1995, 1997) a range of 1.5 – 2.6 ton per ton ethylbenzene can be derived. We use the average of the combined ranges as a representative for Western Europe: 1.6 ton per ton ethylbenzene, corresponding to 1.8 ton per ton styrene, with an energy content of 4.8 GJ.

Investment data were derived from HCPBC (diverse years) and are based on 6 styrene plants built between 1991 and 1997. Fixed costs were calculated as 4% of investments (2% labour and 2% materials). Variable costs refer to catalysts, chemicals and labour (based on Chauvel *et al.*, 1989).

In Table 32 the data for MATTER are summarised.

Table 32 Datasheet for MATTER: Styrene production

MATTER Datasheet Process: **Styrene production**			
		Year:	
	unit	**2000**	**2020**
Input:			
Ethylene	[t]	0.31	0.31
Benzene	[t]	0.83	0.83
Electricity	[GJ_e]	0.33	0.33
hp-steam	[GJ]	5.1	5.1
Fuel	[GJ]	4.9	4.9
Output:			
Products	**[t]**	**1.04**	**1.04**
Styrene	[t]	1	1
Toluene	[t]	0.04	0.04
lp / mp-steam	[GJ]	4.8	4.8
Costs:			
Investments	[ECU_{1994}/t styrene cap.]	677	677
Fixed	[ECU_{1994}/t styrene cap. year]	27	27
including labour	[ECU_{1994}/t styrene cap. year]	*14*	*14*
Variable	[ECU_{1994}/t styrene]	20	20
including labour	[ECU_{1994}/t styrene]	*6*	*6*
Lifetime	[year]	25	25
Availability factor	[-]	0.95	0.95
Residual capacity	[kton styrene / year]	5000	

Polystyrene polymerisation

Of the three types of PS: general purpose PS, high-impact PS and expanded PS, general purpose PS covers the largest part. Therefore we take the polymerisation of general purpose PS as representative. PS can be produced using the liquid phase, solution, suspension or emulsion process. The liquid phase process and the suspension process are used most extensively. It is, however, unknown which is the leading process.

For the MATTER study we do not discern the three types of PS separately, but we concern the Western European PS product mix as a whole. For the input / output data we start from the polymerisation of GPPS. The shares of polybutylene and pentane in the total materials input for PS polymerisation are very small. Therefore polybutylene and pentane inputs are neglected.

Energy data for the polymerisation of PS are given by Boustead (1993). He gives average values for 20 Western European polymerisation plants, 10 of which produce GPPS, 7 produce HIPS and 3 EPS. Total energy requirements (fuel + electricity + steam) derived from these data are: GPPS: 1.53 GJ per ton PS, HIPS: 1.56 GJ per ton PS, EPS: 4.97 GJ per ton PS. The difference between GPPS / HIPS on the one hand and EPS on the other hand are caused by the difference of the amount of steam required, which is much higher for EPS polymerisation (1.67 ton per ton PS) than for GPPS / HIPS polymerisation (0.169 and 0.235 ton per ton PS respectively). Boustead also provides average energy requirement data for all PS polymerisation plants investigated. We will not use these averages, because the product mix (GPPS / HIPS / EPS) produced by those 20 plants differs from the actual total European PS polymerisation product mix. The share of EPS of the plants investigated by Boustead is only 14%, whereas the share of EPS in total Western European PS polymerisation is 26% (APME, 1996). With this we calculated the total average process energy requirement for PS polymerisation at 2.4 GJ per ton PS produced.

Investment data on PS polymerisation are scarce. (HCPBC, 1991) describes two plants, the investments of which range from 879 ECU_{1994} per ton PS to 1538 ECU_{1994} per ton PS. It is not sure whether these figures represent only PS polymerisation or PS polymerisation including styrene production. Also it is not sure whether they include off-site costs or not. Anyway, these figures can not be used to obtain a reliable estimate. The values shown in the datasheet (Table 33) are estimates, based on comparable PE and PP liquid phase and suspension polymerisation processes.

Fixed costs are calculated at 4% of investments. Variable costs are derived from (HCP, 1995) and represent the process chemical costs and labour.

Table 33 Datasheet for MATTER: PS polymerisation

MATTER Datasheet

Process: **PS polymerisation**

		Year:	
	unit	**2000**	**2020**
Input:			
Styrene	[t]	1.02	1.02
Electricity	[GJ_e]	0.65	0.65
Steam	[GJ]	1.54	1.54
Fuel	[GJ]	0.23	0.23
Output:			
Products	**[t]**	**1**	**1**
Polystyrene	[t]	1	1
Costs:			
Investments	[ECU_{1994}/t PS cap.]	800	800
Fixed	[ECU_{1994}/t PS cap. year]	32	32
including labour	[ECU_{1994}/t PS cap. year]	*16*	*16*
Variable	[ECU_{1994}/t PS]	34	34
including labour	[ECU_{1994}/t PS]	*14*	*14*
Lifetime	[year]	25	25
Availability factor	[-]	0.95	0.95
Residual capacity	[kton PS / year]	2900	

2.2.4 Polyvinyl Chloride (PVC)

PVC consumption in Western Europe in 2000 is forecasted at 5100 kton (v. Duin, 1997). We assume that for Western Europe as a whole imports and exports of PVC play no major role compared to inner European trade, so the production of PVC in 2000 can be estimated at 5500 kton too. PVC is consumed for the production of the products that can be read from Table 34.

Table 34 Consumption of PVC, divided between products (Anonymous, 1997)

Product	Share
Pipes and conduits	48%
Front panels	15%
Floor covering	4%
Packaging	4%
Wires and cables	4%
Tube fittings	3%
Windows and doors	3%
Coatings	2%

For PVC, much additives are used: depending on the PVC type (rigid / flexible), an additive content of up to 15% is not uncommon (BUWAL, 1996). An additive content of 10% can be seen as a reliable average (Rubin, 1990). For our analysis, we will, however, confine ourselves to ‘pure’ PVC.

The production of PVC is divided into two steps:

- The production of vinyl chloride monomer (VCM)
- The polymerisation of vinyl chloride monomer to Polyvinyl Chloride (PVC).

VCM Production

All of VCM produced is used for producing PVC (Rubin, 1990). There are various ways to produce vinyl chloride (see for example Chauvel, 1989). In practice however, a limited number of processes is used. VCM is either produced from acetylene or from ethylene. Of the world VCM production capacity, 7% is produced from acetylene, the rest from ethylene. Therefore we start from ethylene as feedstock. The production of VCM from ethylene runs via the intermediate product ethylene dichloride (EDC), which is either produced by chlorination or by oxychlorination of the ethylene. EDC is consequently cracked into VCM and hydrochloric acid (HCl). Chlorination and oxychlorination can be combined and balanced, so that only VCM is formed (see Figure 2). About one third of the world VCM production uses this process. We take this ‘state of the art’ process as representative for VCM production. (According to v. Heijningen (1992), energy use differs only marginally between different VCM production processes). Our analysis concerns VCM production from ethylene, chlorine and oxygen. Chlorine production is analysed in (Gielen, 1997) and is therefore excluded in our analysis. Although it is possible to use either pure oxygen or air for oxychlorination, we only consider the use of pure oxygen, because using air leads to the need for a considerably larger separation and purification unit with higher energy requirement and higher costs. The production of oxygen is excluded from the calculations.

Energy data on the combined chlorination / oxychlorination process to produce VCM (Stauffer process) are given by Chauvel *et al.* (1989) and v. Heijningen *et al.* (1992). Probably the data of Chauvel refer to an older process (overall final energy requirement 10.2 GJ per ton VCM) than the data of v. Heijningen (6.1 GJ per ton VCM). Therefore we take the data of v. Heijningen as representative.

Costs were estimated based on (Chauvel *et al.*, 1989) and data on three VCM plants built between 1991 and 1996 (HCP, 1991, 1996). Data on VCM production is summarised in the datasheet (Table 35).

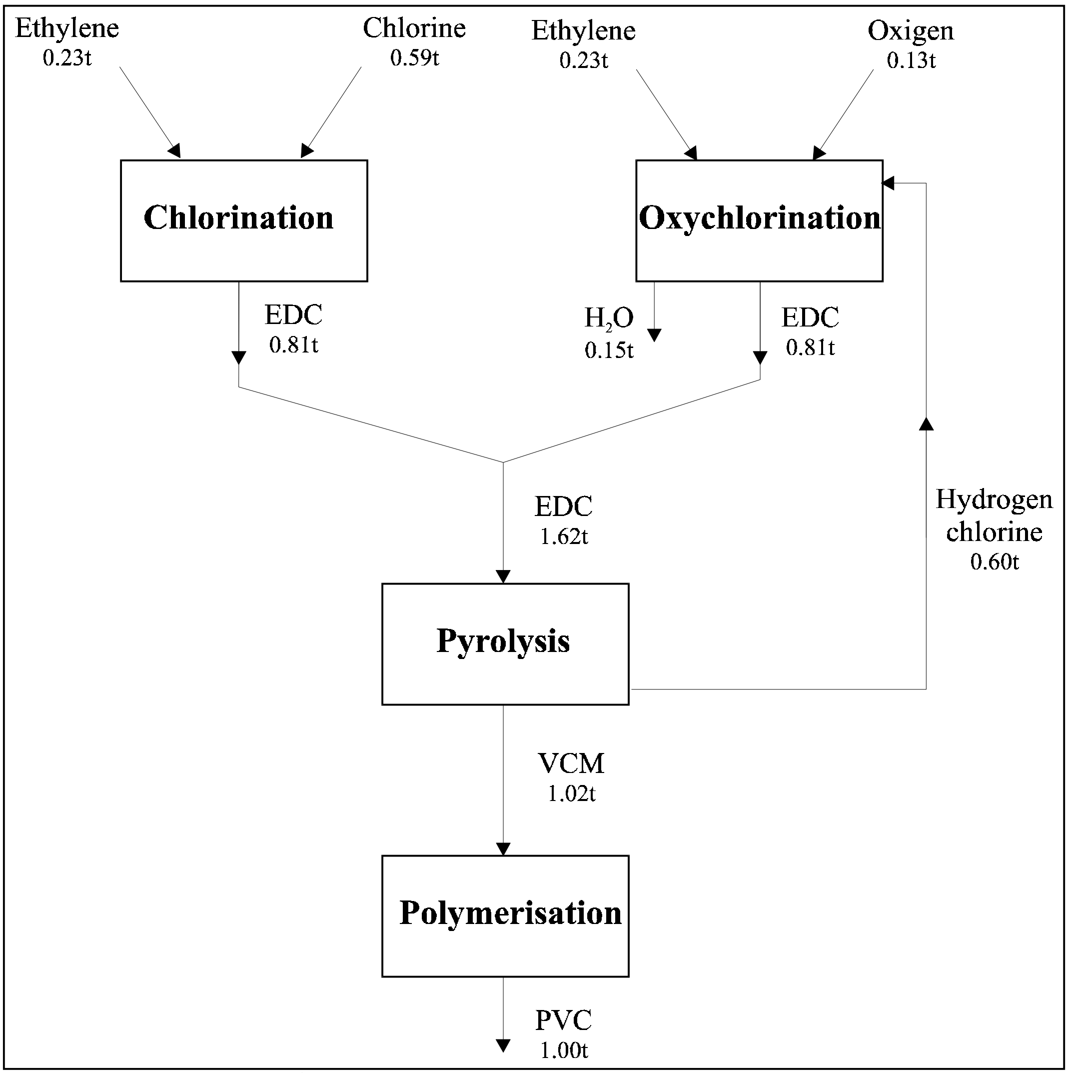


Figure 2 Process scheme of PVC production; 2% material losses in both VCM production and polymerisation

Table 35 Datasheet for MATTER: VCM production

MATTER Datasheet			
Process: **VCM production**			
		Year:	
	unit	**2000**	**2020**
Input:			
Ethylene	[t]	0.47	0.47
Chlorine	[t]	0.59	0.59
Oxygen	[t]	0.13	0.13
Gas	[GJ]	2.9	2.9
Electricity	[GJ_e]	0.9	0.9
Steam	[GJ]	2.3	2.3
Output:			
VCM	**[t]**	**1**	**1**
Costs:			
Investments	[ECU_{1994}/t VCM cap.]	294	294
Fixed	[ECU_{1994}/t VCM cap. year]	10	10
including labour	[ECU_{1994}/t VCM cap. year]	*5*	*5*
Variable	[ECU_{1994}/t VCM]	15	15
including labour	[ECU_{1994}/t VCM]	*2*	*2*
Lifetime	[year]	25	25
Availability factor	[-]	0.95	0.95
Residual capacity	[kton VCM / year]	5100	

Polymerisation

VCM in polymerised to PVC using a suspension, an emulsion, or a bulk process. In Germany, PVC polymerisation is divided between these three processes as: 76% / 13% / 11% respectively (Patel, 1996). For the world in total the division is: 70% / 20% / 10% (Rubin, 1990). It is obvious that the suspension process is the one most extensively used. Therefore we take it as representative.

Energy data on PVC polymerisation can be found in (HCP, 1997), (Patel, 1996) and (v. Heijningen *et al.*, 1992). Comparing the three different processes, it becomes obvious that the emulsion process requires considerably more energy (total final energy requirement: 8-10 GJ per ton PVC) than the suspension process (2.6-6.5 GJ per ton PVC), whereas the bulk process uses still less energy (1.2-2.3 GJ per ton PVC). The bulk process can, however, not be used to produce all PVC, because it leads to PVC with inferior properties (Rubin, 1992). The most recent data on the suspension process indicate a total final energy requirement of 3.0-3.1 GJ per ton PVC for newly built plants (HCP, 1997). Because it is not very likely that in 2000 all Western European plants make use of the newest technology, we use the somewhat older figure of 3.4 GJ as representative for the year 2000. In 2020. however, the new technology is assumed to have become common.

Costs data in the datasheet (Table 36) are estimated values based on information on ten plants built between 1989 and 1997. These estimates were made considering the composition of the plant capacity (suspension / emulsion / bulk polymerisation). Variable costs include costs of additives (estimated at 15 ECU_{1994} per ton PVC).

Table 36 Datasheet for MATTER: PVC polymerisation

MATTER Datasheet

Process: **PVC polymerisation**

		Year:	
	unit	**2000**	**2020**
Input:			
VCM	[t]	1.02	1.02
Electricity	[GJ_e]	0.7	0.7
Steam	[GJ]	2.7	2.4
Output:			
PVC	**[t]**	**1**	**1**
Costs:			
Investments	[ECU_{1994}/t PVC cap.]	555	555
Fixed	[ECU_{1994}/t PVC cap. year]	25	25
including labour	[ECU_{1994}/t PVC cap. year]	*14*	*14*
Variable	[ECU_{1994}/t PVC]	38	38
including labour	[ECU_{1994}/t PVC]	*10*	*10*
Lifetime	[year]	25	25
Availability factor	[-]	0.95	0.95
Residual capacity	[kton PVC / year]	5100	

2.2.5 Polyethylene Therephtalate (PET)

Western European PET consumption is rapidly growing. In 1994, 1971 kton PET were used, including 1171 kton for fibres. In 2000, Western European PET use in 2000 is forecasted at 3000 kton, of which 1500 for fibres. Table 37 shows the division of PET consumption between the products to be made (excluding fibres). With 88%, the use of PET for bottles forms its major application.

Table 37 Consumption of PET, division by applications (Anonymous, 1997)

Application	
Soft drink bottles	83%
Other bottles	5%
Films	5%
Ovenproof dishes	1%
Others	6%

PET polymers can be divided between amorphous and crystalline PET. Amorphous PET is suitable for films and fibres. For bottles crystalline PET is needed, which has better mechanical properties than amorphous PET. Crystalline PET is produced from amorphous PET by adding an extra polymerisation step. (Boustead, 1995). In this report we investigate the production of crystalline (‘bottle-grade’) PET, including this second polymerisation step.

There are two routes to produce Polyethylene Therephtalate (PET): the first route runs via therephtalic acid PTA), the other via dimethyl therephtalate (DMT). In Germany, the DMT route is used for 90% of PET production (Patel *et al.*, 1998). 65% of total Western European PET production runs via the DMT route (Chauvel *et al.*, 1992b). Therefore, we will analyse this route. The production process is rather complex. A process scheme is shown in Figure 3. For the polymerisation of PET, ethylene glycol and DMT are required. The production of ethylene glycol follows the following route: First ethylene is oxidised to ethylene oxide, which is subsequently hydrated to ethylene glycol. For the production of DMT the following route is followed: From the BTX fraction of e.g. a naphtha cracker, the C8 fraction is distilled and subsequently purified by extractive distillation. From the C_8 fraction *p*-xylene is separated via crystallisation (ARCO, modified). The residue, ‘mother liquor’ is converted by isomerisation (ARCO Octafining process) into *p*-xylene, *o*-xylene and some other products. *P-Xylene* is oxidised with methanol into DMT (Witten process). Finally, DMT and ethylene glycol are polymerised, via polycondensation, into PET. In this process, almost all methanol is recovered and recycled to the DMT production.

Energy data were calculated from data on the individual sub-processes (Chauvel *et al.*, 1989a,b), taking into account the respective mass flows needed to produce 1 ton of PET (see Figure 3). We do not, however, discuss all sub-processes separately. In Table 38 data is presented for the whole process together, starting from BTX, ethylene, oxygen and small amounts of hydrogen, water and methanol and ending with 1 ton of PET and a whole range of by-products. The product ‘others’ (Table 38) refers to the by-products of BTX distillation. CO_2 emissions refer to the process CO_2 emissions from the oxidation of ethylene (CO_2 emissions from fuels combustion are excluded). Total final process energy consumption for the whole process amounts to 31.0 GJ per ton PET. This value can be compared to values given by v. Heijningen *et al.* (1992b): 29.3 GJ per ton PET and Patel *et al.* (1998): 14.2 GJ per ton PET. The first value shows good agreement with our calculations, the second one is considerably lower. There are, however, two reasons for this. Firstly, Patel’s data do not include the production of *p*-xylene (10.5 GJ per ton PET). Secondly, Patel’s calculations are based on more recent data. We assume that our values are representative for the average Western European PET production in 2000. Data for the year 2020 is calculated from Patel's values, to which we added the energy required for *p*-xylene production (8.5 GJ per ton PET; 20% reduction compared to 2000 assumed).

Cost data for the whole process were calculated from cost data on the individual sub-processes (Chauvel *et al.*, 1989a,b). 40% of offsite costs are included in investments. Labour costs were calculated based on specifications of the number of operators per shift.

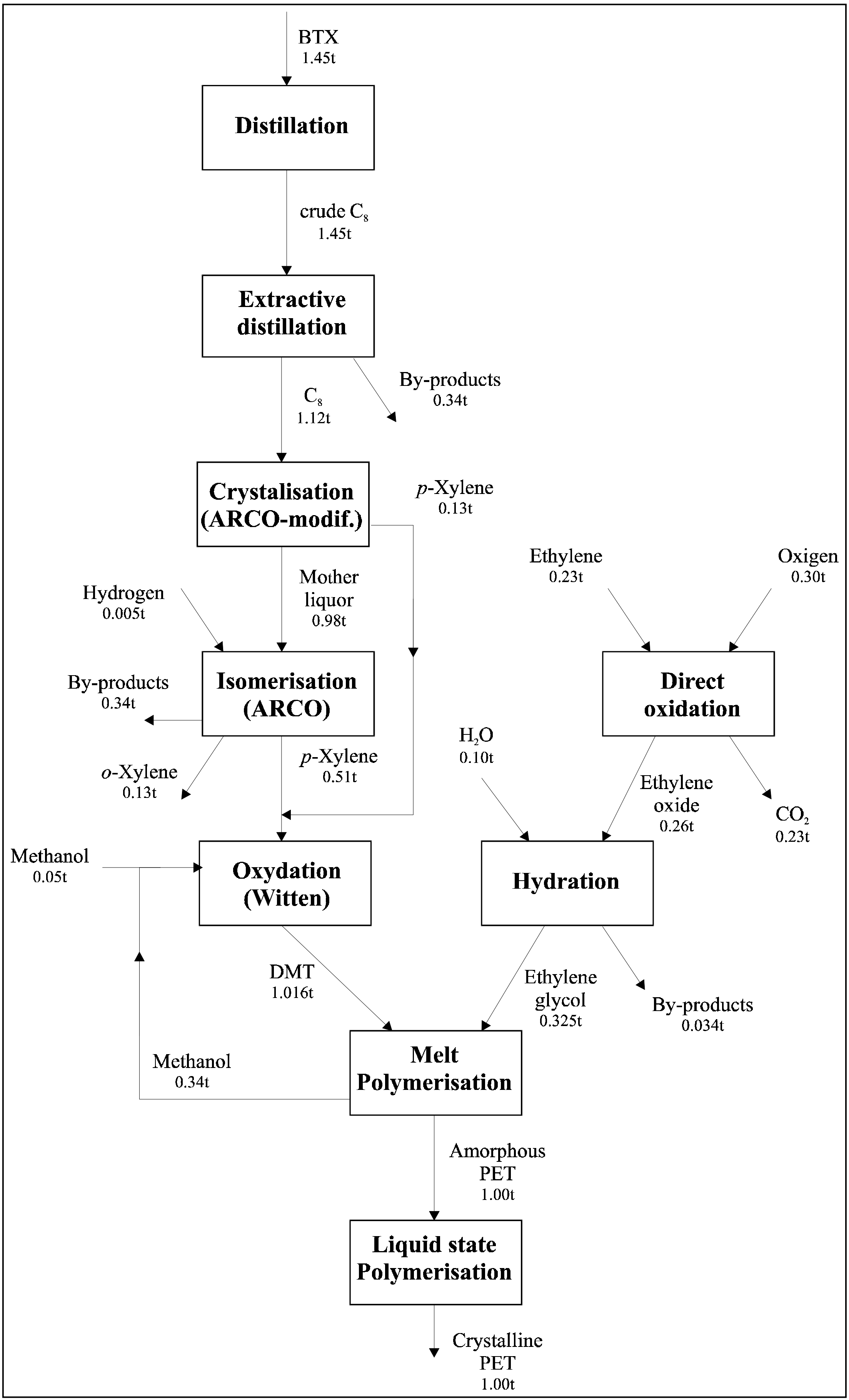


Figure 3 Process tree of PET production

Table 38 Datasheet for MATTER: Production of PET

MATTER Datasheet

Process: **PET production**

		Year:	
	unit	**2000**	**2020**
Input:			
BTX	[t]	1.45	1.45
Ethylene	[t]	0.23	0.23
H_2	[t]	0.005	0.01
Methanol	[t]	0.05	0.05
O_2	[t]	0.30	0.30
H_20	[t]	0.10	0.10
Steam	[GJ/t PET]	14.2	8.8
Electricity	[GJ_e/t PET]	3.3	2.3
Gas	[GJ/t PET]	3.1	5.4
Fuel	[GJ/t PET]	10.4	6.1
Output:			
PET	**[t]**	**1**	**1**
Di-ethylene glycol	[t]	0.033	0.033
Tri-ethylene glycol	[t]	0.002	0.002
o-Xylene	[t]	0.13	0.13
Mixed xylenes	[t]	0.20	0.20
Heavy aromatics	[t]	0.05	0.05
Light aromatics	[t]	0.03	0.03
Fuel gas	[t]	0.06	0.06
Others	[t]	0.34	0.34
CO_2	[t]	0.23	0.23
Costs:			
Investments	[ECU_{1994}/t PET cap]	2384	2384
Fixed	[ECU_{1994}/t PET cap. year]	95	95
Including labour	[ECU_{1994}/t PET cap. year]	*48*	*48*
Variable	[ECU_{1994}/t PET]	106	106
Including labour	[ECU_{1994}/t PET]	*71*	*71*
Miscellaneous:			
Lifetime	[year]	25	25
Availability factor	[-]	0.95	0.95
Residual capacity	[kton PET / year]	3000	

2.2.6 Other thermoplastics (ABS)

In MATTER the polymerisation of ‘other thermoplastics’ is modelled as ABS polymerisation (see paragraph 2.2). Western European Acrylonitril-Butadiene-Styrene consumption amounted to 550 kton (including SAN) in 1994 (APME, 1996) and is expected to grow to 620 kton in 2000 (Frohberg, 1996). Table 39 gives an overview of the applications of ABS.

Table 39 ABS consumption, divided by applications (Frohberg, 1996)

Branch	
Automotive	27%
Consumer electronics	37%
Computer	13%
Extrusion (incl. Refrigeration)	11%
Other	12%

Western European consumption of ‘other thermoplastics’ in 2000 is forecasted at 2800 kton (v. Duin, 1997). Because the datasheet (Table 40) represents the polymerisation of this whole group of plastics (for which the polymerisation of ABS is taken as a representative), residual capacity is increased from 620 kton to 2800 kton. ABS is often applied in combination to other polymers, as copolymer or as blend with for example SAN, PC, PVC *etc*. In this report we restrict ourselves to ABS homopolymers.

The production of ABS is rather complex compared to for example PE, PP or PS. The process scheme is shown in
Figure 4.

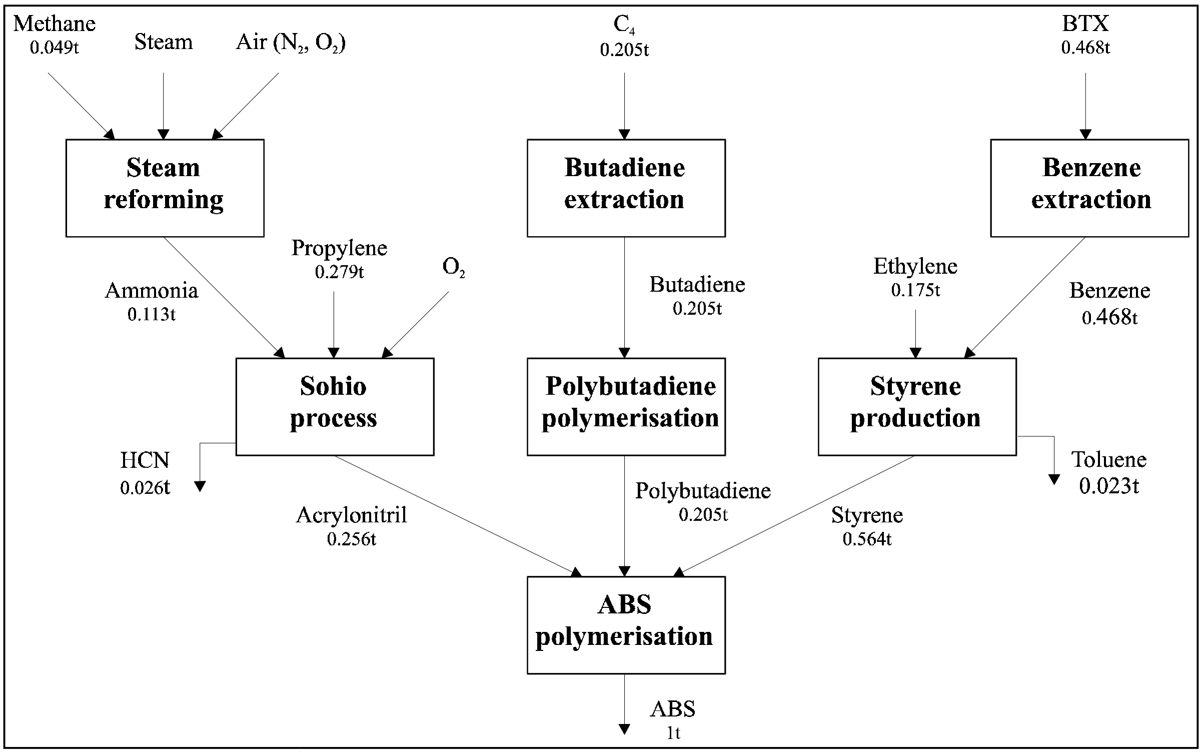


Figure 4 Process scheme of ABS production

Like the name also says, ABS is produced from acrylonitril, butadiene and styrene. ABS polymerisation can be carried out using a liquid phase, suspension or emulsion process.

Emulsion polymerisation is the world most applied process (v. Heijningen *et al.*, 1992b) and is therefore chosen as a representative. It consists of two steps: first butadiene is polymerised to polybutadiene, to which acrylonitril and styrene are added to form the ABS polymer. The shares of acrylonitril, butadiene and styrene can be varied within wide ranges. According v. Heijningen *et al.*, the composition: acrylonitril: 25%, butadiene: 20%, styrene: 55% can be seen as representative average composition. Therefore it is used in our analysis.

The production of ammonia is analysed in (Gielen, 1997) and is therefore not discussed here. Acrylonitril is produced from ammonia, propylene and oxygen using the Sohio process (which is used for 90% of the world ABS production capacity). The raw material for this process, ammonia is produced by steam reforming of natural gas. Butadiene is extracted (solvent extraction) from the C_4 fraction of steamcrackers[3]. Styrene is produced from ethylene and benzene, as is discussed in this report in the paragraph on polystyrene production.

We do not discuss each process separately. Instead, we produce data for the combination of processes to produce ABS. In total, for the production of 1 ton ABS, the combined processes use 0.564 ton styrene, 0.279 ton propylene, 0.113 ton ammonia and 0.205 ton C4 fraction, as well as certain amounts of steam and air. Apart from ABS, 0.026 ton HCN and 0.023 ton toluene are produced as by-products, as well as several negligible amounts of other chemicals.

Energy data were calculated from data on the individual processes (v. Heijningen *et al.*, 1992a, 1992b), (Chauvel *et al.*, 1992) and include acrylonitril production, butadiene extraction, butadiene polymerisation and ABS polymerisation. Benzene extraction, styrene production and ammonia production are not included.

The production of acrylonitril has a number of by-products that are not commercially exploitable. These offgasses and heavy fractions are commonly combusted to produce hp-steam, which can be used for other processes (v. Heijningen *et al.*, 1992b). We assume that the amount of steam produced from the acrylonitril process (2.5 ton per ton acrylonitril, corresponding to 0.65 ton per ton ABS) is approximately equal to the steam used in the polymerisation of ABS. Therefore the total process has no net steam production or consumption. From the combustion of the offgasses and heavy fractions from acrylonitril production CO_2 emissions arise, which are accounted for in MATTER.

Cost data were calculated from data on acrylonitril production and butadiene extraction (Chauvel *et al.*, 1992b) and estimates for ABS polymerisation costs (based on PS polymerisation). Chauvel's investment values were multiplied by 1.40 in order to include offsite costs.

---

[3] Only the part of the C_4 fraction that is converted to butadiene is indicated in **Figure 4**. After butadiene extraction a mixture of butane and butenes remains, which can be further processed to produce butane and butenes. Also energy data in this report only concerns energy for butadiene extraction, *excluding* energy required for further processing of the C_4 fraction.

Table 40 Datasheet for MATTER: polymerisation of 'other plastics' (based on ABS polymerisation)

MATTER Datasheet

Process: **Polymerisation of 'other thermoplastics' (ABS)**

	unit	Year: 2000	2020
Input[a]:			
Styrene	[t]	0.56	0.56
Propylene	[t]	0.28	0.28
C_4	[t]	0.21	0.21
Ammonia	[t]	0.11	0.11
Electricity	[GJ_e]	2.0	2.0
Fuel oil	[GJ]	0.5	0.5
Natural gas	[GJ]	0.4	0.4
Steam	[GJ]	1.2	1.2
Output:			
Products	**[t]**	**1.05**	**1.05**
ABS	[t]	1	1
HCN	[t]	0.03	0.03
Toluene	[t]	0.02	0.02
CO_2	[t]	0.11	0.1
Costs:			
Investments	[ECU_{1994}/t ABS cap.]	1202	1202
Fixed	[ECU_{1994}/t ABS cap. year]	48	48
including labour	[ECU_{1994}/t ABS cap. year]	*24*	*24*
Variable	[ECU_{1994}/t ABS]	52	52
including labour	[ECU_{1994}/t ABS]	*21*	*21*
Lifetime	[year]	25	25
Availability factor	[-]	0.95	0.95
Residual capacity	[kton ABS / year]	2800	

[a] Excluding air

2.2.7 Thermosets (PUR)

Western European consumption of thermosets in 2000 is forecasted at 5100 kton (v. Duin, 1997). In 1994 the consumption of thermosets amounted to 5127 kton. Consumption was divided between the different types of thermoset materials as shown in Table 41. It shows clearly that amino resins and polyurethanes are by far the most important thermosets. In this paragraph we discuss the production of polyurethane (PUR), which we take as representative for the whole group of thermosets.

Table 41 Consumption of thermosets in Western Europe, 1994; division between thermoset types [APME, 1996]

Thermoset type	
Amino resins	35%
Polyurethanes	34%
Phenol resins	12%
Unsaturated polyesters	9%
Alkyd resins	7%
Epoxy resins	5%

In 1995, PUR production in Western Europe amounted to 1895 kton (Anonymous, 1997b). There are four types of PUR: rigid foams, soft foams, elastomers and coatings. A rough estimate of the relative shares, with examples of products can be found in Table 42.

Table 42 Consumption of PUR, by type (Anonymous, 1996, 1997b)

PUR type		**examples of products**
Soft foams	40%	mattresses, furniture, automobile seats
Rigid foams	30%	insulation (building, refrigeration)
Elastomers	20%	bumpers, soles of shoes
Coatings and adhesives	10%	

The production process of PUR is rather complicated. The polymerisation of PUR is based on the polyaddition of polyether-polyols and diisocyanates. Two polyether-polyols are used in PUR production: one produced from ethylene oxide and one produced from propylene oxide. In Germany they make up 39% and 61% of PUR production respectively (Patel *et al.*, 1998). We assume that these percentages are also valid for Western Europe as a whole. Also two types of diisocyanates are used: tolylene diisocyanate (TDI) and diphenylmethane diisocyanate (MDI). The route via TDI (mainly to produce flexible foams) and the route via MDI (mainly to produce rigid foams) each make up about half of PUR production capacity (Patel *et al.*, 1998). In our calculations we used these shares to calculate the mean PUR production energy requirement and costs. Therefore, our values can be seen as representatives for the total Western European PUR production.

The production of TDI contains the following steps:

- Nitration of toluene with nitric acid to dinitrotoluenes
- Reduction of dinitrotoluenes to tolylene diamine (TDA)
- Phosgenation of tolylene diamine to tolylene diisocyanate (TDI)

The production of MDI also contains three steps:

- Nitration of benzene with nitric acid to nitrobenzene
- Reduction of nitrobenzene to aniline
- Phosgenation of aniline to diphenylmethane diisocyanate (MDI)

For each step a number of process variants is available. We do not, however, discuss each sub-process in detail, but present overall values concerning the whole process. Data in the datasheet (Table 43) concern the total PUR production process. Because the process consists of a large number of sub-processes, each with specific inputs, the list of inputs for the total process is also a relatively large one. We calculated the inputs and outputs based on data on the individual sub-processes from (Chauvel *et al.*, 1989b). Some of these sub-processes produce by-products, which are obviously not commercially interesting (Chauvel does not specify them). For this reason the totals of inputs and outputs in the datasheet are unequal. CO_2 emissions are caused by the oxidation of ethylene to ethylene oxide. Blowing agents used to produce PUR foam are not considered in this study.

If the energy requirement for the total process is calculated from the energy requirements of the individual sub-processes given by Chauvel, total final energy requirement amounts to 22.5 GJ per ton PUR. Patel *et al.* (1998) give a much lower value: 15.9 GJ per ton PUR. The main reason for this difference is the fact that the production of propylene oxide is not included fully in Patel's value. Propylene oxide production is a high energy consuming process. Direct oxidation of propylene is not commercially feasible. Therefore, in Western Europe, the chlorohydin process is used to produce 82% of propylene oxide (Weissermel *et al.*, 1994). In this process propylene oxide is produced from propylene, sodium chloride and water. It includes an electrolysis step, which is highly energy consuming. The chlorine produced in this step is needed in the process but finally ends up in the form of worthless salts. Calculations show that the production of propylene oxide uses 13.5 GJ[4] out of 22.5 GJ final energy per ton PUR produced. Chauvel's data concern plants built in 1986, which is a good average for the park of plants in 2000. In 2020 we expect that the mean overall energy requirement for PUR production will have decreased by 20%.

Cost data were obtained the same way as energy data. They were calculated from cost data on the individual sub-processes (Chauvel *et al.*, 1989b). 40% of offsite costs are included in investments. Labour costs were calculated based on specifications of the number of operators per shift.

Residual PUR production capacity in 2000 is expected to be about 2000 kton. However, because in MATTER PUR is used as representative for the whole group of thermosets, the residual capacity in the datasheet was increased to 5100 kton.

---

[4] The value of 13.5 GJ per ton PUR is based on 39% ethylene oxide, 61% propylene oxide and 50% TDI, 50% MDI. The TDI route uses more polyol (0.71 t / t PUR) than the MDI route 0.39 t / t PUR). If only propylene oxide is used, propylene oxide production uses 28.6 and 15.7 GJ per ton PUR for the TDI and MDI routes respectively. Ethylene oxide production, by direct oxidation, is much less energy consuming.

Table 43 Datasheet for MATTER: Polymerisation of thermosets (PUR)

MATTER Datasheet

Process: **Polymerisation of thermosets (PUR)**

	unit	**Year:** 2000	2020
Input:			
Ethylene	[t]	0.19	0.19
Propylene	[t]	0.30	0.30
Benzene	[t]	0.21	0.21
Nitric acid	[t]	0.31	0.31
Carbon monoxide	[t]	0.15	0.15
Toluene	[t]	0.10	0.10
Hydrogen	[t]	0.04	0.04
Oxygen	[t]	0.25	0.25
Formaldehyde	[t]	0.13	0.13
Chlorine	[t]	0.34	0.34
Sodium chloride (NaCl)	[t]	0.10	0.10
Electricity	[GJ_e]	9.1	7.3
Fuel	[GJ]	0.2	0.2
Steam	[GJ]	13.2	10.5
Output:			
PUR	**[t]**	**1**	**1**
Hydrochloric acid	[t]	0.32	0.32
CO_2	[t]	0.19	0.19
Costs:			
Investments	[ECU_{1994}/t PUR cap.]	2548	2548
Fixed	[ECU_{1994}/t PUR cap. year]	102	102
including labour	[ECU_{1994}/t PUR cap. year]	*51*	*51*
Variable	[ECU_{1994}/t PUR]	136	136
including labour	[ECU_{1994}/t PUR]	*97*	*97*
Lifetime	[year]	25	25
Availability factor	[-]	0.95	0.95
Residual capacity	[kton PUR / year]	5100	

2.2.8 Synthetic Rubbers (SBR)

Synthetic rubber consumption in Western Europe in 2000 is estimated at 2200 kton (v. Duin, 1997). We assume that total production equals total consumption (no net exports/imports streams of synthetic rubbers for Western Europe as a whole). So production of synthetic rubbers is also estimated at 2200 kton. From Table 44 Western European consumption of rubbers in 1994 can be read. With a share of 32%, Styrene Butadiene Rubber (SBR) is the most important synthetic rubber. Therefore we take SBR as a representative for the whole group of synthetic rubbers. SBR consumption in 2000 is forecasted at 764 kton. 71% of SBR is used to produce tires (IISRP, 1995).

Table 44 Western European rubber consumption (IISRP, 1995)

Rubber type	1994 consumption [kton]	Share of synthetic rubbers
Synthetic rubbers:		
SBR	693	32%
Carboxyl latex	570	26%
Polybutadiene	280	13%
EPDM	225	10%
Other synthetic rubbers	396	18%
Total	2164	100%
TPE's	299	
Natural rubber	900	
Total	3363	

SBR is produced from butadiene and styrene. According to v. Heijningen *et al.* (1992) it is produced from 75% butadiene and 25% styrene. Butadiene is extracted from the C4 fraction of steamcrackers. Styrene is produced from ethylene and benzene, as is described in this report in the paragraph on PS production. Either an emulsion or a solution polymerisation process is used. The consumption of solution SBR is growing much faster than the consumption of emulsion SBR (Anonymous, 1998).

All data in the datasheet (Table 45) refer to SBR polymerisation including butadiene extraction from C_4 fractions of steamcrackers. Styrene production is excluded. Data on styrene production can be read from Table 32. Energy data were calculated from energy data on butadiene extraction by Chauvel *et al.* (1989a) and an estimate of energy required for SBR polymerisation (based on PVC emulsion and suspension polymerisation processes).

Reliable cost data are not available. In (Hydrocarbon Processing, 1990/1991) investment costs are given for three recent SBR plants, varying from 1509 ECU_{94}/t to 2402 ECU_{94}/t. Probably these figures refer to processes including styrene production. We calculated much lower investment costs, based on cost data on butadiene extraction by Chauvel *et al.* (1989a) and an estimate of the investments for SBR polymerisation (based on investments for PVC emulsion and suspension polymerisation processes).

Table 45 Datasheet for MATTER: Production of synthetic rubbers (SBR)

MATTER datasheet

Process: **Production of Synthetic Rubbers (SBR)**
Styrene production: see PS

		Year:	
	unit	**2000**	**2020**
Input:			
C_4	[t]	0.75	0.75
Styrene	[t]	0.25	0.25
Electricity	[GJ_e]	1.9	1.9
Steam	[GJ]	8.3	8.3
Fuel	[GJ]	1.8	1.8
Output:			
SBR	**[t]**	**1**	**1**
Costs:			
Investments	[ECU_{1994}/t SBR cap.]	877	877
Fixed	[ECU_{1994}/t SBR cap. year]	40	40
including labour	[ECU_{1994}/t SBR cap. year]	*15*	*15*
Variable	[ECU_{1994}/t SBR]	67	67
including labour	[ECU_{1994}/t SBR]	*19*	*19*
Lifetime	[year]	25	25
Availability factor	[-]	0.95	0.95
Residual capacity	[kton SBR / year]	2200	

2.3 Plastics processing

Polymers are processed into plastic products using a variety of plastic processing processes. Table 46 specifies the main plastic processing processes together with their relative importance from a quantitative point of view. The plastic processing process used is strongly connected to the product to be produced. Processes can barely be exchanged to produce the same products. So improvements have to be searched for in improvements or modifications of the processes, rather than in substitution between processes.

Table 46 Western European plastic consumption 1994, by processing process [APME, 1995]

	Plastic consumption [kton]	Share
Film extrusion	6694	25%
Extrusion coating	638	2%
Sheets extrusion	283	1%
Thermoforming	1219	5%
Blow moulding	2456	9%
Injection moulding	4698	18%
Foaming	1980	8%
Tubes extrusion	2289	9%
Profiles extrusion	1090	4%
Cables extrusion	747	3%
Other processes	4162	16%
Total	26256	100%

In practice there are differences between the processing of the different plastic types (PE, PP, PVC, etc.). Processes are not equally suitable for processing individual plastic types. Energy requirement and costs may also differ between processing of the individual plastic types. In this report, however, no distinction is made between the processing of individual plastic types. So all data should be considered as averages for the group of plastic types that are currently being processed using the specific plastic processing process.

Energy data on plastic processing processes were published in (Novem, 1997). The 'standard values' in this publication concern the situation in The Netherlands[5]. 'Standard values' for the energy use of the individual processes can be found in Table 47. These are mean values for each plastic processing process. In practice energy use per ton product (and also costs per ton product) are highly depending on product shape and dimensions, plastic type and machine configuration. For example, electricity use for injection moulding varies between 3.2 and 7.2 GJ_e/ton product (Novem, 1997). For producing small products, more energy is needed (per ton) than for producing larger products. We use, however, the mean values.

---

[5] If the total electricity use in the plastics processing industry in The Netherlands is calculated using the electricity requirements in Table 47, reasonable correspondence is found with national statistics 938 million kWh (calculated) versus 996 million kWh (CBS, 1992), (Eijssen *et al.*, 1993).

Table 47 'Standard values' for energy use of plastic processing processes (Novem, 1997)

	Electricity [GJ_e/ton]	**Gas [GJ/ton]**
Film extrusion	1.9	
Extrusion coating	1.9	
Sheets extrusion	1.8	
Thermoforming	12.6	
Blow moulding	2.2	
Injection moulding	5.2	
Foaming	0.4	1.0
Tubes extrusion	1.4	
Profiles extrusion	1.4	
Cables extrusion	1.8	
Other processes[a]	3.7	0.1

[a] Mean value of the other processes in this table

Costs per kg. products vary considerably with product dimensions. For example: Investments for injection moulding of small products (23 gram) on a 1000 kN. machine are about 1000 ECU_{1994} per ton products (excluding offsite costs) (Tonino, 1996). Investments for injection moulding of larger products (300 gram) on a 4000 kN. machine are about 400 ECU_{1994} per ton products (excluding offsite costs) (Mulder, 1994). Other costs (fixed, variable) differ comparably. This example shows that it is very difficult to determine mean costs per process. As a first approach we use the mean value between injection moulding of small products and large products as mean value for plastic processing: 700 ECU_{1994} per ton products (*excluding* offsite costs) or 875 ECU_{1994} per ton products (*including* 25% offsite costs). Maintenance costs were calculated at 4% of investments (including 2% maintenance labour). Variable materials costs (except plastics) were calculated at 4% of investments. Because plastic processing is relatively labour intensive, we calculated operation labour costs at 10% of investments. Cost estimates can be read from Table 48.

Table 48 Estimated mean costs of plastic processing

	[ECU_{1994} / ton product]
Investments	875
Fixed costs	35
Including labour	*18*
Variable costs	123
Including labour	*88*

In general, energy efficiency improvement has not been cared for yet in the plastics processing industry. Energy costs only make up about 5% of costs (Mulder, 1994). Many plastic processors are not very interested in energy saving measures, which, though energy costs make up only a small part of costs per product, could save a considerable amount of energy if considered by the whole plastic industry. Therefore there is still a large energy efficiency improvement potential in this industry.

Energy savings can be achieved by a whole range of measures[6] (Novem, 1997), each of which apparently has relatively high energy efficiency improvement potentials (14 measures are described, with energy reductions of 10-50% each). Although these savings may be a little optimistic and not even possible for all plants and though combinations of measures may not

---

[6] Insulation of hot machine parts, improved process adjustment, reuse of waste heat, advanced operation of compressors, compressors with variable volume, all electric drive instead of hydraulics, catalytic gas heaters, good housekeeping, *etc*.

lead to an addition of the savings of the individual measures due to mutual influences, it is clear that large energy use reductions are possible.

In this report we do not discuss all possible options separately. Based on descriptions of energy improvement options in (Novem, 1997), (Mulder, 1994), (Van der Leest, 1996) and (Tonino, 1996), we estimate that a mean energy requirement reduction of 30-50% is relatively easy to achieve using (a combination of) the improvement options. Especially for injection moulding and thermoforming (which are currently the most energy consuming processes) interesting improvement options are available (all electric drive and catalytic gas heating respectively). Energy data for ‘enhanced’ processes can be read from Table 49. We estimate that energy efficiency improvement involves an increase of all costs by 30%.

According to the APME (1996) 1838 kton of plastic wastes were produced by Western European plastic processors. This is 7% of the plastics used in this industry. Therefore, 1.07 tons of plastics are needed to produce 1 ton of plastic products. The lifetime of plastic processing plants is estimated at 10 years.

Table 49 Energy use of ‘enhanced’ plastic processing processes

	Energy use reduction	**Electricity [GJ_e/ton]**	**Gas [GJ/ton]**
Film extrusion	30%	1.3	
Extrusion coating	30%	1.3	
Sheets extrusion	30%	1.3	
Thermoforming	50%	1.5	5.0
Blow moulding	30%	1.5	
Injection moulding	50%	2.6	
Foaming	30%	0.3	0.67
Tubes extrusion	30%	1.0	
Profiles extrusion	30%	1.0	
Cables extrusion	30%	1.3	
Other processes	30%	2.6	0.10

2.4 Plastic waste management

Two types of plastic waste are discerned: Firstly post-consumer waste, consisting of all plastic waste from discarding used products (by households and industries) and secondly industrial plastic waste, consisting of the waste arising from the production of plastic products. In 1994, 17505 kton of post consumer plastic waste were produced in Western Europe, as well as 1838 kton of industrial plastic waste from plastic processors (APME, 1996). The largest part (77%) of post consumer plastic waste was disposed of by landfilling. The shares of the other waste management processes: incineration with or without heat recovery, mechanical recycling and back-to-feedstock recycling can be read from Table 50. This table also shows an estimate of the shares of the plastic waste management processes in 2000, mainly based on extrapolation of the growth between 1990 and 1994. Almost all industrial plastic waste (95%) are currently being recycled mechanically (APME, 1996).

Table 50 Western European plastic waste management in 1990, 1994 (APME, 1992, 1996) and 2000 (estimate)

	1990 [kton]	**1994 [kton]**	**2000 [kton]**
Post-consumer plastic waste	**13594**	**17505**	**25000**
Landfilling	9878	13488	20250
Incineration without heat recovery	650	561	450
Incineration with heat recovery	2108	2348	2750
Mechanical recycling of post consumer plastic waste	958	1057	1200
Back To Feedstock recycling	0	51[c]	350
Industrial plastic waste[a]	**1200**	**1838**	**2100**
Mechanical recycling of industrial plastic waste[b]	1140	1746	2000

[a]APME estimates show a growth of ~7% p.a., whereas total plastic consumption grows with only 2.2% p.a. The latter percentage is used for the 2000 estimate; [b]95% of industrial plastic waste; [c]1995: 99 kton, 1996: 251 kton. Plastics injection in blast furnaces is included: 1994: 6 kton, 1995: 50 kton, 1996: 91 kton (Patel *et al.*, 1998).

Roughly speaking there are three types of plastic waste, depending on the condition of the material:

- Unmixed plastic waste (‘high quality’)
- Mixed plastic waste (‘medium quality’)
- Mixed plastic waste in municipal solid waste (‘low quality’)

Unmixed plastic waste consists of only one plastic type. Industrial plastic waste from the plastics processing industry mostly fulfils this condition: Relatively large amounts of waste of one plastic type arise from plastics processing. Another example is formed by multiple use packaging, which is returned to the producer, so as to be finally released in large, sorted quantities. Mixed plastic waste is, for example, obtained by separate collection of plastic packaging waste, like is done with the DSD system in Germany. The waste stream obtained this way contains all types of plastics intermingled. Although the waste stream contains some remnants of food and other dirt, it is far less contaminated as the third type: mixed plastic waste in household waste, which is obtained if no plastic stream is collected separately and which is mixed up with all kinds of other waste materials.

There are a number of plastic processing techniques, which make specific minimum demands on the quality of the plastic waste to be handled. These qualities roughly correspond to the three types of plastic waste discussed above.

Processes that are suited to plastic waste of all qualities are:

- Disposal (‘landfilling’)
- Incineration without heat recovery
- Incineration with heat recovery

Processes that require at least ‘medium quality’ plastic waste are:

- Plastic waste injection in blast furnaces: plastics serve as reducing agent
- Pyrolysis: heating without oxygen
- Gasification: heating in the presence of a controlled amount of oxygen
- Hydrogenation: gasification in the presence of hydrogen
- Selective dissolution

Processes that require at least ‘high quality’ plastic waste are:

- Mechanical recycling (‘re-extrusion’)
- Chemical recycling (methanolysis, glycolysis, hydrolysis *etc.* of polycondensation polymers (PET, PUR, PC, nylon))

‘Low quality’ plastic waste can be upgraded to ‘medium quality’ plastic waste by separating plastics from other waste components. Upgrading of ‘medium quality’ plastic waste to ‘high quality’ plastic waste is practically impossible, because of the huge range of intermingled plastic types and sub-types.

All plastic waste processing processes, except ‘disposal’ and ‘incineration without heat recovery’ aim at obtaining specific usable ‘products’ from the waste stream. These usable ‘products’ may be energy and / or mateials that can either be used to produce new plastic products or serve as feedstocks for the petrochemical industry.

2.4.1 Processes for processing mixed plastic waste in municipal solid waste

Plastic waste in municipal solid waste is heavily contaminated and intermingled with all kind of other waste materials. Material recycling is only possible after extensive sorting, which is generally not commercially feasible. Processes for processing mixed plastic waste in municipal solid waste make only use of (a part of) the *energy* content of the waste plastics, if they make use of anything at all. Processes for processing mixed plastic waste in municipal solid waste are described in another part of the MATTER project. We only give a short description of the processes and focus on the amount of energy that is released and CO_2 emissions involved. This is needed to calculate the share of the CO_2 emissions from plastic waste combustion in the total CO_2 emissions of the Western European plastics system (see paragraph 3). We assume that energy requirement for waste collection is negligible.

Disposal

Disposal (landfilling) is the easiest method to dispose of waste. However, no use is made of the energy and material content of the waste materials and large areas of land are needed during centuries for waste storage. Therefore, governments of a number of European countries (for example The Netherlands and Germany) combat waste disposal with legislative prohibition of disposal of waste that can be disposed of otherwise. Because the rate of decay of plastics is very low, no CO_2 emissions are involved in disposal.

Incineration without heat recovery

A part of the waste combustion installations in Europe does not make use of the energy that is released (see Table 50). CO_2 emissions from combustion depend on the plastic type that is incinerated. Table 51 gives an overview of the CO_2 factors of combustion of the different plastic types as calculated from the combustion reaction equations.

Table 51 CO_2 emission factors of plastics incineration

	CO_2 emission factor [t/t]
PE	3.14
PP	3.14
PS	3.38
PVC	1.42
PET	2.29
ABS	3.13
PUR	2.59
SBR	3.29
Mixed plastic waste[a]	*2.89*

[a] (Patel *et al.*, 1998)

Incineration with heat recovery

For incineration with heat recovery the same CO_2 emission factors are valid as for incineration without heat recovery (Table 51). The only difference is that the heat produced is (partially) transformed into electricity. According to Patel *et al* (1998), plastic waste has a mean lower heating value (LHV) of 38.2 GJ per ton. The energy efficiency of waste incineration plants is estimated at 22% in 2000, growing to 25% in 2030 (Gielen *et al.*, 1994). This means that per ton of plastic waste 8.4 GJ of electricity is produced, growing to 9.5 GJ in 2030. The remaining energy is released as heat that could, in principle, be made use of in industry. There are, however, a number of objections (NIMBY-syndrom, large CHP plants, see (Gielen *et al.*, 1994)), because of which energy delivery to industries is improbable. Therefore we do not consider the use of heat.

Upgrading to 'mixed plastic waste'

'Mixed plastic waste in municipal waste' can be upgraded to 'mixed plastic waste', using a series of sorting and separation processes. According to Patel *et al.* (1998), electricity use involved with these processes amounts to approximately 1.1 GJ_e per ton separated plastic waste. This figure refers to the German DSD, in which five plastic fractions are obtained, of which, however, a mixed fraction makes out the largest part (61%). Sas *et al.* (1994) calculate an electricity use of 0.4 GJ per ton plastic waste, as well as a natural gas use of 0.9 GJ per ton plastic waste. These figures are based on an experimental waste sorting installation of VAM. Sas *et al.* give an uncertainty margin of ±30%, caused by the experimental character of the installation. We assume an electricity use of 0.3 GJ per ton plastic waste and a natural gas use of 0.8 GJ per ton plastic waste. Gielen *et al.* (1994) estimate that the costs involved in plastics separation from municipal solid waste amount to 700 ECU_{1994} in 2000, decreasing to 250 ECU_{1994} in 2030. According to Sas *et al.* (1994) costs are expected to reach this low level much earlier: They estimate the costs around 2000 at 150-210 ECU_{1994} per ton plastic waste.

2.4.2 Processes for processing mixed plastic waste

Mixed plastic waste can be used for Back-To-Feedstock (BTF) recycling. With BTF processes mixed plastic waste is converted into feedstocks, which can be used in the petrochemical industry to produce new plastics or other petrochemical products. Four processes are currently available: plastic waste injection in blast furnaces, pyrolysis, gasification and hydrogenation. In the future also selective dissolution (a Back-To-Polymer (BTP) process) may play a role in mixed plastic waste processing.

Prior to these processes the plastic waste needs preparation. This treatment consist of grinding, separation of non-plastics, sieving, washing, drying and granulation, for which about 1.9 GJ electricity is needed per ton mixed plastic waste (Patel *et al.*, 1998). Furthermore, transportation to the recycling plant requires 0.17 GJ of fuel per ton mixed plastic waste (Patel *et al.*, 1998). These energy requirements are concerned for all processes for processing mixed plastic waste. Plastic waste preparation for recycling costs about 150 ECU_{1994} per ton mixed plastic waste (Dröscher, 1996).

Plastic waste injection in blast furnaces
From a recycling point of view, plastic waste injection is a rather peculiar process. It is injected in blast furnaces to serve as reduction agent for absorbing oxygen from iron ore to produce iron. Normally, heavy oil is used for this purpose. By injection of plastic waste, a part of the heavy oil is saved. At most 30% of heavy oil can be substituted 1:1 by plastic waste. This corresponds to 30 kg mixed plastic waste per ton crude iron (Patel *et al.*, 1998). It is disputable whether the process has to be regarded as material substitution or not. Because 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, we consider this process as material recycling. This is also the vision of the DSD in Germany, which allows plastic waste injection in blast furnaces by virtue of the process's material recycling properties. For the MATTER project we model plastic waste injection in blast furnaces as a dummy process that converts mixed plastic waste, without energy requirement and without costs, into heavy oil, that can subsequently be used as reduction agent in blast furnaces. This way we account for the substitution of heavy oil by mixed plastic waste. The maximum potential of the process is calculated as 3% of crude iron production in blast furnaces. (A description of the Western European metal industry can be found in (Daniëls *et al.,* 1998).

Pyrolysis
Pyrolysis consists of heating the plastic waste without the presence of oxygen in fluidised bed reactors. Kaminsky *et al.* have studied the process since the seventies in detail, at varying temperatures (600-800ºC), at varying waste compositions, with and without the presence of steam. In spite of a ceaseless flow of publications (Kaminsky *et al*., 1992, 1992b, 1995, 1995b, 1996, Kastner *et al.*, 1995, Simon *et al.*, 1996, Kim *et al.*, 1997), only a demonstration plant of 5 kton capacity has been built in Ebenhausen, Germany, which was closed in 1989 for insufficient cost-effectiveness. A 50 kton plant is planned to be built in Leuna, UK.

BASF follows another approach. The BASF pyrolysis process takes place at relatively low temperatures (400ºC). In 1994, a 15 kton pilot plant was built, with the intention to built a 300 kton plant, which would be capable of processing more than half of the German plastic packaging waste. However, because the DSD could not guarantee so large an amount of plastic waste to be delivered annually, the plant has never been built and the pilot plant was closed in 1996.

For the MATTER project we use data from (Patel *et al.*, 1998) on the BASF pyrolysis process, which seems to be the most cost-effective. Products are naphtha, BTX, pyrolysis gas and petcocks. The first two are considered as products, the latter two as fuels.

Gasification

Gasification is the heating of plastic waste to temperatures of 800-1300ºC in the presence of controlled amounts of steam and oxygen. This way plastic waste disintegrates into synthesis gas, which consists of carbon monoxide and hydrogen. Synthesis gas can be used to produce various hydrocarbons (Aurich, 1994) or hydrogen. Patel *et al.* (1998) have investigated gasification with joined methanol synthesis. For the MATTER project we prefer, however, the production of hydrogen. Table 52 shows the inputs and outputs of gasification with coupled hydrogen production from several plastic types (Gielen *et al.*, 1994), together with a calculation for mixed plastic waste, based on the European overall post user plastic waste composition in 1994 (APME, 1996). Hydrogen output as shown in this table is based on the assumption that, in the gasification step, plastic waste only reacts with oxygen (via partial oxidation). According to Patel *et al.* (1998), steam is also involved. The combination of the reactions with oxygen and steam leads to a higher hydrogen output. However, because the share of contribution of the reaction with steam and the effect on energy consumption are not clear, we do not take into account the use of steam.

Table 52 Inputs and outputs of plastic waste gasification with coupled hydrogen production (Gielen *et al.*, 1994); calculation for mixed plastic waste

			Polyolefins	PS	PVC	Other plastics	Mixed plastic waste
	MPW composition[a]		60%	9%	12%	19%	
IN:	Plastic waste	[t]	1	1	1	1	1
	Gas	[GJ/t]	3.8	2.6	1.7	2.9	3.3
	Electricity	[GJ_e/t]			0.7		0.08
	Na(OH)	[t/t]			0.65		0.08
OUT:	Hydrogen	[t/t]	0.29	0.22	0.1	0.17	0.24
	Electricity	[GJ_e/t]	0.3	0.1			0.19
	CO_2[b]	[t/t]	3.14	3.35	1.3	2.3	2.77

[a](APME, 1996); [b]Only process emissions (excluding emissions from fuels combustion)

Hydrogenation

Plastic waste can also be hydrogenated with hydrogen to form ‘syncrude’ that can serve as an alternative for naphtha in steamcracking, a gaseous fraction that can be used as fuel and a hydrogenation residue that can also be used as fuel (Saykowski *et al.*, 1994). The process is exploited by VEBA oil in a plant in Bottrop, which processed 80 kton plastic waste in 1996. In this plant, mixed plastic waste is hydrogenated together with the vacuum residue from crude oil distillation. Plastic waste has a share of about 25%.

The process consists of two steps: First mixed plastic waste is cracked into a heavy fraction (30%) and a light fraction (70%). The light fraction is processed in a hydrotreater into syncrude (synthetic crude oil: comparable to naphtha) and e-gas (energetic gas: comparable to natural gas). The heavy fraction is mixed with Vacuum Residue and led to a VCC. Here it is hydrogenated under high pressure (~300 bar), at a temperature of about 470ºC, into syncrude, e-gas and a hydrogenation residue, which is treated as fuel. Thus, the processing of mixed plastic waste and vacuum residue in the hydrogenation process are coupled. However, data in the datasheet only represents the energy use and costs needed for the processing of mixed plastic waste (the energy use and costs needed for the processing of vacuum residue are excluded).

Selective dissolution

Selective dissolution is based on the differences in solubility between different polymers. The process is developed in the Rensselaer Polytechnic Institute. Before the process can be applied, mixed plastic waste has to be ground, washed and dried. By subsequently bringing mixed plastic waste into contact with solvents of increasing temperatures (20-150ºC), polymers dissolve one by one. This way, PS, LDPE, HDPE, PP, PVC and PET are subsequently extracted from the mixture of plastics. As solvent xylene or tetrahudrofuran is used. The polymers are recovered from the solvents by ‘flash devolatilisation‘, in which most of the solvent is evaporated. The remaining solvent is removed during the extrusion step, from which the polymers arise as regranulate.

Zagouras *et al.* (1995) investigated the economic feasibility of a selective dissolution process that is slightly different. Their process subsequently uses different solvents (which do not need to be heated) to recover the different plastic types (hexane, acetone, methylethylketone). Polymers are recovered from the solution by adding it dropwise to a non-solvent like methanol. This way a suspension is obtained, which is filtrated to recover the polymer. The solvents are recycled. Energy requirement and costs are highly depending on the amount of solvents needed per ton mixed plastic waste and the percentage of solvents that is lost. Both parameters have to be investigated yet. Zagouras *et al.* (1995) estimate that 2200-6600 litres of solvents are needed per ton mixed plastic waste. They also estimate the percentage of solvents that are lost at 0.1-1%. They calculated energy requirement and costs both for 2200 litres per ton / 0.1% loss and 6600 litres per ton / 1% loss, as well as for an ‘intermediate case’ with values in between. We used this ‘intermediate case’ to obtain data for MATTER.

Table 53 summarises for MATTER the data on the processes for mixed plastic waste processing that are already available in 2000. Data on selective dissolution, which is expected to become available in 2010, can be read from Table 54.

Table 53 Datasheet for MATTER: Processing of mixed plastic waste, processes available in 2000

MATTER datasheet

Mixed plastic waste (MPW) processing

	unit	**Blast furnace Injection**[a]	**Pyrolysis**[b]	**Gasification**[c]	**Hydrogenation**[d]
Input:					
Mixed plastic waste	**[t]**	**1.00**	**1.00**	**1.00**	**1.00**
Hydrogen	[t]				0.011
Oxygen	[t]			1.05	
CaO	[t]		0.01		0.001
Na(OH)	[t]			0.08	
Preparation electricity[e]	[GJ$_e$]	1.9	1.9	1.9	1.9
Transportation fuel[e]	[GJ]	0.2	0.2	0.2	0.2
Electricity	[GJ$_e$]		0.4	0.08	0.96
Nat. Gas	[GJ]		3.9	3.3	4.6
Steam	[GJ]				0.11
Output:					
Naphtha	[t]		0.47		0.82
BTX	[t]		0.23		
Hydrogen	[t]			0.24	
Heavy oil	[GJ]	38.2[i]			
CO_2	[t]			2.77	
E-gas / pyrolysis gas	[GJ]		7.3		3.96
Hydrogenation residue	[GJ]				0.88
Petcocks	[GJ]		1.07		
Electricity	[GJ$_e$]			0.19	
Costs:					
Preparation costs[f]	[ECU$_{1994}$/t MPW]	150	150	150	150
Processing costs[g]	[ECU$_{1994}$/t MPW]	0	150	425	225
Lifetime	[year]	25	25	25	25
Availability factor	[-]	0.95	0.95	0.95	0.95
Maximum potential	[kton MPW/year]	[j]			
Residual capacity in 2000[h]	[kton MPW/year]	200	0	50	100

[a] Dummy process to model substitution of heavy oil by mixed plastic waste ;[b] Input-output data: (Patel *et al.*, 1998); [c] Input-output data (except transport and preparation): (Gielen *et al.*, 1994) / own calculations; [d] Input-output data (except transport and preparation): (Sas *et al.*, 1994), values only refer to part allocated to plastic waste processing (excluding processing of vacuum residue); [e] (Patel *et al.*, 1998); [f] (Dröscher, 1996); [g] (Gielen *et al.*, 1994), investments / fixed costs / variable costs not specified; [h] Estimate based on (Patel *et al.*, 1998) and Table 50; [i] To be used as reduction agent in blast furnaces; [j] 30 kg per ton crude iron production in blast furnaces

Table 54 Datasheet from MATTER: Selective dissolution of mixed plastic waste

MATTER datasheet **Selective dissolution of mixed plastic waste (MPW)**		
		Year
	Unit	**2010**
Input:		
Mixed plastic waste	**[t]**	**1.00**
Solvents[e]	[t]	0.04
Methanol	[t]	0.04
Preparation electricity[f]	[GJ_e]	1.9
Transportation fuel[f]	[GJ]	0.2
Electricity	[GJ_e]	[a]
Fuel	[GJ]	4.5
Output:		
Regranulate	[t]	0.62
RDF[d]	[GJ]	7.6
Costs:		
Preparation costs[g]	[ECU_{1994}/t MPW]	150
Investments	[ECU_{1994}/t MPW cap.]	[b]
Fixed	[ECU_{1994}/t MPW cap. year]	[c]
including labour	[ECU_{1994}/t MPW cap. year]	[c]
Variable	[ECU_{1994}/t MPW]	
including labour	[ECU_{1994}/t MPW]	*38*
Lifetime	[year]	25
Availability factor	[-]	0.95
Residual capacity	[kton MPW/year]	

[a]Electricity costs: 14-28 $ per ton MPW; [b]Capital costs: 14-28 $ per ton MPW; [c]Maintenance costs estimated at 4% of investments, including maintenance labour: 2% of investments; [d]Refuse derived fuel: 0.38 ton (paper, wood, plastics other than PE, PP PS and PVC), valued at 20 GJ/ton; [e]Division between the different solvents: acetone: 22 vol%, hexane: 60 vol%; methylethylketone: 18 vol%; [f](Patel *et al.*, 1998); [g](Dröscher, 1996)

2.4.3 Processes for processing unmixed plastic waste

Strictly speaking both mechanical recycling and chemical recycling belong in this category. With mechanical recycling polymers are recovered using only mechanical processes (grinding, extrusion). Chemical recycling uses chemicals to recover the building stones of polycondensation polymers (PUR, PET, PA). In Western Europe a range of different processes is used to recover building stones of polycondensation polymers from specific waste streams, using different chemicals and leading to different building stones. Therefore it is not easy to get an overview on chemical recycling. This, combined with the limited share of chemical recycling in total Western European plastics recycling, made us decide not to confine the analysis to mechanical recycling and not to investigate chemical recycling for the MATTER project

Mechanical recycling

Mechanical recycling of plastic waste is characterised as material reuse while keeping the polymers intact, while using only mechanical processes (grinding, extrusion). Regranulate quality is the main concern in mechanical recycling. However, material quality loss is inevitable. The more inhomogeneous the material is, the more severe is the material quality loss. Therefore, mechanical recycling of plastic waste to obtain (relatively) ‘high quality’ regranulate is only possible if the waste stream consists of one defined plastic type. This is the case with industrial plastic waste from plastic processing. Also separately collected products like deprecated used refillable packaging and building materials (window frames, PVC tubes *etc.*) are pure enough to obtain regranulate of acceptable quality. Regranulate from mechanical recycling of *mixed* plastic waste has very low quality and can only be used to produce thick products like roadside posts and heavy garden furniture, in which plastic waste mainly substitutes wood.

Mechanical recycling of HDPE bottles consists of the following steps (Sas *et al.*, 1994):

- Washing at 100ºC including removal of labels
- Visual inspection to remove strange bottles
- Ferro removal
- Grinding
- Washing
- Hydrocycloning
- Centrifuging
- Thermic drying
- Non-ferro removal
- Degassing
- Melting
- Extruding
- Granulation

Most of these steps are also needed in mechanical recycling of other products (LDPE film, PVC window frames). In the recycling of PET bottles, however, the last four steps are left out because of the limited heat resistance of PET.

According to Sas *et al.* approximately 90% of the input plastic waste can be processed into regranulate, the other 10% ends up as waste.

Sas *et al.* give the following energy requirements (virtually only electricity):

- LDPE film: 2.9 – 4.0 GJ_e per ton plastic waste input
- HDPE bottles: 2.7 – 3.1 GJ_e per ton plastic waste input
- PET bottles: 1.1 – 1.5 GJ_e per ton plastic waste input

According to Patel *et al.* (1998) energy requirement for mechanical recycling of PET bottles amounts to 5 GJ_e per ton plastic waste input. They also give values for the energy requirement of recycling of PVC window frames, floor covering and roofing: 1.3, 3.2 and 2.9 GJ_e per ton plastic waste input respectively. Based on this relatively wide range of values we estimate the mean electricity requirement for mechanical recycling in 2000 at 2.5 GJ_e per ton plastic waste input, decreasing to 2.0 GJ_e per ton plastic waste input in 2020.

These energy requirement figures include waste preparation, as can be seen from the list of process steps. Therefore, no additional energy requirement for preparation has to be added (like is the case for the processes for mixed plastic waste processing; see paragraph 2.4.2).

For cost estimates we rely on Sas *et al.* (1994) who made an economical survey of mechanical recycling of HDPE bottles. According to them, investments amount to 800-925 ECU_{1994} per ton plastic waste input capacity (we use the value of 850 ECU_{1994} per ton plastic waste input capacity). Labour costs amount to 46 ECU_{1994} per ton plastic waste input, whereas 35 ECU_{1994} per ton plastic waste input are needed for auxiliary materials. We estimate the costs for maintenance at 34 ECU_{1994} per ton plastic waste input capacity (4% of investments), including 17 ECU_{1994} per ton plastic waste input capacity maintenance labour (2% of investments).

Because of the serious material quality loss involved in mechanical recycling, only a limited part of plastic products can be produced from regranulate. We estimate that the use of regranulate for plastic products is limited at 20% of plastic products production.

Input data for MATTER are summarised in Table 55.

Table 55 Datasheet for MATTER: Mechanical recycling of unmixed plastic waste (UMPW)

MATTER Datasheet

Process: **Mechanical recycling of unmixed plastic waste (UMPW)**

		Year:	
	unit	**2000**	**2020**
Input:			
Unmixed plastic waste	**[t]**	**1.00**	**1.00**
Electricity	[GJ_e]	2.5	2.0
Output:			
Regranulate	[t]	0.9	0.9
Costs:			
Investments	[ECU_{1994}/t UMPW cap.]	850	850
Fixed	[ECU_{1994}/t UMPW cap. year]	34	34
including labour	[ECU_{1994}/t UMPW cap. year]	*17*	*17*
Variable	[ECU_{1994}/t UMPW]	81	81
including labour	[ECU_{1994}/t UMPW]	*46*	*46*
Miscellaneous:			
Lifetime	[year]	10	10
Availability factor	[-]	0.95	0.95
Maximum potential	[kton UMPW / year]		[a]
Residual capacity	[kton UMPW / year]	3200	

[a] 20% of plastic products production (= 20% of plastics processing)

2.5 Bitumen and lubricants

Bitumen

The main uses of bitumen, also called asphalt, are in the paving industry and for roofing. A number of different asphalt types can be discerned. In ancient times natural asphalt, to be found in lakes was used. Today, however, asphalt is derived from petroleum feedstocks. Asphalt yields from crude oil differ considerably. They range from 7% (Nigerian light crude oil) to 79% (Boscan crude oil) (Speight, 1996). We assume that in Western Europe mainly light crude oils are processed.

Asphalt for paving contains only 4-10% of bitumen, the rest is formed by ceramic materials (note that the word ‘asphalt’ is rather confusing because it is used both for pure bitumen and for paving asphalt, containing only a small amount of bitumen). We discuss the production of ‘pure’ bitumen (without ceramic material) for which we use the terms ‘bitumen’ and ‘asphalt’ alternately.

For paving usually straight-run asphalt is used (Speight, 1996). This is the residue of crude oil distillation. If in distillation heavy crude oils are used, with high asphalt content, only atmospheric distillation is needed. In that case atmospheric residue can be used as asphalt. If, however, lighter types of crude oil are used, the atmospheric residue contains a considerable amount of high boiling gas oil, which has to be removed in an additional vacuum distillation step. In that case the residue of this step, vacuum residue is used as asphalt.

For roofing propane-precipitated asphalt and blown asphalt are used (Speight, 1996). The first type is obtained from deasphalting of atmospheric residue (from heavy crude oils) or vacuum residue (from light crude oils). In this process, primarily used for lubricating oil base stocks (DAO) production (EPA, 1995), asphalt is recovered by solvent extraction. As solvent propane is often used, but also other solvents can be used. Blown asphalt is produced from vacuum residue with air by the asphalt blowing process. Figure 5 summarises the process routes to produce the different types of bitumen.

Petroleum lubricants

Petroleum lubricants contribute 98% of total lubricants production (Booser, 1996). Synthetic lubricants only account for 2% and are currently only used when special properties are needed, like extreme temperature stability, chemical inertness or fire resistance. Their use has, however, been growing rapidly during the last years.

Petroleum lubricants are produced from the vacuum residue (if light crude oils are used) or the atmospheric residue (if heavy crude oil is used) of crude oil distillation. This residue undergoes a series of treatments to make it suitable for high quality lubrication. First asphalt is removed by deasphalting (a solvent extraction process, see above). Subsequently aromatics are extracted (also via solvent extraction), waxes are removed (again via solvent extraction) and the product is finished (via hydrotreating) to remove unwanted chemically active compounds (Gary and Handwerk).

Synthetic lubricants

Although synthetic lubricants have been produced since 1929, major applications date from the last decades. Lots of different synthetic lubricants have been developed and are being developed. However, current production is mainly focussed on poly(α-olefins) (Booser, 1996). Relatively high prices (compared to petroleum lubricants) have inhibited the use of synthetic lubricants for other applications than ‘special purposes’.

Data for MATTER

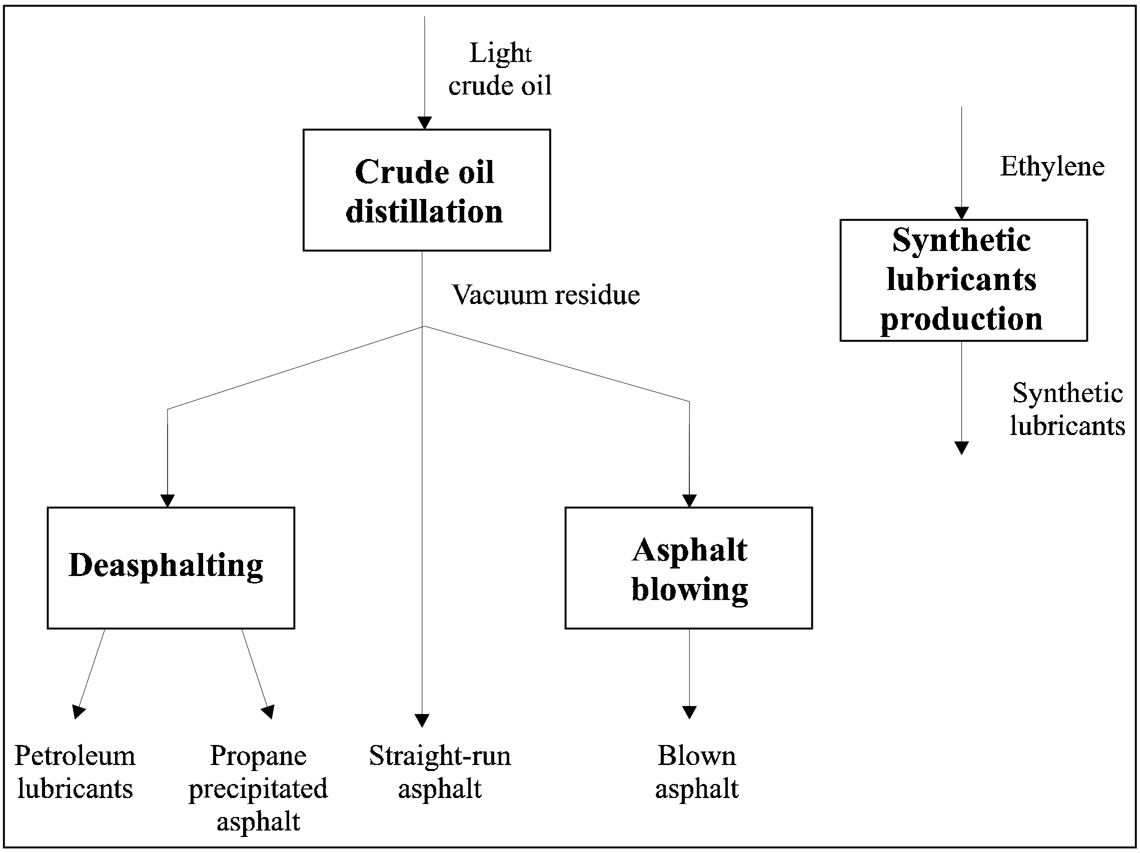
For MATTER four processes to produce bitumen and / or lubricants are of importance (see Figure 5):

- Integrated atmospheric and vacuum distillation of light crude oil to produce vacuum residue, which can be used as asphalt for paving or as feedstock for deasphalting and asphalt blowing
- Deasphalting of vacuum residue to produce petroleum lubricants and propane-precipitated asphalt for roofing
- Asphalt blowing to produce blown asphalt for roofing from vacuum residue
- Production of poly(α-olefins) from olefins

Within the framework of this study it was not possible to investigate all processes to produce lubricants in detail. Therefore, the production of petroleum lubricants was modelled only with the deasphalting process, disregarding the subsequent processes to enhance the quality of the lubricants.

Data for MATTER is summarised in the datasheet (Table 56).

Figure 5 Process tree of bitumen (asphalt) and lubricants production, as modelled for MATTER



Data on crude oil distillation were derived from a description of a Foster Weeler Crude Distillation Unit (HCPR, 1996). Product yields are highly dependent on the crude oil used. We allocated energy requirement and costs to the different products of distillation based on weight distribution. This means that costs and energy requirement per ton are equal for all distillation products. Therefore it is possible to consider only the part of crude oil which is processed into vacuum residue. Maintenance costs were calculated at 4% of investments, including 2% maintenance labour. Operation labour was estimated based on two operators per shift and large throughputs (>1000 kton p.a.).

Investment and energy data on deasphalting were derived from descriptions of four different deasphalting plants (HCPR, 1990, 1996). Mean values were chosen as representatives. Product yields were derived from Van Oostvoorn *et al.* (1989). Product yields depend on the type of crude oil from which the vacuum residue originates. Values in the datasheet (Table 56) refer to light crude oils. Maintenance costs were calculated at 4% of investments, including 2% maintenance labour. Operation labour was estimated based on two operators per shift and large throughputs (1000-1600 kton p.a.).

Data on the asphalt blowing process come from a description of the Snamprogetti process (HCPR, 1990). Investment data are not available. Hence maintenance costs could not be calculated. Operation labour was estimated based on two operators per shift.

Data on the production of poly(α-olefins) is not available. We treated the production of synthetic lubricants as equivalent to polyethylene polymerisation. We assume that the production of synthetic lubricants can be compared to the polyethylene suspension / solution process. Further details on this process can be found in the paragraph on polyethylene production.

Table 56 Datasheet for MATTER: Bitumen and lubricants production

MATTER datasheet

Production of bitumen and lubricants

	unit	**Crude distillation**	**Deasphalting**	**Asphalt blowing**	**synthetic lubricants**
Input:					
Crude oil	[t]	1.0			
Vacuum residue	[t]		**1.0**	1.0	
Ethylene	[t]				1.0
Propylene	[kg]		0.3		
Electricity	[GJ_e]	0.1	0.1	0.1	1.7
Fuel oil	[GJ]	0.75	0.70	0.26	
Steam	[GJ]	0.2	0.37	0.05	1.9
Output:					
Vacuum residue (straight-run asphalt)	[t]	**1.0**			
Petroleum lubricants	[t]		0.47		
Propane-precipitated asphalt (bitumen)	[t]		0.34		
Vacuum gas oil	[t]		0.19		
Blown asphalt (bitumen)	[t]			**1.0**	
Synthetic lubricants	[t]				**1.0**
Investments	[ECU_{1994}/t cap.]	15	26	-	740
Fixed	[ECU_{1994}/t cap. year]	0.6	1.1	-	42
including labour	[ECU_{1994}/t cap. year]	*0.3*	*0.5*	-	*21*
Variable	[ECU_{1994}/t]	1	1	1	43
including labour	[ECU_{1994}/t]	*1*	*1*	*1*	*14*
Lifetime	[year]	25	25	25	25
Availability factor	[-]	0.95	0.95	0.95	0.95
Residual capacity 2000	[kton/year]	-	-	-	-

3. CO_2 EMISSIONS FROM THE WESTERN EUROPEAN SYNTHETIC ORGANICS INDUSTRY

Table 57 shows the relative importance of the processes analysed in this report[7] from a CO_2 emission point of view. CO_2 emissions in this table were calculated using the CO_2 emission factors from Appendix A (Table 59). According to Gielen (1997), total annual Western European CO_2 emissions amount to approximately 3500 Mt. Total CO_2 emissions from the processes analysed in this report amount to 70.0 Mt, which is 2.0% of total CO_2 emissions.

Table 57 shows that 49.5% of CO_2 emissions arise from the production of polymers (including the production of intermediates like styrene and VCM), whereas the production of monomers, plastics processing and plastic waste removal contribute 24.1, 11.9 and 14.5% respectively. Especially the production of PUR and PET make a large contribution (15.1 and 10.7% respectively). Although these are relatively complicated and much energy requiring processes, in interpreting these figures one has to bear in mind that we took PUR as a representative for the category of ‘other thermoplastics’. The production of other thermoplastics might be less energy consuming and therefore, actual CO_2 emissions from thermoplastics production might be lower.

Plastic waste management covers a relatively limited part of CO_2 emissions (10.2%). This is caused by the high share of waste disposal, which involves no CO_2 emissions. In the future, the share of CO_2 emissions from plastic waste management is expected to rise, caused by the trend to replace waste disposal by waste incineration or recycling processes. Especially incineration and gasification show high CO_2 emission factors. However, CO_2 emission factors of plastic waste processing processes can not be used straightforwardly as indicators for ‘greenhouse-contribution’, because products from a number of plastic waste processing processes decrease the amount of products to be produced with ‘conventional’ processes. For example, gasification with combined hydrogen production has a high CO_2 emission factor (3.17 t/t). However, the hydrogen that is produced should otherwise be produced with other processes, which would cause CO_2 emissions as well. This effect has to be accounted for when comparing different plastic waste processing options. Actually, that is one of the aims of the MATTER model, in which the data from this report is intended to be used. The results of the MATTER model must provide a more definite basis for comparing alternative processes with respect to CO_2 emissions.

---

[7] Excluding the production of lubricants and bitumen

Table 57 Overall energy and CO$_2$ balance of synthetic organic materials processes considered in this report, base year 2000; excluding the production of lubricants and bitumen

	Capacity	Electr.[k]	Gas	Oil	Steam[k]	Process CO$_2$	Total CO$_2$	Total CO$_2$	Share
	[kton p.a.]	[GJ$_e$/t]	[GJ/t]	[GJ/t]	[GJ/t]	[t/t]	[t/t]	[Mt p.a.]	[%]
Monomers production:									
Naphtha steamcracking[a]	10716[g]	0.29				1.15	1.18	12.6	18.0
Gas oil steamcracking[a]	1864[g]	0.36				1.15	1.19	2.2	3.2
LPG steamcracking[a]	1708[g]	0.29				0.95	0.98	1.7	2.4
Ethane steamcracking[a]	1242[g]	0.11		0.56		0.25	0.30	0.4	0.5
Oxidative Coupling[a,i]	0[g]	0.20				0.37	0.39	0	0
Methanol to Olefins[a]	0[g]	0.28		2.77	1.14	0.59	0.90	0	0
Biomass pyrolysis[a]	0[g]	0.73		52.5[h]		0.12	0.20	0	0
Total	**15530[g]**							**16.9**	**24.1**
Polymers production[l]:									
LDPE liquid phase polymerisation	4600	3.10					0.31	1.4	2.0
LLDPE gas phase polymerisation	1050	2.00			0.30		0.22	0.2	0.3
LLDPE solution / suspension polymerisation	700	1.70			1.60		0.28	0.2	0.3
HDPE gas phase polymerisation	400	2.00			0.30		0.22	0.1	0.1
HDPE solution / suspension polymerisation	3750	1.70			1.95		0.31	1.1	1.6
PP liquid phase polymerisation	2333	2.10			1.20		0.29	0.7	1.0
PP gas phase polymerisation	2333	2.10			0.80		0.27	0.6	0.9
PP suspension polymerisation	2333	2.10			1.80		0.34	0.8	1.1
PS polymerisation[b]	2900	1.04		6.03	8.17		1.12	3.2	4.6
PVC polymerisation[c]	5100	1.64	2.96		5.02		0.68	3.5	5.0
PET production[a,i]	3000	3.29	3.15	10.41	14.18	0.23	2.49	7.5	10.7
Other thermoplastics production[d]	2800	2.22	0.41	3.71	2.51	0.11	0.80	2.2	3.2
Thermosets production [a,e,i]	5100	9.12		0.43	13.52	0.19	2.08	10.6	15.1
Synthetic rubbers production[f]	2200	2.03		3.21	9.97		1.13	2.5	3.6
Total	**38599**							**34.7**	**49.5**
Plastic processing:									
Film extrusion	6694	1.89					0.19	1.3	1.8
Extrusion coating	638	1.89					0.19	0.1	0.2
Sheets extrusion	283	1.80					0.18	0.1	0.1
Thermoforming	1219	12.60					1.26	1.5	2.2
Blow moulding	2456	2.16					0.22	0.5	0.8
Injection moulding	4698	5.22					0.52	2.5	3.5
Foaming	1980	0.36	0.96				0.09	0.2	0.3
Tubes extrusion	2289	1.44					0.14	0.3	0.5
Profiles extrusion	1090	1.44					0.14	0.2	0.2
Cables extrusion	747	1.80					0.18	0.1	0.2
Other plastic processing processes	4162	3.65	0.14				0.37	1.6	2.2
Total	**26256**							**8.3**	**11.9**
Plastic waste management:									
Disposal	20250						0	0	0
Incineration without heat recovery	450					2.85	2.85	1.3	1.8
Incineration with heat recovery	2750					2.85	2.85	7.8	11.2
Mechanical recycling	3200	2.50					0.25	0.8	1.1
Blast furnace injection	200	1.90		0.20			0.20	0.04	0.1
Pyrolysis	0	2.30	3.90	0.20			0.46	0	0
Gasification / hydrogen production[i]	50	1.98	3.26	0.20		2.77	3.17	0.2	0.2
Hydrogenation	100	2.86	4.63	0.20	0.11		0.57	0.06	0.1
Total	**27000**							**10.2**	**14.5**
Grand total								**70.0**	**100**

[a]Including coproducts; [b]Including benzene and styrene production; [c]Including VCM production, excluding chlorine production; [d]ABS production including benzene and styrene production, excluding ammonia production; [e]PUR production including benzene production, excluding nitric acid, CO, chlorine and NaCl production; [f]SBR production including benzene and styrene production; [g]Ethylene capacity; [h]Biomass combustion: CO$_2$ emissions not accounted for; [i]Excluding oxygen production; [k]Steam and electricity production from the processes are not accounted for; [l]Many of the polymers production processes include the production of intermediates (styrene, VCM *etc.*). See the paragraph 2.2

4. REFERENCES

Anonymous, *Ontwikkelingen in polyurethaan*, Kunststof en Rubber, June 1996, pp.11-13

Anonymous, *Thermoplastische polyesters PET en PEN*, Kunststof en rubber, September 1997, pp. 15-20

Anonymous, *Kunststof top 4; op de derde plaats: PVC*, Kunststoffen en Rubber, June 1997

Anonymous, *PUR in Europa*, Kunststof en Rubber, February 1997(b), p. 41

Anonymous, *Verbruik synthetische rubber*, Kunststof en Rubber, February 1998, p.13

Amenomiya, Y, Birss, V.I., *et al.*, *Conversion of Methane by Oxidative Coupling*, Catal.Rev.-Sci.Eng. 32(3), 1990

APME: *Information system on plastic waste management in Western Europe; 1994 Data*, APME, Brussels, Belgium, 1996.

Aubrey, D.C., *Feedstocks (Petrochemicals)*, in: Kirk-Othmer Encyclopedia of Chemical Technology, fourth edition, Wiley, New York, 1996

Aurich, H.P., *Pyrolyse, Hydrierung, Gaserzeugung*, KGK Kautschuk-Gummi Kunststoffe 47, 1994 (8), pp. 596-601

Avidan, A.A., Krambeck, F.J., Owen, H., Schipper, P.H., *FCC closed-cyclone system eliminates post-riser cracking*, Oil & Gas Journal, March 26, 1990, pp. 56-60

Beer, G., *Polypropylen (PP)*, Kunststoffe 86 (10), 1996, pp.1460-1463

Booser, E.R., *Lubrication and lubricants*, in: Kirk-Omer Encyclopedia of Chemical Technology, fourth edition, Wiley, New York, 1996

Boustead, I., *Eco-profiles of the European plastics industry, Report 4: Polystyrene*, PWMI, Brussels, 1993

Boustead, I., *Eco-profiles of the European plastics industry, report 8: Polyethylene Therephtalate (PET)*, APME, Brussels, Belgium, 1995

BUWAL, *Ökoinventare für Verpackungen, Band 1.* Bundesamt für Umwelt, Wald und Landschaft, Bern, 1996

CBS, *Productiestatistiek kunststofverwerkende industrie 1992*, Statistics Netherlands, Voorburg, The Netherlands

CBS: *Statistisch jaarboek* (in Dutch), Statistics Netherlands, Voorburg / Heerlen, The Netherlands, 1990, 1992, 1996.

Chauvel, A. and Lefebvre, G: *Petrochemical processes, vol. 1: Synthesis-gas derivatives and major hydrocarbons*; *vol. 2: Major oxygenated, chlorinated and nitrated derivatives*, Editions Technip, Paris, 1989.

Chemfacts: *Ethylene and Propylene,* Chemical Intelligence Services, London, 1991.

Chen, J., Thomas, J.M., *MAPO-18 (M=Mg, Zn, Co): a new family of catalysts for the conversion of methanol to light olefins*, J.Chem.Soc., Chem.Commun., 1994, pp. 603-604

Cordi, E.M., Pak, S., Rosynek, M.P., Lunsford, J.H., *Steady-state production of olefins in heigh yields during the oxidative coupling of methane: Utilization of a membrane contractor,* Applied Catalysis A: General 155 (1997), L1-L7

Daniëls, B.W., Moll, H.C., *The base metal industry; Technological descriptions of processes and production routes, status quo and prospects,* IVEM, Groningen University, Groningen, The Netherlands, 1998

Dröscher, M., *Recovery of used plastics in Germany: ecological and economical aspects,* Polymer Recycling 2, 1996 (1), pp. 43-48

Duin, R. v., *From production till end use of materials and products; a 2000-forecast for Western Europe*, Bureau B&G, Emst, The Netherlands, 1997.

Eijssen, P.H.M., Duesmann, H.B., Poel, P. v.d., Koot, J.E., *SPIN kunststofverwerkende industrie* (in Dutch), RIVM, Bilthoven, The Netherlands, 1993

EPA, *Petroleum Refining*, EPA Industry Sector Notebook Project, Washington, September 1995

EPA, *Profile of the Plastic Resin and Manmade Fiber Industries,* EPA Office of Compliance Sector Notebook Project, Washington, September 1997

ECN, *Ready to perform when the price is right*, European Chemical News, April 1997, pp. 16-17

EPN, *New generation polyolefins face bright future*, European Plastics News, March 1996, p. 16

Ferstl, J., Hildebrandt, U., *Ausbeute und Wirtschaftlichkeit der oxidativen Methankopplung,* Linde Berichte aus Technik und Wissenschaft 71. 1994

Frohberg, E., *Acrylonitril-Butadien-Styrol-Copolymerisation (ABS)*, Kunststoffe 86 (10), 1996, pp. 1498-1500

F&S, *Europe's recycling trends in detail,* Frost & Sullivan, European Plastics News, June 1994, p. 17

Gary, J.H., Handwerk, G.E., *Petroleum Refining; Technology and Economics*, Third edition, Marcel Dekker, New York, 19??

Geem, P.C. v.: *Nieuwe routes naar etheen* (in Dutch), in: *Proces Technologie,* april 1992.

Geerts, J.W.M.H., Hoebink, J.H.B.J., Wiele, K. van der, *Ethylene from natural gas: proven and new technologies,* in: Albright, L.F., Crynes, B.L., Nowak, S., *Novel production methods for ethylene, light hydrocarbons and aromatics*, Marcel Dekker, New York, 1992

Gielen, D., Okken, P., *Optimisation of integrated energy and materials systems; Compilation of materials processes,* ECN, Petten, The Netherlands, 1994

Gielen, D.J., Vos, D., van Dril, A.W.N., *The petrochemical industry and its energy use*, ECN, Petten, The Netherlands, 1996.

Gielen, D.J., *Technology characterisation for ceramic and inorganic materials; Input data for Western European MARKAL*, ECN, Petten, The Netherlands, 1997

Hatzmann, G., Jagdmann, S., Klimesch, R.G., *Polyethylen niedriger Dichte (PE-LD, PE-LLD),* Kunststoffe 86 (10), 1996, pp. 1447-1453

HCP, *Petrochemical Processes,* Hydrocarbon processing, diverse years

HCPBC, *HPI Construction Boxcore,* Hydrocarbon processing, diverse years

HCPR, *Refining,* Hydrocarbon Processing, diverse years

Heijningen, R.J.J. v., Castro, J.F.M. de, Worrell, E: *Energiekentallen in relatie tot preventie en hergebruik van afvalstromen* (in Dutch), Utrecht University, department of Science, Technology and Society, Utrecht, 1992a.

Heijningen, R.J.J., Castro, de, J.F.M., Worrell, E., Hazewinkel, J.H.O.: *Meer energiekentallen in relatie tot preventie en hergebruik van afvalstromen*, department of Science, Technology and Society, Utrecht, 1992b.

IISRP, *Verbruik synthetische rubber 1994-1999,* Kunststof en Rubber, May 1995, pp. 44-45

Kaddouri, R., Kieffer, R., Kiennemann, A., *Oxidative Coupling of Methane over* $LnLiO_2$ *Compounds (Ln=Sm,Nd,La),* Applied Catalysis 51. 1989, L1-L6

Kaminsky, W., *Possibilities and limits of pyrolysis*, Macromol. Chem., Macromol. Symp. 57, 1992, pp. 145-160

Kaminsky, W., Rössler, H., *Olefins from wastes*, Chemtech, February 1992b, pp. 108-113

Kaminsky, W., Schlesselmann, B., Simon, C., *Olefins from polyolefins and mixed plastics by pyrolysis*, Journal of Analytical and Applied Pyrolysis, 32, 1995, pp. 19-27

Kaminsky, W., *Pyrolysis with respect to recovering of polymer,* Angewandte Makromolekulare Chemie 232, 1995b, pp. 151-165

Kaminsky, W., Schlesselmann, B., Simon, C.M., *Thermal degradation of mixed plastic waste to aromatics and gas,* Polymer Degradation and Stability 53, 1996, pp. 189-197

Kaps, R., Lecht, R., Schulte, U., *Polyethylene hoher Dichte (PE-HD)*, Kunststoffe 86 (10), 1996, pp. 1454-1458

Kastner, H. Kaminsky, W., *Recycle plastics into feedstocks*, Hydrocarbon Processing, May 1995, pp. 109-112

Kim, J.S., Kaminsky, W., Schlesselmann, B., *Pyrolysis of a fraction of mixed plastic wastes depleted in PVC*, Journal of Analytical and Applied Pyrolysis 40-41, 1997, pp. 365-372

Leest, M. van der, Heijboer, P., *Optimalisatie van de energiestromen bij verwerking van kunststoffen*, Kunststof en Rubber, September 1996, pp. 47-49

Lu, Y., Dixon, A.G., Moser, W.R., Ma, Y.H., *Analysis and Optimization of Cross-Flow Reactors for Oxidative Coupling of Methane*, Ind.Eng.Chem.Res. 36. 1997, p. 559-567

Miguel, M.P., Coronas, J., Menendez, M., Santamaria, J., *Methane oxidative coupling over different alkali-doped catalysts: a comparison of ceramic membrane reactors and conventional fixed bed reactors*, React.Kinet.Catal.Lett., 59(2), 1996, p. 277-284

Mulder, S., *Energiebesparing spuitgietmachines*, Kunststof en Rubber, September 1994, pp.20-22

Netzer, D., *Economically recover olefins from FCC offgases*, Hydrocarbon Processing, April 1997, pp. 83-91

Novem, *Factsheets energy-efficiency: Kunststofverwerkende Industrie*, Novem, Utrecht, The Netherlands, 1997

Oostvoorn, F.v., Kroon, P., Lange, A.V.M. de, *SERUM: een model van de Nederlandse raffinage-industrie*, ECN, Petten, The Netherlands, 1989

Parkyns, N.D., Warburton, C.I., Wilson, J.D., *Natural gas conversion to liquid fuels and chemicals: Where does it stand?*, Catalysis Today, 18. 1993, p. 385-442

Patel, M., Fraunhofer Institut für Systemtechnik und Innovationsforschung, Karlsruhe, unpublished internal report, 1996

Patel, M., Jochem, E. *et al.*, *C-Ströme; Material- und Energieströme des nichtenergetischen Verbrauchs über den Lebenszyclus und* CO_2*-Minderung durch Produkte der Chemischen Industrie – Stand der Perspektiven*, Fraunhofer Institut für Systemtechnik und Innovationsforschung, Karlsruhe, 1998.

Paushkin, Y.M., Lapidus, A.L., Andel'son, S.V., *Plant biomass as raw material for the production of olefins and motor fuels*, Chemistry and Technology of Fuels and Oils, 30 (5-6), 1994, pp. 249-252

Phylipsen, D., Worrell, E. and Blok, K.: *Parameters affecting energy consumption in the petrochemical industry*, ECEEE Summer Study 1995, Utrecht University, department of Science, Technology and Society, Utrecht, 1995.

Redwan, D.S., *Methanol conversion to olefins over high-silica zeolites in continuous flow fixed-bed reactor*, Petroleum Science and Technology, 15(1&2), 1997, p. 19-36

Rubin, I.I. (ed.), *Handbook of plastic materials and technology*, Wiley, New York, 1990

Sas, H.J.W., *Verwijdering van huishoudelijk kunststofafval: analyse van milieu-effecten en kosten; main report + appendices* (in Dutch), Centrum voor energiebesparing en schone technologie, Delft, The Netherlands, 1994.

Saykowski, F., Martin, R., *Kunststoff-Verwertungsalternativen energetisch vergleichen*, Kunststoffe 84, 1994 (9), pp. 1143-1150

Schönfelder, H., Hinderer, J., Werther, J., Keil, F.J., *Methanol to olefins – Prediction of the performance of a circulating fluidized-bed reactor on the basis of kinetic experiments in a fixed-bed reactor*, Chemical Engineering Science 49 (24B), 1994a, pp. 5377-5390

Schönfelder, H., Hinderer, J., Werther, J., Keil, F.J., *Olefinsynthese aus Methanol (MTO) im Reaktor mit Zirkulierender Wirbelschicht*, Chem,Ing,Tech., 66(7) , 1994b, pp.960-963

Seiler, E., *Polypropylen kann noch mehr*, Kunststoffe 85 (8), 1995, pp. 1109-1116

Simon, C.M., Kaminsky, W., Schlesselmann, B., *Pyrolysis of polyolefins with steam to yield olefins*, Journal of Analytical and Applied Pyrolysis 38, 1996, pp. 75-87

Speight, J.G., *Asphalt*, in: Kirk-Omer Encyclopedia of Chemical Technology, fourth edition, Wiley, New York, 1996

Steinberg, M., Fallon, P.T., Sundaram, M.S.: *The flash pyrolysis and methanolysis of biomass (wood) for production of ethylene, benzene and methanol.* In: Novel production methods for ethylene, light hydrocarbons, and aromatics, Marcel Dekker, New York, 1992.

Steinmeyer, D., *The patterns of energy use in the chemical industry*, Proceedings ACEEE Summer Study, 1997

Stijn, A. v., *Meer mans met metalloceen-PE*, Missets Pakblad 9. September 1996, pp. 18-19

Stijn, A. v., *Metalloceen-PP voorbestemd voor de foodsector*, Missets Pakblad 1. January 1997, pp. 22-23

Stratton, A., Hemming, D.F. and Teper, M: *Ethylene production from oil, gas and coal-derived feedstock*, IEA Coal Research, London, 1983.

Tonino, S., *Spuitgietmachine(nieuw)s*, Kunststof en Rubber, May 1996, pp. 13-14

Wagner, D., *Polystyrol (PS, PS-I, SBS)*, Kunststoffe 86 (10), 1996, pp. 1466-1468

Weissermel, K., Arpe, H.J., *Industrielle Organische Chemie; Bedeutende Vor- und Zwischenprodukte*, fourth edition, VCH, Weinheim, Germany, 1994

Zagouras, N.G., Koutinas, A.A., *Processing scheme based on selective dissolution to recycle food packaging and other polymeric wastes and its economic analysis*, Waste Management and Research (13), 1995, pp. 325-333

Zehnder, S., *What are Western Europe's petrochemical feedstock options?*, Hydrocarbon Processing, February 1998

APPENDIX A: HEATING VALUES AND CO_2 EMISSION FACTORS

Table 58 Lower (LHV) and higher heating values (HHV)

	LHV [kJ/g]=[GJ/t]	HHV [kJ/g]=[GJ/t]
Methane	50.0	55.5
Ethane	47.5	51.9
Propane	46.3	50.3
Butane	45.6	49.3
Pentane	45.3	48.9
Benzene	40.6	42.3
Toluene	40.9	42.8
Xylene	41.2	43.3
Ethylene	47.2	50.3
Propylene	45.8	48.9
Butadiene	45.5	47.9
Methanol	21.1	23.9
CO	10.1	10.1
CO2	0	0
Hydrogen	120.0	141.7
Acetylene	48.2	49.9
Naphtha	44	48
Gas oil	42.7	45.7
LPG	46.0	49.8
Biomass (dry)	15	
Mixed plastic waste	38.0	

Table 59 CO_2 emission factors of energy carriers (Gielen, 1997)

	CO_2 emission factor [kg/GJ]
Coal	94
Oil	73
Gas	56
Electricity	100
Steam	70