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Analysis of energy use and carbon losses in the chemical and refinery industries
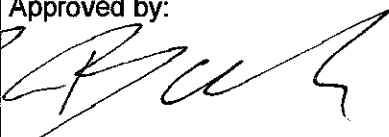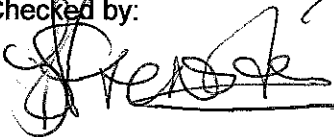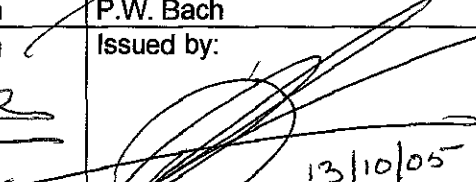
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Preface

Abstract

The chemical and refinery industry are both major consumers of energy. More energy efficient technologies in those industries therefore have the potential to contribute significantly to energy savings and the reduction of CO_2 emissions at the macro-economic level. In order to assess these potentials, it is important to have a proper overview of the structure of energy use and CO_2 emissions in these industries.

In this study an overview based on a spreadsheet model containing process datasets for 68 production processes for the production of 53 of the most important chemicals in terms of production volume and for 16 of the most important processes in the refinery industry is presented. The model also contains production volumes for the chemicals included and process volumes for the various refinery processes for the Netherlands, Western Europe and the world in 2000. The processes cover approximately 70% of the final energy use in the chemical and refinery industries.

For the processes analysed in the *chemical* industry, both the heat effects of the chemical reactions and the energy use of the processes are quantified. The sum of both equals the total energy loss of the processes (i.e. the amount of waste heat to the environment).

The total final energy loss in Western Europe for the processes analysed equals 1620 PJ_f in Western Europe in 2000, the total primary energy loss equals 1894 PJ_p. Total CO_2 emissions are calculated as 111 Mt CO_2, assuming steam and electricity to be produced separately (no cogeneration). Three processes (ethylene, ammonia and chlorine production) contribute approximately 50% to the total energy loss.

The ultimate theoretical energy saving potential of the processes is equal to the total energy loss of the process. The processes with large energy losses in relative (in GJ per tonne of product) and absolute terms (in PJ / year) are identified. The energy losses are split into losses due to non-selectivity, which is an indicator for process selectivity and excess final energy use, which is an indicator for the efficiency of energy use of a process. For the majority of processes the excess final energy contribution is the largest.

Considering those processes for which a Best Available Technology is known, the yearly energy saving potential in Western Europe ranges from 10 to 50% for small and large energy consumers respectively.

For the processes in the *refinery* industry, the analysis is focussed on the energy use of the various processes. The heat effects resulting from the chemical reactions could not be estimated with reasonable accuracy. Total energy use of the processes analysed in 2000 in Western Europe is estimated at 1555 PJ_f and 1654 PJ_p. Total CO_2 emissions are estimated at 137 Mt CO_2. Atmospheric distillation is identified at the largest energy consumer in the refinery (430 PJ_f), followed by catalytic cracking and hydrogen production.

This report presents an analysis at an intermediate (meso) level. The processes have been studied as black boxes without analysing the various unit operations (reactors, separation equipment etc.) within the process. Adding up the results for all processes yields results for the industries as a whole (the macro level). Processes with large theoretical energy saving potentials

in relative and/or absolute terms have been identified. Among these processes are processes that are well known for their large energy use such as the processes to produce ammonia, chlorine and ethylene, but also less well known processes such as the processes to produce acrylonitrile and hexamethylene diamine. These processes could be selected for more detailed analysis at the micro level. In doing so, actual energy saving potentials could be determined, taking into account not only theoretical, but also practical, economic and thermodynamic considerations. The spreadsheet model can also be extended and improved at the meso and macro level. Various recommendations are given for improvements and extensions such as the inclusion of a more sophisticated model section for the production of electricity and steam and the inclusion of dynamic elements in the model to analyse past and to project future energy demand of the chemical and refinery industry.

Keywords

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1. Introduction

Worldwide the industrial sector (including refineries) accounted for a final energy consumption of 101.9 EJ in 2000, 34% of the total energy available for final consumption. Within the industrial sector, the share of the chemical industry was 27% (27.9 EJ of which 13.5 EJ as feedstock) and the share of the refinery industry 10% (10.4 EJ). In the European Union in 2000 (15 countries), these shares were approximately the same. The industrial sector consumed 15.2 EJ of energy (33% of the total final consumption). The chemical and refinery industry accounted for 31% (4.7 EJ of which 2.0 EJ as feedstock) and 11% (1.6 EJ) of this total respectively (all figures from IEA, 2002a and 2002b). Given the large energy use in the chemical and refinery industries, more efficient technologies in these sectors have the potential to contribute significantly to energy savings and the reduction of CO_2 emissions at the macroeconomic level. In order to define energy saving potentials for processes in the chemical and refinery sectors, it is necessary to a have a proper overview of the structure of energy use and CO_2 emissions in these industries.

The thermodynamics of the chemical reactions taking place in the chemical and the refinery industry is an important element of the energy balance of processes in those industries. In detailed studies dealing with saving potentials of individual processes, these reaction effects are for that reason always regarded a key element in understanding the structure of energy use in a process and in determining energy saving potentials. Examples are exergy analyses (e.g. Hinderink et al., 1996 and Radgen, 1997), pinch analyses (e.g. Radgen, 1996) and more theoretical studies on potentials for energy savings in chemical processes (e.g. Leites et al., 2003 and Korevaar, 2004).

In contrast to these detailed studies dealing with individual processes or individual process units, the thermodynamics of the chemical reactions are often not explicitly addressed in overview studies focussing on the energy use in the industries as a whole (e.g. Gielen and van Dril, 1996; DOE/OIT, 1998; DOE/OIT, 2000 and Worrell et al., 2000). In these studies, the focus is mainly on the electricity, fuel and steam input into the various processes. This is also the case for studies aiming to calculate life cycle energy use and CO_2 emission data for important intermediates and plastics (e.g. APME, 1994-2003; Joosten, 2001 and Patel, 2003). An exception is a study by Lange (2001) in which the heat effect of reaction is considered an important element in understanding the cost structure of processes in the chemical industry. In his study, however, no totals are given for the processes studied and only a few specific processes are individually discussed. In studies by Tonkovich et al. (1995) and Lange (2002), carbon losses resulting from chemical reactions are quantified for a large number of processes, but these losses are not related to the thermodynamic effects of the reactions taking place.

The purpose of this study is therefore to present an overview of the structure and breakdown of energy use and CO_2 emissions in the chemical and refinery industries by studying the thermodynamics of the chemical reactions in relation to the total fuel, electricity and steam use of the processes. By doing so, ultimate theoretical energy saving and CO_2 emission reduction potentials will be identified. We limit ourselves to an energy analysis and do not explicitly take into account aspects related to the second law of thermodynamics, as is done in for example the exergy and pinch analyses mentioned above. Central research questions are:
- What are the heat effects of the chemical reactions taking place in the processes in the chemical and refinery industries?
- What is the energy use of the processes in the chemical and refinery industries and how does this energy use relate to the heat effect of the chemical reactions taking place?

- How do the reaction effects and the energy use relate to ideal processes without energy and carbon losses, i.e. what are the theoretical energy saving en CO_2 emission reduction potentials?

The research questions will be answered both at the level of individual processes and for the totals of the processes studied. For the latter, we use production data for three geographical areas for the year 2000: the Netherlands, Western Europe and the World. The individual processes will be analysed as black boxes, i.e. we only look at the flows going in and out of the process and not at the flows between the various unit operations (reactors, separation equipment etc.) inside the process. We refer to this as a *meso*-level of analysis.

We discuss the research approach and input data in Chapter 2. For the chemical industry, we limit ourselves to processes in the organic chemical industry, complemented with ammonia and chlorine production. As will be shown, these processes cover approximately 70% of the total final energy use of the chemical sector. In Chapter 3, we give the results of our analyses for the chemical industry and in Chapter 4, the results for the refinery industry are discussed. We end with conclusions and recommendations in Chapter 5.

2. Research approach, input data and basic assumptions

2.1 Overview of the Chapter

To answer the research questions raised in the introduction, we use a spreadsheet model containing in total approximately 300 process datasets from open literature for:

- 68 processes applied in the chemical industry for the production of 53 of the most important chemical commodities in terms of production volume[1].
- 16 processes applied in the refinery industries.

The chemical commodities for which the production processes are included and the refinery processes included in the model are given in Appendix B. In Section 2.2, we present the variables that are included for each of the datasets and discuss the system boundaries chosen in the analysis.

The model also contains production figures for the chemical commodities included and for the process volume of the refinery processes for three geographical regions in the year 2000:

- Netherlands (NL)
- Western Europe (WE), defined as the EU-15[2] + Switzerland and Norway
- World.

For the chemicals for which different process routes are included in the analysis, also the share of these processes in the total production is included in the model. The input data for production volumes and process shares are given in Appendix E.

In Section 2.3 we introduce the indicators relevant with respect for energy efficiency, energy saving potentials that are calculated in the model. Results for these indicators are shown in Chapter 3 and 4. In cases where more than one dataset was available for a given process route, we made a choice for one dataset to be included in our analysis. We discuss this choice in Section 2.4.

2.2 System boundaries: variables included

The spreadsheet model contains data on the raw materials, the desired products and the by-products of the processes included as well as data on steam, fuel and electricity use. The general structure of the model is shown in Figure 2.1. In the next two Sections, we discuss the system boundary choices made for the processes in the chemical industry (Section 2.2.1) and in the refinery industry (Section 2.2.2).

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[1] When a chemical commodity can be produced via more than one process route (using a different raw material), we include process datasets for all the process routes applied.

[2] Austria, Belgium, Denmark, Finland, France, Germany, Great Britain, Greece, Ireland, Italy, Luxemburg, Netherlands, Portugal, Spain and Sweden.
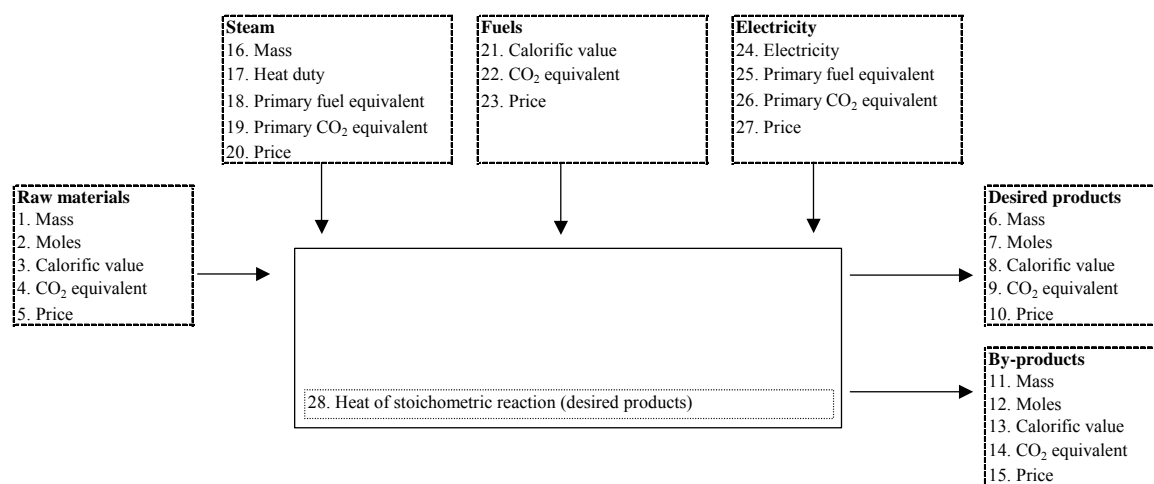
Figure 2.1 *Overview of variables included in the datasets*

2.2.1 Chemical industry

In most of the processes of the chemical industry, raw materials are converted into products having a different chemical structure. In some processes, the raw material used is a commodity, which is included in energy statistics. Examples are the use of naphtha in olefin production or the use of natural gas in ammonia production[3]. In the majority of processes included, however, the raw material applied is a basic or intermediate chemical commodity with a uniform and well-defined chemical structure, which is further converted to another chemical commodity (e.g. the conversion of ethylene to ethylene oxide). In the model, the heat effect of the stoichometric reaction from raw material to the desired product or products (in case of co-production of several chemical commodities in the same process) is included (variable 28).

In some processes, not only the desired products are produced, but also small amounts of by-products. In the model, we only include sellable chemical-grade commodities as by-products of a process and not the production of undesired fuel-grade by-products[4]. For the raw materials, products and by-products of a process, the mass, molar quantity, calorific value and price are included. In the datasets from open literature that are the basis of the model, normally only the flows in mass units are given. We explain the assumptions made in estimating the remaining variables from these mass flows in Appendix C. We also include the energy use of the processes, split into direct fuel use, steam use and electricity use. For electricity and steam use, final energy use, primary fuel equivalents, CO_2 equivalents and price is included. Final energy use is expressed throughout this report with subscript f (steam / fuels) or e (electricity), primary energy equivalents with subscript p. The assumptions made for energy prices, energy conversion efficiencies and CO_2 emissions factors are explained in Appendix D. Additional non-energy inputs into the process that are not part of the conversions taking place such as cooling water and catalysts are not included in the model.

2.2.2 Refineries

Contrary to the process in the chemical industry, the various raw material and product flows in the refinery industry do not have a well-defined and uniform structure. An additional complicating factor is that the terminology used to distinguish between the various refinery

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[3] In international energy statistics (e.g. IEA, 2002a), the use of energy commodities as raw material in the chemical industry is included as a memo item under the final consumption of the chemical industry and is referred to as feedstock use in the chemical industry.

[4] An exception is made for the steam cracking process for which we included all products, including the fuel by-products. See Chapter 3 for details.

flows very much differs between the data sources from which datasets are taken[5]. We could therefore not determine the calorific value, price and carbon content of the various refinery flows with sufficient accuracy to calculate the related indicators given in Section 2.3 and we therefore only focus in Chapter 4 on the indicators related to the energy use of the processes. For some of the processes, we will, however, add some qualitative and quantitative remarks on the chemical conversions. As for the processes in the chemical industry, we also include the energy use, split into direct fuel, steam and electricity use. Final energy (expressed throughout the report with subscript f for steam / fuels and e for electricity) and primary fuel equivalents (expressed throughout the report with subscript p) are included as well as CO_2 equivalents and price. The assumptions made in determining these variables are discussed in Appendix D.

2.3 Indicators

Using the variables given in Figure 2.1, we can calculate various indicators relevant with respect to energy efficiency, CO_2 emissions and process profitability for each of the datasets included. In Table 2.1, we give the definition of all indicators for which results are shown in the Chapters 3 and 4. In the following 3 Sections, we give some background on the energy indicators (Section 2.3.1), CO_2 emission indicators (Section 2.3.2) and financial indicators (Section 2.3.3). A worked out example, explaining how the various indicators are calculated, is given in Appendix G.

Table 2.1   *Definition of indicators*

No.	Indicator name (unit)	Formula (numbers refer to the variables in Figure 2.1).
1	Heat of stoichometric reaction (J_f)	28
2	Electricity use (J_e)	24
3	Fuel use (J_f)	21
4	Steam use (J_f)	17
5	Total final energy use (J_f)	17+21+24
6	Total primary energy use (J_p)	18+21+25
7	Heat effect of reaction (J_f)	3-8-13
8	Total final energy loss (J_f)	17+21+24+3-8-13
9	Total primary energy loss (J_f)	18+21+25+3-8-13
10	Excess final energy use (J_f)	17+21+24-28
11	Losses due to non-selectivity (J_f)	3-8-13+28
12	Energy efficiency, final (%)	(8+13) / (3+17+21+24)
13	Energy efficiency, primary (%)	(8+13) / (3+18+21+25)
14	Carbon losses, energy use, primary (t CO_2)	19+22+26
15	Carbon losses, reaction (t CO_2)	4-9-14
16	Total carbon losses, primary (t CO_2)	4-9-14+19+22+26
17	Carbon efficiency, reaction (%)	(9+14) / (4)
18	Total carbon efficiency (%)	(9+14) / (4+19+22+26)
19	Energy costs (€)	20+23+27
20	Value added reaction (€)	10+15-5
21	Total value added (€)	10+15-5-20-23-27
22	Value added reaction, % of product value (%)	(10+15-5) / (10+15)
23	Total value added, % of product value (%)	(10+15-5-20-23-27) / (10+15)

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[5] A way to circumvent these problems would be to use a single refinery model with a detailed specification of the flows used in the model. We tried to use the Serum model developed by ECN for this purpose (van Oostvoorn et al., 1989). In this model, the terminology used to distinguish between the various refinery flows is indeed uniform for all processes. However, calorific values and carbon content of the flows are not specified.

2.3.1 Energy indicators 1-13

From the final electricity, fuel and steam use (indicator 2, 3 and 4), the total energy use in final (indicator 5) and primary units (indicator 6) is calculated. The heat effect of reaction (indicator 7) is calculated by deducting the calorific value of the products and by-products from the calorific value of the raw material. The heat effect of reaction is, opposite to the normal convention, positive in case of an exothermic reaction, whereas it is negative in case of an endothermic reaction[6]. The total energy loss of the process (indicator 8 and 9) is the total difference between energy coming out and energy going into the process and equals the sum of energy use (in either final or primary units) and the heat effect of reaction.

With indicator 10 and 11, the energy use of the process is compared to a theoretical process without energy losses. In such a process, the actual heat effect of reaction (indicator 7) would be equal to the negative of the heat of the heat of the stoichometric reaction from the raw materials to the desired products (indicator 28). The difference between the stoichometric heat of reaction and the actual observed heat effect of reaction is therefore an indicator for the losses due to non-selectivity (indicator 11). Processes without energy losses, and a heat of reaction equal to the stoichometric heat of reaction would have an energy use equal to the heat of the stoichometric reaction. For an exothermic reaction, this would mean that the process exports an amount of energy. For an endothermic reaction, this would mean that the process requires an amount of energy. The difference between the heat of the stoichometric reaction and the observed energy use is therefore an indicator for the excess final energy use (indicator 10). It should be emphasised that these statements are all based on the first law of thermodynamics, not taking into account aspects related to the quality of energy (the second law of thermodynamics). In practice, the heat effect of an exothermic reaction might become available at low temperature, making the heat unusable from a practical point of view. Furthermore, these statements do not take into account that some energy will always be required for separation etc. The excess final energy use calculated should therefore be regarded as purely theoretical. We also calculate the energy efficiency of the processes by dividing the total energy output by the total energy input (indicator 12 and 13). These efficiency indicators as defined in Table 2.1 could, however, only be calculated if all raw materials and products have positive calorific values[7].

For the processes in the refinery industry, for which we do not include the calorific values and carbon content of the various flows as explained in Section 2.2.2, only indicators 2-6 are therefore calculated.

2.3.2 CO$_2$ emission indicators (14-18)

Using the various variables included, we are also able to quantify the CO_2 emissions related to the energy use of a process (indicator 14) and related to the carbon losses resulting from the reaction (indicator 15), together resulting in the total carbon losses from the process (indicator 16). The carbon efficiency of the reaction is calculated by dividing the carbon content of the products by the carbon content of the raw material (indicator 17). The total carbon efficiency is calculated by dividing the carbon content of the products by the total carbon input, both in the raw materials and resulting from the energy use (indicator 18).

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[6] We defined the heat effect of reaction opposite to the normal convention of defining the heat of reaction, since our main interest is in the energy available from and lost in the reaction. Exothermic reactions have a positive heat effect of reaction, whereas endothermic processes have a negative heat effect of reaction in our approach.

[7] If chemicals contain other elements than carbon, hydrogen and sulphur, the calorific value as calculated according to Equation 1 in Appendix 3 can become negative. This does not lead to errors in indicators 1-11 (as long as the balances for the elements are closed, the negative values cancel out), but does lead to errors in the efficiency indicators 12 and 13. For some processes, these indicators could for this reason not be calculated.

2.3.3 Financial indicators (19-23)

Since also the energy costs and the prices of raw materials and products is included in the model, we are also able to calculate some simple financial indicators for the processes included such as the energy costs (indicator 19), the 'value added' of the reaction (indicator 20, defined as the difference in value between products and raw materials) and the total 'value added' (indicator 21). Both the 'value added' of the reaction and the total 'value added' are also calculated as percentage of the value of the products (indicator 22 and 23). It should be noted that only raw materials, products and energy costs are included in the 'value added' calculations and not the other cost factors such as capital costs, labour costs and costs for additional materials such as catalysts and cooling water.

2.4 Choice of dataset when multiple datasets were available

In the model, approximately 300 datasets are included. For process routes for which several datasets are available, we use the dataset most likely representing the average technology in use in Western Europe in 2000 in the analyses shown in this report; this choice is based on own judgements. In cases, where only one process dataset was available, we use this dataset in the analysis without adjusting for process improvements that might have taken place over time. In cases where explicit information is available on Best Available Technologies (BAT), we also give the process data for these BAT processes. We discuss the uncertainties in the results in Section 3.6 (chemical industry) and 4.6 (refinery industry).

3. Results for the chemical industry

3.1 Overview of the Chapter

In this Chapter, we present an overview of the process indicators introduced in Table 2.1 for the processes included in the model. The numerical values for all indicators shown in this Chapter are given in Appendix H. We focus in this study on energy and CO_2 emission indicators, but give in Appendix H also the financial indicators. In Section 3.2, we study the effects of the reactions taking place and in Section 3.3, we analyse the energy use of the processes in relation to these reactions. In Section 3.4, an overview of total energy losses and CO_2 emissions is presented. We will relate our results to directions for energy saving possibilities in Section 3.5. The uncertainties in the results are discussed in Section 3.6, in which we also compare our results with other available sources. Throughout this chapter, we refer to the indicators shown in Table 2.1 without explicitly referring to this table.

3.2 Heat effect and carbon losses of reaction

We first focus on the heat effect and carbon losses resulting from the conversion of raw materials to products. In Figure 3.1, we show for the processes included in the analysis the actual heat effect of reaction (indicator 7) as a function of the negative[8] value of the heat of the *desired* stoichometric reaction from raw material to products (indicator 1).

Figure 3.1 *Heat effect of reaction (indicator 7) as a function of stoichometric heat of reaction (indicator 1). Vertical distance between the data-points and the y=x line equal the losses due to non-selectivity (indicator 11). Numbers refer to Table 3.1*

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[8] Exothermic reactions have a positive heat effect of reaction in our approach. See footnote 6 for details.

Processes that would have a 100% conversion from raw materials to desired products according to the stoichometric reaction would be on the y=x line shown in Figure 3.1, having a heat effect of reaction exactly equal to the negative value of the heat of the stoichometric reaction.

From the figures it becomes clear that most processes included in the model are exothermic; the products of the process have a calorific value, which is lower than the calorific value of the raw material going into the process. Exceptions are the steam cracking process to produce ethylene, propylene and aromatics[9], the production of chlorine and the dehydrogenation of ethylbenzene to styrene and isopropanol to acetone. These conversions are endothermic, i.e. the products have a higher calorific value than the raw material. It should be noted that Figure 3.1 does not give any information on whether the heat available from the reaction is used within the process or is recovered and exported from the process (e.g. in the form of steam). This link between the heat effect of reaction and the energy use of the processes is made in the next section.

In practice, a part of the raw material is not converted to the desired products, but is lost. We refer to these as losses due to non-selectivity (indicator 11), defined as the difference between the heat effect of reaction (indicator 7) and the negative value of the stoichometric heat of reaction (indicator 1). The losses can either be the result of the formation of undesired non-valuable fuel grade by-products, often referred to as off-specs[10], but can also be the result of over-oxidation of the hydrocarbon raw materials, leading to direct CO_2 emissions (e.g. in ethylene oxide production). In the second case, the energy becomes directly available as process heat within the reactor, whereas in the first case, the energy is embodied in non-valuable by-products, which might be burned with energy recovery. It is not always clear whether this second type of energy recovery is netted off in the process datasets as found in literature. Part of the losses due to non-selectivity might therefore be double counted in our analysis, both as losses due to non-selectivity and once more as final energy use. We will come back to this possible double counting in Section 3.6.2.

It should be noted that the effect of raw material losses on the heat effects of reaction is substantial. If 0.01 tonne of a hydrocarbon raw material is lost per tonne of product, the heat effect of reaction increases by $0.1 - 0.5$ GJ$_f$ / tonne[11], either in the form of heat or in the form of non-valuable by-products. This is a significant fraction of the heat of reaction of most processes as becomes clear from Figure 3.1. In Figure 3.1, we numbered the 10 processes having losses due to non-selectivity exceeding 5 GJ$_f$ / tonne of product. They are summarised in Table 3.1. The table shows that especially oxidation reactions are often difficult to control in a selective way. In ethylene oxide production, for example, 18 mass % of the ethylene is burned rather than converted to ethylene oxide, causing the heat effect of reaction to be 9.1 GJ$_f$ / tonne ethylene oxide rather than the 2.4 GJ$_f$ / tonne in case of a stoichometric conversion from ethylene to ethylene oxide.

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[9] The steam cracking process to produce ethylene, propylene and aromatics is included in such a way that the internal use of part of the fuel products is visible. No ideal desired stoichometric reaction is defined, because it would be an arbitrary choice, which of the multiple products produced are regarded desired products. Instead, the stoichometric heat of reaction is set equal to the heat effect of reaction, which is calculated as the difference between the total cracker output and the cracker input. Part of the cracker output (the fuel by-products) is used to fuel the process. This amount is given under final energy use in Figure 3.3. The resulting figures are all expressed per tonne of total products produced. In the production of ammonia and methanol by steam reforming or partial oxidation, the raw material is also used both as fuel and as feedstock. In these processes, we did not define a stoichometric heat of reaction, since it would involve an arbitrary choice between the amount used as fuel and the amount used as feedstock. Instead, we allocated an amount of input equal to the calorific value of the product to raw material use (resulting in a heat effect of reaction equal to 0) and included the remainder of the raw material use as final energy use of the input (Figure 3.3).

[10] Some processes might be valuable, but the concentrations might be too low to justify a complicated and/or expensive product separation and purification train.

[11] Considering that the calorific value of the hydrocarbons used as raw materials range between 10 and 50 GJ / tonne.

We can convert the heat effects of reaction and the losses due to non-selectivity per tonne of product to total losses per year, taking into account the production volumes of the chemical commodities and the shares of the various process routes that are also included in the model. An overview is presented in Table 3.2. Ethylene and chlorine, the two most important endothermic processes are given separately to show their large contribution to the totals. The total cumulative heat effect of reaction for Western Europe is 151 PJ_f / year, whereas it would be 13 PJ_f / year if all processes would take place according to the stoichometric reactions to the desired products. Excluding ethylene and chlorine production, the total losses due to non-selectivity of the processes analysed amount to 138 PJ_f in Western Europe, which is 40% of the observed heat effect of reaction. We show the cumulative graph for Western Europe in Figure 3.2. In the Figure, we also list the 10 processes with the largest losses due to non-selectivity per year.

It is beyond the scope of this study to go into the details of specific processes and to specify possibilities and directions for energy savings at the level of the individual process unit operations (reaction, separation equipment etc.). Some general directions for energy savings possibilities will be summarised in Section 3.5, including some examples taken from literature. The processes presented in Table 3.1 and Figure 3.2 are processes with large energy saving potentials related to inefficiencies in the chemical conversions, either in relative (per tonne of product) or absolute (in PJ_f per year) terms.

The losses due to non-selectivity are closely related to the carbon losses of reaction (indicator 15), which we estimate at 9.1 Mt CO_2 per year in Western Europe in the year 2000, 1.6 Mt CO_2 in the Netherlands and 39.1 Mt CO_2 worldwide. Part of this CO_2 is lost in the form of direct CO_2 emissions to the atmosphere (e.g. in ethylene oxide production), part indirectly leads to CO_2 emissions via the production of non-valuable by-products, which are burned and part is lost in other ways (e.g. via waste water flows).

Table 3.1 *Processes having losses due to non-selectivity exceeding 5 GJ_f / tonne. Numbers refer to the numbers in Figure 3.1. Processes in italics are uncertain estimates based on single sources from before 1990 (see Section 3.6.1 for more details)*

No	Product	Process	Losses due to non-selectivity, indicator 11 (GJ_f / tonne product)
1	Acrylonitrile	Ammoxidation of propylene	13.2
2	*Phenol*	*Oxidation of toluene*	*11.1*
3	Hexamethylene diamine	Hydrogen cyanide with butadiene	10.4
4	*Toluene diisocyanate (TDI)*	*Nitration of toluene and phosgenation to TDI*	*9.9*
5	Caprolactam	From cylohexane	9.6
6	Phthalic anhydride	Oxidation of o-xylene	7.8
7	*Adipic acid*	*Oxidation of cyclohexane*	*7.6*
8	Ethylene oxide	Oxidation of ethylene	6.8
9	*Propylene oxide / tert-butanol*	*Indirect oxidation via tert-butyl hydroperoxide*	*6.0*
10	Hexamethylene diamine	Ammonia with adipic acid	5.3

Table 3.2 *Overview of the cumulative heat effect of reaction and the losses due to non-selectivity*

Indicator	NL PJ_f per year	WE PJ_f per year	World PJ_f per year
Heat effect of reaction, indicator 7	**32**	**151**	**658**
Of which:			
- Ethylene production (all processes)[1]	-17	-129	-531
- Chlorine production (all processes)	-3	-68	-283
- Other processes	53	342	1472
Heat of stoichometric reaction, indicator 1	**8**	**13**	**89**
Of which:			
- Ethylene production (all processes)[1]	-17	-129	-531
- Chlorine production (all processes)	-3	-68	-283
- Other processes	29	204	903
Losses due to non-selectivity, indicator 11	**24**	**138**	**569**
Of which			
- Ethylene production (all processes)[1]	0	0	0
- Chlorine production (all processes)	0	0	0
- Other processes	24	138	569

[1] See footnote 9 for an explanation on how ethylene production by steam cracking is included in the model.

10. Dimethylterephthalate — 5.0
9. Polyethylene — 5.0
8. Phthalic anhydride (from o-xylene) — 5.1
7. Vinylchloride — 5.5
6. Phenol / acetone — *6.3*
5. Adipic acid — *6.8*
4. Propylene oxide / tert butanol — 11.2
3. Caprolactam (from cyclohexane) — *14.6*
2. Ethylene oxide — 14.7
1. Acrylonitrile — 14.9

Figure 3.2 *Cumulative losses due to non-selectivity (indicator 11) in Western Europe in 2000 for the processes included in the analysis, ranked in the order of decreasing losses due to non-selectivity. Processes in italics are uncertain estimates based on single sources from before 1990 (see Section 3.6.1 for more details). Processes for which the losses due to non-selectivity could not be calculated are not shown (see notes in Appendix H)*

3.3 Energy use

The energy use of the process is also related to the heat of the reaction involved. We show the energy use as a function of the negative value of the heat of the desired stoichometric reaction in final units (indicator 5) in Figure 3.3 and in primary fuel equivalents (indicator 6) in Figure 3.4.
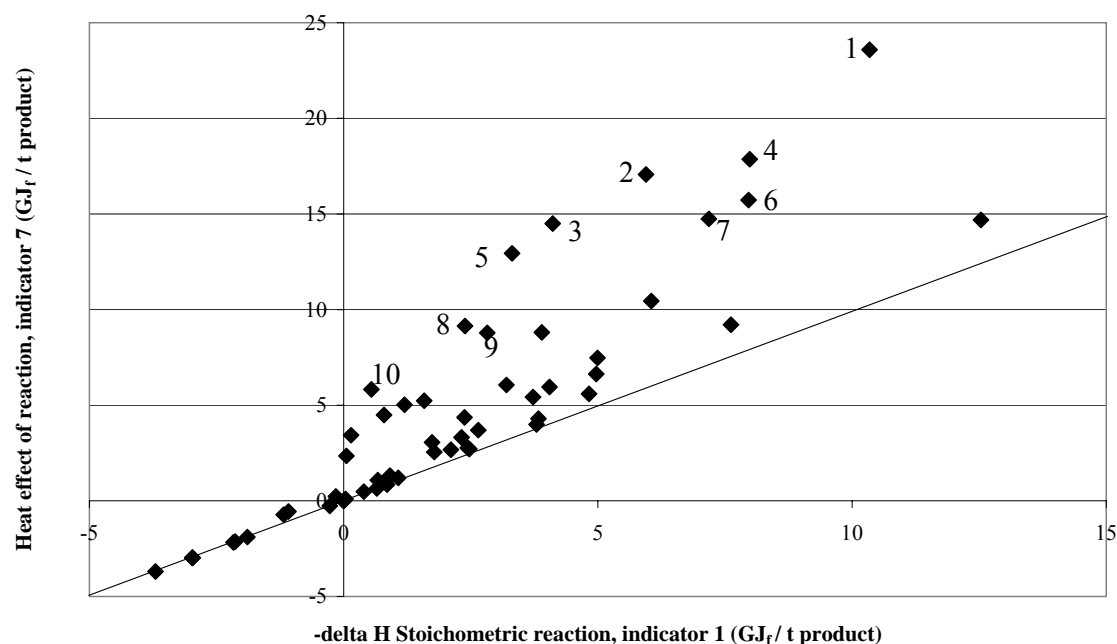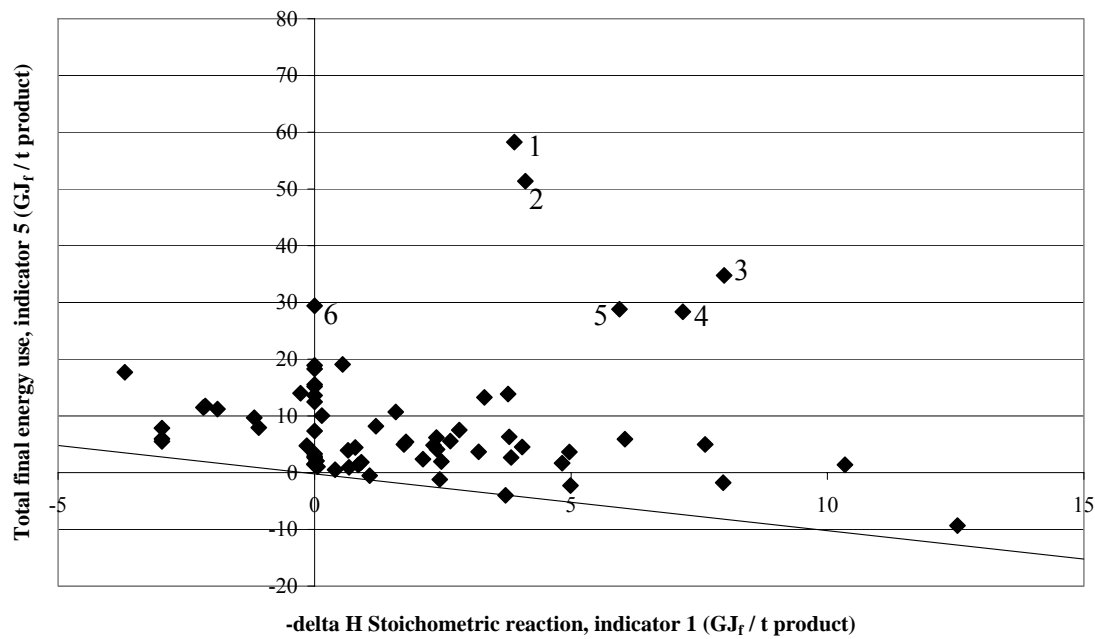

Figure 3.3 *Total final energy use (indicator 5) as a function of stoichometric heat of reaction (indicator 1). Vertical distance between the data-points and the y= –x line equal the excess final energy use (indicator 10)*
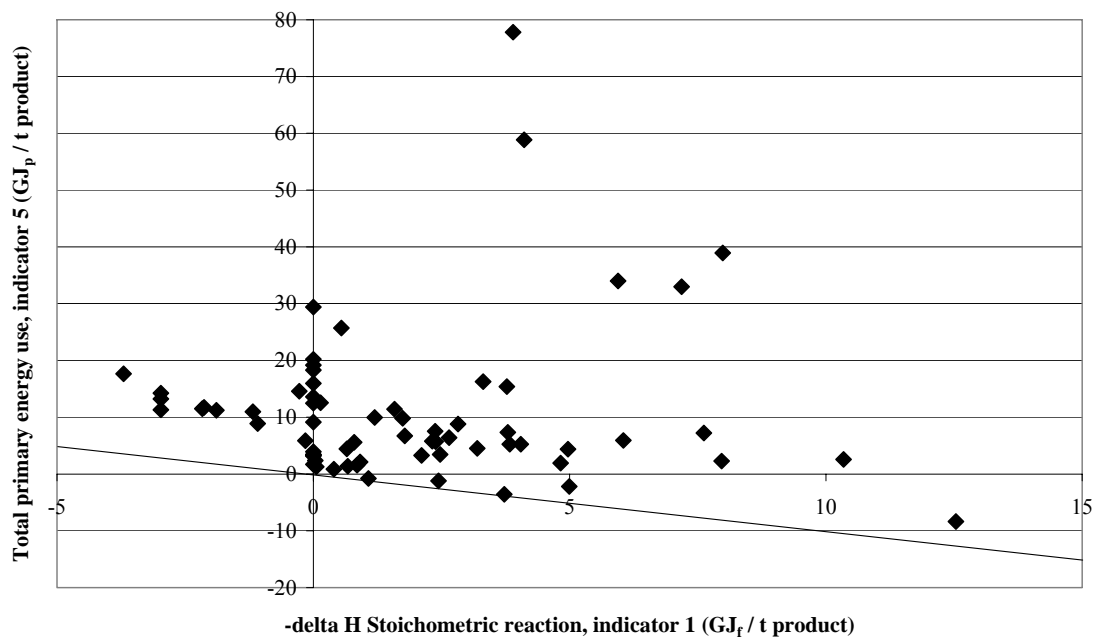
Figure 3.4 *Total primary energy use (indicator 6) as a function of stoichometric heat of reaction (indicator 1)*

In the ideal case of zero energy losses, endothermic processes would use just the amount of energy required to sustain the desired stoichometric endothermic reaction and an exothermic processes would fully recover the amount of energy available from the desired stoichometric reaction. These processes would lie on the y= –x line shown in Figure 3.3. The figure shows that some of the processes involving exothermic reactions indeed recover energy to the extent that they become net exporters of energy in the form of steam. The majority of processes, however, are net consumers of energy. We define the excess final energy use of a process (indicator 10) as the difference between the final energy use and the stoichometric heat of reaction (indicator 1). We numbered the six processes having an excess final energy use exceeding 20 GJ_f / tonne of product and summarise them in Table 3.3. For a limited number of processes we could not calculate the heat of the stoichometric reaction and the reaction effects with sufficient accuracy, because data was not available (see Appendix H for details). For those processes we set the excess final energy use equal to the total final energy use.

We can again convert the indicators shown in GJ per tonne of product to total PJ per year, taking into account production volumes and shares of the various process routes. We present this overview in Table 3.4. Ethylene, ammonia and chlorine production are given separately to show their large contribution to the total. The cumulative total final energy use of the processes included in the analysis is 1469 PJ_f per year for Western Europe in 2000. Since the cumulative heat of the stoichometric reactions is 13 PJ_f, the cumulative excess final energy use is 1482 PJ_f. In the endothermic ethylene and chlorine production, the excess final energy use is lower than the observed final energy use (part of the energy use cannot be avoided, because the endothermic reaction requires a certain amount of energy). For the remainder of the processes for which the cumulative total heat effect of reaction is positive (exothermic reactions), the cumulative excess final energy use exceeds the observed final energy use, because theoretically, these processes could be net energy exporters. We show the cumulative graph for Western Europe in 2000 in Figure 3.5. In the figure, we also list the 10 processes with the largest excess final energy use per year.

It is beyond the scope of this study to go into the details of specific processes at the level of process unit operations. This would be required to specify in which way possible energy savings could be accomplished and to judge how likely this energy saving possibilities are in view of thermodynamic, practical and economic considerations. We did, for example, not take into account the fact that the heat from an exothermic reaction might become available at low temperatures (e.g. below 323 K), making it very difficult to find a useful application for this heat. Furthermore, not all the excess final energy use can be avoided, because some energy will be required for separation and purification etc. In Section 3.5, we give some general directions for energy saving possibilities, including some examples from literature. The lists of processes presented in Table 3.3 and Figure 3.5 are processes with large energy saving potentials in either relative (per tonne of product) or absolute (in PJ per year) terms, when looking at the processes from a black box perspective.

Using the assumptions summarised in Appendix D, we can also estimate the total CO_2 emissions related to the energy use of the processes (indicator 14). These total CO_2 emissions are for Western Europe estimated to be 102 Mt CO_2 per year in 2000 and for the Netherlands and the World 15 and 566 Mt CO_2 respectively.

Table 3.3 *Overview of processes having an excess final energy use exceeding 20 GJ$_f$/ tonne of product. Numbers refer to the numbers in Figure 3.3. Processes in italics are uncertain estimates based on single sources from before 1990 (see Section 3.6.1 for more details)*

No	Product	Process	Excess final energy use, indicator 10 (GJ$_f$/ tonne product)
1	Hexamethylene diamine	Hydrogenation of acrylonitrille	62.2
2	Hexamethylene diamine	Hydrogen cyanide with butadiene	55.5
3	*Toluene diisocyanate (TDI)*	*Nitration of toluene and phosgenation to TDI*	*42.8*
4	*Adipic acid*	*Oxidation of cyclohexane*	*35.6*
5	*Phenol*	*Oxidation of toluene*	*34.8*
6	Ammonia	Partial oxidation of coal	29.4

Table 3.4 *Overview of cumulative total final and primary energy use and excess final energy use. For processes for which the heat of the stoichometric reaction and the heat effects of reaction are not included (see Appendix H), we set the excess final energy use equal to the final energy use*

Indicator	NL	WE	World
	PJ per year	PJ per year	PJ per year
Total final energy use, indicator 5	**218**	**1469**	**7946**
Of which:			
- Ethylene production (all processes)[1]	93	689	2828
- Ammonia production (all processes)[1]	37	152	2061
- Chlorine production (all processes)	7	131	667
- Other processes	82	497	2390
Total primary energy use, indicator 6	**246**	**1743**	**9124**
Of which:			
- Ethylene production (all processes)[1]	93	689	2828
- Ammonia production (all processes)[1]	37	152	2061
- Chlorine production (all processes)	15	273	1279
- Other processes	102	629	2956
Heat of stoichometric reaction, indicator 1	**8**	**13**	**89**
Of which:			
- Ethylene production (all processes)[1]	-17	-128	-531
- Ammonia production (all processes)[1]	0	0	0
- Chlorine production (all processes)	-3	-62	-283
- Other processes	29	204	903
Excess final energy use, indicator 10	**227**	**1482**	**8035**
Of which:			
- Ethylene production (all processes)[1]	75	561	2297
- Ammonia production (all processes)[1]	37	152	2061
- Chlorine production (all processes)	4	69	384
- Other processes	111	701	3293

[1] See footnote 8 for an explanation on how ethylene production by steam cracking and ammonia production are included in the model.

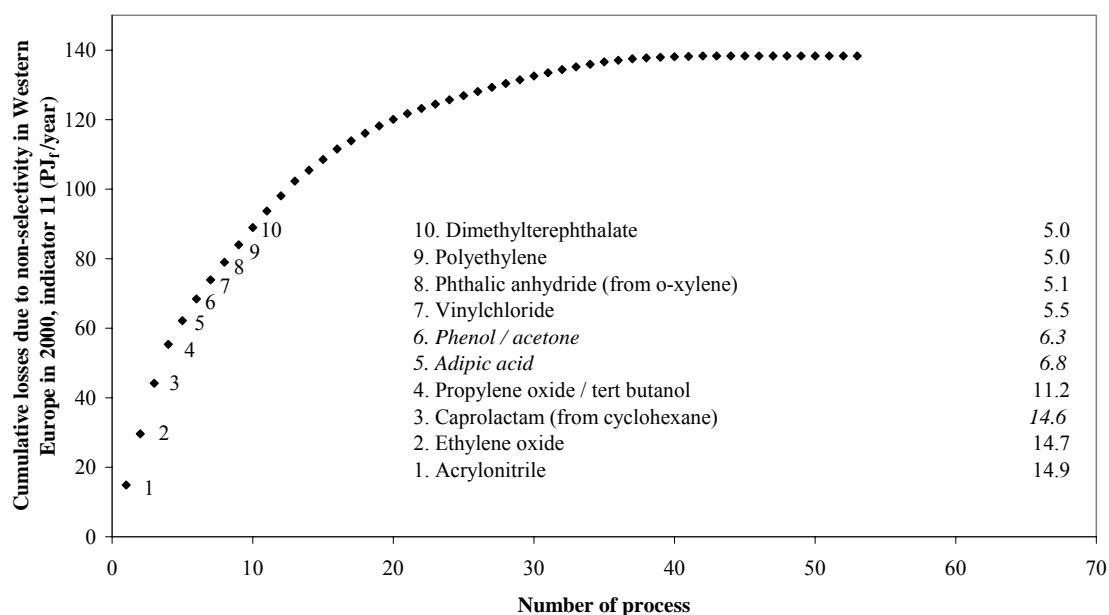|	
10. *Adipic acid*	*32*
9. Methanol (natural gas)	36
8. Vinylchloride	39
7. Ethylene (propane)	40
6. Benzene (from pyrolysis gasoline)	49
5. Chlorine (all processes)	69
4. Polyethylene	69
3. Ethylene (gas oil)	76
2. Ammonia (from natural gas)	132
1. Ethylene (from naphtha)	428
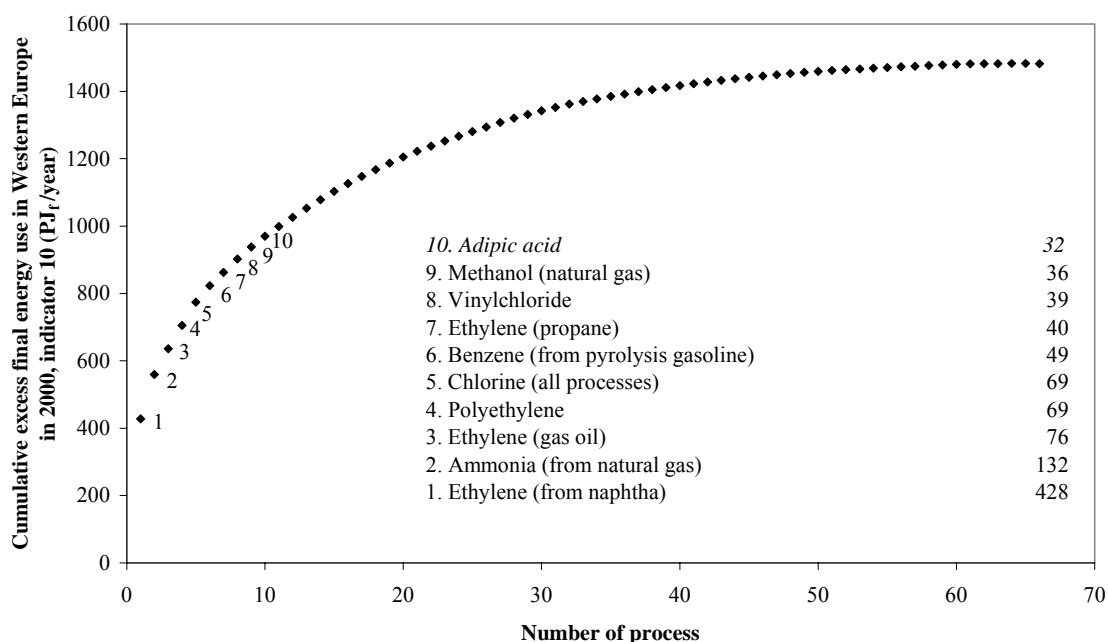
Figure 3.5 *Cumulative excess final energy use (indicator 10) in Western Europe in 2000 for the processes included in the analysis, ranked in the order of decreasing total excess final energy use. Processes in italics are uncertain estimates based on single sources from before 1990 (see Section 3.6.1 for more details). For processes for which the heat of the stoichometric reaction and the heat effect of reaction are not included (see Appendix H), we set the excess final energy use equal to the total final energy use*

3.4 Total energy loss and CO_2 emissions

The total final energy loss of the processes (indicator 8) equals the sum of the heat effect of reaction (indicator 7, Table 3.2) and the total final energy use (indicator 5, Table 3.4). The total primary energy loss (indicator 9) equals the sum of the heat effect of reaction and the total primary energy use of the processes (indicator 6, Table 3.4). By definition, the total final energy loss is also equal to the sum of losses due to non-selectivity (indicator 10, Table 3.2) and excess final energy use (indicator 11, Table 3.4).

The contribution of losses due to non-selectivity and excess final energy use to the total final energy loss of the processes is shown in Figure 3.6. The diagonal lines are lines with a constant total final energy loss. From the 68 processes included in the analysis, 38 have a total final energy loss lower than 10 GJ_f / tonne of product, 21 a total final energy loss between 10 and 20 GJ_f / tonne of product and 9 a total final energy loss exceeding 20 GJ_f / tonne of product. The processes having a total final energy loss exceeding 10 GJ_f / tonne of product are specified in Figure 3.7. The processes with large losses due to non-selectivity (given in Table 3.1) and a large excess final energy use (given in Table 3.3) are readily identified in the two figures.

We convert the indicators shown in GJ per tonne of product to total PJ per year, taking into account production volumes and shares of the various process routes. The cumulative total final and total primary energy loss for Western Europe in 2000 is shown in Figure 3.7. In the Figures, we also list the 10 processes with the largest total final energy loss. We show the contribution of heat effects of reaction and final energy use to the total final energy loss in Figure 3.9 and the resulting CO_2 emissions in Figure 3.10.
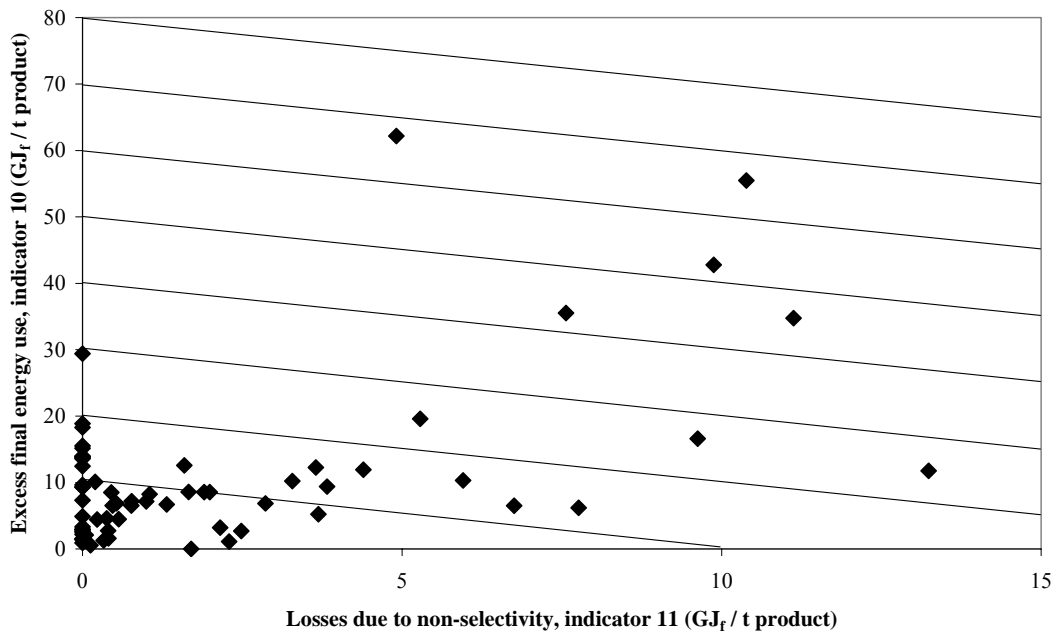
Figure 3.6 *Excess final energy use (indicator 10) as a function of losses due to non-selectivity (indicator 11). The lines shown are lines of equal total final energy loss (indicator 8). For processes for which the heat of the stoichometric reaction and the reaction effects are not included (see Appendix C), we set the excess final energy use equal to the total final energy use and the losses due to non-selectivity to 0*
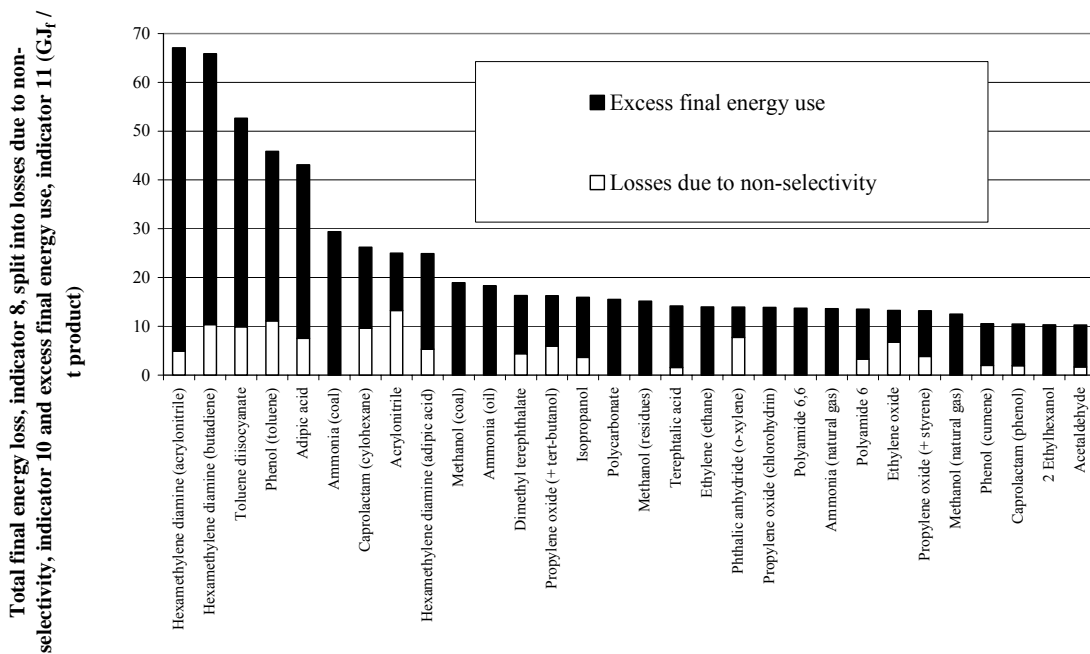
Figure 3.7 *Processes with total final energy loss (indicator 8) exceeding 10 GJ_f / tonne, split into losses due to non-selectivity (indicator 10) and excess final energy use (indicator 11). For processes for which the heat of the stoichometric reaction and the reaction effects are not included (see Appendix H), we set the excess final energy use equal to the total final energy use and the losses due to non-selectivity to 0*
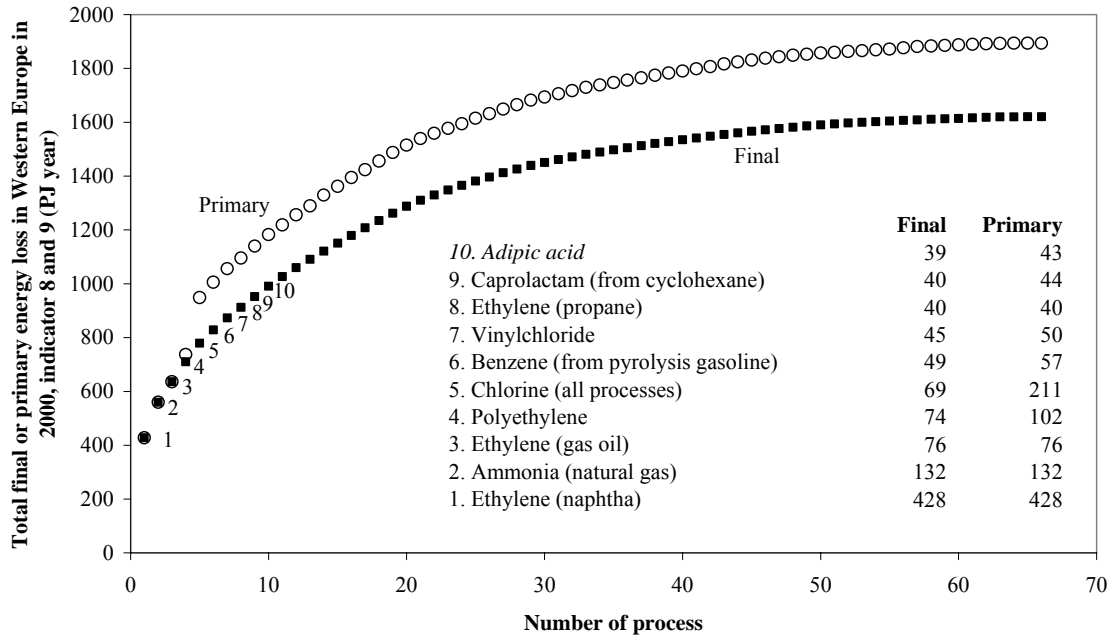
Figure 3.8 *Cumulative total final and total primary energy loss (indicator 8 and 9) in Western Europe in 2000 for the processes included in the analysis, ranked in the order of decreasing total final energy loss. Processes in italics are uncertain estimates based on single sources from before 1990 (see Section 3.6.1 for more details). For processes for which the heat of the stoichometric reaction is not included (see Appendix C), we set the total final and primary energy loss equal to the total final or primary energy use*
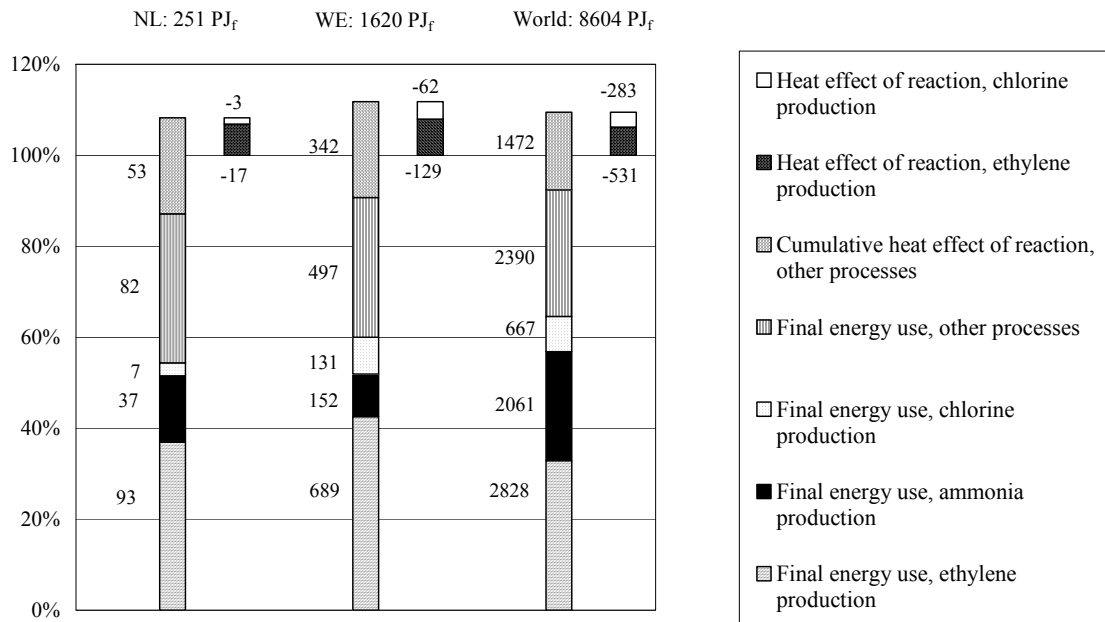
Figure 3.9 *Overview of cumulative total final energy loss (indicator 8), split into final energy use (indicator 5) and heat effects of reaction (indicator 7). Ethylene, ammonia and chlorine production are given individually to show their major contribution to the totals*

NL: 16.6 Mt CO$_2$ WE: 111 Mt CO$_2$ World: 606 Mt CO$_2$
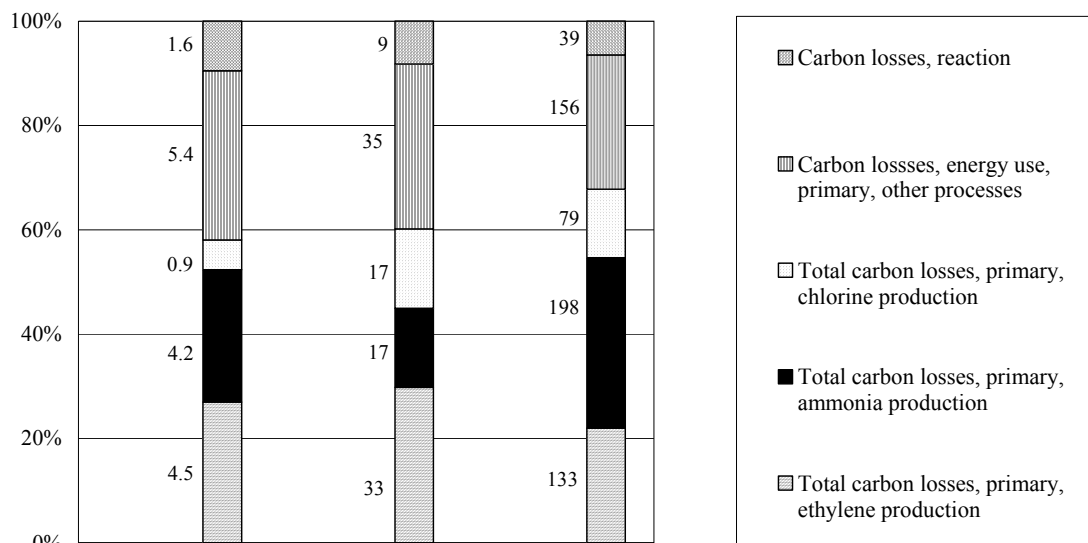
Figure 3.10 *Overview of cumulative total final carbon loss, primary (indicator 16), split into carbon losses, energy use, primary (indicator 14) and carbon losses, reaction (indicator 15). Ethylene, ammonia and chlorine production are given individually to show their major contribution to the totals. Ammonia emissions are corrected for sequestration in urea*

From Figure 3.9, the energy profile of the petrochemical industry becomes visible. First, petrochemical feedstocks (naphtha, gas oil, LPG, ethane) are converted into ethylene, propylene and aromatics in the endothermic steam cracking process[12]. We estimate the overall heat effect of reaction of the steam cracking process in Western Europe as –129 PJ (endothermic) per year in 2000. The endothermic reaction is sustained by burning 689 PJ$_f$ of fuels, leading to a total of 33 Mt CO$_2$ emissions. The total final energy loss in the steam cracking process is therefore estimated as 560 (=689 – 129 PJ) per year in 2000.

The heat effect of reaction of chlorine production, the other important endothermic reaction in Western Europe, is estimated as 62 PJ$_f$ per year in Western Europe in 2000. This reaction is sustained by supplying 131 PJ$_f$ per year of final energy (273 PJ$_p$ of primary energy), resulting, under the assumptions given in Appendix D, in a total of 17 Mt CO$_2$ emissions.

In the remainder of the chemical industry, heteroatoms are added to the double bonds in the olefins and aromatics in conversions that are almost all exothermic. The cumulative heat effect of reaction of these more downstream processes together is estimated as 342 PJ$_f$ (exothermic) per year in 2000 in Western Europe. The cumulative stoichometric heat of reaction in those processes only equals 204 PJ$_f$ per year in 2000 in Western Europe (Table 3.2). Therefore, more than 40% of the heat effect of reaction results from losses due to non-selectivity (138 PJ$_f$ per year = 342 – 204). Carbon losses resulting from these losses due to non-selectivity are estimated as 9.1 Mt CO$_2$ per year in Western Europe[13]. Rather than exporting energy as could be expected on basis of the stoichometric reactions, the processes are considerable energy consumers. Final energy use in ammonia production is estimated as 152 PJ$_f$ per year in Western Europe in 2000[14], resulting in a total of 33 Mt CO$_2$ emissions per year in 2000. The remaining processes have a final energy use of 497 PJ$_f$ per year (620 PJ$_p$ of primary energy), resulting in 35 Mt CO$_2$

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[12] Part of the aromatics and a small part of the propylene are also recovered in refineries and not via steam cracking.

[13] The emissions from ammonia and methanol production are excluded from this total.

[14] Excluding feedstock use, which we defined as the LHV of the ammonia product.

emissions. With the overall exothermicity of the desired stoichometric reactions given above (204 PJ_f), we can calculate the excess final energy use in those processes as 701 PJ_f (=497 + 204) of energy. In other words, the processes would *produce* 204 PJ_f of energy if they would run 100% according to the defined stoichometric reactions and without energy losses; in practice they *consume* 497 PJ_f.

The total final energy loss for all the processes equals 1620 PJ_f and the total primary energy loss equals 1894 PJ_p for Western Europe in 2000. The results clearly show that the heat effect and carbon losses of reaction contribute significantly to the overall energy loss and CO_2 emission of the chemical industry. These effects are often not explicitly addressed or quantified in overview studies on the chemical industry, but should be considered in order to get a proper overview of the energy use and energy saving and CO_2 reduction possibilities in the chemical sector.

3.5 Energy saving potentials

3.5.1 General directions for energy savings

We stressed already several times that it is beyond the scope of this study to go inside the black box of the processes studied and to study the actual energy saving potentials for the various processes in more detail, for example at the level of individual process units (reactors, separators etc.). We also stressed that our analysis is based on the first law of thermodynamics and does not distinguish between various qualities of energy like is done in for example exergy or pinch analysis. In this section, we will therefore only give general directions for energy saving possibilities without going into the details of specific processes, which would require a more detailed analysis taking into account more detailed characteristics such as temperature and pressure levels of the various flows within the process.

We analysed the *energy* content of the various flows into and out of the processes included in the model and defined the difference as the energy loss of a process. According to the first law of thermodynamics, energy cannot really be lost and the energy losses calculated in our analysis therefore equals the flow of waste heat from the processes to the environment in the form of cooling water, hot off-gases from furnaces etc. A first energy saving possibility is therefore to find a suitable use for this waste heat. In industrial practice, heat integration within and between processes is already common practice. In pinch analysis, for example, the heating and cooling requirements of individual process steps are balanced in such a way that the heating and cooling requirements of the total process are minimised. One limitation of heat integration between different processes is the resulting interdependency of the various processes. When one process shuts down (for maintenance or for other reasons), this also affects the energy system of the other process. Back-up facilities are in such a case required to avoid a shutdown of all integrated processes.

Whether or not waste heat can be used for applications such as heat pumps, heating of buildings etc. depends among other things on the temperature level of the waste heat flow to the environment. Without looking inside the processes, it is not possible to analyse the temperature of the waste heat disposal. Other studies (e.g. Carp and Bach, 2001 and Spoelstra et al., 2002) show that at least part of the waste heat becomes available at temperature levels suitable for such useful applications (exceeding 323 K). One example of such an application is the use of waste heat from the chemical industry for the heating of buildings as will be done in the Rotterdam area (Energiemanagement, 2004). This is an example of heat integration, which goes beyond the borders of individual processes, companies and industries. It might be an interesting option to locate industrial and municipal areas on basis of their waste heat availability and heat requirements. An example of such thinking is the co-siting program initiated in Rotterdam port area (Port of Rotterdam, 2005).

When we look at the individual processes we can conclude that only by looking at the *energy* balance of the process, the ultimate potential for *energy* savings in the processes analysed equals the calculated total *energy* loss. These potentials are purely theoretical, because they do not take into account thermodynamic, practical and economic limitations related to energy saving possibilities. Furthermore, the potentials identified are *energy* saving potentials, not taking into account aspects related to quality (entropy) of the various energy flows. We split the total energy losses of the processes into losses related to the chemical conversions and related to the energy use of the processes. We identified those processes having large losses due to non-selectivity (Section 3.2), a large excess final energy use (Section 3.3) and large total energy losses, being the sum of the two (Section 3.4). Both processes having large losses in relative terms (per tonne of product), and in absolute terms (in PJ / year or Mt CO_2 / year) are identified.

Based on the two types of energy losses distinguished in this study, we can also distinguish energy saving possibilities in two interlinked directions:
1. Improvements aiming at lowering the losses due to non-selectivity of processes.
2. Improvements aiming at lowering the excess final energy use of processes.

The two are interlinked, because improving the selectivity from raw materials to desired products might substantially change the process lay-out (pressure and temperature levels, separation requirements etc.), thereby influencing also the energy use of the processes. Furthermore it should be realised that improvements in the selectivity in the reactions decreases the raw material requirements, thereby also resulting in energy savings in the more upstream process to produce this raw material. Some examples of potential energy saving technologies are:
- *The use of (more selective) catalysts*
  Catalysts can help to increase the selectivity of a process towards the desired product, thereby reducing the losses due to non-selectivity. Catalysts can help to overcome kinetic limitations in processes, thereby increasing the degree of conversion per pass through the reactor, decrease the size of separation equipment etc. A good example of process improvements resulting from more selective catalysts is the production of ethylene oxide from ethylene. Molar selectivity increased from around 70% in the sixties to more than 80% nowadays (Lange, 2001).
- *Novel process routes*
  Another way to reduce both losses due to non-selectivity and excess final energy use is the shift towards completely other process routes, using other raw materials. As is shown by Lange (2001), past changes in raw material choice, often resulted in a lower heat effect of reaction, thereby also resulting in lower energy losses. Another option would be to make use of biomass raw materials or bioconversion technologies, such as enzymatic conversions and/ or fermentation. The potentials for such routes have been studied in several projects (see e.g. van Tuil et al., 2002 and Crank et al., 2004).
- *Novel process concepts such as membrane reactors or heat exchange reactors*
  At the level of individual process units (reactors, separators, etc.), various energy saving technologies are possible. Examples are the use of heat exchange reactors in which the functions of a chemical reactor and a heat exchanger are integrated (Hugill, 2003) and the use of membrane reactors in which the function of a chemical reactor and product separation are combined (van Dorst and van Veen, 2002).

3.5.2 Improvement potential from implementing Best Available Technologies

So far, we compared actual processes in place with theoretical processes according to the desired stoichometric reactions and without energy losses. For a limited amount of processes we also included Best Available Technique (BAT) processes (Appendix H). For those processes, we are able to calculate potentials for energy efficiency improvement of the average processes

compared to these BAT processes. By doing so, we get an idea of energy saving potentials already achievable by implementing BAT processes. We give an overview in Table 3.5.

Table 3.5 *Energy saving potential from implementing BAT processes in Western Europe*

Product[1]	Feedstock	Total final energy use, average	Total final energy use, BAT	Energy saving potential	Energy saving potential	Energy saving potential, WE, 2000
		GJ_f / tonne product	GJ_f / tonne product	GJ_f / tonne product	%	PJ_f / year
Ammonia	Natural gas	13.6	8.4	5.2	38	50
Ammonia	Oil	18.3	16.5	1.8	10	2
Ammonia	Coal	29.4	23.4	6.0	20	-
Ethylene	Naphtha	11.5	6.8	4.7	41	215
Ethylene	Gas oil	11.8	6.2	5.6	47	44
Ethylene	Propane	11.2	8.1	3.1	28	13
Ethylene	Ethane	17.7	11.1	6.6	37	8
Methanol	Natural gas	12.5	9.4	3.1	25	8

1. See footnote 9 and Appendix H for an explanation on how the ethylene, ammonia and methanol production are included in the mode.

It should be stressed that both the average final energy use figures used in our analysis and the BAT figures are subject to uncertainties of up to at least 10% (see also next section), making it difficult to draw robust conclusions about potentials for energy savings related to the implementation of BAT processes. If we, however, assume these examples to be representative for all processes included, we can conclude that the potentials for energy savings related to the difference between the final energy use in current average processes and in BAT processes ranges from 10 to 50% for small and large energy consumers respectively. [15].

3.5.3 Financial impact of energy saving potentials

The model contains also information on energy costs and on the prices of the various raw materials, products and by-products of the processes. We are therefore also able to convert the estimated theoretical energy saving potentials into financial units. For Western Europe in 2000, we estimated the total final energy loss to be 1620 PJ_f (Figure 3.9), consisting of an excess final energy use of 1482 PJ_f (Table 3.4) and losses due to non-selectivity of 138 PJ_f (Table 3.2). Using an energy price of 5 Euro / GJ and an ethylene[16] price of 13 Euro / GJ to convert these losses into financial units, we can estimate the total theoretical energy saving potential to be approximately 9 billion Euros in Western Europe. By analogy, worldwide and Dutch theoretical potentials are estimated at 48 billion and 1.4 billion Euros respectively. These figures show that the financial impact of even small energy efficiency improvements can be in the order of millions of Euros. It would, however, require more detailed techno-economic analyses to determine financial profitability (pay-back times etc.) of various energy saving technologies in more detail.

3.6 Discussion

In this paragraph, we will discuss the uncertainties in the results and we will relate our results to the energy use of the chemical industry as a whole as it can be found in international energy statistics and other studies. We will pinpoint shortcomings of our analysis and identify areas for

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[15] It would require more detailed analysis to define these potentials for more individual processes, which is beyond the scope of the current study.

[16] We use the price of ethylene as an approximation of the price of raw materials lost due to non-selectivity. We assumed an ethylene price of 593 Euro / tonne (based on Statistisches Bundesamt, 2001), which is equivalent to approximately 13 Euro / GJ, using a calorific value (LHV) for ethylene of 47.2 GJ / tonne. 1Billion Euros is 10^9 Euros.

further additional research. We will end the section with a general conclusion on how the results of this analysis should be regarded given the uncertainties involved.

3.6.1 Uncertainties in process data, production volumes and shares of production routes

The number of datasets available per process ranged from 1 to more than 10. In cases where more than one dataset was available, we selected the dataset most likely representing average Western European plants currently in place, a choice made on own insights. In cases were only one dataset was available, we used this dataset in the analysis without correcting for energy efficiency improvements. All process information is based on open literature rather than on highly energy-integrated chemical plants. For this reason, the results for the individual processes should be used with a significant uncertainty range. Based on the number of process datasets available and on the types of sources used, we marked with "1" in Appendix H those processes for which we estimate the final energy use data shown in Figure 3.3 to have an uncertainty of less than +/-10%. For the remaining processes, we estimate the uncertainty to be between +/-10 and +/-30% and marked those processes with "2" in Appendix H. The high uncertainty range of 30% is thought to be representative for process data based on single old source before 1990 (e.g. Chauvel and Lefebvre, 1989), which are marked with "3" in Appendix H.

We did not account for geographical differences in energy efficiency between and within the three regions included. Instead, we based all analyses on process energy data that are thought to be representative for Western Europe. However, we do take into account differences in the various process routes applied to produce a certain product (e.g. a larger fraction of ammonia produced from coal worldwide compared to Western Europe). Some insight in the ranges observed in practice can be obtained by looking at literature ranges for processes in place. For steam cracking to produce olefins, ranges of 15-25 GJ/tonne ethylene for ethane cracking, 25-40 GJ/tonne for naphtha cracking and 40-50 GJ/tonne for gas oil cracking are reported for European steam crackers (IPTS, 2003a). There is no clear indication that European steam crackers are clearly more energy efficient compared to the worldwide average (Phylipsen, 2000), so these ranges can also be regarded as indicative for the worldwide situation for this process. Since such comparative data are not available for most of the processes included, it is difficult to draw robust conclusions about the geographical differences in energy efficiency based on the current set of data.

The production volumes and the shares of the various process routes as they are included in the model in the year 2000 have been taken from various sources and are sometimes calculated using linear inter- and extrapolations using data from years close to 2000 and by applying default capacity utilisation factors (see Appendix E). It is hard to estimate the exact uncertainties resulting from the method used, but we have indications that the uncertainty in some of the production volumes might be in the order of about 10-20% and the uncertainties in the shares of the various process routes is in the order of about 5-10%[17].

3.6.2 Double counting of losses due to non-selectivity

As already mentioned in Section 3.2, some of the losses due to non-selectivity are in the form of non-valuable fuel grade by-products, often referred to as off-specs. These fuel by-products might be burned under the recovery of energy. This energy recovery might not be deducted from the energy use of the process, thereby resulting in double counting of energy use, both as losses due to non-selectivity and, once more, as final energy use. The same is true for carbon losses from reaction. From Table 3.2 and Figure 3.10 we can conclude that this double counting

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[17] We base this range on the capacity data and production volumes from different sources which are included in the model.

for Western Europe is maximally 138 PJ_f or 9 Mt CO_2/year on a total final energy loss and total CO_2 emissions of 1620 PJ_f and 111 Mt CO_2, approximately 8%. In reality, the double counting will be less, because in some of the processes (e.g. ethylene oxide production), the losses due to non-selectivity are the result of over-oxidation of the feedstock, leading to direct CO_2 emissions and to the formation of heat, which comes available within the process. Since we do not know the form of the losses due to non-selectivity for most of the processes included, it is difficult to estimate the amount of carbon and energy lost in the form of direct CO_2 and process heat within the process or via the intermediate production of non-valuable fuel grade by-products. We leave this exercise and the position of the non-valuable fuel-grade by-products in the energy statistics (see next section) as an area for further research.

3.6.3 Comparison with international energy statistics and other sources

We can compare the results for the total of all processes covered in this study with the energy use of the chemical sector as it can be found in the international energy statistics (IEA, 2002a and 2002b). We show this comparison in Table 3.6 and also show the relation with the total final energy loss shown in Figure 3.9. We split the final energy use into electricity, fuel and heat use to allow a better comparison.

Table 3.6 *Comparison of final energy use according to model calculations and the energy statistics for 2000 and relation to the total final energy loss as shown in Figure 3.9*

	Model PJ_f	Energy statistics 2000, PJ_f[1]	Coverage %	Final energy loss (Figure 3.9) PJ_f
The Netherlands				
Electricity	18	43	42	18
Fuels [2]	88	146	73	155
Heat	45	36		45
Feedstock [2]	298	306	97	-
Heat effect of reaction	-	-	-	32
Total	449	531	85	251
Western Europe				
Electricity	197	674	29	197
Fuels [3]	306	1337	42	987
Heat	285	58		285
Feedstock [4]	2246	2752	82	-
Heat effect of reaction	-	-	-	151
Total	3034	4821	63	1620
World				
Electricity	829	3131	26	829
Fuels [3]	3005	9194	43	5665
Heat	1452	1155		1452
Feedstock [4]	12379	14414	86	-
Heat effect of reaction	-	-	-	658
Total	17665	27894	63	8604

1. Energy statistics-data based on IEA (2002a and b).
2. Based on detailed information from Statistics Netherlands (2003), we allocated 24 PJ of the natural gas use in ammonia production to fuel use, the remainder of the input to feedstock use. 32 PJ of the fuel use in steam crackers is part of the decentral heat and power sector in the energy sector and is therefore excluded from fuel use and feedstock figures, 47 PJ of the fuel use in steam crackers is reported as fuel use, the remainder as feedstock use. 65 PJ of the feedstock use in steam crackers is in the international energy statistics reported as non-energy use of other petroleum products and is therefore deducted from the feedstock use.
3. The fuel use in olefin production is included in the feedstock use, except for 40% of the fuel use in ethane crackers, which are energy self-sufficient (9 PJ in Western Europe, 168 PJ Worldwide).
4. The feedstock use in ammonia and methanol production (defined as the LHV of the ammonia and methanol produced) plus the total raw material input into steam cracking minus the backflows to the refineries reported in the energy statistics (631 PJ in Western Europe; 1108 PJ worldwide).

The comparison is complicated by the unclear definition of feedstock use in the international energy statistics. In the steam reforming and steam cracking processes, the raw material (e.g. natural gas or naphtha) is used partly as feedstock and partly as fuel. The use as fuel can take place via either the intermediate production of fuel gas (steam cracking) or directly (e.g. natural gas in ammonia production). It is unclear from the outset which part of the raw material is reported as feedstock use and which part is reported as final consumption of fuels in the international energy statistics[18].

In Table 3.6, we tried to ensure consistency with the methodology chosen in the energy statistics. For the Netherlands, we used information available from the detailed national energy statistics. For the European and worldwide figures, we assumed a gross definition of feedstock use for olefin production (allocating the total input into the crackers to non-energy use, corrected for reported backflows to refineries) and a net definition of feedstock use for methanol and ammonia production (allocating only the calorific value of the products to feedstock use). Based on a detailed comparison on the level of individual fuels, this definition choice proved to yield the most reasonable results[19].

We can conclude that the processes included cover approximately 30% of the electricity use of the chemical sector (NL: 42%) and approximately 70% of the combined fuel and feedstock use in the chemical sector (NL: 88%). This energy coverage is consistent with other sources:

- According to DOE/OIT (2000), more than 50% of electricity use in the US is consumed in other sub-sectors of the chemical industry apart from the industrial organic industry (industrial gases, industrial inorganic chemicals excluding chlorine, phosphatic fertilisers) not covered in this analysis. In the Netherlands, the fertiliser industry (excluding ammonia), the inorganic basic chemical industry (excluding chlorine), the other basic chemical industry and the chemical products industry, which are not covered in this study, also consume approximately 50% of the chemical industry's electricity use (Statistics Netherlands, 2003).
- According to DOE/OIT (2000), 47% of total energy use in the US chemical industry is consumed in the drugs (6%), soaps/cleaners (3%), agricultural (9%), inorganics (25%) and other subsectors (4%), which are to a large extent not covered by our analysis.
- The heat reported in the international energy statistics only represents heat bought from third parties. The fuel reported under final consumption includes fuel used for direct fuel applications (e.g. in furnaces) as well as fuel used for steam generation, either in stand-alone steam boilers or in cogeneration plants, but excludes the amount of fuel used for the generation of electricity in cogeneration units, which should be reported in the energy conversion sector[20]. As a result, the fuel consumption figures in the energy statistics include losses in steam generation, which are not included in the dataset figures. The same is true for further losses in the steam system (see also Section 3.6.4).

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[18] These issues are currently being studied in a research project financed by the European Commission (NEU-CO$_2$, 1999-2006). In Neelis et al. (2003), the Dutch non-energy use accounting is discussed.

[19] When a net definition would have been applied for steam cracking, excluding the fuel use in the crackers, one would expect a major final use of chemical rest gas in the chemical industry. This is indeed the case for the Netherlands (where a net definition is applied), but not for many other countries.

[20] This practice raises the question of how the fuel input in auto-producer CHP plants is allocated to the electricity and heat produced. In the electricity and heat survey, the countries are asked to use national methodologies. In cases, where an adequate national method is lacking, it is recommended by the IEA to allocate the input between electricity and heat in proportion to the energy content of the heat and electricity produced (IEA, 2003). This latter method leads to steam generation efficiencies equal to the overall efficiency of the cogeneration units, which is in the European Union 72% on average in the chemical industry (Table 3-7). When we apply this efficiency to the steam generated in CHP plants (Table 3.7) we can conclude that the final fuel use according to the energy statistics includes 136 PJ of energy lost in steam generation. Deducting this amount from the reported final fuel use would lead to a coverage of 47% in Western Europe.

- In the Netherlands, the basic chemical industry is relatively important compared to other subsectors in the chemical industry, which can at least partly explain the higher coverage for the Netherlands[21].

In view of the shortcomings and uncertainties involved in both our model and the international energy statistics, we consider our results of total final energy use to be consistent with energy statistics and other reports and leave further bottom-up comparison between datasets from open literature and international statistics as an area for further research.

The estimates for energy and carbon losses in the chemical industry as summarised in Figure 3.9 and Figure 3.10 are consistent with the very few other sources that could be found in literature. In Tonkovich et al. (1995), the carbon losses from reaction in the US Chemical industry in 1992 were for a comparable set of processes calculated to be equivalent to 9.5 Mt CO_2, which is in the same order as the calculated losses for Western Europe in this study (9 Mt CO_2). Since the US and Western European chemical industry are comparable in size, this is consistent with our study. For Flanders (Belgium), CO_2 emissions from non-valuable by-products (excluding steam cracking) are estimated to be 1-1.5 Mt CO_2 (Theunis et al., 2003), which is in the same order as the calculated carbon losses of reaction (1.6 Mt CO_2) for the Netherlands, having a chemical industry comparable in size.

As explained in Section 3.5, energy cannot really be lost according to the first law of thermodynamics, and the energy losses summarised in Figure 3.9 can therefore be regarded as estimates for the total disposal of waste heat into the environment. For the US Chemical industry, a total waste heat disposal of 2100 PJ is mentioned in Vision 2020 (2004), although based on an old source from the early eighties. This is in the same order as the total energy loss in Western Europe calculated in this study (1620 PJ_f). A bottom-up survey in the Dutch chemical industries identified a waste heat potential at temperature exceeding 323 K of 53_f PJ / year for the Dutch organic chemical industry (Carp and Bach, 2001). This is approximately one fifth of the total amount of waste heat (indifferent of temperature) calculated in this study (251 PJ_f).

3.6.4 Uncertainties related to the production of electricity and steam

The main focus of this study is on final energy use, excluding losses due to the production and transport of electricity and steam. We calculated in a simplified way the CO_2 emissions from steam and electricity using the conversion factors to primary energy use and the emission factors given in Table D.1 of Appendix D. In practice, a considerable fraction of the heat and power used in the chemical industry is produced in combined heat and power (CHP) plants rather than is separate systems. An overview of key data is presented in Table 3.7.

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[21] According to CEFIC (2004), the basic chemical industry accounted for 38% of the sales in the chemical industry in 2003, whereas this percentage was 60% in the Netherlands.

Table 3.7   *Combined heat and power generation in the Dutch and EU-15 chemical industry*

Row no.		Unit	NL[1]	EU[2]	Formula[3]
1	Fuel input into CHP units	PJ	143	781	-
2	Electricity production	PJ	37	215	-
3	Heat production	PJ	78	350	-
4	Power to heat ratio	-	0.47	0.61	2/3
5	Overall efficiency	%	80	72	(2+3)/1
6	Total final consumption of electricity[4]	PJ	43	636	-
7	Maximum fraction of CHP electricity in electricity consumption	%	86	34	2/6
8	Total consumption of fuels/heat[4]	PJ	182	1359	-
9	Minimal fraction of CHP heat in total fiels/heat consumption[5]	%	43	26	3/8

1. Data for the Netherlands from Statistics Netherlands (2004).
2. Data for the European Union from Loesonen (2004).
3. Numbers refer to the row numbers given in the first column.
4. Data for the European Union differ from Table 3.5, because Switzerland and Norway are excluded to allow a fair comparison with CHP data.
5. See text for further explanation.

The fraction of the electricity consumption that is produced in CHP plants as it is derived in the table represents a maximal value, since part of the auto-produced electricity might be sold back to the grid. For comparison, the share of auto-produced electricity in the total consumption of electricity in the US chemical industry in 1994 was 22% (DOE/OIT, 2000). The share of heat produced in CHP plants on the other hand represents a minimal value, since the total final fuels/heat consumption according to the international energy statistics also include conversion losses resulting from the production of heat in CHP unit units. If we assume all countries to equally divide the conversion losses in proportion of the electricity and heat produced, the percentage for the Dutch chemical industry would go up to 48%.

Producing electricity and heat with CHP units having the efficiencies given in Table 3.7 results in primary energy savings of 26 PJ_p for the Netherlands and 86 PJ_p for the European Union compared to producing the same electricity and heat according to our reference case of separate generation with efficiencies of 45% (electricity) and 90% (heat), see Appendix D. The comparison between the Netherlands and the European Union shows that there is room for energy savings from further penetration of CHP in the European Union and most probably also worldwide. Increasing the amount of electricity produced by CHP units in the European Union to 547 PJ_e (equal to the Dutch share of 86%), thereby using CHP units having the same overall efficiency (72%) and power to heat ratio (0.61) as the CHP units installed in 2000 in the European Union would lead to primary energy savings of 125 PJ_p compared to producing the same heat and electricity separate with efficiencies of 45% (electricity) and 90% (heat).

Another element not addressed in this study are losses in the steam system. According to Patel (2003), losses in the steam system are assumed to be 7.5%. In Vision 2020 (2004), distribution losses of 9% are reported. Studying those elements of energy loss is beyond the scope of the current study and we leave it as a area of further research.

3.6.5   Conclusion – how to use the results of this study given the uncertainties involved

The purpose of the analysis was to show the structure and breakdown of energy use and CO_2 emissions in the chemical industry for the processes included in the model. Based on the comparison with the energy statistics and with other available sources, we are confident that we have been able to do so. At the same time, we do realise that the uncertainties in our results are

large. Uncertainties result from the limited availability of up-to-date process data and data on production volumes and from the simplifying assumptions made for the production of electricity and steam. In this section, we have tried to quantify some of the uncertainties involved. Users of this report and of the model should take these uncertainties in the process data and the basic assumptions made with respect to electricity and steam generation into account, especially when using results for the individual processes included in the model.

4. Results for the refinery industry

4.1 Overview of the Chapter

In this Chapter, we present an overview of the process indicators introduced in Table 2.1 for the processes included in the model. The numerical values for all indicators shown in this chapter are given in Appendix I. As with the chemical industry, we first look at the effects of the reactions taking place (Section 4.2) followed by an analysis of the energy use of the processes included (Section 4.3). An overview of total energy losses and CO_2 emissions is presented in Section 4.4. Directions for energy saving possibilities are presented in Section 4.5, followed by a discussion of the results in Section 4.6.

4.2 Heat effect and carbon losses of reaction

In a petroleum refinery, crude oil is first separated into various fractions in the primary and vacuum distillation units. These processes are separation processes rather than processes involving chemical conversions. The concept of an idealised reaction (for use in indicators 1, 10 and 11) is therefore irrelevant for these processes.

In the subsequent process steps of the refinery, the various fractions are upgraded and blended to get the desired refinery output. To quantify the heat effects of the multiple reactions taking place in these conversions, one would need detailed information on the energy content of all refinery flows. As explained in Section 2.2.2, this information is not readily available from the literature sources. This is in contrast with the well-defined pure compounds used and produced in the processes in the chemical industry. It was therefore not possible to analyse the differences in energy content between feedstock and product flows for the refinery processes with reasonable accuracy based on the process descriptions found in literature and we will therefore not present an analysis as in Section 3.2.

The reactions involved are the rearrangement of the hydrocarbon molecules (cracking, isomerisation, polymerisation etc.) and the removal of small amounts of impurities like sulphur. The heat effects of these reactions per unit of feedstock are generally moderate (less than 3 GJ / tonne) compared to some of the processes in the chemical industry involving for example oxidation reactions (e.g. 10 GJ / tonne for acrylonitrile, compare Figure 3.1 for absolute values). An exception is the recovery of sulphur from hydrogen sulphide (overall reaction: $H_2S + \frac{1}{2} O_2 \rightarrow H_2O + S$). This is a clearly exothermic process with an overall heat effect of reaction of +6.9 GJ_f / tonne of sulphur. Other exothermic processes are hydrotreating and hydrocracking. The reactions involved in these processes are hydrogenations of heteroatoms such as nitrogen and sulphur and the hydrogenation of some of the double bonds. Alkylation (formation of higher branched alkanes from alkenes and isobutane) and isomerisation (formation of higher branched alkanes from linear alkanes) are other examples of exothermic processes.

Thermal cracking, catalytic cracking, catalytic reforming and coking are endothermic processes. In catalytic cracking, the necessary heat to sustain the endothermic reaction is generated by burning the coke, which is formed on the catalyst, making the overall heat effect of reaction (defined as calorific value of process inputs – outputs) exothermic. Per tonne of throughput, depending on the feedstock used, between 5 and 13 mass % of coke is formed (van Oostvoorn et al., 1989), resulting in $0.16 - 0.22$ ton of CO_2 per tonne of feedstock (IPTS, 2003b). Together with hydrogen production, catalytic cracking is the only process leading to significant carbon losses resulting from the overall reaction. Similar heat integration is performed in fluid and

flexicoker units, where part of the cokes formed is gasified. In this process, a very low calorific fuel gas is formed which is used elsewhere as fuel.

Petroleum refineries are to a large extent energy self-sufficient and are, as such, good examples of energy integration, where low value by-products of certain processes are used as fuel in other processes.

Examples of these low-value by-products are refinery gas, propane and butane, which are produced in atmospheric distillation (~2 wt. %), catalytic cracking (~20%), catalytic reforming (~10%), hydro cracking (~10%), thermal cracking (~5%) and coking (~10%). Another fuel used is heavy fuel oil produced in e.g. the thermal processes.

4.3   Energy use

We plot the final energy use in the refinery processes as a function of the Western European process volume in Figure 4.1. Process volume is defined as tonne of product for alkylation, isomerisation, lubricants and sulphur recovery and per tonne of feedstock for the other processes.

We did not show the production of hydrogen (final energy use of 21.7 GJ_f / tonne of hydrogen, excluding feedstock use) to improve the readability of the figure.
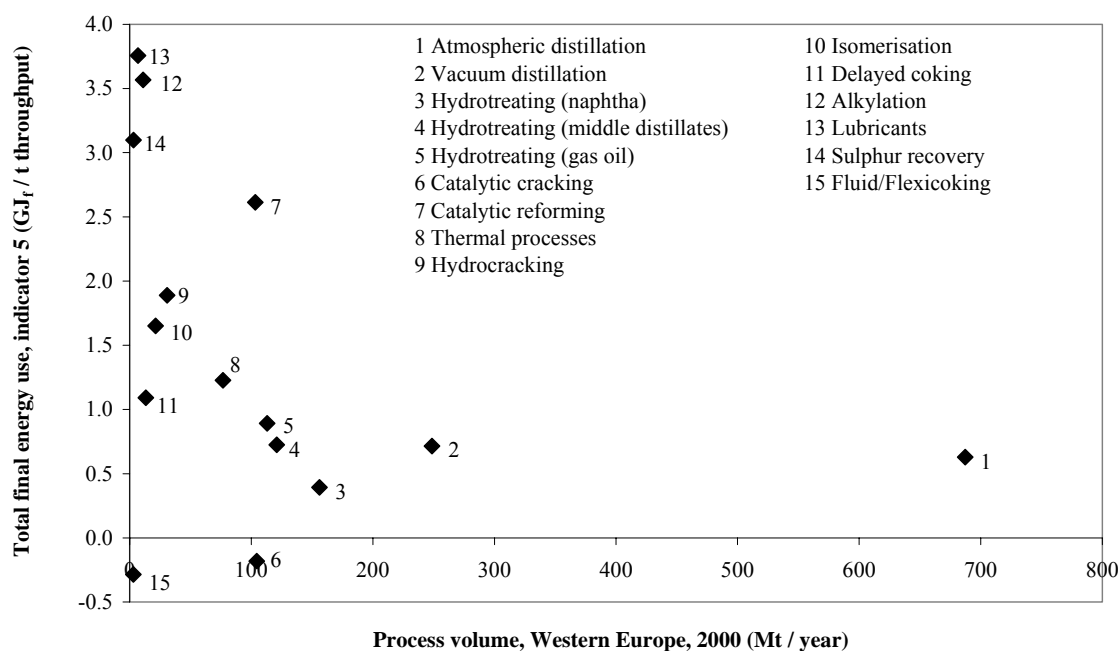
Figure 4.1   *Total final energy use (indicator 5) as a function of the Western European process volume in 2000*

Compared to the processes in the chemical industry, the refinery processes have a much lower total final energy use (compare Figure 3.3). Two processes (Fluid/Flexicoking and catalytic cracking) are net exporters of energy in the form of steam. It should be realised, however, that these are also the only two processes in which part of the process output (the cokes formed) are burned as inherent part of the process lay-out and are therefore also two processes with a significant exothermic heat effect of reaction, which could not be quantified for the reasons explained in the previous section.

4.4 Total energy use and CO_2 emissions

Due to the large process volumes in the refinery industry, the total final energy use in the refinery industry is comparable to the chemical industry, despite the lower specific final use of the processes. The absolute figures for total final energy use and total final CO_2 emissions are given in Figure 4.2 and Figure 4.3. Since we were unable to derive heat effects of reaction in an accurate way, we did not include them in the figure. These reaction effects are much lower compared to the chemical industry and we therefore expect these effects to be of less importance compared to the chemical industry (compare Figure 3.9 and Figure 3.10). The processes included account for a total final energy use of 1555 PJ_f in Western Europe in 2000. Heat is far more important than electricity (heat to power ratio approximately 20:1). The total primary energy use equals 1654 PJ_p (NL: 145 PJ_p; World: 8843 PJ_p), using the conversion efficiencies given in Appendix D.
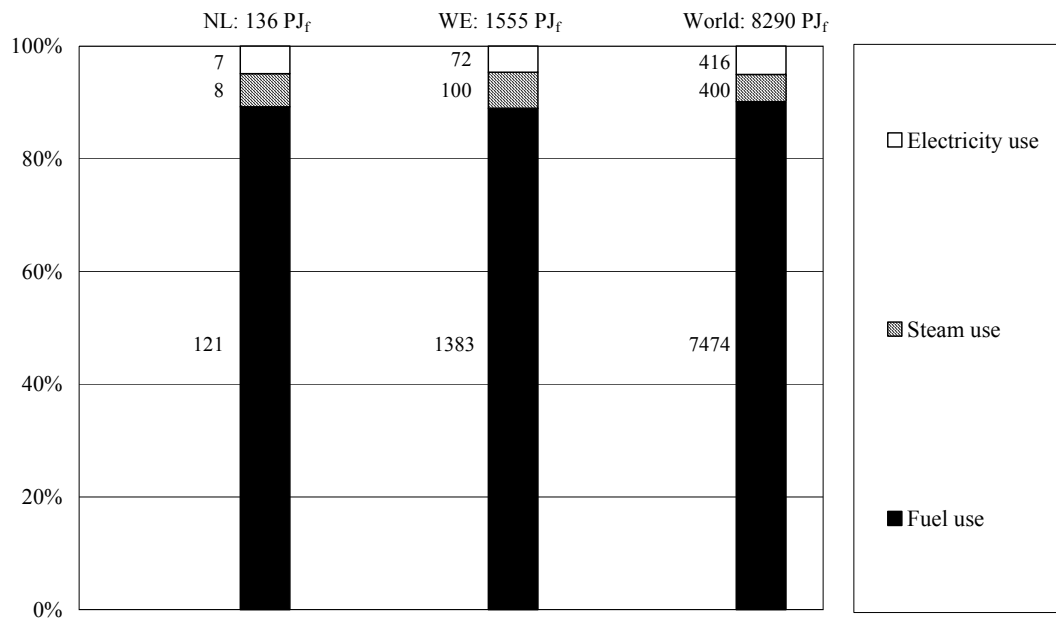
Figure 4.2 *Overview of the cumulative total final energy use, split into fuel, steam and electricity use. Fuel use includes the total input into hydrogen production, including the feedstock use*
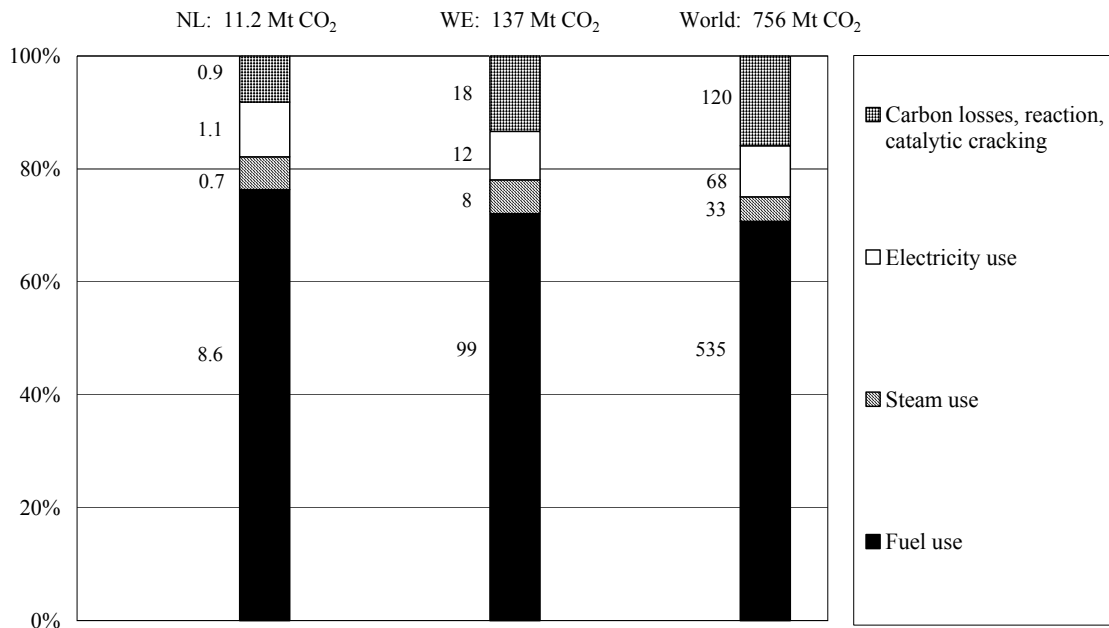
Figure 4.3 *Overview of cumulative total CO_2 emissions, split into fuel, steam and electricity use and the emissions from catalytic cracking. Total emissions from hydrogen production are included under fuel use*

The overview of CO_2 emissions shows comparable results. Total CO_2 emissions of the refinery industry in Western Europe in 2000 are estimated at 137 Mt with fuel and steam (including hydrogen production) contributing 78%, electricity 9% and the direct CO_2 emissions from catalytic cracking 13%. The contribution of the individual processes to the total energy use is shown in Figure 4.4.
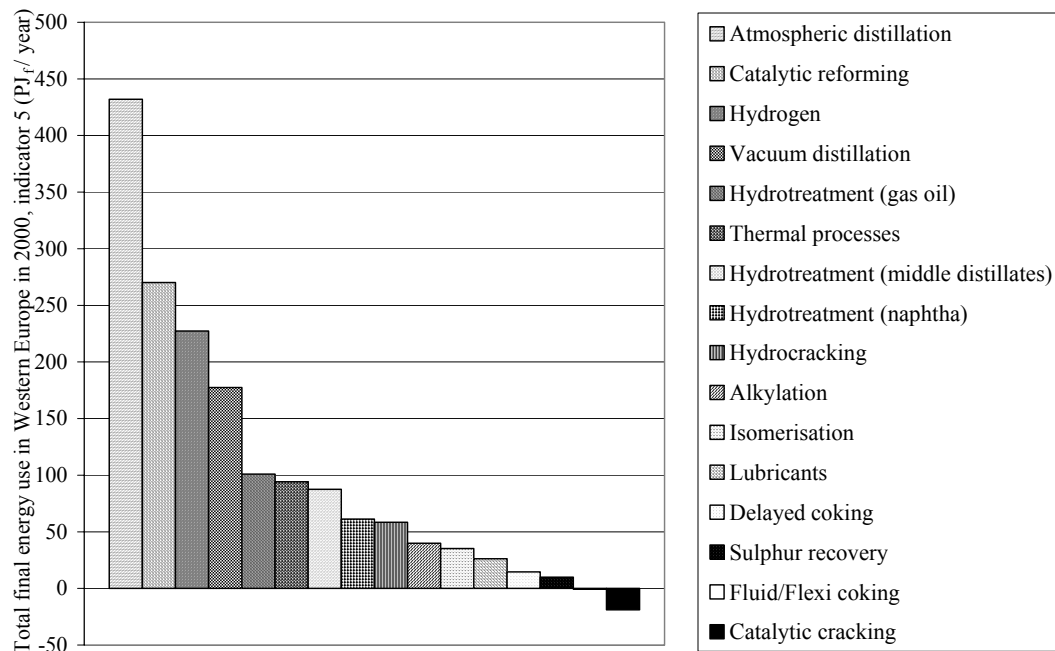
Figure 4.4 *Total final energy use (indicator 5) in Western Europe in 2000 for the processes included in the analysis, ranked in the order of decreasing total final energy use. The figure for hydrogen includes the total fuel input into the process, including the feedstock use*

Atmospheric distillation of crude oil, despite having a final energy use of only 0.6 GJ$_f$ per tonne of crude oil input, consumed as much as 0.43 EJ$_f$ of energy in Western Europe in 2000, which is more than any of the chemical process included in this analysis.

4.5   Energy saving potentials

The general remarks made and general directions for energy savings given for the chemical industry in Section 3.5 are also valid for the refinery industry. We analysed the processes as black boxes, just looking at the energy flows into the processes and did not take into account differences in quality of energy, as is done in for example exergy or pinch analysis. Since according to the first law of thermodynamics, energy cannot really be lost, the energy use as calculated equals the flow of waste heat to the environment[22]. The overview presented can be used to select those processes with large potentials for energy savings in relative and / or absolute terms, but without going inside the black boxes of the various process units analysed, it is hard to make more specific recommendations taking into account thermodynamic, practical and economic considerations of various energy saving possibilities.

4.5.1   Financial impact of energy saving potentials

Using the energy prices of 5 Euro / GJ for fuels, 5.5 Euro / GJ for steam and 19 Euro / GJ for electricity given in Appendix D, we estimate the total energy costs of the Dutch, Western European and worldwiderefinery industry in 2000 at respectively 0.8, 8.8 and 47.5 billion Euros, using the estimates for fuel, steam and electricity use given in Figure 4.2. These figures show that already very small energy savings in relative terms (e.g. 1%) can have financial impacts in the order of millions of Euros. It would, however, require more detailed techno-economic analyses to determine financial profitability (pay-back times etc.) of various energy saving technologies in more detail.

4.6   Discussion

In this paragraph, we will discuss the uncertainties in our results and we will relate our results to the results from other available sources. We will end the section with a general conclusion on how the results of this analysis should be regarded given the uncertainties involved.

4.6.1   Uncertainties in process data, production volumes and shares of production routes

In this report, we presented a rather simple overview of a petroleum refinery in which we distinguished only 16 different processes and only a very limited amount of different refinery flows. The actual process characteristics heavily depend on site-specific conditions such as the type of crude oil used, the fractions of the various petroleum products in the refinery output and the sulphur fractions allowed in these outputs. According to van Oostvoorn et al. (1989), for example, the type of crude oil uses influences the energy requirements of the atmospheric distillation unit by approximately +/-25%. Based on an analysis of all process datasets available, we regard this as a suitable uncertainty range for the figures used in our analysis.

As with the chemical industry, we are unable to assess geographical difference in energy efficiency based on the current set of data. International comparison of refineries is difficult, because of the incomparability of individual refineries (Phylipsen et al., 1998).

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[22] We neglected the heat effects of the reactions taking place, which are assumed to be small (Section 4.2).

The process volumes of the various processes included in the model for 2000 are based on one single data source with capacity data that already take into account regular scheduled downtime of refineries (Oil and Gas Journal, 1999). Shares of the various process types were taken from various sources like (IPTS, 2003b). It is difficult to estimate the uncertainty in the resulting figures, but we expect the uncertainties to be in the same range as the ones derived from the chemical industry (i.e. between 10 and 20% for the process volumes and between 5 and 10% for the shares of the various process routes).

4.6.2 Comparison with international energy statistics and other sources

We compare the results for the total of processes with the energy use according to the international energy statistics in Table 4.1. The processes included in our analysis cover approximately 70% of the electricity use in the refineries and approximately 80% of the fuel/steam use (Table 4.1). The comparison is complicated by the limited reliability of the energy statistics, which becomes most visible in the row transformation losses. This row can include for example coke burning in catalytic cracking and flaring of refinery gas. However, the system boundary between losses and final energy use is difficult to make (e.g. the energy from burning coke is not lost, but used within the process). Surprisingly, the transformation losses for the Netherlands and Western Europe are negative (i.e. more energy is produced than consumed), which might be the result of uncertainties in heating values used within the international energy statistics. As was the case in the chemical industry, the final energy use figures in the energy statistics include losses in steam generation, which can partly explain the somewhat low coverage[23]. In view of the shortcomings and uncertainties involved in both our model and the international energy statistics, we are satisfied with these results and leave further bottom-up comparisons between datasets from open literature and international energy statistics as an area for further research.

Table 4.1 *Comparison of final energy use between the datasets and the energy statistics*

	Model PJ$_f$[1]	Energy statistics 2000, PJ$_f$[2]	Coverage %
The Netherlands			
Electricity	7	9	72
Fuels [3]	121	171	76
Heat	8	0	
Transformation losses	-	-26	-
Total	136	154	88
Western Europe			
Electricity	72	95	76
Fuels [2]	1383	1585	93
Heat	100	2	
Transformation losses	-	-139	-
Total	1555	1544	101
World			
Electricity	416	621	67
Fuels [2]	7474	9306	80
Heat	400	503	
Transformation losses	-	1455	-
Total	8290	11885	70

1. The total final energy use can be seen as an approximation of total final energy loss if we assume the overall effect of the reactions taking place to be small, see Section 4.2.
2. Energy statistics based on IEA (2002a and b).
3. Including feedstock use for hydrogen production (NL: 16 PJ; WE: 141 PJ; World: 720 PJ).

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[23] As explained in footnote 14, the default method suggested by the IEA to allocate the fuel input into CHP units to steam and electricity leads to steam generation efficiencies equal to the overall efficiency of the cogeneration units, which is in the European Union 76% on average in the chemical industry (Table 4-2). When we apply this efficiency to the steam generated in CHP plants (Table 4-2) we can conclude that the final fuel use according to the energy statistics includes 73 PJ of energy lost in steam generation. Deducting this amount from the reported final fuel use would increase the coverage to 98% in Western Europe.

As already stated in Section 4.5, the final energy use as calculated with our model equals the amount of waste heat disposed to the environment. We are unable to estimate the temperature level of this waste heat disposal given the level of detail of our analysis. A bottom-up survey in the Dutch refinery sector identified as total waste heat potential at temperatures exceeding 323 K of 44 PJ_f / year (Carp and Bach, 2001). This is approximately one third of the total amount of waste heat (indifferent of temperature) calculated in this study (136 PJ_f).

4.6.3 Uncertainties related to the production of electricity and steam

Similar to the chemical industry, we focussed our analysis on the final energy use figures so far and did not pay much attention to the energy conversion steps. We disregarded the combined production of heat and power, which is a well-established technology in the refinery industry and assumed separate production of heat and power instead. We present an overview of combined heat and power generation in the refinery industry in Table 4.2.

Table 4.2 *Combined heat and power generation in the Dutch and EU-15 refinery industry*

Row no.		Unit	NL[1]	EU[2]	Formula[3]
1	Fuel input into CHP units	PJ	51	451	-
2	Electricity production	PJ	11	109	-
3	Heat production	PJ	33	232	-
4	Power to heat ratio	-	0.33	0.47	2/3
5	Overall efficiency	%	86	76	(2+3)/1
6	Total final consumption of electricity[4]	PJ	9	93	-
7	Maximum fraction of CHP electricity in electricity consumption[5]	%	122	117	2/6
8	Total consumption of fuels/heat[4]	PJ	171	1542	-
9	Minimal fraction of CHP heat in total fiels/heat consumption[5]	%	19	15	3/8

1. Data for the Netherlands from Statistics Netherlands (2004).
2. Data for the European Union from Loesonen (2003).
3. Numbers refer to the row numbers given in the first column.
4. Data for the European Union differ from Table 3.5, because Switzerland and Norway are excluded to allow a fair comparison with CHP data.
5. See text for further explanation.

CHP plants installed at refineries even produce more electricity than consumed within the refinery, both in the Netherlands and in the European Union as a whole. Producing electricity and heat with CHP units having the efficiencies given in Table 4.2 results in primary energy savings of 10 PJ_p (the Netherlands) and 49 PJ_p (European Union) compared to producing the same electricity and heat according to our reference scenario of separate generation. As with the chemical industry, we leave the analysis of the total energy system (including conversion losses) for total refineries as an area for further research.

4.6.4 Conclusion – how to use the results of this study given the uncertainties involved

The aim of this study is to show the structure and breakdown of energy use and CO_2 emissions in the refinery industry. As for the chemical industry, we are confident that we have been able to do so, based on the comparison with the international energy statistics. At the same time we realise that we analysed the refinery in a rather simplified way by just looking at 16 different processes. Therefore and because of the limited availability of up-to-date process data, the uncertainties in our results are large. Furthermore, we made assumptions with respect to the production of electricity and steam, which are simplification compared to the actual practice in the refinery industry. In this section, we tried to quantify the uncertainties. Users of this report

and of the model should take these uncertainties and the assumptions made into account, especially when using results for individual processes in a model.

5. Conclusions and recommendations

5.1 Conclusions

We presented an analysis of the structure and breakdown of energy use and CO_2 emissions in the chemical and refinery industry based on process data from open literature.

We used a spreadsheet model containing process datasets for 68 production processes for the production of 51 of the most important organic chemicals in terms of production volume, complemented with the two inorganic gases ammonia and chlorine. For the refinery industry, 16 of the most important processes are included. For each of the process datasets, data on raw materials, products and by-products and data on the energy use of the process is included. With the model we are able to make energy and carbon balances of the processes and to calculate various indicators relevant with respect to energy and carbon efficiency. Only first law contributions are considered. Evaluations as to the value (exergy) of heat streams are beyond the scope of this report.

The processes are analysed as black boxes, i.e. we only look at the in- and outgoing of the process, without analysing the individual process units (reactors, separation equipment etc.).

The model also contains production figures of the chemicals included and throughput volumes of the refinery processes for the Netherlands, Western Europe and the world in 2000. The processes cover approximately 70% of the total final energy use in the chemical and refinery industry according to international energy statistics. We therefore conclude that our model is quite comprehensive and at the same time allows conducting quite detailed analyses at the level of individual processes.

5.1.1 Chemical industry

For the processes analysed in the chemical industry, we quantified both the heat effects of the chemical reactions (defined as the calorific value of raw materials minus the calorific value of the products and by-products of a process) and the energy use. The sum of reaction effects and energy use equals the difference between energy flows into and out of the process and therefore equals the total energy loss of the process (i.e. the amount of waste heat to the environment). The total final energy loss in Western Europe in 2000 for all processes together was estimated as 1620 PJ_f and total CO_2 emissions were estimated as 111 Mt CO_2.

Three processes (ethylene, ammonia and chlorine production), contribute about half of this total. Energy loss in the production of ethylene is 560 PJ_f. In this process, 689 PJ_f of fuels are used, but 129 PJ_f of this is converted into chemical energy (the reaction is endothermic). Chlorine production is analogous. The process uses 131 PJ_f (mainly in the form of electricity), but 62 PJ_f is converted to chemical energy and the total energy loss therefore equals only 69 PJ_f. Total energy loss in ammonia production is 152 PJ_f. The total energy loss in the sum of all the other processes is 839 PJ_f. In these processes, which are mainly exothermic, the total heat effect of reaction is 342 PJ_f and on top of that, the processes use 497 PJ_f of energy. We can therefore conclude that the heat effect of reaction, which is often not explicitly addressed in overview studies of the chemical industry, is an important part of the total energy loss of the process.

The ultimate energy saving potential of the processes analysed equals the total final energy loss of the process and equals the amount of waste heat disposal to the environment. We split the total loss into undesired reaction losses and excess final energy use by comparing the actual heat

effect of reaction and energy use with the heat effect of the desired stoichometric reaction from raw materials to products. For the majority of processes the excess final energy contribution is the largest.

The comparison of the actual heat effect of reaction with the heat effect of the desired stoichometric reactions results in an estimate of total losses due to non-selectivity. The cumulative heat effect of the desired stoichometric reaction, excluding ethylene, chlorine and ammonia production, is 204 PJ_f. Since the actual heat effect of reaction is 342 PJ_f, we can estimate the total losses due to non-selectivity as 138 PJ_f, which is 40% of the observed heat effect of reaction. These losses due to non-selectivity result in a total of 9 Mt CO_2 emissions, either in the form of direct CO_2 emissions or indirectly via the formation of non-valuable fuel-grade by-products. This is approximately 8% of the total CO_2 emissions of the processes included (111 Mt CO_2). The remainder of the CO_2 emissions result from the energy use of the processes. If the total heat effect of the desired stoichometric reaction would be exported from the process to be used elsewhere, these processes would export 204 PJ_f of energy. Instead, they use 497 PJ_f of energy. The excess final energy use in these processes therefore equals 701 PJ_f. Following the same argumentation, the theoretical excess final energy use in ethylene, chlorine and ammonia production is calculated as 560, 152 and 69 PJ_f respectively.

We identified processes with large energy losses per tonne of product (relative units) and in PJ_f / year (absolute units). Examples of processes having large losses due to non-selectivity in PJ_f / year are acrylonitrile, ethylene oxide and caprolactam production from cyclohexane, which all have losses due to non-selectivity of approximately 15 PJ_f / year. Processes with a large excess final energy use are, besides the three processes already mentioned, also polyethylene production (69 PJ_f), aromatics production from pyrolysis gasoline (49 PJ_f), vinylchloride (39 PJ_f), methanol production from natural gas (36 PJ_f) and adipic acid production (32 PJ_f).

Considering the processes for which a Best Available Technology is known, the yearly energy saving potential in Western Europe ranges from 10 to 50% for small and large energy consumers respectively.

The processes mentioned could be selected for further analyses to identify actual saving potentials taking into account no only theoretical, but also thermodynamic, economic and practical considerations. This would require more in depth studies at the process unit level (reactors, separation equipment) in which also aspects related to the second law of thermodynamics should be taken into account. In our study, we gave some general directions for energy savings such as the use of the waste heat available from the various processes, the use of (more selective) catalysts to reduce losses due to non-selectivity, the use of totally new process routes based on biomass or via biotechnological conversions (enzymatic or fermentation) or the use of novel process concepts such as membrane or heat exchange reactors.

5.1.2 Refinery industry

For the processes in the refinery industry, we did not quantify the heat effects resulting from the chemical reactions in the refinery, because the calorific values of the various flows mentioned in the process datasets could not be estimated with reasonable accuracy. However, since most of the chemical reactions within the refinery are reactions in which hydrocarbon molecules are rearranged (cracking, isomerisation, alkylation etc.), we expect the heat effects in these processes to be lower than the ones found in the chemical industry involving for example oxidation reactions. We did quantify the energy use of the processes. The total final energy use of the processes analysed in 2000 in Western Europe is 1555 PJ_f with fuels and heat contributing 95% and electricity only 5%. Total CO_2 emissions of the processes are estimated to be 137 Mt CO_2. We ranked the processes in the order of decreasing energy use and showed that atmospheric distillation consumes by far the most energy of all processes included (430 PJ_f),

followed by catalytic cracking (270 PJ_f), hydrogen production (227 PJ_f, including feedstock) and vacuum distillation (177 PJ_f).

5.2 Recommendations for further research

We presented an analysis of the structure and breakdown of energy use and CO_2 emissions in the refinery and organic chemical industry. We thereby used a model in which the processes were regarded as black boxes. We refer to this as a *meso*-level of analysis. Summation over all processes yields results for the chemical and refinery industry as a whole, i.e. at a *macro*-level. In our model, we do not look inside the black boxes at the level of process unit operations (reactors, separation equipment etc.), which we refer to as analysis at the *micro*-level. The analysis presented here can be used for further research at all of the three levels. Below we give some recommendations for research directions.

In order to specify actual energy saving potentials, taking into account practical, economic and thermodynamic limitations, it is necessary to extend the analysis as performed in this study to the *micro*-level. The processes with large theoretical energy saving potentials as identified in this study (see the previous section and the result chapters) could be selected for this kind of analysis. Among the data requirements for such *micro*-level analysis are data on the temperature and pressure level of the various flows, data on the performance of the various unit operations such as reactors, heat exchangers etc. This kind of information could be stored within the model, which we applied in this study, but can also be done independent of this model. Such analyses at the micro level should link up with existing literature on energy saving potentials at the process unit level rather than at the process level such as the Icarus database (Alsema and Nieuwlaar, 2001) and various ECN reports (e.g. van Delft et al., 2001 and van Veen et al., 2001). Based on such micro level analyses, it might be possible to identify interesting combinations of processes or industries with respect to heat integration (e.g. locating a paper factory with a large demand of low temperature heat next to a chemical process disposing waste heat of this temperature).

Various possibilities are available to improve and extend the model at the *meso* and *macro*-level. Examples are:
- Reducing the uncertainties in the results by finding more process data. The detailed data required to more fair international comparisons on energy efficiency are for example currently not available. Generally, the availability of process data from open literature is rather limited (compared to e.g. the steel industry). It might be worthwhile trying to improve this data situation, e.g. by cooperation with organisations like the European Chemical Industry Council (CEFIC).
- Inclusion of production volumes for several more countries or regions, allowing to estimate energy losses in more separate countries or regions.
- Inclusion of a more sophisticated model section (e.g. various scenarios) for the production of electricity and steam, which are currently modelled in a rather simple way.
- Using the financial variables included in the model to analyse the financial performance of processes.
- Including time-dependant variables into the model such as production volumes over time, energy efficiency improvements over time etc. In doing so, a dynamic model of energy use in the chemical industry could be made, analysing past and projecting future energy demand and CO_2 emissions.
- Coupling the data for various processes to get life cycle energy use and CO_2 emission data for various chemicals such as polymers. Since we quantified both energy use and reaction losses, these could also be separately identified in the life cycle data, which could be a worthwhile addition to conventional Life Cycle Analysis (LCA).

References

Alsema, E.A. and E. Nieuwlaar (2001): *ICARUS-4. A Database of Energy-Efficiency Measures for the Netherlands, 1995-2020*. Utrecht Centre for Energy Research / Deptartment of Science, Technology and Society, Utrecht University / Ecofys Energy and Environment, Utrecht.

APME (1994-2003): *Eco-Profiles of the European Plastics industry. Various reports on different types of plastics*. Prepared by Dr. I. Boustead for the Association of Plastics Manufacturing in Europe (APME).

Appl, M. (1997): *Ammonia, methanol, hydrogen, carbon monoxide, modern production technologies - a review*. Published by Nitrogen - The Journal of the World Nitrogen and Methanol industries, London.

Aspen Technology (2001): *Aspen Properties, part of Aspen Engineering Suite 11.1*. Aspen Technology Inc., Cambridge, Massachusetts.

Brandrup, J. and E.H. Immergut (editors) (1989): *Polymer Handbook – Third Edition*. John Wiley and Sons, New York.

Boustead, I. (1997): *Eco-profiles of the European Plastics Industry, Report 9: Polyurethane precursors (TDI, MDI, Polyols)*. For ISOPA (European Isocyanate Producers Association), Brussels.

Boustead, I. (2002): *Eco-profiles of the European plastics industry, Polyethylene terephthalate*. A report for the European Centre for Plastics in the Environment, Brussels.

Carp, J.A. and P.W. Bach (2001): *Market potential for thermohydraulic engines using waste heat sources*. Energy Research Centre of the Netherlands, Petten.

Chauvel, A. and G. Lefebvre (1989a and b): *Petrochemical processes, technical and economic characteristics; Part 1: Synthesis-gas derivatives and major hydrocarbons (a) and Part 2: Major oxygenated, chlorinated and nitrated derivatives (b)*. Editions Technip, Paris.

Chemical Market Reporter (1998-2004): *various issues.*

Chemical Week (1998-2004): *various issues.*

CEFIC (2004): *Sectoral breakdown of EU chemical industry sales*. CEFIC facts and figures, electronic source, www. cefic.org, accessed on 27 October 2004.

Crank, M., M.K. Patel, F. Marscheider-Weidemann, J. Schleich, B. Hüsing and G. Angerer (2004): *Techno-economic feasibility of large-scale production of bio-based polymers in Europe (PRO-BIP)*. Copernicus Institute, Department of Science, Technology and Society, Utrecht University and Fraunhofer Institute for Systems and Innovation Research (FhG-ISI), Utrecht/Karlsruhe.

DOE/OIT (1998): *Energy and environmental profile of the US petroleum refining industry*. US Department Of Energy, Office of Industrial Technologies (DOE/OIT), Washington DC.

DOE/OIT (2000): *Energy and environmental profile of the US chemical industry*. US Department Of Energy, Office of Industrial Technologies (DOE/OIT), Washington DC.

Dorst, E.M. van and H.M. van Veen (2002): *The application of hydrogen-selective membranes in industrial processes*. Energy Research Centre of the Netherlands, Petten.

ECN (2001a): *Energie verslag Nederland 2000*. Energy Research Centre of the Netherlands, Petten

EFMA (2000): *Best Available Techniques for Pollution Prevention and Control in the European Fertlizer Industry, Booklet 1-8*. European Fertilizer Manufacturers' Association, Brussels.

Energiemanagement.net (2004): *Eerste stap in nieuw warmtedistributienet in Rotterdam*. Electronic source: http://www.energiemanagement.net. Date 16 September 2004, accessed on 6 April 2005.

European Chemical News (1998-2004): *various issues.*

FhG-ISI (1999): *C-Ströme. Abschätzung der Material-, Energie- und CO_2-ströme für modellsysteme in Zusammenhang mit dem nicht-energetischen verbrauch, orientiert am lebensweg - Stand und Szenarienbetrachtung. Band-I Abchätzungen dur das Gesamtsystem.* Fraunhofer-Institut fur Systemtechnik und Innovationsforschung (FhG-ISI), Karlsruhe (in German).

Gielen, D.J., D. Vos and A.W.N. van Dril (1996): *The petrochemical industry and its energy use, prospects for the Dutch energy intensive industry*. Energy Research Centre of the Netherlands, Petten.

Hinderink, A.P., F.P.J.M. Kerkhof, A.B.K. Lie, J. de Swaan Arons and H.J. van der Kooi (1996): *Exergy analysis with a flowsheeting simuluation - II. Application; Synthesis Gas production from natural gas*. Chemical Engineering Science, 51 (20), pp. 4701-4715.

Hugill, J.A. (2003): *HEX-reactor applications in the Netherlands - A non-confidential summary*. Energy Research Centre of the Netherlands, Petten.

Hydrocarbon Processing (2003): *Petrochemical processes 2003*. Hydrocarbon processing, 82 (3), pp. 72-124.

IDEA (1991): *An international database for Ecoprofile analysis.* International Institute for Applied Systems Analysis, Laxenburg.

IEA (2001): *Annual statistical supplement to the IEA monthly Oil Data Service.* International Energy Agency, Paris.

IEA (2002a): *Extended energy balances of OECD countries, 2002 edition.* International Energy Agency, Paris.

IEA (2002b): *Extended energy balances of Non-OECD countries, 2002 edition.* International Energy Agency, Paris.

IEA (2002c): *CO_2 emissions from fuel combustion, 1971-2000 (2002 edition).* International Energy Agency, Paris.

IEA (2003): *Electricity and Heat: Annual questionnaire*. International Energy Agency, Paris.

IPCC/IEA/OECD/UNEP (1997): *Revised 1996 IPCC Guidelines for National Greenhouse Gas Inventories Programme, Volume 1-3*. IPCC WGI Technical Support Unit, Bracknell, UK.

IPTS (1996): *Best Available Techniques Reference Document on Ammonia Production*. European Commission, Joint Research Centre, Institute for Prospective Technological Studies, Seville.

IPTS (2001): *Reference Document on Best Available Techniques in the Chlor-Alkali Manufacturing Industry*. European Commission, Joint Research Centre, Institute for Prospective Technological Studies, Seville.

IPTS (2003a): *Reference Document on Best Available Techniques in the Large Volume Organic Chemical Industry*. European Commission, Joint Research Centre, Institute for Prospective Technological Studies, Seville.

IPTS (2003b): *Reference Document on Best Available Techniques for Mineral Oil and Gas Refineries.* European Commission, Joint Research Centre, Institute for Prospective Technological Studies, Seville.

Joosten, L (2001): *The Industrial Metabolism of Plastics - Analysis of Material Flows, Energy Consumption and CO_2 Emissions in the Lifecycle of Plastics*. PhD thesis, Utrecht University, Utrecht.

Korevaar, G. (2004): *Sustainable Chemical Processes and Products - new design methodology and design tools*. PhD thesis, Delft University of Technology, Delft.

Lange, J.P. (2001): *Fuels and chemicals manufacturing - guidelines for understanding and minimizing the production costs*. Cattech, 5 (2), pp. 82-95.

Lange, J.P. (2002): *Sustainable development: efficiency and recycling in chemicals manufacturing*. Green Chemistry, 4 (6), pp. 546-550.

Leites, I.L., D.A. Sama and N. Lior (2003): *The theory and practice of energy saving in the chemical industry: some methods for reducing thermodynamic irreversibility in chemical technology processes*. Energy, 28, pp. 55-97.

Loesoenen, P. (2003): *Combined Heat and Power (CHP) Plant Statistics in the EU, 2000, Statistics in Focus, Theme 8*. Eurostat, Luxemburg.

Neelis, M., M. Patel and M. de Feber (2003): *Improvement of CO_2 emission estimates from the non-energy use of fossil fuels in the Netherlands.* Utrecht University, Department of Science, Technology and Society, Utrecht University, Utrecht.

NEU-CO_2 (1999-2006): *Non-energy use and CO_2 emissions.* Project funded by the European Commission. project web-site: http://www.chem.uu.nl/nws/www/nenergy/.

Nieuwlaar, E. (2001): *ICARUS-4: Sector Study for the Chemical Industry*. Department of Science, Technology and Society, Utrecht University, Utrecht.

Oostvoorn, F. van, P. Kroon and Lange, A.V.M. de (1989): *SERUM: Een model van de Nederlandse raffinage-industrie*. Energy Research Centre of the Netherlands, Petten.

Oil and Gas Journal (1999): *Special Issue on Worldwide Refining*. Oil and Gas Journal, December 20, 1999, pp. 50-89.

Patel, M. (1998): *Personal Communication with industry.*

Patel, M. (2003): *Cumulative Energy Demand (CED) and cumulative CO_2 emissions for products of the organic chemical industry*. Energy, 28, pp. 721-740.

Phylipsen, G.J.M., K. Blok and E. Worrell (1998): *Handbook on International Comparisons of Energy Efficiency in the Manufacturing Industry*. Department of Science, Technology and Society, Utrecht University, Utrecht.

Phylipsen, G.J.M. (2000): *International Comparisons and National Commitments; Analysing energy and technological differences in the climate debate*. Department of Science, Technology and Society, Utrecht University, Utrecht.

Plinke, E., R. Schüssler and K. Kämpf: *Konversion Chlorchemie, Endbericht*, Prognos AG, Basel (in German).

Port of Rotterdam (2005): *Co-siting*. Electronic source: http://www.portofrotterdam.com/Business/UK/Industry/Oil_and_Chemicals/Setting_up_new_activities/siterelatedinformation/Index.asp. Accessed on 6 April, 2005.

Radgen, P. (1996): *Pinch and exergy analysis of a fertilizer complex, part 1*. Nitrogen, 224, pp. 30-38.

Radgen, P (1997): *Pinch and exergy analysis of a fertilizer complex, part 2*. Nitrogen, 225, pp. 27-39.

Spoelstra, S., W.G. Haije and J.W. Dijkstra (2002): *Techo-economic feasibility of high-temperature high-lift chemical heat pumps for upgrading industrial waste heat*. Applied Thermal Engineering, 22, pp. 1619-1630.

Statistisches Bundesamt (2001): *Aussenhandel, Fachserie 7, Aussenhandel nach Waren und Landern (Spezialhandel). Dezember und Jahr 2000, Endgultige Ergebnisse*. Statistisches Bundesamt, Wiesbaden (in German).

Statistics Netherlands (2001): *Toelichting op Z029, aardoliegrondstoffen en aardolieproducten*. Centraal Buro voor de Statistiek (Statistics Netherlands, Voorburg/Heerlen.

Statistics Netherlands (2003): *Dutch Energy balances (NEH) for 2000*. Personal communication with Statistics Netherlands Voorburg, 15 September 2003.

Statistics Netherlands (2004): *Productie middelen electriciteit*. Statline, electronic source: www.cbs.nl. Accessed on 9 June 2004.

Szargut, J., D.R. Morris and F.R. Steward (1988): *Exergy analysis of thermal, chemical and metallurgical processes*. Springer Verlag, Berlin.

Tebodin (1996): *Milieu-effectrapport voor de oprichting van de Basell styreen monomeer / propeenoxidefabriek in Moerdijk*. Tebodin, Consultants and Engineers, Den Haag.

Theunis, J., H. Joul and H. van Rompaey (2003): *Vlaamse koolstofbalans voor het niet-energetisch verbruik*. VITO.

Tonkovich, A.L.Y. and M.A. Gerber (1995): *The Top 50 commodity chemicals: impact of catalytic process limitations on energy, environment, and economics*. Pacific Northwest Laboratory, Richland.

Tuil, R. van, E. de Jong, E. Scott, R. Weusthuis, S. Vellema, I. de Keizer and H. Croezen (2002): *Biomass for the chemical industry*. ATO / CE, Wageningen/Delft.

Veen, H.M. van (2001): *Reduction of energy comsumption in the process industry by pervaporation with inorganic membranes : techno-economical feasibility study*. Energy Research Centre of the Netherlands, Petten

Vision 2020 (2004): *Opportunities for Innovative Energy Systems in the US Chemical Industry*. Chemical Industry Vision 2020 Technology Partnership (Vision 2020)'s Challenge Technical Committee, http://www.chemicalvision2020.org/.

VNCI (2003): *Jaarverslag 2003*. Vereniging van de Nederlandse Chemische Industry, Leidschendam.

Weissermel, K. and H.J. Arpe (2003): *Industrial Organic Chemistry, fourth, Completely Revised Edition*. Wiley-VCH, Weinheim.

Worrell, E., D. Phylipsen, D. Einstein and N. Martin (2000): *Energy Use and Energy Intensity of the U.S. Chemical Industry*. Ernest Orlando Lawrence Berkeley National Laboratory, Energy Analysis Department, Environmental Energy Technologies Division, Berkeley.

Appendix A   Abbreviations and glossary

BAT	Best Available Technology
By-products	sellable chemical-grade commodities produced in process that are not intended when looking at the stoichometric reaction
Carbon efficiency, reaction	carbon content of desired products and by-products divided by carbon content of raw materials into a process
Carbon losses, energy use, primary	carbon losses associated with the energy use of a process
Carbon losses, reaction	difference between the carbon content of desired products and by-products and the carbon content of the raw materials of a process
CHP	Combined Heat and Power
Desired products	intended products of a process according to the stoichometric reaction
Energy efficiency, final	calorific value of desired products and by-products divided by the final energy use and the calorific value of the raw material
Energy efficiency, primary	calorific value of desired products and by-products divided by the primary energy use and the calorific value of the raw material
Excess final energy use	difference between the final energy use and the stoichometric heat of reaction of a process
Heat effect of reaction	difference between calorific value of raw materials and the calorific value of the desired products and by-products of a process
Heat of stoichometric reaction	the difference between enthalpy of raw materials and the enthalpy of desired products according to the stoichometric reaction
HP	High Pressure
LHV	Lower Heating Value
Losses due to non-selectivity	difference between the heat effect of reaction and the negative value of the heat of stoichometric reaction of a process
LP	Low Pressure
MP	Middle Pressure
Process volume	used for processes in the refinery industry. Tonne of product for alkylation, isomerisation, lubricants and sulphur recovery; tonne of feedstock for the other processes

Total carbon efficiency	carbon content of the products and by-products of a process divided by the carbon content of the raw materials and the carbon losses associated with the energy use of a process
Total final energy loss	difference between the calorific value of raw materials + the final energy use and the calorific value of the desired products and by-products of a process
Total primary energy loss	difference between the calorific value of raw materials + the primary energy use and the calorific value of the desired products + by-products of a process
Total value added	difference between value of products + by-products and the value of raw materials + energy costs
Total value added, % of product value	difference between value of products + by-products and the value of raw materials + energy costs divided by the value of products + by-products
Value added, reaction	difference between value of products + by-products and the value of raw materials
Value added, reaction, % of product value	difference between value of products + by-products and the value of raw materials divided by the value of products + by-products

Appendix B Chemical commodities and refinery processes included in the model

Table B.1 *Chemical commodities for which the production processes are included in the model. In cases where a commodity can be produced via more than one process route, the number of process routes included is given between brackets.*

Acetaldehyde	Ethylene oxide	Polyvinylchloride
Acetic acid (2)	Formaldehyde	Propylene (4)
Aceton (2)	Hexamethylene diamine (3)	Propylene oxide (3)
Acrylonitrile	Isopropanol	Styrene (2)
Adipic acid	Methanol (3)	Terephthalic acid
Ammonia (3)	Methyl tert butyl ether	Toluene (3)
Aniline	Methylene diisocyanate	Toluene diisocyanate
Benzene (3)	N Butanol	Urea
Bisphenol A	Nitrobenzene	Urea Formaldehyde resin
Butadiene	Phenol (2)	Vinylchloride
Caprolactam (2)	Phthalic anhydride (2)	m-Xylene (3)
Chlorine (3)	Polyamide 6	o-Xylene (3)
Cum ene	Polyamide 66	p-Xylene (3)
Cyclohex ane	Polycarbonate	
Dimethyl terephthalate	Polyetherpolyols	
Dioctylphthalate	Polyethylene	
Ethylbenzene	Polyethylene terephthal ate	
Ethylene (4)	Polypropylene	
Ethylene glycol	Polystyrene	
Ethylhex anol (2)	Polyurethane (2)	

Note: The number of processes (86) given in this table exceeds the 68 processes mentioned in the text, because some of the chemicals are produced via the same process (e.g. ethylene and propylene via steam cracking).

Table B.2 *Refinery processes included in the model*

Alkylation	Hydrotreatment (naphtha)
Atmospheric distillation	Hydrotreatment (middle distillates)
Catalytic cracking	Hydrotreatment (vacuum distillate)
Catalytic reforming	Isomerisation
Coking (delayed coking)	Lubricants production
Coking (fluid/flexicoking)	Sulphur recovery
Hydrocracking	Thermal processes
Hydrogen production	Vacuum distillation

Appendix C Assumptions for properties of raw materials, products and by-products

For chemical commodities having a uniform and well-defined chemical structure, we convert the consumption of the raw material and the production of the desired and by-products in mass units (variable 1,6 and 11 in Figure 2.1) to molar quantities (variable 2,7 and 12) and CO_2 equivalents (variable 4, 9 and 14) using the molecular formulas of the commodity. We mainly base the calculation of the calorific values (variable 3,8 and 14) for these commodities on the Heat of Formation of pure substances taken from Aspen Plus flow sheeting software (Aspen Technology, 2001). The calorific value (Lower Heating Value, LHV) for a chemical commodity with chemical formula $C_xH_yS_z$ is calculated from this Heat of Formation using the following formula:

$$LHV = x * \Delta H_{formation, CO2\,(g)} + (y/2) * \Delta H_{formation, H2O\,(g)} + z * \Delta H_{formation, SO2\,(g)} - \Delta H_{formation, compound} \qquad \text{Equation 1}$$

By using this formula, one calculates the calorific value by converting carbon, hydrogen and sulphur to CO_2, H_2O and SO_2, which are the products in reacting carbon, hydrogen and sulphur with oxygen. Other elements present in the commodity are implicitly assumed to be converted to their elemental state (which has a heat of formation equal to 0). As a result, the 'calorific' value for commodities containing elements other than carbon, hydrogen and sulphur like sodium chloride can become negative. As a result, some indicators given in Section 2.3 cannot be calculated as is explained there. For some of the polymers, we calculated the LHV based on the heat of polymerisation given in Brandrup and Immergut (1989) or using estimation methods given by Szargut et al. (1988). The prices for the chemical commodities are derived from German trade statistics for the year 2000 (Statistisches Bundesamt, 2001) by dividing the traded physical quantity by the traded monetary quantity for both imports and export. If the derived import and export prices differ less than 25%, we use the average of import and export price. In cases where import and export prices differ more than 25%, we use the price representing the largest quantity. When trade statistics were unavailable, we use other source like the European Chemical News (1998-2004) and Chemical Market Reporter (1998-2004) for price data. For the raw materials in the chemical industry, of which the chemical structure is not well defined (e.g. naphtha, coal), we took calorific values and CO_2 emission factors from IPCC/IEA/OECD/UNEP (1997) and prices for the year 2000 from ECN (2001) and IEA (2001). For obvious reasons, we did not include molar quantities for these commodities.

Appendix D Assumptions for properties of electricity, fuels and steam

Fuels

The overall CO_2 emission factors for the fuels reported as final consumption in the chemical and refinery industry in the international energy statistics (IEA, 2002a and 2002b) are derived in Appendix F. From this overview it becomes clear that natural gas is the dominant fuel in the chemical industry, whereas refinery gas dominates in the refinery industry. We use the emission factors derived in Appendix F for Western Europe (62 kg CO_2 / GJ for the petrochemical industry and 74 kg CO_2 / GJ for the refinery industry) for calculating the associated CO_2 emissions of the fuel use reported in the datasets. For the fuels used in the steam cracking and steam reforming processes, we use process specific emission factors, which are explained Chapter 3. We use a fuel price of 5 Euro / GJ reflecting a reasonable average of the Western European situation in 2000 (ECN, 2001).

Electricity and steam

In order to accurately calculate the primary fuel equivalent and associated CO_2 emissions related to the electricity use, one would need to know for every single plant worldwide the background of the electricity used such as the fraction of auto-generated electricity (with or without the co-generation of steam) versus the fraction purchased from the public grid. By analogy, for steam one would need to know the amount produced in stand-alone boilers versus the amount produced in cogeneration units or via heat integration. If steam consumption is reported only in tonnes, one needs to know in addition the exact temperature and pressure level of the steam used in order to determine the heat content of this steam. Data at this low level of aggregation is not available. We therefore made the following assumptions. We distinguish between three temperature and pressure levels of steam based on Patel (1998) and calculated the heat content of steam using Statistics Netherlands (2001):

- Low Pressure (LP) steam of 4 bar and 175 °C, having a heat content of 2.8 GJ / tonne compared to liquid water of 25°C.
- Middle Pressure (MP) steam of 10 bar and 280 °C, having a heat content of 3.0 GJ / tonne compared to liquid water of 25°C.
- High Pressure (HP) steam of 40 bar and 400 °C, having a heat content of 3.2 GJ / tonne compared to liquid water of 25°C.

To better reflect the actual heat duty of a tonne of steam, we deduct from the heat content of steam given above the heat content of hot condensate, which is normally returned to steam boilers. We assume this return condensate to be hot water of 100 °C, having a heat content of 0.4 GJ / tonne compared to liquid water of 25 °C (Statistics Netherlands, 2001). The resulting heat duty is referred to as the final energy use of steam. We assume this heat duty to be produced from fossil fuels with a boiler having an energy efficiency of 90%. For the CO_2 emission factors and the price of the fuels used we use the characteristics of the fuels used within the chemical and refinery industry derived above. In cases, where the type of steam was not specified in the dataset used, we used the properties of MP steam.

We assume the electricity to be generated from fossil fuels with and energy efficiency of 45%. For the CO_2 emission factors, we use again the same characteristics as assumed for the direct fuel use (62 and 74 kg CO_2 / GJ for the chemical and refinery industry, respectively). We use an electricity price of 19 Euro / GJ_e being a reasonable average of the Western European situation in 2000 (ECN, 2001). A summary of the assumptions made is given in Table D.1.

Table D.1 *Overview of assumptions for primary fuel equivalents and specific CO_2 emissions for steam and electricity use*

	Steam, primary fuel equivalent	Steam, specific primary CO_2 emissions[1]	Electricity, primary fuel equivalent	Electricity, specific primary CO_2 emissions[1]
	GJ_p / GJ_f	kg CO_2 / GJ_f	GJ_p / GJ_e	kg CO_2 / GJ_e
Chemical industry	1.11	69	2.22	138
Refinery industry	1.11	82	2.22	164

[1] Using emission factors of 62 kg CO_2 / GJ and 74 kg CO_2 / GJ for respectively the chemical and the refinery industry.

Appendix E Sources for production data and for shares of production processes

The majority of production figures for the year 2000 for the chemicals included were obtained from the following three magazines:

- Chemical Profile pages from Chemical Market Reporter (1998-2004)
- Product Profile pages from European Chemical News (1998-2004)
- Product Focus pages from Chemical Week (1998-2004)

These sources were complemented with data from grey literature and textbooks on the organic chemical industry (e.g. Weissermel and Arpe, 2003). In some cases, also publicly available company data were used. If only data for years close to 2000 were available, we used linear inter- and extrapolations to obtain production data for 2000 or applied growth rates mentioned in the literature sources used. In cases where only capacity data was available, we used capacity utilization rates mentioned in the literature source or otherwise a default capacity utilization rate of 86%, a value based on the Netherlands for the period 1999-2003 (VNCI, 2003). For chemicals produced via more than one process route, the shares of the various process routes was in most cases obtained from Weissermel and Arpe (2003), complemented with other sources like the three magazines given above. For the throughput figures in the refinery industry, we use figures from the Oil and Gas Journal (1999).

Appendix F Fuel mix in chemical and refinery industries

Table F.1 *Final energy use in the chemical industry in 2000 by fuel type, excluding feedstock use (IEA, 2002a and 2002b)*

	Emission factor [1]	Netherlands			Western Europe			World		
	kg CO_2 / GJ	PJ_f	%	kt CO_2	PJ_f	%	kt CO_2	PJ_f	%	kt CO_2
Hard Coal	94.6	1	1%	127	31	1%	2899	1530	11%	144756
Lignite / Brown Coal / Sub-bituminous Coal	101.2				3	0%	292	61	0%	6186
Coke oven coke / Lignite coke	108.2	1	0%	77	4	0%	430	135	1%	14641
BKB / Peat briquettes	94.6				4	0%	345	7	0%	646
Gas works gas [2]	47.7				1	0%	28	24	0%	1146
Coke oven gas	47.7				6	0%	293	26	0%	1223
Industrial waste [2]	73.3				9	0%	648	48	0%	3496
Primary solid biomass	0.0				4	0%	0	22	0%	0
Natural gas	56.1	90	40%	5024	978	47%	54863	5016	37%	281426
Refinery gas	66.7	51	23%	3384	62	3%	4169	610	5%	40706
Liquefied Petroleum Gas	63.1	2	1%	114	30	1%	1867	129	1%	8146
Other kerosene	71.9				3	0%	241	24	0%	1730
Gas / Diesel oil	74.1	0	0%	19	19	1%	1371	384	3%	28464
Heavy fuel oil	77.4	0	0%	23	94	5%	7298	802	6%	62086
Naphtha	73.3				52	2%	3780	203	2%	14897
Petroleum coke	100.8				4	0%	414	36	0%	3664
Other petroleum products [2]	100.8	1	1%	135	34	2%	3410	128	1%	12868
Other fuels [2]	73.3				1	0%	55	8	0%	565
Total final fuel use		*146*	*65%*	*8901*	*1337*	*65%*	*82402*	*9194*	*68%*	*626646*
Average emission factor fuels used		*61 kg CO_2 / GJ*			*62 kg CO_2 / GJ*			*68 kg CO_2 / GJ*		
Heat	0.0	36	16%	0	58	3%	0	1155	9%	0
Electricity	0.0	43	19%	0	674	33%	0	3131	23%	0
Total final energy use		*225*	*100%*	*8901*	*2068*	*100%*	*82402*	*13480*	*100%*	*626646*

1. Emission factors from IEA (2002c) unless otherwise stated.
2. Emission factors are own estimates.

Table F.2 *Final energy use in the refinery industry by fuel type in 2000 (IEA, 2002a and 2002b)*

Fuel	Emission factor [1]	Netherlands			Western Europe			World		
	kg CO_2 / GJ	PJ_f	%	kt CO_2	PJ_f	%	kt CO_2	PJ_f	%	kt CO_2
Hard Coal	94.6							13	0%	1228
Coke oven coke / Lignite coke	108.2							4	0%	457
Gas works gas [2]	47.7							15	0%	721
Coke oven gas	47.7				5	0%	218	5	0%	220
Industrial waste [2]	73.3							5	0%	347
Natural gas	56.1	31	17%	1731	74	4%	4179	1488	14%	83502
Crude oil	73.3							27	0%	2011
Natural Gas liquids	63.1							7	0%	454
Refinery gas	66.7	105	58%	7024	815	48%	54393	4468	43%	298141
Ethane	61.6				2	0%	147	3	0%	138
Liquefied Petroleum Gas	63.1	2	1%	114	20	1%	1262	127	1%	8006
Motor gasoline	69.3				0	0%	29	42	0%	2884
Other kerosene	71.9							10	0%	695
Gas / Diesel oil	74.1				12	1%	865	133	1%	9849
Heavy fuel oil	77.4	11	6%	836	417	25v	32285	1980	19%	153191
Naphtha	73.3				5	0%	396	10	0%	752
Petroleum coke	100.8				127	8%	12804	807	8%	81407
Other petroleum products [2]	100.8	24	13%	2393	107	6%	10787	161	2%	16244
Total final fuel use		*171*	*95%*	*11984*	*1585*	*94%*	*117365*	*9306*	*89%*	*660292*
Average emission factor fuels used		*70 kg CO_2 / GJ*			*74 kg CO_2 / GJ*			*71 kg CO_2 / GJ*		
Heat	0.0	0	0%	0	2	0%	0	503	5%	0
Electricity	0.0	9	5%	0	95	6%	0	621	6%	0
Total final energy use		*180*	*100%*	*11984*	*1683*	*100%*	*117365*	*10430*	*100%*	*660292*

1. Emission factors from IEA (2002c) unless otherwise stated.
2. Emission factors are own estimates.

Appendix G   Research approach, example for vinyl chloride

Calculation of variables included in the model

As an example of our research approach we would like to give the production of vinyl chloride (VC) from ethylene, chlorine and oxygen. The stoichometric reaction equation is:

$$4\ C_2H_4\ (g) + 2\ Cl_2\ (g) + O_2\ (g) \rightarrow 4\ C_2H_3Cl\ (g) + 2\ H_2O\ (g)^{[24]}$$
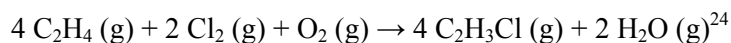
The heat of this reaction $\Delta H_{reaction}$ is –2.32 GJ / t VC (variable 28 from Figure 2.1). According to IPTS (2003a), pp. 293, the typical raw material and energy requirement per tonne of VC product are:

- Ethylene   0.47 tonne
- Chlorine   0.60 tonne
- Oxygen   0.14 tonne
- Electricity   0.2 MWh
- Natural gas 1 MWh
- Steam   0.2 tonne

The molecular formulas of ethylene (C_2H_4), chlorine (Cl_2), oxygen (O_2) and VC (C_2H_3Cl) are used to convert the mass units into molar units. Calorific values for the chemicals are calculated using heat of formation values from Aspen Plus Flowsheeting software (Aspen Technology, 2001). Price data for 2000 are taken from German trade statistics (Statistisches Bundesamt, 2001). An overview of the resulting variables is given in Table G.1.

Table G.1   *Variables included for the raw materials and products in VC production*

	Ethylene	Chlorine	Oxygen	VC
Mass (t / t VC)	0.47	0.60	0.14	1.00
Moles (kmole / t VC)	16.75	8.39	4.38	16.00
Calorific value (GJ / t VC)	22.17	0.00	0.00	18.85
Carbon content (t CO_2 / t VC)	1.47	0.00	0.00	1.41
Value (€ / t VC)	278.59	105.04	7.49	576.23

Using the assumptions summarised in Appendix D, we can convert the energy use as given in the data source (IPTS, 2003a) to the variables summarised in Table G.2.

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[24] We take water in the gaseous state to be consistent with the Lower Heating Values used as calorific value. If water would be taken in the liquid state, we should include liquid water as one of the products of the process (with a calorific value of –2.44 GJ / tonne) to avoid errors in the calculation of the heat effect or reaction.

Table G.2 *Variables included for the energy use in VC production*

Steam

Mass (t / t VC)	0.20
Heat duty (GJ$_f$ / t VC)	0.51
Primary fuel equivalent (GJ$_p$ / t VC)	0.57
Primary CO_2 equivalent (t CO_2 / t VC)	0.04
Value (€ / t VC)	2.86
Fuel use	
Calorific value (GJ$_f$ / t VC)	3.60
CO_2 equivalent (t CO_2 / t VC)	0.22
Value (€ / t VC)	18.00
Electricity	
Electricity use (GJ$_e$)	0.72
Primary fuel equivalent (GJ$_p$)	1.60
Primary CO_2 equivalent (t CO_2)	0.10
Value (€)	14.00

Calculation and interpretation of indicators
We can now calculate all the indicators listed in Table 2.1 for this process (Table G.3).

Table G.3 *Overview calculated indicators for the production of VC*

No.	Indicator name	Value	Unit
1	Heat of stoichometric reaction	-2.32	GJ$_f$ / t VC
2	Electricity use	0.72	GJ$_e$ / t VC
3	Fuel use	3.60	GJ$_f$ / t VC
4	Steam use	0.52	GJ$_f$ / t VC
5	Total final energy use	4.84	GJ$_f$ / t VC
6	Total primary energy use	5.77	GJ$_p$ / t VC
7	Heat effect of reaction	3.32	GJ$_f$ / t VC
8	Total final energy loss	8.16	GJ$_f$ / t VC
9	Total primary energy loss	9.09	GJ$_p$ / t VC
10	Excess final energy use	7.16	GJ$_f$ / t VC
11	Losses due to non-selectivity	1.00	GJ$_f$ / t VC
12	Energy efficiency, final	70	%
13	Energy efficiency, primary	67	%
14	Carbon losses, energy use, primary	0.36	t CO_2 / t VC
15	Carbon losses, reaction	0.06	t CO_2 / t VC
16	Total carbon losses, primary	0.42	t CO_2 / t VC
17	Carbon efficiency, reaction	96	%
18	Total carbon efficiency	77	%
19	Energy costs	34.86	€ / t VC
20	Value added reaction	185.11	€ / t VC
21	Total value added	150.25	€ / t VC
22	Value added reaction, percentage of product value	32	%
23	Total value added, percentage of product value	26	%

A graphical representation of some of the energy indicators is given in Figure G.1. The total final energy **loss** (indicator 8, 8.16 GJ / t VC) consists partly of final energy **use** (indicator 5, 4.84 GJ / t VC) and partly of the heat effect of reaction (indicator 7, 3.32 GJ / t VC). The negative of the heat of the stoichometric reaction given by Equation 2 is only 2.32 GJ / t VC. The losses due to non-selectivity therefore equal 1.00 GJ / t VC. This result can also be derived from the molar quantities given in Table G.1. The molar efficiency from ethylene to VC is 96%

(16.00/16.75). Per tonne of VC, 0.75 kmole of ethylene is therefore lost, which is equal to 0.021 tonne and 1.00 GJ[25]. Without looking inside the black box of the process, we cannot say in which way the energy is lost. Losses can occur due to the formation of non-valuable by-products (off-specs) or from over-oxidation of the feedstock.

The energy efficiency indicators (indicator 12 and 13) are directly calculated by dividing the energy going out of the process (the VC product) by the energy going into the process (the raw materials + the energy use).
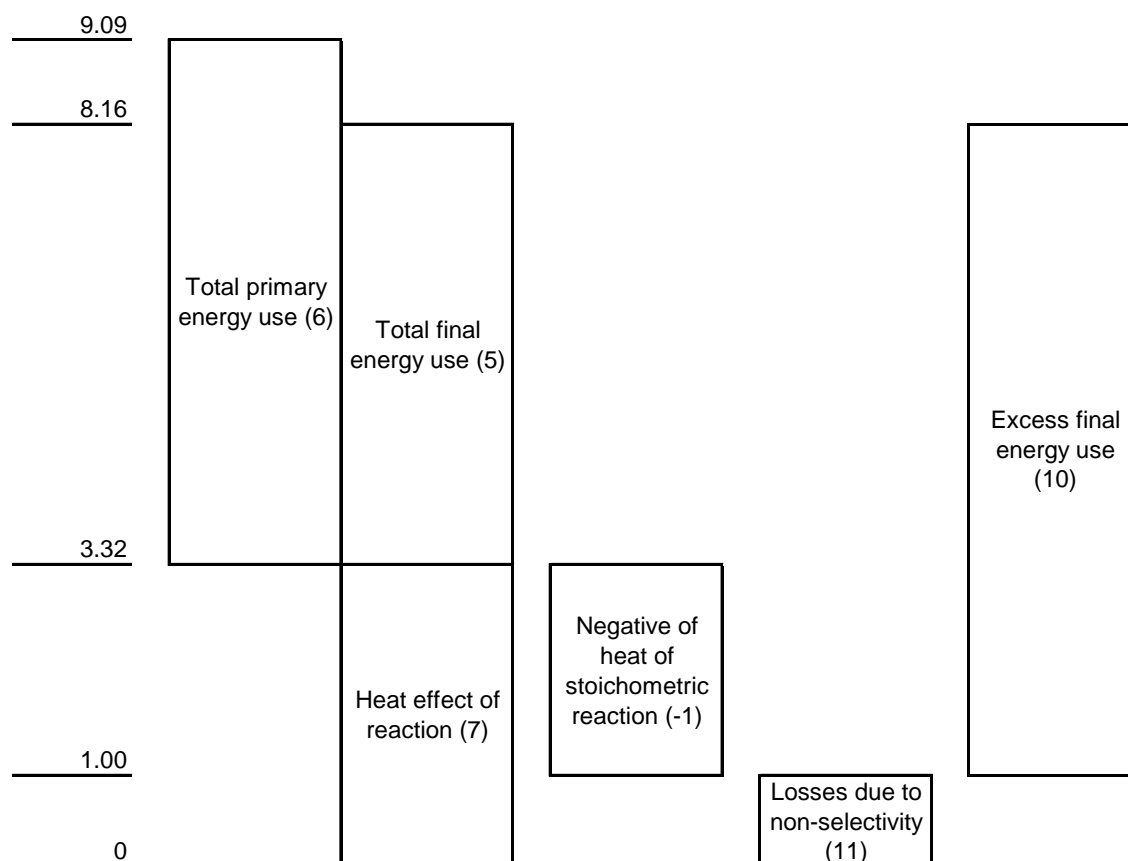
Figure G.1 *Graphical interpretation of energy related indicators for the production of VC. Numbers are in GJ / tonne of product. Indicator number is shown between brackets*

The interpretation of the carbon and financial indicators is more straightforward. The total CO_2 emissions of the process (indicator 16, 0.42 t CO_2 / t VC) are the sum of reaction losses (indicator 15, 0.06 t CO_2 / t VC) and CO_2 emissions resulting from the energy use of the process (indicator 14, 0.36 t CO_2 / t VC). The carbon efficiency of reaction (indicator 17) is directly calculated by dividing the carbon in the product by the carbon embodied in the raw materials. The total carbon efficiency (indicator 18) is calculated by dividing the carbon in the product by the total carbon input into the process (in raw materials and resulting from the energy use). The value added of the reaction (indicator 20) is calculated by comparing the value of the product with the value of the raw materials. Deducting the energy costs from this value added of reaction yields the total value added of the process (indicator 21). With indicator 22 and 23, these value added figures are related to the product value.

We can calculate all indicators (except for the efficiency indicators 12/13, 17/18 and 22/23) in absolute units per year (per year) by multiplying the indicators in specific units (per tonne of product) with the total production of the product (tonne per year) and the share of the process

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[25] The molar mass for ethylene is 28.02 g and the calorific value for ethylene is 47.2 GJ / t.

route in the total production of the product (%). Production in 2000 is estimated to be 430 ktonne in the Netherlands (based on Chemical Week, 1998-2003), 5500 ktonne in Western Europe (Weissermel and Arpe, 2003) and 26746 ktonne worldwide (based on (Chemical Week, 1998-2003). According to Patel (1998), almost all VC is produced via this process, so the share of this process in the total production of VC is 100% for all regions included.

Appendix H   Process characteristics chemical industry

Characteristic	Unit	Ammonia — Steam reforming of natural gas (Average)	Steam reforming (BAT)	Partial oxidation of oil (Average)	Partial oxidation of oil (BAT)	Partial oxidation of coal (Average)	Partial oxidation of coal (BAT)
Production volume, the Netherlands	[ktonne / year]	2689					
Production volume, Western Europe	[ktonne / year]	10787					
Production volume, World	[ktonne / year]	134330					
Reaction route		Steam reforming of natural gas		Partial oxidation of oil		Partial oxidation of coal	
Reaction		-		-		-	
Share, the Netherlands		100%		0%		0%	
Share, Western Europe		90%		10%		0%	
Share, World		83%		9%		9%	
Source for process data		Nieuwlaar (2001), pp. 19	EFMA (2000), booklet 1, pp. 22	EFMA (2000), booklet 1, pp. 22	EFMA (2000), booklet 1, pp. 22	IPTS (1996), pp. 29	IPTS (1996), pp. 29
Type of process		Average	BAT	Average	BAT	Average	BAT
Uncertainty indicator energy use values (see Section 4.1.1 for explanation)		1	1	1	1	1	1
Heat of stoichometric reaction	[GJf / t of main product]	-	-	-	-	-	-
Electricity use	[GJe / t of main product]	0.00	0.00	0.00	0.00	0.00	0.00
Fuel use	[GJf / t of main product]	13.60	8.40	18.30	16.50	29.40	23.40
Steam use	[GJf / t of main product]	0.00	0.00	0.00	0.00	0.00	0.00
Total primary energy use	[GJp / t of main product]	13.60	8.40	18.30	16.50	29.40	23.40
Heat effect of reaction	[GJf / t of main product]	-	-	-	-	-	-
Total final energy loss	[GJf / t of main product]	13.60	8.40	18.30	16.50	29.40	23.40
Total primary energy loss	[GJp / t of main product]	13.60	8.40	18.30	16.50	29.40	23.40
Excess final energy use	[GJf / t of main product]	-	-	-	-	-	-
Losses due to non-selectivity	[GJf / t of main product]	-	-	-	-	-	-
Energy efficiency, final	[%]	58%	69%	50%	53%	39%	44%
Energy efficiency, primary	[%]	58%	69%	50%	53%	39%	44%
Carbon losses, energy use, primary	[t CO2 / t main product]	-	-	-	-	-	-
Carbon losses, reaction	[t CO2 / t main product]	-	-	-	-	-	-
Total carbon losses, primary	[t CO2 / t main product]	1.81	1.51	2.84	2.70	4.64	4.06
Carbon efficiency, reaction	[%]	-	-	-	-	-	-
Total carbon efficiency	[%]	0%	0%	0%	0%	0%	0%
Energy costs	[€ / t main product]	-	-	-	-	-	-
Value added reaction	[€ / t main product]	-	-	-	-	-	-
Total value added	[€ / t main product]	40	61	1	9	78	90
Value added reaction, % of product value	[%]	-	-	-	-	-	-
Total value added, % of product value	[%]	23%	35%	1%	5%	45%	52%
Notes							[1]

Characteristic	Unit	Urea	Ethylene			
Production volume, the Netherlands	[ktonne / year]	881	2666			
Production volume, Western Europe	[ktonne / year]	4988	19788			
Production volume, World	[ktonne / year]	118436	91000			
Reaction route		Reaction of ammonia with CO2	Steam cracking of naphtha		Steam cracking of propane	
Reaction		2NH3 (g) + CO2 (g) → CH4ON2(s) + H20(g)	-		-	
Share, the Netherlands		100%	83%		12%	
Share, Western Europe		100%	75%		10%	
Share, World		100%	51%		21%	
Source for process data		EFMA (2000), booklet 5, pp. 21	Neelis (2003), pp. 24	Neelis (2003), pp. 24 (yields), Phylipsen (1998), pp. 168 (BAT energy values)	Neelis (2003), pp. 24	Neelis (2003), pp. 24 (yields), Phylipsen (1998), pp. 168 (BAT energy values)
Type of process		Average	Average	BAT	Average	BAT
Uncertainty indicator energy use values (see Section 4.1.1 for explanation)		1	1	1	1	1
Heat of stoichometric reaction	[GJf / t of main product]	-0.04	6.69	6.69	4.07	4.07
Electricity use	[GJe / t of main product]	0.08	0.00	0.00	0.00	0.00
Fuel use	[GJf / t of main product]	0.00	35.50	21.00	24.10	17.50
Steam use	[GJf / t of main product]	1.97	0.00	0.00	0.00	0.00
Total primary energy use	[GJp / t of main product]	2.37	35.50	21.00	24.10	17.50
Heat effect of reaction	[GJf / t of main product]	0.09	-6.69	-6.69	-4.07	-4.07
Total final energy loss	[GJf / t of main product]	2.14	28.81	14.31	20.03	13.43
Total primary energy loss	[GJp / t of main product]	2.46	28.81	14.31	20.03	13.43
Excess final energy use	[GJf / t of main product]	2.09	28.81	14.31	20.03	13.43
Losses due to non-selectivity	[GJf / t of main product]	0.05	0.00	0.00	0.00	0.00
Energy efficiency, final	[%]	83%	83%	91%	84%	89%
Energy efficiency, primary	[%]	81%	83%	91%	84%	89%
Carbon losses, energy use, primary	[t CO2 / t main product]	0.05	1.73	1.02	1.04	0.76
Carbon losses, reaction	[t CO2 / t main product]	0.02	0.00	0.00	0.00	0.00
Total carbon losses, primary	[t CO2 / t main product]	0.07	1.73	1.02	1.04	0.76
Carbon efficiency, reaction	[%]	98%	100%	100%	100%	100%
Total carbon efficiency	[%]	91%	85%	90%	86%	90%
Energy costs	[€ / t main product]	12	148	87	100	73
Value added reaction	[€ / t main product]	47	725	725	255	255
Total value added	[€ / t main product]	35	578	638	154	182
Value added reaction, % of product value	[%]	17%	50%	50%	25%	25%
Total value added, % of product value	[%]	13%	40%	44%	15%	18%
Notes						[2]

Characteristic	Unit	Ethylene			
Production volume, the Netherlands	[ktonne / year]	2666			
Production volume, Western Europe	[ktonne / year]	19788			
Production volume, World	[ktonne / year]	91000			
Reaction route		Steam cracking of ethane		Steam cracking of gas oil	
Reaction		-		-	
Share, the Netherlands		0%		5%	
Share, Western Europe		5%		10%	
Share, World		21%		7%	
Source for process data		Neelis (2003), pp. 24	Neelis (2003), pp. 24 (yields), Phylipsen (1998), pp. 168 (BAT energy values)	Neelis (2003), pp. 24	Neelis (2003), pp. 24 (yields), Phylipsen (1998), pp. 168 (BAT energy values)
Type of process		Average	BAT	Average	BAT
Uncertainty indicator energy use values (see Section 4.1.1 for explanation)		1	1	1	1
Heat of stoichometric reaction	[GJf / t of main product]	4.61	4.61	8.52	8.52
Electricity use	[GJe / t of main product]	0.00	0.00	0.00	0.00
Fuel use	[GJf / t of main product]	22.00	13.80	47.00	24.80
Steam use	[GJf / t of main product]	0.00	0.00	0.00	0.00
Total primary energy use	[GJp / t of main product]	22.00	13.80	47.00	24.80
Heat effect of reaction	[GJf / t of main product]	-4.61	-4.61	-8.52	-8.52
Total final energy loss	[GJf / t of main product]	17.39	9.19	38.48	16.28
Total primary energy loss	[GJp / t of main product]	17.39	9.19	38.48	16.28
Excess final energy use	[GJf / t of main product]	17.39	9.19	38.48	16.28
Losses due to non-selectivity	[GJf / t of main product]	0.00	0.00	0.00	0.00
Energy efficiency, final	[%]	79%	87%	82%	92%
Energy efficiency, primary	[%]	79%	87%	82%	92%
Carbon losses, energy use, primary	[t CO2 / t main product]	0.95	0.60	2.29	1.21
Carbon losses, reaction	[t CO2 / t main product]	0.00	0.00	-	-
Total carbon losses, primary	[t CO2 / t main product]	0.95	0.60	2.29	1.21
Carbon efficiency, reaction	[%]	100%	100%	100%	100%
Total carbon efficiency	[%]	79%	86%	85%	91%
Energy costs	[€ / t main product]	91	57	195	103
Value added reaction	[€ / t main product]	403	403	699	699
Total value added	[€ / t main product]	311	345	503	595
Value added reaction, % of product value	[%]	48%	48%	39%	39%
Total value added, % of product value	[%]	37%	41%	28%	33%
Notes					[2]

Characteristic	Unit	Chlorine			Polyethylene
Production volume, the Netherlands	[ktonne / year]	537			1331
Production volume, Western Europe	[ktonne / year]	9704			10658
Production volume, World	[ktonne / year]	44084			40856
Reaction route		Electrolysis of sodium chloride (diaphragma cells)	Electrolysis of sodium chloride (mercury cathode)	Electrolysis of sodium chloride (membrane)	Addition polymerisation of ethylene
Reaction		2NaCl (s) + 2H2O (g) → Cl2 (g) + H2 (g) + 2NaOH (s)	2NaCl (s) + 2H2O (g) → Cl2 (g) + H2 (g) + 2NaOH (s)	2NaCl (s) + 2H2O (g) → Cl2 (g) + H2 (g) + 2NaOH (s)	n C2H4(g) → (C2H4)n (s)
Share, the Netherlands		22%	66%	11%	100%
Share, Western Europe		22%	58%	20%	100%
Share, World		60%	20%	20%	100%
Source for process data		IPTS (2001), pp. 35	IPTS (2001), pp. 35	IPTS (2001), pp. 35	DOE/OIT (2000), pp. 72
Type of process		Average	Average	Average	Average
Uncertainty indicator energy use values (see Section 4.1.1 for explanation)		1	1	1	2
Heat of stoichometric reaction	[GJf / t of main product]	6.41	6.41	6.41	-3.83
Electricity use	[GJe / t of main product]	10.69	12.82	10.04	2.04
Fuel use	[GJf / t of main product]	0.00	0.00	0.00	0.00
Steam use	[GJf / t of main product]	6.27	0.00	1.85	0.64
Total primary energy use	[GJp / t of main product]	30.73	28.48	24.38	5.24
Heat effect of reaction	[GJf / t of main product]	-6.41	-6.41	-6.41	4.30
Total final energy loss	[GJf / t of main product]	10.56	6.40	5.48	6.98
Total primary energy loss	[GJp / t of main product]	24.32	22.07	17.97	9.54
Excess final energy use	[GJf / t of main product]	10.56	6.40	5.48	6.51
Losses due to non-selectivity	[GJf / t of main product]	0.00	0.00	0.00	0.47
Energy efficiency, final	[%]	-	-	-	86%
Energy efficiency, primary	[%]	-	-	-	82%
Carbon losses, energy use, primary	[t CO2 / t main product]	1.91	1.77	1.51	0.33
Carbon losses, reaction	[t CO2 / t main product]	0.00	0.00	0.00	0.03
Total carbon losses, primary	[t CO2 / t main product]	1.91	1.77	1.51	0.36
Carbon efficiency, reaction	[%]	-	-	-	99%
Total carbon efficiency	[%]	-	-	-	90%
Energy costs	[€ / t main product]	243	249	206	43
Value added reaction	[€ / t main product]	377	377	377	326
Total value added	[€ / t main product]	135	128	172	283
Value added reaction, % of product value	[%]	92%	92%	92%	35%
Total value added, % of product value	[%]	33%	31%	42%	31%
Notes				[3]	

Characteristic	Unit	Benzene from py-gas (aromatics)	Benzene from toluene (aromatics)	p-xylene from reformate (aromatics)	Methanol		
Production volume, the Netherlands	[ktonne / year]	1402	1402	430	731		
Production volume, Western Europe	[ktonne / year]	6966	6966	1591	3270		
Production volume, World	[ktonne / year]	30200	30200	16000	27900		
Reaction route		Benzene separation from py gas	Hydrodealkylatoin of toluene from py-gas	p-Xylene from C8 aromatics cut	Steam reforming of natural gas		Partial oxidation of residues
Reaction		-	C7H8(l) + H2(g) → C6H6(l) + CH4(g)	-	-		-
Share, the Netherlands		66%	5%	100%	100%		0%
Share, Western Europe		66%	5%	100%	88%		9%
Share, World		39%	5%	100%	88%		9%
Source for process data		IPTS (2003a), pp. 208	IPTS (2003a), pp. 208	IPTS (2003a), pp. 208	Appl (1997), pp. 88	Appl (1997), pp. 88	Appl (1997), pp. 96
Type of process		Average	Average	Average	Average	BAT	Average
Uncertainty indicator energy use values (see Section 4.1.1 for explanation)		2	2	2	1	1	1
Heat of stoichometric reaction	[GJf / t of main product]	Separation	-0.48	Separation	-	-	-
Electricity use	[GJe / t of main product]	0.92	0.30	0.66	0.00	0.07	0.65
Fuel use	[GJf / t of main product]	2.67	0.00	1.37	12.47	9.37	14.51
Steam use	[GJf / t of main product]	7.01	0.31	6.74	0.00	0.00	0.00
Total primary energy use	[GJp / t of main product]	12.50	1.02	10.33	12.47	9.53	15.95
Heat effect of reaction	[GJf / t of main product]	Separation	0.48	Separation	-	-	-
Total final energy loss	[GJf / t of main product]	10.60	1.09	8.77	12.47	9.44	15.16
Total primary energy loss	[GJp / t of main product]	12.50	1.50	10.33	12.47	9.53	15.95
Excess final energy use	[GJf / t of main product]	10.60	1.09	8.77	-	-	-
Losses due to non-selectivity	[GJf / t of main product]	Separation	0.00	Separation	-	-	-
Energy efficiency, final	[%]	79%	98%	85%	62%	68%	57%
Energy efficiency, primary	[%]	76%	97%	83%	62%	68%	56%
Carbon losses, energy use, primary	[t CO2 / t main product]	0.77	0.06	0.64	-	-	-
Carbon losses, reaction	[t CO2 / t main product]	-	0.00	-	-	-	-
Total carbon losses, primary	[t CO2 / t main product]	0.77	0.06	0.64	0.44	0.28	1.37
Carbon efficiency, reaction	[%]	-	100%	-	-	-	-
Total carbon efficiency	[%]	81%	98%	87%	76%	83%	50%
Energy costs	[€ / t main product]	70	8	57	-	-	-
Value added reaction	[€ / t main product]	-	-	-	-	-	-
Total value added	[€ / t main product]	-	-	-	48	60	9
Value added reaction, % of product value	[%]	-	-	-	-	-	-
Total value added, % of product value	[%]	-	-	-	26%	33%	5%
Notes				[4]			[1]

Characteristic	Unit	Methanol	Polypropylene	Polyvinylchloride	Vinylchloride	Methyl tert butyl ether	Ethylbenzene
Production volume, the Netherlands	[ktonne / year]	731	888	447	430	934	1210
Production volume, Western Europe	[ktonne / year]	3270	6558	5269	5500	3360	5183
Production volume, World	[ktonne / year]	27900	27833	25398	26746	20867	20351
Reaction route		Partial oxidation of coal	Addition polymerisation of propylene	Addition polymerisation of vinylchloride	Integrated chlorination and oxychlorination of ethylene	Reaction of isobutene and methanol	Alkylation of benzene
Reaction		-	n C3H6 (g) → (C3H6)n (s)	n C2H3Cl (g) → (C2H3Cl)n (s)	4C2H4(g) + 2Cl2(g) + O2(g) → 4C2H3Cl(g) + 2H2O(g)	C4H8(g) + CH4O(l) → C5H12O(l)	C6H6(l) + C2H4(g) → C8H10(l)
Share, the Netherlands		0%	100%	100%	100%	100%	100%
Share, Western Europe		3%	100%	100%	100%	100%	100%
Share, World		3%	100%	100%	100%	100%	100%
Source for process data		FhG-ISI (1999)	Hydrocarbon processing (2003), pp. 124	Hydrocarbon processing (2003), pp. 129	IPTS (2003a), pp. 293	IPTS (2003a), pp. 122	Hydrocabon Processing (2003), pp. 92
Type of process		Average	Average	Average	Average	Average	Average
Uncertainty indicator energy use values (see Section 4.1.1 for explanation)		1	2	2	1	1	2
Heat of stoichometric reaction	[GJf / t of main product]	-	-2.47	-2.11	-2.32	-0.65	-1.07
Electricity use	[GJe / t of main product]	0.22	1.15	0.58	0.72	0.06	0.07
Fuel use	[GJf / t of main product]	18.67	0.00	0.00	3.60	0.00	2.51
Steam use	[GJf / t of main product]	0.00	0.80	1.80	0.51	3.86	-3.10
Total primary energy use	[GJp / t of main product]	19.16	3.45	3.28	5.77	4.41	-0.77
Heat effect of reaction	[GJf / t of main product]	-	2.70	2.68	3.32	0.65	1.20
Total final energy loss	[GJf / t of main product]	18.89	4.65	5.05	8.15	4.56	0.68
Total primary energy loss	[GJp / t of main product]	19.16	6.15	5.96	9.09	5.06	0.43
Excess final energy use	[GJf / t of main product]	-	4.42	4.49	7.15	4.57	0.56
Losses due to non-selectivity	[GJf / t of main product]	-	0.23	0.57	1.00	0.00	0.13
Energy efficiency, final	[%]	51%	90%	77%	70%	89%	98%
Energy efficiency, primary	[%]	51%	88%	74%	67%	87%	99%
Carbon losses, energy use, primary	[t CO2 / t main product]	-	0.21	0.20	0.36	0.10	-0.05
Carbon losses, reaction	[t CO2 / t main product]	-	0.02	0.04	0.07	0.00	0.01
Total carbon losses, primary	[t CO2 / t main product]	2.39	0.23	0.25	0.42	0.10	-0.04
Carbon efficiency, reaction	[%]	-	100%	97%	96%	100%	100%
Total carbon efficiency	[%]	36%	93%	85%	77%	96%	101%
Energy costs	[€ / t main product]	-	27	21	35	23	-5
Value added reaction	[€ / t main product]	-	311	228	185	342	47
Total value added	[€ / t main product]	102	284	207	150	319	51
Value added reaction, % of product value	[%]	-	39%	28%	32%	44%	9%
Total value added, % of product value	[%]	56%	35%	25%	26%	41%	10%
Notes		[1]					

Characteristic	Unit	Styrene	Terephthalic acid	Ethylene oxide	Polystyrene	Ethylene glycol	Cumene
Production volume, the Netherlands	[ktonne / year]	1243	249	353	396	237	344
Production volume, Western Europe	[ktonne / year]	4588	1959	2176	3028	1170	2678
Production volume, World	[ktonne / year]	20067	17000	13410	13244	12200	9631
Reaction route		Dehydrogenation of ethylbenzene	Oxidation of p-xylene	Oxidation of ethylene	Addition polymerisation of styrene	Hydration of ethylene oxide	Alkylation of propylene with benzene
Reaction		$C8H10(l) \rightarrow C8H8(l) + H2(g)$	$C8H10(l) + 3O2(g) \rightarrow C8H6O4(l) + 2H2O(g)$	$2C2H4(g) + O2(g) \rightarrow 2C2H4O(g)$	$n\ C8H8(l) \rightarrow (C8H8)n\ (s)$	$C2H4O(g) + H2O(g) \rightarrow C2H6O2(l)$	$C3H6(g) + C6H6(l) \rightarrow C6H12(l)$
Share, the Netherlands		29%	100%	100%	100%	100%	100%
Share, Western Europe		85%	100%	100%	100%	100%	100%
Share, World		85%	100%	100%	100%	100%	100%
Source for process data		Patel (1998)	Boustead (2002), pp. 24	Patel (1998)	Hydrocarbon processing (2003), pp. 125	Patel (1998)	Hydrocarbon processing (2003), pp. 88-89
Type of process		Average	Average	Average	Average	Average	Average
Uncertainty indicator energy use values (see Section 4.1.1 for explanation)		2	1	2	2	2	2
Heat of stoichometric reaction	[GJf / t of main product]	1.11	-7.62	-2.39	-0.67	-2.65	-0.91
Electricity use	[GJe / t of main product]	0.22	1.69	1.02	0.37	0.26	0.04
Fuel use	[GJf / t of main product]	1.68	1.63	0.00	0.53	0.94	0.00
Steam use	[GJf / t of main product]	6.19	1.65	3.09	0.01	4.37	1.80
Total primary energy use	[GJp / t of main product]	9.05	7.21	5.69	1.38	6.38	2.10
Heat effect of reaction	[GJf / t of main product]	-0.57	9.21	9.14	1.08	3.70	1.31
Total final energy loss	[GJf / t of main product]	7.53	14.18	13.25	2.00	9.27	3.16
Total primary energy loss	[GJp / t of main product]	8.48	16.43	14.83	2.45	10.08	3.41
Excess final energy use	[GJf / t of main product]	6.98	12.58	6.49	1.59	8.22	2.76
Losses due to non-selectivity	[GJf / t of main product]	0.54	1.59	6.75	0.41	1.05	0.40
Energy efficiency, final	[%]	85%	57%	68%	95%	67%	93%
Energy efficiency, primary	[%]	84%	53%	65%	94%	66%	92%
Carbon losses, energy use, primary	[t CO2 / t main product]	0.56	0.45	0.35	0.09	0.40	0.13
Carbon losses, reaction	[t CO2 / t main product]	0.05	0.15	0.45	0.03	0.05	0.03
Total carbon losses, primary	[t CO2 / t main product]	0.61	0.60	0.80	0.12	0.45	0.16
Carbon efficiency, reaction	[%]	98%	93%	82%	99%	97%	99%
Total carbon efficiency	[%]	85%	78%	71%	97%	78%	95%
Energy costs	[€ / t main product]	48	50	37	10	34	11
Value added reaction	[€ / t main product]	266	258	259	348	-20	116
Total value added	[€ / t main product]	218	208	222	338	-54	105
Value added reaction, % of product value	[%]	33%	42%	34%	32%	-3%	21%
Total value added, % of product value	[%]	27%	34%	29%	31%	-9%	19%
Notes		[5]					

Characteristic	Unit	Butadiene	Polyethylene terephthalate (PET)	Polyurethane		Acetic acid	
Production volume, the Netherlands	[ktonne / year]	352	185	187	187	0	0
Production volume, Western Europe	[ktonne / year]	1839	3268	2797	2797	1214	1214
Production volume, World	[ktonne / year]	7868	7800	7720	7720	7310	7310
Reaction route		From steam cracking	Esterification of terephthalic acid with ethylene glycol	Reaction of TDI with polyols	Reaction of MDI with polyols	Oxidation of acetaldehyde	Carbonylation of methanol
Reaction		-	n C8H6O4(l) +n C2H6O2(l) → (C10H8O4)n (s) + 2n H2O(g)	-	-	2C2H4O(g) + O2(g) → 2C2H4CO2(l)	CH3OH(l) + CO(g) → C2H4O2(l)
Share, the Netherlands		100%	100%	50%	50%	-	-
Share, Western Europe		100%	100%	50%	50%	20%	80%
Share, World		100%	100%	50%	50%	20%	80%
Source for process data		Chauvel (1989a), pp. 207	Boustead (2002), pp. 30	Boustead (1997)	Boustead (1997)	Patel (1998)	Patel (1998)
Type of process		Average	Average	Average	Average	Average	Average
Uncertainty indicator energy use values (see Section 4.1.1 for explanation)		2	1	1	1	2	2
Heat of stoichometric reaction	[GJf / t of main product]	Separation	0.15			-4.83	-1.78
Electricity use	[GJe / t of main product]	0.90	0.70	1.50	1.50	0.02	0.63
Fuel use	[GJf / t of main product]	0.00	1.63	0.00	0.00	0.00	0.00
Steam use	[GJf / t of main product]	6.43	2.42	0.00	0.00	1.67	4.77
Total primary energy use	[GJp / t of main product]	9.14	5.87	3.33	3.33	1.90	6.71
Heat effect of reaction	[GJf / t of main product]	Separation	0.22	-	-	5.59	2.55
Total final energy loss	[GJf / t of main product]	7.33	4.97	-	-	7.28	7.96
Total primary energy loss	[GJp / t of main product]	9.14	6.09	-	-	7.49	9.26
Excess final energy use	[GJf / t of main product]	7.33	4.59	-	-	6.52	7.19
Losses due to non-selectivity	[GJf / t of main product]	Separation	0.38	-	-	0.76	0.77
Energy efficiency, final	[%]	86%	81%	-	-	65%	63%
Energy efficiency, primary	[%]	83%	78%	-	-	64%	59%
Carbon losses, energy use, primary	[t CO2 / t main product]	0.57	0.36	0.21	0.21	0.12	0.42
Carbon losses, reaction	[t CO2 / t main product]	0.00	0.04	-	-	0.06	0.11
Total carbon losses, primary	[t CO2 / t main product]	0.57	0.40	-	-	0.18	0.52
Carbon efficiency, reaction	[%]	-	98%	-	-	96%	93%
Total carbon efficiency	[%]	85%	85%	-	-	89%	74%
Energy costs	[€ / t main product]	53	35	29	29	10	39
Value added reaction	[€ / t main product]	-	432	298	586	-113	342
Total value added	[€ / t main product]	-	396	269	557	-123	303
Value added reaction, % of product value	[%]	-	37%	16%	31%	-26%	78%
Total value added, % of product value	[%]	-	34%	14%	30%	-28%	69%
Notes			[6]		[7]		

Characteristic	Unit	Formaldehyde	Phenol		Cyclohexane
Production volume, the Netherlands	[ktonne / year]	351	103		232
Production volume, Western Europe	[ktonne / year]	1850	2065		1255
Production volume, World	[ktonne / year]	6450	5586		5100
Reaction route		Oxydehydration of methanol	Oxidation of cumene	Oxidation of toluene	Hydrogenation of benzene
Reaction		$2CH_3OH(l) + O_2(g) \rightarrow$ $2CH_2O(g) + 2H_2O(g)$	$C_9H_{12}(l) + O_2(g) \rightarrow$ $C_6H_6O(l) + C_3H_6O(l)$	$2C_7H_8(l) + 3O_2(g) \rightarrow$ $2C_6H_6O(l) + 2CO_2(g)$	$C_6H_6(l) + 3H_2(g) \rightarrow$ $C_6H_{12}(l)$
Share, the Netherlands		100%	0%	100%	100%
Share, Western Europe		100%	95%	5%	100%
Share, World		100%	96%	4%	100%
Source for process data		IPTS (2003a), pp. 253	Chauvel (1989b), pp. 124	Chauvel (1989b), pp. 124	Patel (1998)
Type of process		Average	Average	Average	Average
Uncertainty indicator energy use values (see Section 4.1.1 for explanation)		1	3	3	2
Heat of stoichometric reaction	[GJf / t of main product]	-3.72	-3.82	-5.95	-2.44
Electricity use	[GJe / t of main product]	0.77	0.94	2.16	0.09
Fuel use	[GJf / t of main product]	0.00	0.00	3.50	0.00
Steam use	[GJf / t of main product]	-4.77	9.00	23.14	-1.28
Total primary energy use	[GJp / t of main product]	-3.60	12.08	34.01	-1.21
Heat effect of reaction	[GJf / t of main product]	5.43	7.03	17.07	2.77
Total final energy loss	[GJf / t of main product]	1.42	16.97	45.87	1.59
Total primary energy loss	[GJp / t of main product]	1.83	19.11	51.08	1.56
Excess final energy use	[GJf / t of main product]	-0.28	13.76	34.75	1.25
Losses due to non-selectivity	[GJf / t of main product]	1.70	3.21	11.12	0.33
Energy efficiency, final	[%]	93%	74%	41%	96%
Energy efficiency, primary	[%]	91%	72%	38%	97%
Carbon losses, energy use, primary	[t CO2 / t main product]	-0.22	0.75	2.11	-0.08
Carbon losses, reaction	[t CO2 / t main product]	0.12	0.26	1.17	0.02
Total carbon losses, primary	[t CO2 / t main product]	-0.11	1.01	3.28	-0.06
Carbon efficiency, reaction	[%]	93%	94%	71%	99%
Total carbon efficiency	[%]	108%	81%	46%	102%
Energy costs	[€ / t main product]	-12	68	188	-5
Value added reaction	[€ / t main product]	-44	-136	199	-88
Total value added	[€ / t main product]	-32	-204	11	-83
Value added reaction, % of product value	[%]	-26%	-22%	32%	-18%
Total value added, % of product value	[%]	-19%	-33%	2%	-17%
Notes				[8]	

Characteristic	Unit	Propylene oxide			Polyetherpolyols	Acrylonitrile
Production volume, the Netherlands	[ktonne / year]	602			413	172
Production volume, Western Europe	[ktonne / year]	1656			1337	1125
Production volume, World	[ktonne / year]	4877			4816	4704
Reaction route		Indirect oxidation via chlorohydrin	Indirect oxidation via tert-butyl hydroperoxide	Indirect oxidation via ethylbenzene hydroperoxide	Polyaddtion of epoxies to an initiator	Ammoxidation of propylene
Reaction		$C_3H_6(g) + Cl_2(g) + NaOH(s) \rightarrow C_3H_6O(l) + HCl(g) + NaCl(s)$	$1.89C_4H_{10}(g) + C_3H_6(g) + 1.45\ O_2(g) \rightarrow 1.89C_4H_{10}O(l) + C_3H_6O(l)$	$1.34C_8H_{10}(l) + C_3H_6(g) + 1.17O_2(g) \rightarrow 1.34C_8H_8(l) + C_3H_6O(l) + 1.34H_2O(g)$		$2C_3H_6(g) + 2NH_3(g) + 3O_2(g) \rightarrow 2C_3H_3N(l) + 6H_2O(g)$
Share, the Netherlands		0%	36%	64%	100%	100%
Share, Western Europe		46%	33%	21%	100%	100%
Share, World		51%	30%	19%	100%	100%
Source for process data		Chauvel (1989b), pp. 19	Chauvel (1989b), pp. 19	Tebodin (1996), p. 144	Chauvel (1989b), pp. 361	Patel (1998)
Type of process		Average	Average	Average	Average	Average
Uncertainty indicator energy use values (see Section 4.1.1 for explanation)		3	3	2	3	2
Heat of stoichometric reaction	[GJf / t of main product]	-3.78	-9.73	-3.94	-	-10.34
Electricity use	[GJe / t of main product]	0.00	1.44	3.18	0.13	0.90
Fuel use	[GJf / t of main product]	0.00	0.00	5.74	0.00	0.00
Steam use	[GJf / t of main product]	13.86	24.43	18.02	1.29	0.50
Total primary energy use	[GJp / t of main product]	15.40	30.34	32.83	1.71	2.55
Heat effect of reaction	[GJf / t of main product]	-	30.28	16.53	-	23.58
Total final energy loss	[GJf / t of main product]	-	56.15	43.46	-	24.98
Total primary energy loss	[GJp / t of main product]	-	60.62	49.35	-	26.14
Excess final energy use	[GJf / t of main product]	-	35.60	30.88	-	11.74
Losses due to non-selectivity	[GJf / t of main product]	-	20.55	12.59	-	13.24
Energy efficiency, final	[%]	-	68%	74%	-	57%
Energy efficiency, primary	[%]	-	66%	71%	-	56%
Carbon losses, energy use, primary	[t CO2 / t main product]	0.95	1.88	2.04	0.11	0.16
Carbon losses, reaction	[t CO2 / t main product]	0.33	1.28	0.68	-	0.71
Total carbon losses, primary	[t CO2 / t main product]	1.28	3.16	2.71	-	0.87
Carbon efficiency, reaction	[%]	88%	87%	94%	-	79%
Total carbon efficiency	[%]	65%	73%	79%	-	75%
Energy costs	[€ / t main product]	77	164	191	10	20
Value added reaction	[€ / t main product]	-	997	928	102	289
Total value added	[€ / t main product]	-	833	737	93	269
Value added reaction, % of product value	[%]	-	49%	35%	10%	32%
Total value added, % of product value	[%]	-	41%	28%	9%	30%
Notes				[9]	[10]	

Characteristic	Unit	Caprolactam		Acetone	Phthalic anhydride	
Production volume, the Netherlands	[ktonne / year]	189		129	69	
Production volume, Western Europe	[ktonne / year]	1000		1280	695	
Production volume, World	[ktonne / year]	4160		3900	3200	
Reaction route		From cyclohexane	From Phenol	Dehydrogenation of isopropanol	Oxidation of o-xylene	Oxidation of naphthalene
Reaction		$2C_6H_{12}(l) + 3O_2(g) + 8.16\ NH_3(g) + 3.08\ H_2SO_4(l) \rightarrow 2C_6H_{11}ON(l) + 4H_2O(g) + 3.08(NH_4)_2SO_4(l)$	$2C_6H_5O(l) + 17.08\ NH_3(g) +3H_2(g) +4.52\ S(s) + 3.02\ H_2SO_4(l) + 6.78O_2(g) + 4.52\ H_2O(g) \rightarrow 2C_6H_{11}ON(l) + 7.54(NH_4)_2SO_4(s)$	$C_3H_8O(l) \rightarrow C_3H_6O(l) + H_2(g)$	$C_8H_{10}(l) + 3O_2(g) \rightarrow C_8H_4O_3(l) + 3H_2O(g)$	$2C_{10}H_8(l) + 9O_2(g) \rightarrow 2C_8H_4O_3(l) + 4CO_2(g) + 4H_2O(g)$
Share, the Netherlands		0%	100%	100%	100%	0%
Share, Western Europe		54%	46%	17%	94%	6%
Share, World		54%	46%	10%	85%	15%
Source for process data		Patel (1998)	Chauvel (1989b), pp. 272	Chauvel (1989b), pp. 135	Patel (1998)	Chauvel (1989b), pp. 316
Type of process		Average	Average	Average	Average	Average
Uncertainty indicator energy use values (see Section 4.1.1 for explanation)		2	3	3	2	3
Heat of stoichometric reaction	[GJf / t of main product]	-9.27	-21.86	1.21	-7.97	-12.53
Electricity use	[GJe / t of main product]	3.96	1.08	0.20	3.81	1.80
Fuel use	[GJf / t of main product]	0.80	0.10	0.00	0.00	0.00
Steam use	[GJf / t of main product]	32.40	23.14	9.77	-5.57	-11.14
Total primary energy use	[GJp / t of main product]	45.59	28.21	11.30	2.28	-8.38
Heat effect of reaction	[GJf / t of main product]	36.23	32.14	-0.75	15.73	14.69
Total final energy loss	[GJf / t of main product]	73.38	56.47	9.22	13.97	5.35
Total primary energy loss	[GJp / t of main product]	81.82	60.36	10.55	18.00	6.31
Excess final energy use	[GJf / t of main product]	46.43	46.19	8.76	6.20	3.19
Losses due to non-selectivity	[GJf / t of main product]	26.95	10.28	0.47	7.76	2.16
Energy efficiency, final	[%]	-	-	78%	61%	80%
Energy efficiency, primary	[%]	-	-	76%	55%	77%
Carbon losses, energy use, primary	[t CO2 / t main product]	2.83	0.71	0.70	0.14	-0.52
Carbon losses, reaction	[t CO2 / t main product]	0.88	0.25	0.03	0.60	0.78
Total carbon losses, primary	[t CO2 / t main product]	3.71	0.96	0.73	0.74	0.26
Carbon efficiency, reaction	[%]	73%	90%	99%	80%	75%
Total carbon efficiency	[%]	39%	71%	76%	77%	90%
Energy costs	[€ / t main product]	261	150	58	43	-27
Value added reaction	[€ / t main product]	411	602	45	178	271
Total value added	[€ / t main product]	150	451	-13	135	297
Value added reaction, % of product value	[%]	31%	37%	6%	31%	50%
Total value added, % of product value	[%]	11%	28%	-2%	23%	55%
Notes			[11]	[12]		

Characteristic	Unit	Dimethyl terephthalate	Aniline	Dioctylphthalate	Acetaldehyde	Nitrobenzene	2 Ethylhexanol
Production volume, the Netherlands	[ktonne / year]	103	0	0	0	0	0
Production volume, Western Europe	[ktonne / year]	1128	875	432	470	1225	775
Production volume, World	[ktonne / year]	3096	3010	2880	2566	2468	2408
Reaction route		Oxidation of p-xylene, esterification with methanol	Hydrogenation of nitrobenzene	Esterification of phthalic anhydride with 2-ethylhexanol	Oxidation of ethylene	Nitration of benzene	Hydroformylation of propylene
Reaction		C8H10(l) + 3O2(g) +2CH4O(l) → C10H10O4(l) + 4H2O(g)	C6H5NO2 (l) + 3H2(g) → C6H7N(l) + 2H2O(g)	C8H4O3(l) + 2C8H18O(l) → C24H38O4(l) + H2O(g)	2C2H4(g) + O2(g) → 2C2H4O(g)	C6H6(l) + HNO3(l) → C6H5NO2(l) + H2O(g)	2C3H6(g) +2CO(g) + 4H2(g) → C8H18O(l) + H2O(g)
Share, the Netherlands		100%	-	-	-	-	-
Share, Western Europe		100%	100%	100%	100%	100%	100%
Share, World		100%	100%	100%	100%	100%	100%
Source for process data		Patel (1998)	Chauvel (1989b), pp. 356	Patel (1998)	Patel (1998)	Chauvel (1989b), pp. 356	Patel (1998)
Type of process		Average	Average	Average	Average	Average	Average
Uncertainty indicator energy use values (see Section 4.1.1 for explanation)		2	3	2	2	3	2
Heat of stoichometric reaction	[GJf / t of main product]	-6.05	-4.99	-0.06	-4.97	-0.85	-3.80
Electricity use	[GJe / t of main product]	0.02	0.29	0.09	0.29	0.05	0.29
Fuel use	[GJf / t of main product]	5.86	0.00	0.00	0.00	0.00	0.00
Steam use	[GJf / t of main product]	0.00	-2.57	0.95	3.34	1.29	6.02
Total primary energy use	[GJp / t of main product]	5.90	-2.22	1.27	4.35	1.55	7.33
Heat effect of reaction	[GJf / t of main product]	10.44	7.47	2.35	6.63	0.85	3.99
Total final energy loss	[GJf / t of main product]	16.32	5.19	3.40	10.26	2.19	10.30
Total primary energy loss	[GJp / t of main product]	16.35	5.26	3.62	10.98	2.40	11.32
Excess final energy use	[GJf / t of main product]	11.93	2.71	1.10	8.60	2.19	10.10
Losses due to non-selectivity	[GJf / t of main product]	4.40	2.48	2.30	1.66	0.00	0.20
Energy efficiency, final	[%]	58%	87%	91%	71%	-	80%
Energy efficiency, primary	[%]	58%	87%	90%	70%		78%
Carbon losses, energy use, primary	[t CO2 / t main product]	0.37	-0.14	0.08	0.27	0.10	0.45
Carbon losses, reaction	[t CO2 / t main product]	0.34	0.06	0.17	0.11	0.00	0.00
Total carbon losses, primary	[t CO2 / t main product]	0.71	-0.08	0.24	0.38	0.10	0.45
Carbon efficiency, reaction	[%]	87%	98%	94%	95%	100%	100%
Total carbon efficiency	[%]	76%	103%	92%	84%	96%	87%
Energy costs	[€ / t main product]	30	-9	7	24	8	39
Value added reaction	[€ / t main product]	227	156	56	304	303	110
Total value added	[€ / t main product]	197	165	49	280	294	71
Value added reaction, % of product value	[%]	37%	13%	8%	43%	47%	18%
Total value added, % of product value	[%]	32%	13%	7%	40%	46%	11%
Notes						[13]	

Characteristic	Unit	Bisphenol A	Polyamide 66	Polyamide 6	Methylene diisocyanate (MDI)	Urea Formaldehyde resin	Adipic acid
Production volume, the Netherlands	[ktonne / year]	280	133	133	241	145	0
Production volume, Western Europe	[ktonne / year]	641	496	496	813	814	898
Production volume, World	[ktonne / year]	2300	2237	2237	2159	2129	2100
Reaction route		Condensation of phenol with acetone	Polycondensation of adipic acid with hexamethylenediamine	Polymerisation of caprolactam	Condensation of aniline with formaldehyde, phosgenation to MDI	Condensation of urea with formaldehyde	Oxidation of cyclohexane
Reaction		2C6H6O(l) + C3H6O(l) → C15H16O2(l) + H20(g)	nC6H10O4(l) + nC6H16N2(l) → (C12H22O2N2)n (s) + 2nH20(g)	n C6H11ON(l) → (C6H11ON)n (s)	2C6H7N(l) + CH2O(g) + 2Cl2(g)+2CO(g) → C15H10N2O2(l) + H2O(g) + 4HCl(g)	-	2C6H12(l) + 5O2(g) → 2C6H10O4(l) + 2H2O(g)
Share, the Netherlands		100%	100%	100%	100%	100%	-
Share, Western Europe		100%	100%	100%	100%	100%	100%
Share, World		100%	100%	100%	100%	100%	100%
Source for process data		IDEA (1991), pp. 75	Patel (1998)	Patel (1998)	Patel (1998)	Patel (1998)	Chauvel (1989b), pp. 244
Type of process		Average	Average	Average	Average	Average	Average
Uncertainty indicator energy use values (see Section 4.1.1 for explanation)		2	2	2	2	2	3
Heat of stoichometric reaction	[GJf / t of main product]	-0.79	0.27	-0.14	-1.74	-	-7.18
Electricity use	[GJe / t of main product]	0.58	0.40	0.40	3.88	0.18	1.44
Fuel use	[GJf / t of main product]	0.00	13.02	9.66	0.00	0.00	1.20
Steam use	[GJf / t of main product]	3.86	0.60	0.00	1.07	2.51	25.71
Total primary energy use	[GJp / t of main product]	5.57	14.56	12.53	9.82	3.19	32.97
Heat effect of reaction	[GJf / t of main product]	4.49	-0.27	3.43	3.06	-	14.75
Total final energy loss	[GJf / t of main product]	8.92	13.74	13.48	8.01	-	43.10
Total primary energy loss	[GJp / t of main product]	10.06	14.29	15.96	12.87	-	47.72
Excess final energy use	[GJf / t of main product]	5.23	13.74	10.20	6.69	-	35.54
Losses due to non-selectivity	[GJf / t of main product]	3.69	0.00	3.28	1.32	-	7.56
Energy efficiency, final	[%]	79%	69%	69%	78%	-	29%
Energy efficiency, primary	[%]	77%	68%	65%	69%	-	27%
Carbon losses, energy use, primary	[t CO2 / t main product]	0.35	0.90	0.65	0.61	0.20	2.04
Carbon losses, reaction	[t CO2 / t main product]	0.37	0.00	0.26	0.14	-	0.55
Total carbon losses, primary	[t CO2 / t main product]	0.72	0.90	0.91	0.75	-	2.59
Carbon efficiency, reaction	[%]	89%	100%	90%	95%	-	77%
Total carbon efficiency	[%]	80%	72%	72%	78%	-	41%
Energy costs	[€ / t main product]	33	76	56	81	17	177
Value added reaction	[€ / t main product]	243	680	564	864	-3	717
Total value added	[€ / t main product]	210	604	508	783	-20	540
Value added reaction, % of product value	[%]	25%	31%	31%	45%	-1%	66%
Total value added, % of product value	[%]	22%	27%	28%	40%	-6%	50%
Notes						[14]	

Characteristic	Unit	Isopropanol	Polycarbonate	Hexamethylene diamine			Toluene Diisocyanate (TDI)
Production volume, the Netherlands	[ktonne / year]	215	103	0			0
Production volume, Western Europe	[ktonne / year]	520	488	435			425
Production volume, World	[ktonne / year]	1806	1500	1346			1213
Reaction route		Hydration of propene	Polycondensation of bisphenol-A with phosgene	Hydrogenation of acrylonitrile	Ammonia with adipic acid	Hydrogen cyanide with butadiene	Nitratiopn of toluene, phosgenation to TDI
Reaction		C3H6(g) + H2O(g) → C3H8O(l)	-	2C3H3N(l) + 5H2(g) → C6H16N2(l)	C6H10O4(l) + 2NH3(g) + 4H2(g) → C6H16N2(l) + 4H2O(g)	C4H6(g) + 2CHN(g) + 4H2(g) → C6H16N2(l)	C7H8(l) + 2HNO3(l) +6H2 (g) + 2Cl2(g) + 2CO(g) → C9H6N2O2(l) + 6H2O(g) + 4HCl(g)
Share, the Netherlands		100%	100%	-	-	-	-
Share, Western Europe		100%	100%	23%	52%	25%	100%
Share, World		100%	100%	23%	52%	25%	100%
Source for process data		Chauvel (1989b), pp. 79	Plinke, pp. IV-30	Patel (1998)	Patel (1998)	Patel (1998)	Chauvel (1989b), pp. 342
Type of process		Average	Average	Average	Average	Average	Average
Uncertainty indicator energy use values (see Section 4.1.1 for explanation)		3	2	2	2	2	3
Heat of stoichometric reaction	[GJf / t of main product]	-1.58		-3.90	-0.54	-4.11	-7.99
Electricity use	[GJe / t of main product]	0.09	2.66	12.60	4.28	4.14	2.76
Fuel use	[GJf / t of main product]	5.20	0.00	8.37	2.10	25.54	24.76
Steam use	[GJf / t of main product]	5.40	12.86	37.29	12.67	21.70	7.25
Total primary energy use	[GJp / t of main product]	11.40	20.20	77.80	25.70	58.85	38.94
Heat effect of reaction	[GJf / t of main product]	5.24	-	8.81	5.83	14.50	17.86
Total final energy loss	[GJf / t of main product]	15.93	-	67.07	24.88	65.88	52.63
Total primary energy loss	[GJp / t of main product]	16.64	-	86.61	31.53	73.35	56.81
Excess final energy use	[GJf / t of main product]	12.27	-	62.16	19.60	55.49	42.75
Losses due to non-selectivity	[GJf / t of main product]	3.65	-	4.91	5.28	10.39	9.88
Energy efficiency, final	[%]	66%	-	35%	59%	35%	33%
Energy efficiency, primary	[%]	65%	-	29%	53%	33%	32%
Carbon losses, energy use, primary	[t CO2 / t main product]	0.71	1.25	4.83	1.59	3.65	2.42
Carbon losses, reaction	[t CO2 / t main product]	0.25	-	0.54	0.40	0.76	0.44
Total carbon losses, primary	[t CO2 / t main product]	0.96	-	5.37	2.00	4.40	2.86
Carbon efficiency, reaction	[%]	90%	-	81%	85%	75%	85%
Total carbon efficiency	[%]	70%	-	30%	53%	34%	46%
Energy costs	[€ / t main product]	58	123	494	164	329	218
Value added reaction	[€ / t main product]	242	-	550	-223	330	1251
Total value added	[€ / t main product]	185	-	56	-387	2	1033
Value added reaction, % of product value	[%]	39%	-	34%	-14%	20%	59%
Total value added, % of product value	[%]	29%	-	3%	-24%	0%	49%
Notes			[15]				

Characteristic	Unit	n Butanol
Production volume, the Netherlands	[ktonne / year]	0
Production volume, Western Europe	[ktonne / year]	314
Production volume, World	[ktonne / year]	1019
Reaction route		Hydroformulation of propylene, hydrogenation of buteraldehyde
Reaction		$C3H6(g) + CO(g) + 2H2(g) \rightarrow C4H10O(l)$
Share, the Netherlands		-
Share, Western Europe		100%
Share, World		100%
Source for process data		Patel (1998)
Type of process		Average
Uncertainty indicator energy use values (see Section 4.1.1 for explanation)		2
Heat of stoichometric reaction	[GJf / t of main product]	-3.20
Electricity use	[GJe / t of main product]	0.40
Fuel use	[GJf / t of main product]	0.00
Steam use	[GJf / t of main product]	3.27
Total primary energy use	[GJp / t of main product]	4.51
Heat effect of reaction	[GJf / t of main product]	6.06
Total final energy loss	[GJf / t of main product]	9.73
Total primary energy loss	[GJp / t of main product]	10.57
Excess final energy use	[GJf / t of main product]	6.87
Losses due to non-selectivity	[GJf / t of main product]	2.86
Energy efficiency, final	[%]	79%
Energy efficiency, primary	[%]	77%
Carbon losses, energy use, primary	[t CO2 / t main product]	0.28
Carbon losses, reaction	[t CO2 / t main product]	0.17
Total carbon losses, primary	[t CO2 / t main product]	0.45
Carbon efficiency, reaction	[%]	94%
Total carbon efficiency	[%]	85%
Energy costs	[€ / t main product]	26
Value added reaction	[€ / t main product]	85
Total value added	[€ / t main product]	59
Value added reaction, % of product value	[%]	15%
Total value added, % of product value	[%]	10%
Notes		

Notes
General
The results are expressed per tonne of the chemical commodity mentioned (main product). In Chapter 3, we express the results for processes where more than one product is produced per tonne of total products. For these processes, the production of by-products is given in the notes below. The absolute figures can easily be calculated using the production volumes and the shares of the various process routes. Processes are ranked in the order of decreasing worldwide production volume. The three processes to produce aromatics are grouped.

Per process

[1]   We did not specify a stoichometric reaction for ammonia and methanol production, because it would involve an arbitrary choice between the amount of hydrogen produced from the raw material and the amount of hydrogen produced from steam. We allocate an amount of raw material equivalent to the ammonia and methanol product (18.6 GJ / tonne and 19.9 GJ / tonne respectively) to feedstock use, the remainder to fuel use. To obtain a value for the total raw material input, the calorific value of ammonia and methanol should be added to the reported fuel use.

We use the emission factors of the raw materials used to calculate CO_2 emissions from ammonia and methanol production instead of the general fuel emission factor given in Appendix D.

Import and export of electricity and steam are not separately given in the literature sources used. They are small compared to the fuel input.

[2]   We did not specify a desired stoichometric reaction for the production of ethylene, because of the multiple products produced. We use the actual observed heat effect of reaction as the heat of the stoichometric reaction.

In Chapter 3, we express the results per tonne of total products in which we regard the total output of the cracker as products. To obtain the results per tonne of total products (including e.g. propylene), we multiplied the values per tonne of ethylene given here with the ethylene yield (0.324 for naphtha, 0.250 for gas oil, 0.803 for ethane, 0.465 for propane). Parts of the products are used to fuel the process. These amounts are given under fuel use. We used an emission factor of 48.7 kg CO_2 / GJ for naphtha and gas oil cracking and emission factor of 43.3 kg CO_2 / GJ for ethane and propane cracking (Neelis et al., 2003) instead of the emission factor given in Appendix D to account for the fact that the fuels used contain mainly methane and hydrogen.

[3]   We assume stoichometric conversion of sodium chloride, because it is unclear in which way the excess sodium chloride is lost. In Chapter 3, we express the results per tonne of total products, including 0.028 tonne of hydrogen and 1.128 tonne of sodium hydroxide. The energy efficiency indicators could not be calculated, because the input (sodium chloride) has a negative 'calorific value'.

[4]   With these three generic process configurations, we cover the total aromatics production (IPTS, 2003a). The benzene not produced from py-gas or toluene is produced as by-product in the production of p-xylene from reformate. Toluene, o-xylene and m-xylene are produced as by-products of the three processes given. In Chapter 3, we express the result per tonne of total products in which we regard the total output of the processes as product. To obtain these values, we multiplied the values per tonne of benzene given here with the benzene yield (0.275 for benzene from py-gas and 0.83 for benzene from toluene). The values per tonne of p-xylene from reformate are multiplied with the p-xylene yield (0.380).

[5]   The remaining styrene is produced as co-product in the production of propylene oxide. In Chapter 3, we express the results per tonne of total products, including 0.02 tonne of hydrogen.

[6]   No detailed process description was available for the production of PET from dimethylterephthalate. We therefore use a share of 100% for PET production from terephthalic acid.

[7]   Calorific value and heat of polymerization for polyurethane depends on the type of polyurethane produced and could not be calculated with sufficient accuracy. The heat effects of reaction and related indicators are therefore not calculated.

[8]   In Chapter 3, we express the results per tonne of total products, including for cumene oxidation 0.61 tonne of acetone.

[9]   The only process description for the chlorohydrin route available includes also the electrolysis of chlorine. To avoid double counting, we estimated the electricity and steam use for chlorine production by assuming that for every mole of propylene, one mole of chlorine is required and deducted this amount from the reported electricity and steam use. The resulting electricity and steam use is given in the table. The consumption of some of the raw materials is not given in the literature source and the heat effects of reaction and related indicators could therefore not be calculated.

        The stoichometric reactions in the two hydroperoxide routes are based on the molar ratio of the inputs. In Chapter 3, we express the results per tonne of total products, including 2.45 tonne tert-butyl alcohol (indirect oxidation via tert-butyl-hydroperoxide) or 2.29 tonne of styrene (indirect oxidation via ethylbenzene hydro peroxide).

[10]   The calorific value and heat of polymerization for polyetherpolyols depends on the type of polyether polyols produced and could not be calculated with sufficient accuracy. The heat effects of reaction and related indicators are therefore not calculated.

[11]   The stoichometric reactions include the production of ammonium sulphate by-product. In Chapter 3, we express the results per tonne of total products, including 1.8 tonne (from cyclohexane) or 4.4 tonne (from phenol) ammonium sulphate. The energy efficiency indicators could not be calculated, because one of the inputs (sulphuric acid) has a negative 'calorific value'.

[12]   The remaining acetone is produced as co-product in the production of phenol and is covered there. In Chapter 3, we express the results per tonne of total products, including 0.03 tonne of hydrogen.

[13]   The energy efficiency indicators could not be calculated, because one of the inputs (nitric acid) has a negative 'calorific value'.

[14]   The calorific value and heat of polymerization for urea formaldehyde resins are unknown. The heat effects of reaction and related indicators are therefore not calculated.

[15]   Only data on electricity and steam use were available. The heat effects of reaction and related indicators are therefore not calculated.

Appendix I   Process characteristics refinery industry

Characteristic	Unit	Atmospheric distillation Value	Vacuum distillation Value	Catalytic cracking Value	Catalytic reforming Value	Hydro cracking Value	Thermal processes Value	Coking Value	Coking Value	Hydrotreatment Value	Hydrotreatment Value
Volume, the Netherlands	[ktonne / year]	59392	21528	5220	8587	5408	6065	1833	1833	32278	32278
Volume, Western Europe	[ktonne / year]	687174	248571	104541	103312	30887	76703	16328	16328	390206	390206
Volume, World	[ktonne / year]	4077490	1335058	687965	552661	201015	188793	187251	187251	1834628	1834628
Reaction route		Atmospheric distillation of crude oil	Vacuum distillation of atmospheric residue	Catalytic cracking of vacuum destillate	Catalytic reforming of heavy naphtha	Hydrocracking of vacuum destillate	Visbreaking of vacuum residue	Delayed Coking	Fluid/Flexicoking	Naphtha	Middle destillates
Share, the Netherlands		100%	100%	100%	100%	100%	100%	0%	100%	50%	30%
Share, Western Europe		100%	100%	100%	100%	100%	100%	82%	18%	40%	31%
Share, World		100%	100%	100%	100%	100%	100%	82%	18%	40%	31%
Source for process data		IPTS (2003b), pp. 71, 139, 461-463	IPTS (2003b), pp. 71, 139, 461-463	DOE/OIT (1998), pp. 55,63	van Oostvoorn (1989), pp. A2-25-28	van Oostvoorn (1989), pp. A2-36-39	van Oostvoorn (1989), pp. A2-40	IPTS (2003b), pp. 35-37, 108, 464	van Oostvoorn (1989), pp. A2-41	IPTS (2003b), pp. 53-59, 124-126	IPTS (2003b), pp. 53-59, 124-126
Type of process		Average	Average	Average	Average	Average	Average	Average	Average	Average	Average
Electricity use	[GJe / t]	0.02	0.01	0.10	0.05	0.29	0.02	0.09	0.31	0.03	0.05
Fuel use	[GJf / t]	0.54	0.60	0.48	2.40	1.50	1.00	1.00	0.00	0.28	0.40
Steam use	[GJf / t]	0.07	0.10	-0.76	0.17	0.10	0.21	0.00	-0.59	0.09	0.27
Total final energy use	[GJf / t]	0.63	0.71	-0.18	2.61	1.89	1.23	1.09	-0.29	0.39	0.72
Total primary energy use	[GJp / t]	0.66	0.74	-0.15	2.69	2.25	1.28	1.20	0.02	0.43	0.82
Carbon losses, energy use, primary	[t CO2 / t]	0.05	0.05	-0.01	0.20	0.17	0.09	0.09	0.00	0.03	0.06
Carbon losses, reaction	[t CO2 / t]	-	-	0.17	-	-	-	-	-	-	-
Total carbon losses, primary	[t CO2 / t]	-	-	0.16	-	-	-	-	-	-	-
Energy costs	[€ / t]	3	4	0	14	13	7	7	2	2	4
Notes	[1]										

Characteristic	Unit	Hydrotreatment	Isomerisation	Alkylation	Sulphur_recovery	Lubricants	Hydrogen
		Value	Value	Value	Value	Value	Value
Volume, the Netherlands	[ktonne / year]	32278	685	633	307	580	133
Volume, Western Europe	[ktonne / year]	390206	21372	11193	3200	6957	1180
Volume, World	[ktonne / year]	1834628	70899	91347	20464	41142	6000
Reaction route		Vacuum destillate and gas oil	Isomerisation of naphtha	Alkylation of olefins	Sulphur recovery	Lubricants	Steam reforming of natural gas
Share, the Netherlands		20%	100%	100%	100%	100%	100%
Share, Western Europe		29%	100%	100%	100%	100%	100%
Share, World		29%	100%	100%	100%	100%	100%
Source for process data		IPTS (2003b), pp. 53-59, 124-126	van Oostvoorn (1989), pp. A2-30	IPTS (2003b), pp. 25-26, 96-97,	IPTS (2003b), pp. 337-340	IPTS (2003b), pp. 27-28, 98-99	Appl (1997), pp. 106
Type of process		Average	Average	Average	Average	Average	Average
Electricity use	[GJe / t]	0.07	0.10	0.15	0.51	0.59	0.68
Fuel use	[GJf / t]	0.55	1.13	2.00	1.30	3.16	51.05
Steam use	[GJf / t]	0.27	0.42	1.41	1.29	0.00	-30.02
Total final energy use	[GJf / t]	0.89	1.65	3.57	3.10	3.76	21.72
Total primary energy use	[GJp / t]	1.01	1.82	3.91	3.87	4.48	19.21
Carbon losses, energy use, primary	[t CO2 / t]	0.07	0.13	0.29	0.29	0.33	-
Carbon losses, reaction	[t CO2 / t]	-	-	-	-	-	-
Total carbon losses, primary	[t CO2 / t]	-	-	-	-	-	7.24
Energy costs	[€ / t]	5	7	20	22	26	57
Notes	[1]						

Notes

[1]   The figures for alkylation, isomerisation, lubricants and sulphur recovery are per tonne of product produced. The figures for all other processes are per tonne of feedstock. Absolute figures can easily be calculated using the process volumes and the shares of the various process routes. Processes are ranked in the order of decreasing worldwide process volume.