Economic and Environmental Aspects of Integration in Chemical Production Sites

Zur Erlangung des akademischen Grades eines
Doktors der Wirtschaftswissenschaften

(Dr. rer. pol.)

von der Fakultät für
Wirtschaftswissenschaften
der Universität Karlsruhe (TH)

genehmigte

DISSERTATION

von

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Tag der mündlichen Prüfung: 10. Juli 2008
Referent: Professor Dr. Otto Rentz
Korreferent: Professor Dr. Henning Bockhorn

2008 Karlsruhe

Acknowledgements

I had the pleasure of completing this dissertation while working in the chemical industry in Asia, based in Singapore. My sincerest thanks go to my supervisor, Professor Dr. Otto Rentz, for giving me the opportunity to undertake this project from afar and for providing his support and expertise. I would also like to express my gratitude to all my industry contacts who entrusted me with valuable information and answered my many questions. Additionally, I would like to thank my colleagues at the ‘Institut für Industriebetriebslehre und Industrielle Produktion, Universität Karlsruhe’ for their kind support.

Karlsruhe, July 2008 Nicola Kimm

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Abbreviations

Units

a	Annum
h	Hour
J	Joule
K	Thousand
MW	Megawatt
t	Tons

Acronyms

AA/AE	Acrylic Acid / Acrylic Esters
AN	Aniline
ASU	Air Separation Unit
BA	Butylacrylate
C#	Carbon compound with # Carbon atoms, eg. C2 ethylene
CAA	Crude Acrylic Acid
CHP	Combined Heat and Power plant
EA	Ethylacrylate
2-EHA	2-Ethylhexyl Acrylate
EO/EG	Ethylene Oxide / Ethylene Glycol
GTCC	Gas Turbine Combined Cycle
ICPS	Integrated Chemical Production Site
LCA	Life Cycle Assessment
LDPE	Low Density Polyethylene
LPG	Light Petroleum Gas
MA	Methylacrylate
MDI	Methylene Diphenylene Isocyanate
MFA	Material Flow Analysis
NB	Nitrobenzene
PA	Polyacrylates
PIOT	Physical Input-Output Tables
PFO	Pyrolysis Fuel Oil
S#	Case study scenario, eg. S1, S2, or S3
SA	Stand-Alone Chemical Production Site
Semi-ICPS	Semi-Integrated Chemical Production Site
Syngas	Synthesis gas
WWT	Waste Water Treatment

Symbols

ε	Efficiency, %
σ	Standard deviation, -

Abbreviations

C	Cost, €/a
c	Specific cost, €/t
D	Distance, km
e	Specific energy, KJ/Kg
E	Energy flow, KJ/a
F*f*	Factor fuel, $t_f/(t_{prod}\cdot km)$
F*t*	Factor t, €/$(t_{prod}\cdot km)$
F*em,pp*	Factor em,pp, t_{em}/MWh
F*em,t*	Factor em,t, $t_{em}/(t_{prod}\cdot km)$
h	Enthalpy, KJ/Kg
M	Mass flow, t/a
S	Savings, €/a
v	Value, €/t
x	Normed integration factor, -
X	Integration factor, -

Indices

b	boiler
bp	by-product
c	captive use material
cw	cooling water
d	disposal of waste
dm	demineralised water
em	emissions
el	electrical
eq	equipment
f	fuel
fac	facilities
h2O	water
hr	heat recovery
hs	heated stream
in	incineration
infras	infrastructure
l	logistics
lm	logistics management
p	packaging
pp	power plant
rm	raw material
s	sales product
sp	all sales products for site
st	steam
t	transport
th	thermal
u	useable by-product
u,d	u for disposal
u,i	u for incineration
u,s	u for sales
v	value chain
w	waste
wd	waste for disposal
wi	waste for incineration
ww	waste water
we	waste emissions

1 Introduction

Various types of chemical production sites exist throughout the world. At one end of the spectrum are stand-alone sites consisting of a single production plant and at the other end, large sites consisting of several production plants, each with their associated infrastructure. Sites consisting of several production plants are often referred to as chemical parks or chemical clusters. Chemical clusters consist of several plants located close to one other in order to derive some benefit. The benefit may be as simple as the shared use of land and infrastructure or extend to the sharing of resources or the exchange of materials.

As the scale of chemical sites increases, co-location becomes of greater importance. Large chemical production facilities consist of world-scale chemicals producers and exist in various parts of the world, typically strategically located at coastal areas or waterways for port and water access. Such sites consist of individual chemical production plants which are integrated with one another in different ways and to different degrees. This integration involves individual plants exchanging feeds or products with one another. Value chains link production plants where each plant achieves a successively higher level of processing, leading to chemical products which are ultimately used to make consumer products. The linkages in such sites are not limited to materials, but extend to energy, shared facilities, and resources. Most often, several companies are involved in such a network.

Since the types of chemical sites vary considerably, research into the benefits of co-location must specify the type of production site. The focus of this work is the Integrated Chemical Production Site (ICPS), which is defined here as a kind of chemical cluster in which production plants form an integrated network via ties in production, logistics, and energy. This site represents a special kind of industrial cluster where its members are physically linked to one another via pipeline. Further, members of an ICPS share facilities such as those for utilities, energy provision, and waste water treatment. Also, these sites may benefit from pooled resources and services such as raw material procurement, IT systems, personnel training, and more.

It is the premise of this work that integration in such sites leads to significant cost savings and environmental benefits due to the use of chemical by-products, the onsite transport of materials, energy integration, and the shared use of facilities. The benefit of integration for an ICPS is expected to vary depending on the types of processes onsite and the site configuration; that is, if the site utilises all potentials for integration, such as available by-products or the transfer of excess heat.

The aim of this work is to provide an approach for quantifying the economic and environmental benefits of integration for either a site or a plant. This research is novel and purposeful, as it aims to provide a methodology to support strategic decision-making for site planning, optimisation, or investigating alternative production scenarios.

Outline and Approach

The approach of this work is as follows. The objectives of the study are defined from which research questions are derived. Next, relevant literature is reviewed in order to provide a theoretical framework from which to derive a methodology. This methodology is applied to case studies in order to answer the research questions and meet the objectives of the research.

An application-based, case-study approach is followed. Through application of the methodology, the abstract concepts of integration are put into quantifiable terms. The methodology is first applied to one integrated site to determine the overall economic and environmental benefits of integration for the site and to investigate which aspects of integration are most significant. This is followed by application of the methodology on the plant level. This is to demonstrate how integration affects a specific plant. Two plant level case studies are selected in order to highlight different aspects of integration. Finally, an approach is proposed to assess a particular process' suitability for location within an integrated site.

Objectives

A methodology is proposed to determine the economic and environmental implications of integration. The objectives of the work are to:

- Introduce the concept of the ICPS

- Describe types of integration present at the ICPS
- Develop methodologies to:
  - quantify the overall advantages of a particular ICPS
  - evaluate different integration scenarios for a particular plant
  - evaluate the suitability for a particular plant to be built in an ICPS
- Apply the methodologies to case studies

The main research questions to be answered are:

- Does an ICPS provide significant economic and environmental benefits compared to less integrated chemical production sites?
- What are the main contributors to the potential savings: materials integration, energy integration, or shared infrastructure?
- What considerations are important for the integration of a particular plant?

Implications of the Work

The methodology may be used by the management of an existing integrated site to quantify the economic and environmental benefits according to a site's current configuration and identify potentials for increased integration. Also, the methodology may be employed for the planning of an ICPS in order to compare alternative scenarios, such as in the evaluation of different production capacities or competing process technologies leading to different by-products or energy streams. Further, the resulting economic and environmental benefits may be utilised promotionally to increase acceptance of a chemical production site.

The work aims to provide a new perspective on describing and highlighting the advantages of integration in the ICPS. Also, the work may provide a useful approach for further application or as a basis for future studies.

Scope and Limitations

Organisational integration forms such as knowledge sharing and integrated internal processes, which may also contribute to cost savings, will not be addressed as they are less clearly quantifiable and out of the scope of this work. The research will focus on chemicals producers. Plants at the refining end of chemical production where fossil fuels are broken down into feedstock chemicals are not the focus of this work. The types of integrated sites addressed in this work consist of world-scale plants producing various types of chemical products. The research will not investigate to a detailed degree the technology behind the processes investigated. The degree of integration within a particular ICPS inevitably depends on the process technologies present, as the use of some technologies may benefit an ICPS more than others. However, this is not the main focus of this work.

Research Method

The case study research method is used for this work, as it is considered to be the most appropriate for the research topic as discussed below. An overview of the case study approach and reasons for its suitability are given below.

The use of case studies is widely adopted as a "*research strategy which focuses on understanding the dynamics present within single settings*" (Eisenhardt, 1989, p.534). Case studies are empirical investigations which rely on multiple data sources, which through corroboration, can enhance a study's validity. For example in an ICPS, the product flow rates cited by two inter-connected production plants ensures consistency in the data.

According to Stake (1994), to follow a case study approach is not a choice of methodology, but rather the selection of an object of study. The most compelling reason for the application of the case study approach for this topic is that it is suitable for investigating the unique character of a particular system which is also representative of other cases (Stake, 1994). However, case studies may have some disadvantages. The selection of the case may be biased and there is a risk of improper interpretation (Gable, 1994). Further, due to the large amount of data and the specific characteristics of a case, an overly complex and narrow theory may be developed (Eisenhardt, 1989).

The case studies in this work are particular sites or production plants. For each case study, one scenario represents an actual case and the other scenario is conceived for comparison purposes. A disadvantage of using an actual case is the problem of confidentiality regarding company data. Alternatively, the cases may be represented by design data, such as through process simulation software. This may be appropriate to support decisions in site design or plant location. However, in a simulated system, it must be ensured that the decisions made regarding process and energy streams are realistic and not overly optimistic. In applying the methodology to an actual setting, the routing of various flows is already determined and therefore the methodology is expected to yield valid results.

2 The Concept of Industrial Clusters

This chapter introduces the different perspectives on clusters. Thus, relevant literature was derived from various fields of study to provide the background and theoretical foundation for this study.

Below, an introduction and overview of this chapter is given. First, the terms 'cluster' and 'chemical cluster' are defined based on their use in the literature. Then a term defined for this work is introduced, the 'Integrated Chemical Production Site', a specific kind of chemical cluster where its members are physically linked to one another. Then, a review of the most important literature on clusters is given in order to illuminate relevant theories. This is followed by an introduction to the inter-disciplinary field of Industrial Ecology, in which the approach of Ecology (mapping of flows) is combined with Industrial Economics (Duchin and Hertwich, 2003). As Industrial Ecology deals explicitly with linked systems, it is useful in describing the interconnectedness of an ICPS. Related concepts are introduced, such Material Flow Analysis (MFA), which is used to track flows in industrial systems. Also, industrial settings which benefit from the application of Industrial Ecology principles, such as the closing of material loops, are highlighted.

The literature on clusters is mainly focussed on the investigation of cooperative advantages, while Industrial Ecology focuses primarily on environmental benefits. The literature from both of these fields is helpful in providing a framework with which to develop the methodology for this work, where the tools of Industrial Ecology are applied to the chemical cluster setting to determine the economic and environmental benefits of integration.

2.1 Definitions

2.1.1 The Cluster

The Oxford Dictionary defines a cluster as a "close group of things" (The Concise Oxford Dictionary, 1982). However, various theories on clusters define 'close' and 'things' in different ways. Porter (1998, p.199) defined a cluster as "*a geographically proximate group of interconnected companies and associated institutions in a particular field, linked by commonalities and complementarities*" and "*a system of interconnected firms and institutions the whole of which is greater than the sum of the parts*". Also, Roelandt and den Hertog (1999, p.1) noted that "*economic clusters can be characterised as networks of strongly interdependent firms (including suppliers) linked to each other in a value-adding production chain*."

2.1.2 The Chemical Cluster

Applying Porter's definition (1998, p.199) to the chemicals industry, the chemical cluster describes a geographically proximate group of interconnected chemical companies which may be linked to one another through 'commonalities and complementarities' such as customer/supplier relationships, technology, labour, or distribution. These customer/supplier relationships may be manifested in the transfer of materials or sharing of energy. However, the term chemical cluster does not insist that the individual members of the cluster are physically linked through material or energy flows. For example, the term chemical cluster may also describe an agglomeration of chemical companies which are co-located to derive a benefit, such as proximity to customers, a port, or a shared labour pool. Since this research investigates a specific form of chemical cluster in which material and energy flows physically link its members, another term is required. Thus the Integrated Chemical Production Site (ICPS) is defined.

2.1.3 The Integrated Chemical Production Site

An Integrated Chemical Production Site (ICPS) is defined here as a network of chemical producers in close physical proximity of one another in which the transfer of material and energy flows connects the individual chemical producers. The members of an ICPS are individual production plants or site facilities such as utilities. These members work together as an integrated network and rely on one another in order for daily production to function. This network combines production, energy, waste disposal, logistics, and shared infrastructure.

2.2 Clusters in the Literature

Industry cluster concepts date from the last century, but they have only become a popular topic in the literature over the last decade (Bergman and Feser, 1999). Marshall (1890) is commonly cited as the first to describe the occurrence of spatially concentrated industries. He described concentrated industrial districts as places where firms enjoy the benefits of large, skilled pools of labour, greater opportunities for intensive specialisation (a finer division of labour), and heightened diffusion of industry-specific knowledge and information (knowledge spill-overs). Also he highlights the social, cultural, and political factors, including trust, business customs, social ties, and other institutional considerations (Bellandi, 1989).

Michael Porter's "The Competitive Advantage of Nations" (1990) acted as an impulse or seed for much literature on clusters. On account of Porter's article and the apparent success of clusters around the world, the study of clusters has increasingly become a subject of literature. Research on clusters has attracted scholars from different disciplines and has led to a "*geographical turn in economics*" (Martin, 1999, p.67).

Below, the most important theories related to clusters are presented, pertaining to: the development of clusters, categorisation of clusters, identification of clusters, and advantages of clusters. Finally, the relevance of this literature for the ICPS is discussed.

2.2.1 Development of Clusters

Marshall (1890) attributed agglomeration to the following factors: a shared labour pool, input-output dependency (firms supplying intermediate products or services to each other), and knowledge spill-overs (benefits derived from the sharing of knowledge). Today, location theory is normally used to explain why clusters develop. Summarised below are the main theories describing the motivation behind cluster formation.

According to Maggioni (2002, p.2), reasons for industrial clustering found in the literature can be grouped into three main categories:

- To benefit from local sources of raw materials, intermediate inputs, or demands
- To reduce search costs and to tackle location risk and uncertainty
- To benefit from agglomeration economies

Agglomeration economies refer to economies which are external to a firm but internal to the industry such as a greater availability of specialised services, a larger pool of trained workers, public infrastructure, financial markets familiar with the industry, or inter-firm information or technology transfer.

Least Cost

Weber (1929) is the founder of the 'least cost approach' and attributes the co-location of manufacturing firms to the interaction of three factors: transportation costs, labour costs, and agglomeration forces. In his theory, Weber explains that firms choose a location in order to minimise transport costs between required material inputs and outputs for the marketplace. Then, the influence of the two other factors, labour costs and agglomeration forces, will determine the final location. Agglomeration forces are defined as the reduction of production and marketing costs which result from an increasing number of firms at a site.

Location Equilibrium

Location Equilibrium theories assume that price interactions are the fundamental cause of spatial agglomeration. According to Kanemoto (1990, p.47), market transactions of intermediate inputs can create clustering if accompanied by indivisibility in production: "*Combining the market exchange of intermediate inputs with indivisibility, [..] creates externalities in location decisions. For example, suppose that two firms interact with each other and they equally share the interaction costs. If one firm moves closer to the other firm, the interaction costs for both firms decrease*." Krugman (1991, p.1) theorises that industry location depends on the interaction of the expenditure in manufactured goods, transportation costs, and the extent of scale economies. To realise economies of scale while minimising transportation costs, manufacturing firms tend to locate in regions with larger demand.

Industrial Geography

The above theories are based on the premise that industry chooses a location based on external factors (Maggioni, 2002). In contrast, Industrial Geography Theory states that industries create their own conditions for growth based on the dynamic economy of production, both internal and external to the firm, leading to the agglomeration of firms at a certain location. For example, once a company chooses a location, this leads to a labour and investment influx (Storper, 1989).

Porter's Competitive Advantages

Porter (1990) bases his theory on the argument that there are four determining factors in an industry's success:

1. Factor conditions (natural resources, labour, infrastructure, etc.)
2. Demand conditions (customers)
3. Related and supporting industries (suppliers or competitors)
4. Firm strategy (encouraging investment and upgrading)

Porter extrapolates this to explain that "*regional clusters grow because of several factors: concentration of highly specialized knowledge, inputs and institutions; the motivational benefits of local competition; and often the presence of sophisticated local demand for a product or a service*" (Porter, 1996, p.87).

Below, Maggioni (2002, p.26) summarises the location theories introduced here and how they explain cluster formation.

Table 2.1 Summary of Location Theories for Clusters

Theory	Advantages	Disadvantages	Clustering explained by
Least Cost	Supply-side orientation, distance related variables, multiple equilibria	Overlooks demand-side, perfect competition	Resources location; labour force pool; agglomeration economies
Location Equilibrium	Non-price interactions; monopolistic competition	Lack of a unifying framework	Demand-supply interactions among firms
Industrial Geography	Existence of windows of locational opportunity; industries produce regions	No explicit formal modelling	Dynamic economies of production; horizontal integration
Porter's Competitive Advantages	Use of case-studies; heuristic and pragmatic approach	Must be reduced in order to be empirically tested	Localisation economies; beneficial effects of local competition; local concentration of demand

2.2.2 Types of Clusters

Different types of clusters proposed in the literature are reviewed below.

Meso- vs. Micro-cluster

Hoen (2001) describes two groups of clusters: micro-clusters, composed of firms which cooperate and diffuse knowledge, and meso-clusters, composed of firms which have buyer-supplier relationships. Normally the work on micro-clusters is theoretical or interview-based and focuses on the innovative nature of the cluster, whereas studies on meso-clusters tend to be empirical. Below, further sub-categories of meso-clusters are introduced.

Value Chain Cluster

A term which is aligned with the concept of the meso-cluster is the value chain cluster, which Roeland and den Hertog (1999) define as a cluster with an extended input-output or buyer-supplier chain. It is comprised of final market producers and first, second, and third tier suppliers which directly and indirectly engage in trade. This is consistent with Enright's vision of a cluster in which members are bound together by "*buyer-supplier relationships, or common technologies, common buyers or distribution channels, or common labour pools* " (Enright, 1996, p.191).

Markusen (1996) further defines four types of clusters according to the types of firms they are composed of and their interactions, described as follows.

Marshallian Clusters

Marshallian clusters are composed of locally owned, small and medium sized firms concentrated in craft-based, high technology, or manufacturing industries. Substantial trade is transacted between firms and specialised services, labour markets, and institutions develop to serve these firms. Firms network to solve problems (Markusen, 1996).

Industrial District

Brusco (1986) defines the industrial district as a territorial agglomeration of small to medium sized independent firms which are engaged in a similar activity and represent a type of Marshallian cluster. The members benefit from the collaboration and competition of the relationships which bind them. Examples in the United States are Silicon valley and the electronics, multimedia, and cultural products clusters in California (Scott, 1996). Further examples are the textile, ceramic tile, and machine tools clusters in northern and central Italy (Paniccia, 1998). A German example is given by the technology-intensive industrial regions in Baden-Württemberg (Sabel et al., 1989; Herrigel, 1993).

Hub and Spoke District

Here, one or few large firms act as an anchor, attracting other companies to it. The smaller firms which gather around the anchor firm may supply raw materials or utilise products produced by the anchor firm. The small companies cooperate with the anchor company, however, the small companies may compete with one another and do not cooperate as in the Marshallian cluster. Examples are the clusters around GM in Detroit, Boeing in Seattle, or Toyota city in Japan (Markusen, 1996).

Satellite Platform

The satellite platform is a congregation of firms which are branch facilities of externally based firms. The members operate independently and there is little cooperation between them. Satellite platforms normally develop through the recruitment of members to share land specifically allocated for industrial use (Markusen, 1996).

2.2.3 Identification of Clusters

Input-output tables may be used to identify clusters in that they describe the relations between firms in a cluster. Analysis of input-output patterns to identify clusters began in the 1960's, became of less interest in the 1970's, and had a resurgence in the 1990's. Hoen (2001) used input-output tables to identify clusters in Europe, North America, and Asia in the following sectors: agro-food, mining, energy, construction, metal, chemicals, electronics, and auto manufacturing. Lindqvist et al. (2003) identified clusters in 40 different industries, such as chemicals, textiles, pharma, and plastics. The clusters were identified according to an agglomeration coefficient determined as a function of the fraction of employees in a region in a particular industry relative to the total for that industry.

2.2.4 Advantages of Clusters

According to Barkley and Henry (2001, pp.5-6), there are three main advantages of clusters:

1. Clustering strengthens localisation economies. There is a greater availability of specialised input suppliers and business services and a larger pool of trained workers and public infrastructure.

2. Clustering facilitates industrial reorganisation. Specialisation and adoption of new production technologies is facilitated. Proximity between more specialised firms and their input suppliers and product markets enhances the flow of goods through linked systems and enables firms to more quickly adapt to market changes.
3. Clustering encourages networking among firms. Links between firms are facilitated, activities are integrated, resources or knowledge in areas such as new product development and technological upgrading are shared.

Isard (1956) highlights the following advantages of firm proximity: the increased market power through brokered buying and selling, the better availability and use of specialised repair facilities, shared infrastructure, and reduced risk and uncertainty for aspiring entrepreneurs.

Rosenfeld (1995, p.20) cites ‘tailored infrastructure’ as an advantage of the cluster based on scale economy logic: "*As industry concentration increases, individual businesses benefit from the development of sophisticated institutional and physical infrastructure tailored to the needs of specific industry*."

Doeringer and Terkla (1997) cite two examples of the benefits of clusters. First, the efficiency of just-in-time inventory and delivery systems for closely located firms, such as Japanese manufacturers and their suppliers. Second, the speed and frequency of interactions between firms. The more frequent and rapid the interaction, the more likely it is that niche markets and new specialised products can be identified. They characterise such dynamics as *"collaboration economies or the ability to participate in, and respond rapidly to changing design and manufacturing practices among firms that buy and sell from one another* “ (1997, p.182).

In a study by Ribas et al. (2003), the performance of chemical companies inside and outside of clusters in Tarragona, Spain was analysed. The study investigated whether clustering leads to higher returns and performance. Two groups were identified: 34 companies clustered in the Tarragona chemical industrial estate and 175 non-clustered companies in the same state of Catalonia, all producers of basic chemicals. Higher returns (on investment, equity, and sales) and 35% higher productivity (firm earnings/personnel cost) were found for companies in a cluster compared to non-clustered companies. These advantages are hypothesised to arise from the relationships and the sharing of resources among cluster members.

Similarly, Signorini (1994) used business data to confirm that higher production levels and profits were achieved for firms in a cluster compared with firms outside of a cluster for the wool industry. Other authors have investigated the performance of firms inside and outside of clusters for the industrial districts of Italy and Spain with similar results (Hernandez-Sanchez and Soler-Marco, 2002).

2.2.5 Applicability of Cluster Literature to this Work

The research on clusters has focussed on explaining how clusters develop, defining cluster types, identifying clusters, and determining the advantages of clusters. In this work, the clusters consist of individual production plants. This is considered a justified application of the concept of the cluster, as the plants in an ICPS function in a similar way to members of a cluster. The plants in an ICPS are considered cluster members which cooperate through shared resources and input/output relationships, but also compete with one another for resources, such as personnel, investment allocation, utilities, and material inputs. All publications on clusters reviewed consider the clusters as agglomerates of different firms and none investigate clusters belonging to a single company, which is possible in the ICPS.

Theories describing localisation economies, in which agglomeration arises through the benefits of shared labour, input-output dependency, specialised services, infrastructure, information transfer, and knowledge spill-overs apply to an ICPS. However, these theories imply that a cluster develops over time due to these factors, whereas, a chemical site is normally consciously planned from the start with these advantages in mind. Weber's least cost approach (1929) is particularly appropriate with regard to transport costs, as chemical production plants would optimally be located in close proximity to one another as a cluster to minimise transport costs. Kanemoto's (1990) theory is equally relevant for chemical producers, as each interconnected member benefits from lowered interaction costs. Industrial Geography Theory, which states that a company creates its own favourable conditions is also applicable, since the large investment of a chemical site will attract workers and perhaps further investment in the area.

Porter's (1990) four determining factors for success are also applicable to the ICPS:

1. Factor conditions: plants share resources, labour, and infrastructure
2. Demand conditions: interconnected plants are each other's customers
3. Related and supporting industries: eg. utilities provision, waste management
4. Firm strategy: management support of integration efficiencies

The type of cluster considered in this work may be considered to be a meso-cluster or value chain cluster in which its members are connected through buyer-supplier like relationships. According to the cluster types identified by Markusen (1996), the Marshallian cluster or the industrial district comes closest to describing an ICPS. These cluster types as well as the ICPS rely on strong connections, trust, and interdependencies between its members.

The tools used for the identification of clusters aim to identify relationships between more dispersed cluster members. However, they can also be applied to the input/output relationships between chemical plants at one site. The advantages of clusters cited in the literature such as improved industrial organisation and increased market power also apply to the ICPS. However, often the advantages given in the literature focus primarily on the qualitative, cooperative, and social aspects of the cluster, which are not addressed in this work. The literature on clusters explains the motivation behind cluster formation and the advantages of clusters.

However, the special characteristic of the ICPS in that its members are physically linked to one another, is not specifically addressed in the cluster literature. The literature reviewed next addresses this aspect. The following section introduces theory and accompanying tools which can be used to describe the material and energy linkages in an ICPS.

2.3 Industrial Ecology

Industrial Ecology is a young interdisciplinary field which aims to describe industrial settings with the tools of engineering and ecology. It is mainly concerned with tracking flows and stocks of materials or energy in industrial systems as a basis for reducing the impact of the production process on the environment. Mathematical tools are used to describe industrial systems and to analyse future scenarios (Duchin and Hertwich, 2003). The geographical scope of studies in Industrial Ecology varies. A study may be global (Socolow, 1994), regional (Rhine river basin: Stigliani, et al. 1993), or focus on individual industries (Frosch and Gallopoulos 1989) or companies (Greadel and Allenby, 1995; Van Berkel and Lafleur, 1997).

Among the first to implement the term and philosophy were Japanese research groups aiming to reduce Japan’s dependence on resources (Watanabe, 1972). On the frontier of this field was a Belgian study on national energy and material flows (Billen et al., 1983) as well as a manual on cleaner production and material cycling by a German industrialist (Winter, 1988). Industrial Ecology was really popularised through Frosch and Gallopoulos’ groundbreaking article “Strategies for Manufacturing” (1989). This article proposed that new ways of thinking about industrial production are necessary due to increasing environmental constraints. “*Throughout history, human economic activity has been characterized by an open and linear system of materials flows, where materials are taken in, transformed, used and thrown out*” (Frosch, 1997, p.37). Frosch and Gallopoulos argued that the traditional model of industrial activities where individual manufacturing processes take in raw materials and generate sales products and waste should be transformed into a more integrated system, an industrial ecosystem, with the aim of reducing waste. “*The industrial system ought to be modified to mimic the natural ecosystem in its overall operation*” (Frosch and Gallopoulos, 1992, p.271).

Industrial Ecology aims to make industrial systems more efficient and sustainable like natural systems. Traditional industrial processes in which fossil fuels are linearly transformed into sales products and wastes are modified into closed, cyclical processes where the waste from one sector is used as an input for another. The ultimate goal is to reduce the environmental impact of industrial systems. The flow of industrial materials is compared to the flows of nutrients in biological ecosystems and the industrial network is seen as a system of mutually dependent transformation processes. In an industrial ecosystem "*the consumption of energy and materials is optimised and effluents of one process [..] serve as the raw materials of another process*" (Frosch and Gallopoulos, 1989, p.94). The overall consumption of energy and materials is minimised and the effluents of one process serve as the raw materials for another process (Thomas, et al., 2003).

Three levels of Industrial Ecology have been defined by Duchin and Hertwich (2003): the micro, meso, and macro levels. The micro and meso levels can also be described as the tools of Industrial Ecology; the micro level focuses on physical balances (such as Industrial Metabolism or Material Flow Analysis) and the meso level adopts a wider view, for example, the Life-Cycle Assessment, introduced below. The macro level represents the widest view and describes processes used to evaluate industrial options employed by key decision makers.

2.3.1 Tools of Industrial Ecology

Below, the tools most commonly employed in Industrial Ecology are presented.

Industrial Metabolism

Industrial Metabolism (Ayres, 1989) is fundamental to Industrial Ecology and is defined as the study of flows of materials and energy in industrial systems and their transformations into products, by-products, and wastes (Garner and Keoleian, 1995). According to Ayres (1989), the optimal Industrial Metabolism would minimise the extraction of virgin natural resources, reduce the loss of materials as waste, and increase the reuse and recycling of resources. Ayres (1989) distinguishes Industrial Metabolism from its parent concept Industrial Ecology. He considers Industrial Metabolism as the study of mass flows and transformations, analogous to the metabolic processes of an organism and considers Industrial Ecology the industrial analogue of an ecosystem, consisting of a network of firms processing one another's wastes.

Material Flow Analysis

An analytical tool used to describe Industrial Metabolism is Material Flow Analysis (MFA), also called Substance Flow Analysis. It is derived from the first law of thermodynamics, the conservation of mass (Duchin and Hertwich, 2003). The quantities of a particular (normally environmentally relevant) substance are tracked through a particular system as the amount entering the boundary of a system, flowing through various parts of the production system, and ending up as waste. The flows within the system are determined according to process engineering principles and the conservation of mass. The materials balanced may be elements or composite materials (Duchin and Hertwich, 2003). MFA studies have been carried out for different substances. Metals considered to pose a human health threat such as lead or mercury have been focussed on as well as copper (Graedel, 2002). Also, MFA has been used to study flows in a particular geographic region, for example the Rhine Valley (Stigliani et al., 1993). MFA can be applied to production processes in order to identify inefficiencies which may be improved through process innovations, contributing to the goals of Cleaner Production and Pollution Prevention concepts.

Use of Physical Input-Output Tables

Input-output economics study the interdependence of different parts of an economic system. Similarly, input-output models have been used in Industrial Ecology to track the use of materials and energy and the generation and possible re-use of waste. In order to distinguish these from economics applications, they have also been called physical input-output tables or PIOT (Stahmer et al., 1998). Normally in Industrial Ecology, the PIOT is used to track flows between industries in mass units. The development of PIOTs has benefited from the experience of economic input-output tables regarding the careful accounting of flows to ensure that a particular flow is not counted more than once. The data used for PIOTs are average values which give a snapshot representation of a system. PIOTs have been used extensively in the literature. Several articles by Duchin use input-output tables to evaluate alternative technological assumptions (1990, 1992, 1994). The inventory modelling of some Life Cycle Assessment (LCA) software tools use input-output analysis (e.g. Frischknecht et al., 1996; Heijungs 1994). Studies with direct relevance for Industrial Ecology include the investigation of carbon emissions (Proops et al., 1993), the recycling of plastics (Duchin and Lange, 1998), waste management (Nakamura and Kondo, 2002), and water use (Duarte et al., 2002).

Life Cycle Assessment

LCA is the most popular application of Industrial Ecology and is represented by a large body of literature. The objective of LCA is to quantify the environmental impact of a given industrial product or process. It involves measuring or estimating the material and energy inputs and outputs for a given process. LCA builds on MFA by attempting to quantify the environmental impact of a process. For example, if a product is investigated, all stages will be mapped: the extraction of inputs, the production process, the product's use, and its disposal. LCA quantifies environmentally relevant factors such as emissions and resource use relative to a functional unit of the product. It is normally carried out using average process values. The resulting environmental profile of a product can be used for comparison against competing products or for suggesting ways to improve a process or product design. A fundamental challenge in an LCA is determining the system boundaries for the particular process or product and identifying all environmentally significant production steps. Often the boundaries are defined in administrative terms such as a country or region (den Hond, 2000).

Macro-level: Decision Making

One of the primary objectives of Industrial Ecology is to influence industrial decision making. Concepts such as Design for the Environment (DfE), Cleaner Production, and Pollution Prevention aim to incorporate Industrial Ecology principles during the planning stage. Today, environmental considerations are incorporated into many routine corporate decision-support tools and management information systems with the aim of closing production loops and decreasing environmental damage (Duchin and Hertwich, 2003). This helps identify problem areas, evaluate processing trade-offs, and design new production sites according to Industrial Ecology principles. According to Tibbs (1993), the incorporation of these principles is necessary to ensure a company's future success. "*The benefit offered by Industrial Ecology is that it provides a coherent framework for shaping and testing strategic thinking about the entire spectrum of environmental issues confronting industry. Executives and policymakers who take steps to absorb and appreciate this new mode of thinking now will find themselves and their organizations at a very real advantage in the world of the future"* (Tibbs, 1993, p.26).

2.3.2 Restructuring the Industrial System

According to Suren Erkman (2001), the strategy for implementing industrial ecology is referred to as 'eco-restructuring' and consists of four main elements:

1. Optimising the use of resources. This involves analysing individual processes in order to eliminate unnecessary losses and is also part of the concepts of Cleaner Production and Pollution Prevention.
2. Closing material loops and minimising emissions. This involves reviewing the complete lifecycle of a product to determine where wastes can be recycled. This may prove difficult, as wastes may be of no value or some by-products may be dispersed along with an end-product after its use, such as fertilisers and detergents. Closing material loops in industry may involve a new process and most probably energy consumption.
3. Dematerialisation activities. This involves minimising the total flow of matter and energy used to provide equivalent services. A distinction is made between relative dematerialisation – obtaining more services from a given quantity of matter, and absolute dematerialisation – reducing the resource requirements for the industrial system.
4. Reducing dependence on non-renewable sources of energy. This involves increasing the energy efficiency of processes through such things as co-generation or energy cascading.

Closing Material Loops

The concept of closing material loops through the use of by-products is very relevant for this work. By determining the value of a given by-product stream and determining its possible further use, Industrial Ecology is put into practice. The closing of material loops is central to the philosophy of Industrial Ecology. This idea is not new. Talbot (1920, p.19) wrote: "*The German, when he encounters a waste, does not throw it away or allow it to remain an incubus. Saturated with the principle that the residue from one process merely represents so much raw material for another line of endeavour, he at once sets to work to attempt to discover some use for refuse*." Clemen, an American economist, wrote about the packing industry (1927, p.vii): "*from the viewpoint of individual business, this manufacture of by-products has turned waste into such a source of revenue that in many cases the by-products have proved more profitable per pound than the main product*". Further, the relation between reusing by-products and decreasing pollution was recognised: "*the greatest proportion of environmental pollution is a* *direct consequence of an underdeveloped materials economy*" and therefore that the goal of a "*closed material cycle*" should be set (Maier and Roos, 1974, pp.32-35). Reasons underlying the motivation for reusing by-products are given by Desrochers (2002, p.1042):

1. The value of some by-products could be close to nothing for the producer, but of much greater value to somebody else.
2. A lot of processing has already gone into the production of by-products, therefore lowering further processing costs.
3. By-products are often produced much closer to their potential buyers than virgin materials, therefore lowering transportation costs.

Joint Production

The concept of Joint Production is introduced here, as it explains why the production of by-products is inevitable. Simply put, more than one output must emerge from a single production process. The principles behind Joint Production are described as follows. "*From a thermodynamic point of view one can describe the process of production as a transformation of a certain number of inputs into a certain number of outputs, each of which is characterised by its mass and its entropy. Typical industrial production processes [..] use a low entropy material fuel [..] to transform a high entropy raw material into a low entropy desired product. […] Since the by-products are characterised by high specific entropy they will generally be considered as useless waste*" (Baumgärtner et al., 2002, p.4). This results due to the first and second laws of thermodynamics[1] (Baumgärtner et al., 2002).

However, the characterisation of a by-product as either something useful or as a waste is subjective and dependent on the potential uses for the material. Wastes generated as dispersed material in the form of air-borne emissions are not easily recovered and are best reduced through process improvements. On the other hand, by-products in waste water may be potentially recovered through the closing of material loops.

[1] The first law states that energy and matter are conserved in an isolated system, thus raw materials and fuels are converted into products and by-products. The second law states that entropy is generated, thus the increase in entropy following a production process means that it is irreversible.

Joint Production can describe the following aspects of the production system:

1. Irreversibility: since the production process generates entropy
2. Limits to substitution: the conversion of high entropy raw materials to low entropy desired goods requires low entropy fuel for energy
3. The ubiquity of waste: the joint production of high entropy, often embodied as waste
4. Limits to growth, as a result of the combination of the above points (Baumgärtner et al., 2001)

Joint production applies to chemical transformation processes and separation processes (Oenning, 1997). The input-output techniques from Industrial Ecology can be used to describe Joint Production through a set of linear or non-linear algebraic systems. Models from computer science, process engineering, and chemistry can be used to balance the material and energy flows in joint production processes (Spengler, 1999).

2.4 Industrial Symbiosis and Eco-Industrial Parks

Many terms are used to describe the implementation of the concepts of Industrial Ecology, such as: eco-industrial development, eco-industrial cluster, eco-industrial network, industrial symbiosis, by-product synergy, by-product exchange, green twinning, environmentally balanced industrial complex, integrated resource recovery system, eco-industrial park, localised industrial ecosystems, industrial bio-system, zero-emission cluster, and eco-factory.

2.4.1 Industrial Symbiosis

Research in Industrial Symbiosis tends to focus either on identifying possible synergies at existing industrial locations or on the greater scope of site planning. Various researchers have investigated potentials for improving energy or materials management through case studies. Suren Erkman conducted research in India to map material flows with the aim of better utilising existing resources, such as the incineration of textile and paper wastes rather than scarce firewood and the use of sugar mill waste as a raw material for paper-making (Erkman, 2000). Michael Frank (2003) investigated the economic and ecological effects of inter-company energy supply concepts by focussing on linked energy flows between six companies close to the Rhine harbour of Karlsruhe separated by a maximum of four kilometres. He identified technical solutions of inter-company energy supply concepts to identify the benefits of economies of scale and Cleaner Production through joint installations. Further studies carried out by the Institute for Industrial Production (IIP) of the University of Karlsruhe employ models to investigate the interconnection of energy and material flows to enable a quantitative assessment of questions related to energy systems on a company, national, or regional level (Rosen, 2007, p.97).

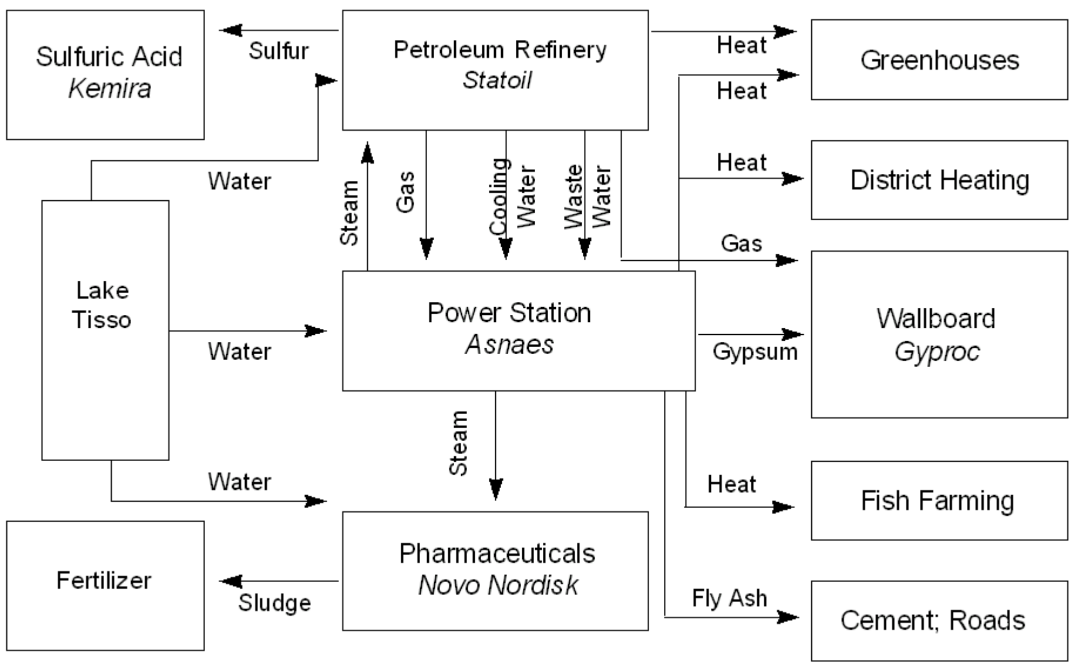
In practice, governmental agencies may aid companies to match under-valued waste or by-product streams with potential users to help create new revenues or savings while simultaneously reducing environmental impact. This is termed ‘by-product synergy’ and is a focus of the United States Business Council for Sustainable Development. Also, an initiative by Germany’s Fraunhofer Institute entitled CuRa (Cooperation für umweltschonenden Ressourcenaustausch) attempts to locate uses for waste residues, such as the use of organic waste from the food industry in a municipal fermentation plant (Schön et al., 2003).

2.4.2 The Eco-Industrial Park

The concept of the eco-industrial park was developed in the early 1990’s. It is a setting in which businesses cooperate to efficiently share resources (materials, water, energy, infrastructure, etc.) leading to economic and environmental gains. Expressed another way, eco-industrial parks consist of members which are in industrial symbiosis. The objectives of Industrial Ecology are applied to minimise waste, close material loops, and maximise resource efficiency. Industrial symbiosis may involve transferring waste generated by one firm to another where it is used as a raw material. Energy usage may be optimised through cogeneration (using otherwise wasted heat from electrical generation) or heat recovery (where excess heat from one business is utilised elsewhere). Two prominent examples of eco-industrial parks are given below.

Examples of Eco-Industrial Parks

The best-known example of Industrial Ecology in practice is in the port city of Kalundborg, Denmark. Kalundborg’s network of materials and energy exchanges began to evolve in the 1970’s. The motivation behind most of the exchanges was financial, to find uses for wastes or unused energy. Later, the members realised that these exchanges also generate environmental benefits. This industrial ecosystem consists of six main partners: a power station, an oil refinery, a biotechnology company, a producer of plasterboard, Kalundborg city, and a soil remediation company. Waste heat from the power plant provides residential heating to the city, sludge from various producers is used as fertiliser for nearby farms, farmers use excess yeast from the biotech firm for pig food, and excess refinery gas, fly ash, gypsum, and liquid sulphur are traded among the companies (The Kalundborg Centre for Industrial Symbiosis, 2007). The linkages between the partners are shown schematically below.



(Allenby and Graedel, 1994)

Figure 2.1 Industrial Ecosystem at Kalundborg, Denmark

As a result, surplus gas is no longer flared, some coal has been substituted with desulphurised gas and the city's district heating system has replaced 3500 oil furnaces, formerly a significant source of air pollution. Each year, 30 kt of coal and 20 kt of oil are saved. Carbon dioxide emissions are reduced by 130 kt/a and water consumption is reduced by 25%. It was estimated that the 75 million USD investment in infrastructure to transport energy and materials corresponds to savings of approximately 15 million USD/a (Christensen, 2006, p.1).

A second example is given by the Austrian province of Styria, where strict regulations and high waste disposal costs have motivated approximately 50 companies to sell or share their by-products. Industries involved in this network include agriculture, food processing, plastics, fabrics, paper, energy, metal processing, wood working, building materials, and a variety of waste processors and dealers.

The Bruce Energy Centre is an example of an eco-industrial park which focuses on energy exchanges. Various firms are located around a nuclear power plant to take advantage of waste heat and steam generation. The site includes a greenhouse, a food processing company, a feed dehydration company, an alcohol company, and a polypropylene company.

A further exchange network exists in Germany's Ruhr area involving a steel company, a power plant, and various companies including cement and road construction companies. These and other examples of eco-industrial parks may be found in Cote and Cohen-Rosenthal (1998) and Fleig (2000).

2.4.3 Eco-Industrial Parks as Clusters

Both eco-industrial parks and industrial clusters are based on the idea that manufacturers develop cooperative relationships in order to derive benefits. Eco-industrial parks emphasise environmental benefits, while industrial clusters emphasise networking benefits such as knowledge transfer and financial benefits. Both require geographical proximity for their services or functions to be interrelated in some way. In a cluster, this interrelation is often based around a particular industrial sector to optimise buyer-supplier relationships, while eco-industrial parks may consist of very diverse industries. Eco-industrial parks benefit from the same cooperation and proximity benefits which clusters do. Networking in eco-industrial parks may not only occur in material and energy flows, but also in transportation services, human resources, safety, and technical services.

2.4.4 Applicability of Industrial Ecology to this Work

The ICPS is viewed as both a cluster and an eco-industrial park in this work. The ideas behind Industrial Ecology are useful in explaining the motivation and environmental benefits behind an ICPS. The work in Industrial Ecology has focussed more on the flow of specific elements than on categorised flows as this work does. Also, geographic administrative regions are often used as boundaries rather than site boundaries. However, the ideological framework and tools are suitable for this study.

Erkman's (2001) eco-restructuring elements are relevant to the ICPS: 1) the linking of plants to optimise resources by exploiting by-products, 2) the closing of material loops to minimise waste, 3) the aim to reduce overall matter and energy requirements, and 4) the aim to reduce dependence on non-renewable energy sources. The use of physical input-output tables in Material Flow Analysis to describe the flows of mass and energy in a given system is appropriate to describe the flows in an ICPS.

The flow of materials and energy which link production plants in an ICPS can be described as industrial symbiosis. Hence, the concept of the eco-industrial park and the tools of Industrial Ecology are thought to be the most suitable for investigating the various types of integration which exist in such sites. Thus, the analogy of the ICPS and the eco-industrial park is drawn.

3 The Integrated Chemical Production Site

This chapter begins with an overview of process types in the chemical industry, followed by the focus of chemical companies and supply of olefin feedstocks. This is followed by a description of the ICPS, locations of major sites, and examples of sites. Finally, the different types of integration that exist in such sites are explained.

3.1 Process Types in the Chemical Industry

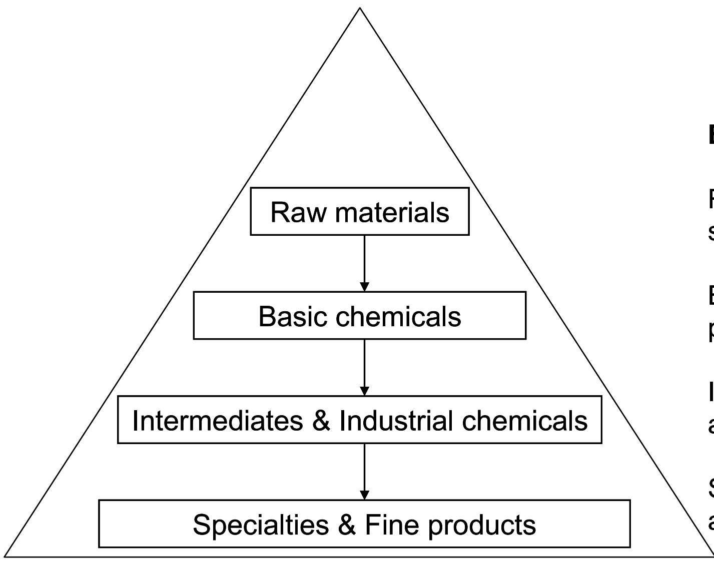
The chemical industry is recognised as a complex industrial sector with an incredible number and diversity of products. "*Some 70,000 chemical compounds are produced world-wide, and each has a distinct chemical nature, production route(s) and end use*" (European Commission, 2003, pxli). Typically in an ICPS, few raw materials are the source for successive levels of chemical refinement. Few natural sources of carbon (crude oil, natural gas, and coal) are used to produce a limited number of high volume raw materials for the chemical industry, such as naphtha. Oil and gas are the main sources of organic chemicals produced in the world today. Few originate from the declining carbon source of coal or the emerging source of renewable biomass. These carbon sources together with water, air, and elements and minerals such as sulphur, phosphate, rock salt, and ores are the building blocks for the chemical industry.

ICPS are generally based on large-scale organic chemical synthesis processes. The term 'Large Volume Organic Chemicals' has been used in literature (European Commission, 2003, pxli) to describe production plants characterised by:

- Basic chemicals used in large quantities as raw materials in the synthesis of other chemicals and rarely consumer products in their own right
- Production in continuously operated plants
- Products not produced in a range of products or formulations, compositions, or grades
- Products which have a relatively low added value
- Products which have a less stringent purity tolerance than fine chemicals

The term ‘large’ does not have a threshold value, but it has been suggested that capacities of 100 kt/a may characterise a plant as large; in Europe, a threshold of 100 kt/a would classify approximately 90 chemical products as ‘large’ (European Commission, 2003, pxli).

The figure below shows products corresponding to levels of refinement in the chemical industry and examples of these product categories.



Examples and approximate number of substances

Raw materials (~10): natural gas, naphtha, water, air, sulphur, phosphate, salt, ores

Basic chemicals (~12): cracker products (ethylene, propylene), benzene, acetylene, syngas, ammonia

Intermediates & Industrial chemicals (hundreds): aniline, butanediol, formeldahyde, solvents

Specialties (thousands): polymers, surfactants, agro chemicals, pharma, colourants, coatings

Figure 3.1 Pyramid of Levels of Refinement in Chemical Production

Basic chemicals are most commonly produced from steam cracking and refinement processes. Processing of these basic chemicals, such as introducing functional groups allows many more intermediates to be formed, such as alcohols, aldehydes, ketones, acids, nitriles, amines, and chlorides. Additionally, industrial chemicals such as formaldehyde are produced, which are used in various processes. Further processing of intermediates leads to the synthesis of specialties with a high level of functionalism and high commercial value, such as:

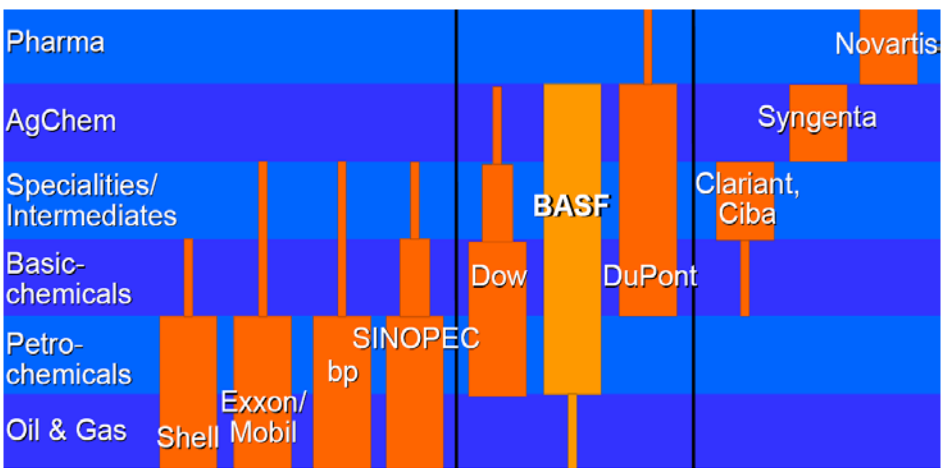
- Agricultural products, cosmetics, aroma chemicals, nutritional products, or pharmaceuticals
- Polymer dispersions for adhesives, construction, paper chemicals, etc.
- Specialty chemicals for detergents, textiles, leather, coatings, etc.
- Plastics for automotive, electrical, household, mechanical / industrial parts

3.2 Focus of Large Chemical Companies

The focus of large chemical companies in the 1990's can be categorised as petrochemicals, specialities / life-sciences, or diversified, exemplified by:

- Petrochemical: BP, Shell, ExxonMobil
- Specialties / life-science: Ciba / Novartis, Clariant, Degussa, Rohm & Haas
- Diversified: BASF, Bayer, Dow, DuPont

However, in 2000, many of the large chemical companies underwent restructuring driven by analyst and investor pressure for higher returns and demands for more transparency in the valuing of companies. Restructuring in the chemicals industry saw life-sciences split into agricultural and pharmaceutical sectors. Bayer and Dupont announced compartmentalisation (or de-integrating), creating spin-offs of either pure specialities or pure basics. Hence, fewer companies, such as BASF and Dow, were committed to a diversified strategy.



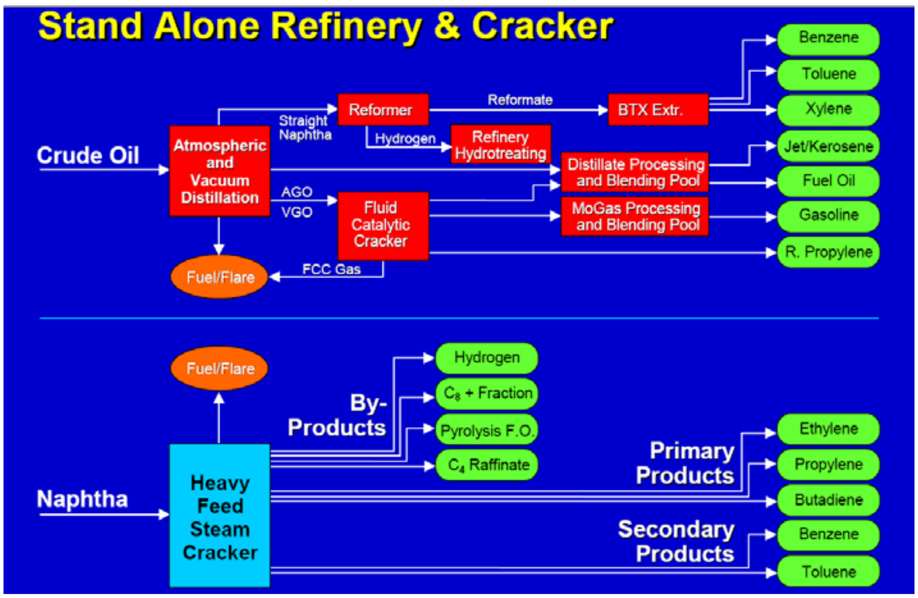
(BASFa, 2001)

Figure 3.2 Focus of Large Chemical Companies

The bars in the above figure represent increasing levels of refinement in the chemical industry, from oil and gas to pharma. These levels contain production plants which pass products to subsequent downstream processes.

3.3 Importance of Location and Feedstock Availability

The feedstocks of a refinery and cracker provide the building blocks for the value chains in a chemical production site. A refinery breaks down crude oil through distillation and catalytic cracking to benzene, toluene, xylene, kerosene, fuel oil, gasoline, and propylene. Steam crackers break down either ethane or naphtha into different fractions: primary products ethylene (C2), propylene (C3), and butadiene (C4), secondary aromatics products benzene and toluene, as well as by-products such as hydrogen and fuels. The relative generation of products depends on how the cracker is operated (pressure, temperature, and residence time). An integrated refinery and cracker break down both crude oil and naphtha to make a full, combined range of feedstocks, as shown below.



(BASFb, 2001)

Figure 3.3 Feedstock Preparation via Refinery and Steam Cracker

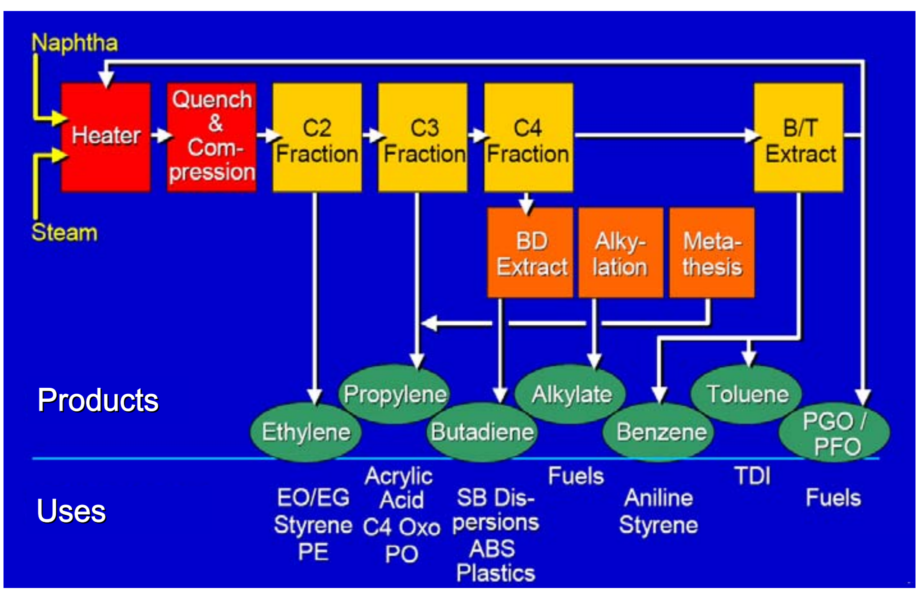
In Western Europe, liquid naphtha from crude oil refining is the most important starting material in the chemical industry and accounts for 73% of ethylene production (European Commission, 2003, p.144). In Asia, naphtha is the main feedstock, whereas, ethane, due to its availability, is used in Saudi Arabia. In the United States, both ethane and naphtha are common feedstocks. A naphtha cracker has a higher feedstock flexibility and provides a greater variety of products, hence is a better basis for integration, as is shown in the following table.

Table 3.1 Cracker Products based on Different Feedstocks

Product	Feedstock				
	Ethane	Propane	Butane	Naphtha	Gas-oil
Hydrogen	4.3	1.3	1.2	0.8	0.5
Methane	4.2	25.2	20.1	13.5	10.9
Acetylene	0.4	0.5	0.8	0.7	0.2
Ethylene	56	40.9	40.4	28.4	20.6
Ethane	30	3.6	3.5	3.9	4.8
Propadiene	0.1	0.5	1.2	0.4	0.5
Propylene	1	11.5	14.4	16.5	14
Propane	0.2	5	0.1	0.5	0.8
Butadiene	1.6	4.5	4.3	4.9	4.9
Butylenes	0.2	1	1.3	5.2	3.9
Butane	0.2	0.1	2	1	0.1
C5/C6	1.8	5.9	10.7	3.9	1.9
C7+ non-aromatics				1.2	2.1
Aromatics				10.5	12.5
< 430°C				5.2	2.6
> 430°C				3.4	19.7
Total	100	100	100	100	100

(European Commission, 2003, p.154)

Various separation processes following the cracker provide different fractions used to produce a variety of chemical products, as shown below.



(BASFb, 2001)

Figure 3.4 Fractions from Naphtha Cracker and their use in an ICPS

Steam crackers have increased in size over the years, from around 200 kt/a in the 1960's (Exxon Baton Rouge, Louisiana), to around 700 kt/a in the 1980's and 1990's (Freeport, Texas), and expanding to over 1000 kt/a in 2000 (Port Arthur, Texas and Iran). Production capacities per region are given below.

Table 3.2 Steam Cracker Production per Region in 2005

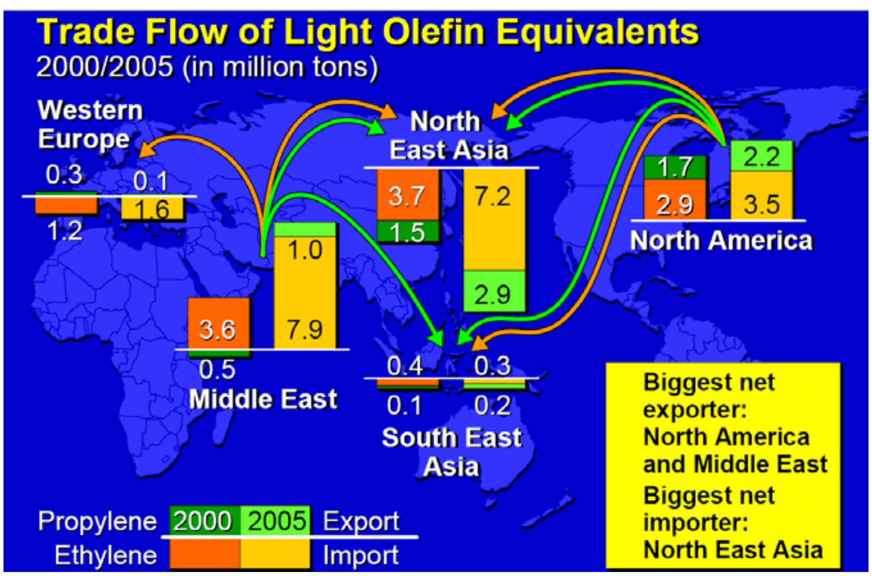
Capacity (mil t/a)	Asia	W. Europe	N. America	S. America
Ethylene	15.8	21.6	28.7	3.9
Propylene	11.3	15.4	16.6	1.9
Benzene	8.7	8.4	7.6	1.1

(Association of Petrochemicals Producers in Europe, 2007)

New steam crackers are being built in China to accommodate its rapidly expanding chemicals market. For example, China's ethylene demand is growing by 10% annually, twice the world's average, and is expected to reach 37 million tons in 2015 (Dow Jones Energy Service, 2006).

3.3.1 Distribution of Olefins

An onsite cracker is warranted for large-scale sites requiring a wide range of cracker products. However, as liquid feeds predominate in Europe due to their relative abundance and ability to be easily transported, it may not be essential to co-locate a cracker (European Commission, 2005, p.144). Olefins are transported globally, as shown by the trade flow schematic below.

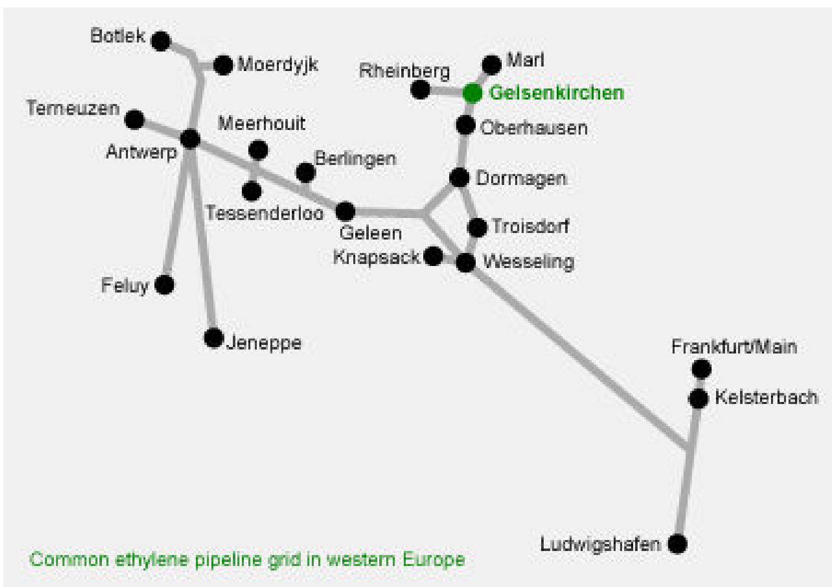


(BASFa, 2001)

Figure 3.5 Trade Flow of Light Olefin Equivalents

On the other hand, ethane, extracted from natural gas, is difficult to transport, requiring special refrigerated ships.

Pipelines are commonly used to distribute olefins from refineries and crackers to chemical companies which use them as feedstocks. One example is the West European pipeline network. The ethylene pipeline from Antwerp, shown below, is tapped by Exxon, Dow, and DSM on its way to Cologne, then diverges in Germany to the Ruhr in the North (Bayer, Wacker, Solvay, Ruhr-chemie, Veba Oel, Huels) and the Rhine in the South (ROW, RWE, Frankfurt, BASF Ludwigshafen). Another example is the olefin pipeline which starts at the integrated refinery and cracker in Port Arthur, Texas. This serves the sites west of it along the Texan shore and east of it in Louisiana along the Mississippi river.



(British Petroleum, 2005)

Figure 3.6 West European Ethylene and Propylene Pipelines

3.4 Location of Major Integrated Chemical Production Sites

The strategic location of integrated chemical production sites is optimally chosen with respect to two main aspects: 1) the availability of feedstocks, and 2) the ability to transport sales products. An ICPS should have easy access to raw materials, such as ethylene (via an onsite cracker or pipeline) and natural gas, as well as utility provisions, such as water and electricity (for backup provision). Also, an ICPS benefits from being located close to a sea port for easy access to sea freight, as shipping is an important mode of transport in the chemicals industry. The availability of surrounding land is important in case further expansion is required. Lastly, proximity to customers, generally producers of finished goods, is an important consideration. Finally, the site should be able to rely on outside infrastructure, such as communications systems and be able to provide for personnel.

The locations of the most important integrated sites worldwide are shown in the map below. North America’s largest integrated chemical production area is along the Gulf Coast. The Port Arthur steam cracker supplies 830 kt/a of ethylene and 860 kt/a of propylene to numerous large-scale chemicals producers located in the region (BASFb, 2001). South America’s largest chemical sites are located in Brazil, in Sao Paulo and Rio de Janeiro, as well as in Venezuela.

(BASF, 2000)

Figure 3.7 Location of Important ICPS

Europe’s major chemical sites, shown in the following map, are located in: Belgium (Antwerp), Holland (Rotterdam, Moerdijk), Germany (Ruhr and Rhine in the west, other sites in the east), United Kingdom (Wilton/Teeside in the northeast, Baglan Bay in the northwest), Spain (Tarrangona in the south), and France (Le Havre and Dunkerque in the north and Marseille in the south).

(Czytko, 1999)

Figure 3.8 Location of ICPS in Western Europe

Antwerp is "*probably the most diversified and integrated chemical production site of its kind*" with 10 of the world's top 20 chemical producers and four steam crackers (Short, 2001, p.18). Atofina's cracker provides feedstocks (ethylene, propylene, benzene, and toluene) to the value chains of various companies. Antwerp is the hub from which about 100 pipelines carry natural gas, ammonia, butadiene, isobutylene, chlorine, ethylene, propylene, nitrogen, fluid hydrocarbons, oxygen, and hydrogen (Short, 2001). Exxon Mobil uses ethylene to produce low density polyethylene, Borealis uses ethylene to produce high and low density polyethylene, and propylene to produce polypropylene. BP Amoco has value chains based on xylene, ethylene, and acetic acid, to produce olefins and acetates, among other products. Major chemical companies located here are Bayer, Dow, BASF, and Solvay. Antwerp and Rotterdam are Europe's two largest ports in terms of tonnage and the chemical industries here are closely linked. "*In the roughly 60-mile stretch between Antwerp and Rotterdam, enough chemical operations have been established that it is easy to accept Antwerp's claim to be the world's second largest chemical industry cluster after Houston*" (Short, 2001, p.18).

Hauthal (2003) reviewed 25 of Germany's major chemical sites, listing their size, the number of firms on site, the infrastructure supplier, and the type of production. Germany's major sites are located around the west European ethylene pipeline: Chemsite in North Rhine Westfalia (Marl, Gelsenkirchen), Bayer in Leverkusen, Hoechst by Frankfurt, and BASF on the Rhein in Ludwigshafen. Also, three large sites are located in the east: Bitterfeld, Leuna and Schkopau.

In the Middle East, Saudi Arabia, with its rich oil reserves, is the location of two major integrated sites, the Yanbu site on the west coast and the Al-Jubail site on the east coast, which receive their feeds from Aramco. The Al-Julail site is the largest and most diversified site and consists of strong integration between various daughter companies of SABIC. Here polyethylene, polyvinylchloride, polypropylene, methyl tertiary-butyl ether, among other basic chemicals are produced. Yanbu, a second integrated site, has two major value chains which produce polyethylene, ethylene glycol, poly-ethylene-terephthalate, and polyether-sulfone, among others. A second middle-eastern country in which integrated petrochemical sites can be found is Iran.

South East Asia's major chemical sites are located in Malaysia and Singapore. Malaysia's Kerteh site is centred around the national oil company Petronas, with BP as a major partner. Kuantan, a second Malaysian site just south of Kerteh, is home to an integrated site consisting of Petronas, BP, and BASF. Singapore's Jurong Island site is the location of companies such as ExxonMobil, Shell, Sumitomo, Celanese, Ellba, Eastman, Dupont, and Chevron Phillips.

As China is increasingly becoming more industrially developed, chemical clusters are developing along the Chinese coastal region, shown in the following map provided by BASF AG in 2005. These consist of various joint ventures involving international players such as: Dupont, BASF, BP, Huntsman, Bayer, Akzo Nobel, Dow, DSM, Atofina, and others. The largest sites are in Nanjing and Shanghai, as well as south in Ningbo and Daya Bay, and north in Beijing and Tianjin. Other chemical production sites can be found along the Pacific Rim, such as in South Korea (Yeosu, Ulsan).

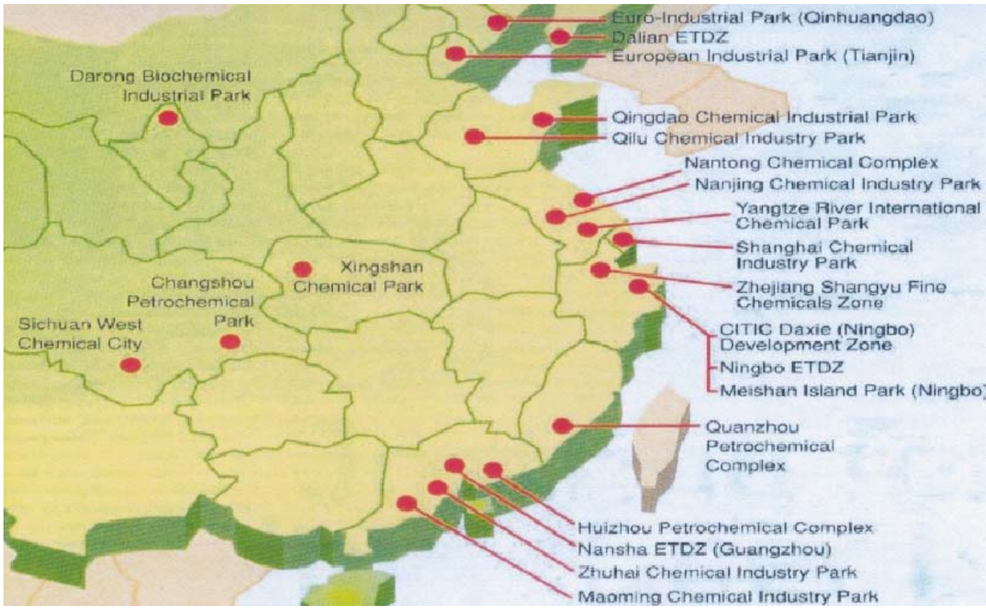


Figure 3.9 Location of Chemical Clusters in China

3.5 Examples of Integrated Sites

Examples of integrated chemical production sites are given below. First, BASF's integration philosophy and its Ludwigshafen site are introduced, followed by examples of multi-company integrated sites. Aerial photos of these sites can be found in Appendix A.

BASF

BASF is one of the world's largest chemical companies and was founded in 1865. It refers to its integrated production philosophy as 'Verbund' or 'network' in German. Integration is one of BASF's most important strengths and a cornerstone of the company's strategy. BASF believes that the most efficient way to manage chemical production is through large, fully integrated sites that spread production costs over a large asset base. Its aim in physically integrating production chains is to ensure the lowest cost of production for bulk chemicals, thereby leading to subsequent advantages in downstream products. BASF believes that such integration reduces cyclicity (or financial vulnerability) and enables more controlled capacity expansions and better environmental control. BASF has remained committed to its integrated philosophy, which allows for the production of a diversified spectrum of chemical products. Also, BASF remains one of the top players in virtually all chemicals sectors (Isaac and Comer, 2000).

The BASF Ludwigshafen site, where the company was founded, produces approximately 8500 sales products and consists of over 7 km² of site area and 2000 buildings. This is the largest single-company integrated chemical production site in the world. The enormity of the Ludwigshafen site, which grew historically starting in the late 1800's, is an exception today due to the huge investment required. According to Isaac and Comer (2000, p.35), *"we have no doubt that there are genuine benefits to integration, particularly at Ludwigshafen; however, a difficulty arises when expansion of the concept is required. The unparalleled infrastructure already in place and high levels of asset depreciation mean new projects have difficulty competing with the earnings currently achievable at Ludwigshafen".* BASF has concentrated on expanding its integration strategy on a global level. In addition to Ludwigshafen, BASF has integrated sites in Antwerp Belgium, Tarragona Spain, Freeport Texas, Geismar Louisiana, Kuantan Malaysia, and Nanjing China (BASF, 2007).

The Jurong Island Site in Singapore

Jurong Island, located on the south tip of Singapore, is a chemical site consisting of more than 70 companies, including chemical and petrochemical companies such as BP, Celanese, ExxonMobil, Dupont, Mitsui Chemicals, Ellba, Chevron Oronite, Shell, and Sumitomo Chemical. The main members of the site are refineries, upstream and downstream petrochemical and chemical plants, and logistics companies. The site has infrastructure including a fire department and third party providers of utilities, tanks and terminal facilities, warehouses, and maintenance and repair centres (Jurong Town Corporation, 2006).

ChemSite's Marl Chemical Park in Germany

ChemSite is the umbrella company which manages six large ICPS in Germany along the Rhine river and was founded in 1997. The Marl site is ChemSite's largest site having an area of 6.5 km². It is comprised of various companies: Degussa, Air Liquide, Bayer Buna, BP, Sasol, ISP, Linde, and others and benefits from an extensive materials flow network. A range of basic chemicals and specialties are produced based on benzene, ethylene, propylene, butadiene, acetylene, syngas, phenol, fatty alcohols, and chlorine (ChemSite Initiative, 2006).

3.6 Description of the ICPS

Integrated Chemical Production Sites consist of several chemical production plants linked in terms of: materials, energy, logistics, infrastructure, and organisation. These types of integration will be explained in the next sections. A general schematic showing the material and energy flows is shown below. Raw materials and energy enter the site to be transformed into sales products, by-products, or wastes and emissions. By-products may potentially be used as raw materials in further processes, wastes may be incinerated or disposed of, and energy may be recovered from processes producing excess heat or from waste incineration.

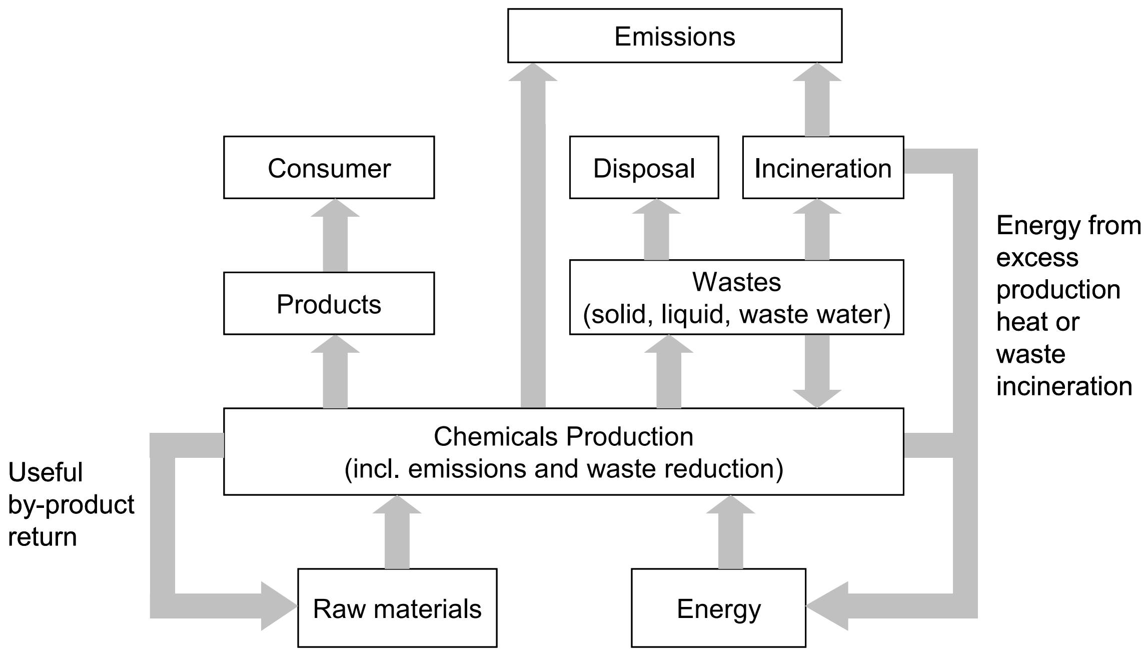


Figure 3.10 Schematic of Materials and Energy Flows in an ICPS

The core of the ICPS is its network of production plants and utilities providers, linked through materials and energy streams, shown in the following schematic. In addition, the ICPS relies on a management system to ensure the receipt and storage of raw materials and handling, storage, and transport of products.

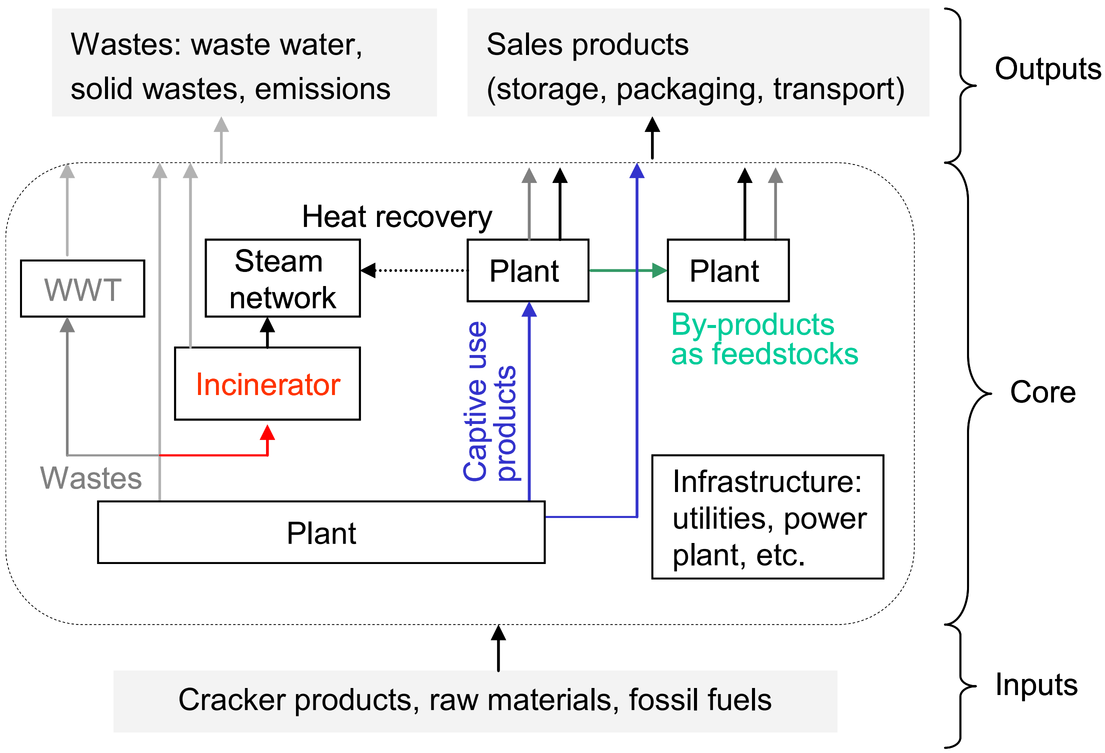


Figure 3.11 Schematic of Input, Core and Output Systems of an ICPS

Inputs to the site include raw materials provided by external suppliers, such as fossil fuels, water, and potentially cracker products. Outputs are waste streams, which can be either emitted to the atmosphere, remain in treated waste water or are transported to an offsite disposal site, and external sales products and their associated logistical processes.

3.7 Types of Integration

Integration in this work refers to the shared use of facilities or the transfer of energy or materials streams for further use in physical and chemical processes. Integration may exist on different levels in the chemical industry. For example, energy or materials streams may be transferred within a unit operation, a plant, or a site in order to improve production efficiency. This is shown through various examples in the following table.

Table 3.3 Integration on Different Levels in the Chemical Industry

Level	Type of integration	Example
Unit operation	Energy	Dryer with return of heated off-gas stream.
	Material	Reactor with separation and return of product-containing waste stream.
Process	Energy	Reactor with heat exchanger to produce steam for use in other process section (eg. distillation).
	Material	Separation of components (eg. VOCs by selective adsorption) and return.
Several processes	Energy	Re-use of cooling water from one process for another process. Transfer of a heated reactant stream to a downstream process.
	Material and Energy	Incineration of waste from one process to produce steam for use in another process.
	Material	Use of by-product from one process as a reactant in another process.

Thus, optimisation can be carried out in terms of energy and materials integration on different levels. This work focuses on integration on the site level resulting from the co-location of several processes.

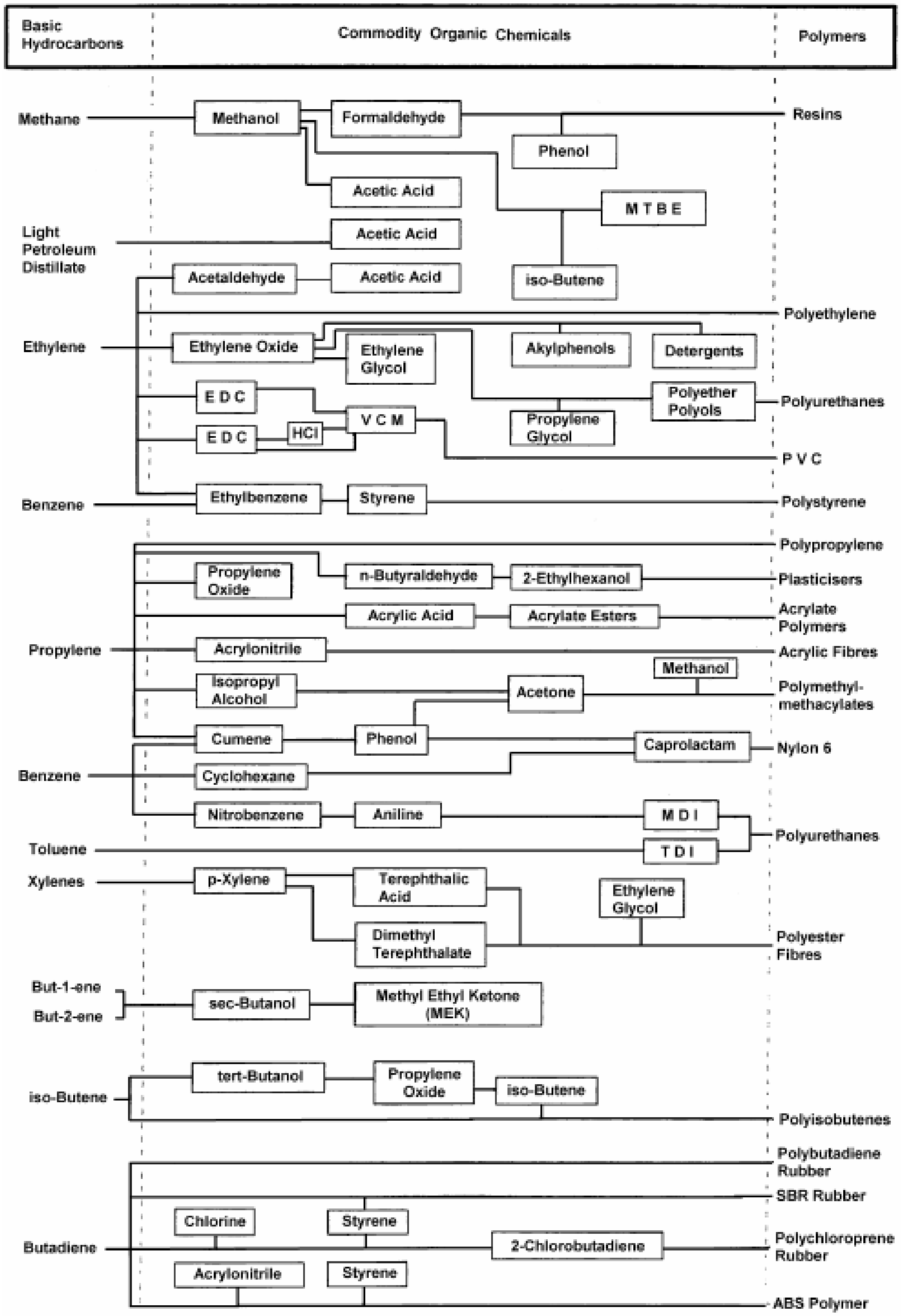
In the sections which follow, the types of integration found in an ICPS are introduced. Integration is manifested in the material and energy flows between site members, referred to as ‘materials integration’ and ‘energy integration’. Also, integration exists on account of the physical proximity of the members of the site allowing for onsite transfer of materials, referred to as ‘logistics integration’.

3.7.1 Materials Integration

In this section, materials integration is described and two types of materials integration are defined. This is followed by examples of materials integration at companies and examples of specific cases of materials integration.

Materials integration occurs if a product from one plant provides a feedstock for another plant. These connections may be part of a value chain. A value chain in the chemical industry represents the transformation of a basic feedstock into a consumer-near product through successively higher levels of refinement.

For example, selected value chains for the polymer industry are shown below.



(European Commission, 2003, p.3)

Figure 3.12 Selected Value Chains for Polymer Production

Each process step, normally represented by one production plant, is one link in the value chain. As such, these linkages are deliberate and based on the strategic design and construction of a value chain within an ICPS. Other material flows may be less intentional, linking two plants within an ICPS from different value chains.

These two kinds of materials integration are defined here as:

- Vertical materials integration: the transfer of main products between plants in a value chain. Main products from one plant (eg. ethylene, methanol) may by be part of different value chains. Thus, one plant may be part of more than one value chain.
- Horizontal materials integration: the transfer of secondary products (normally by-products or intermediates) from one value chain for use as raw materials in another value chain.

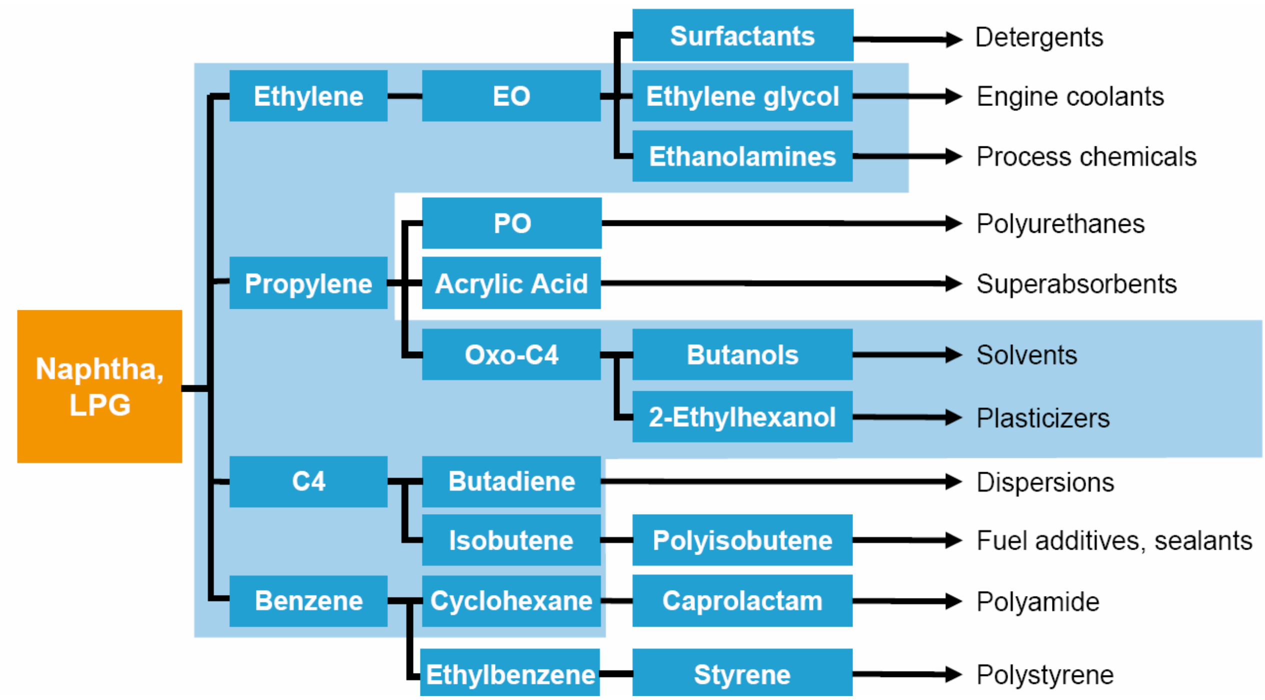
Materials integration may benefit a site in several ways. First, the chemical use of by-products or intermediates which would otherwise be considered as wastes means that these streams are not incinerated or disposed of. Second, the transfer of products between onsite plants, most often by pipeline, means these streams do not need to be transported to offsite customers. This type of integration is described in more detail under ‘logistics integration’ in the next section. Furthermore, the linkages may not be limited to chemical product streams, but may also consist of utilities such as water, which is covered under ‘shared infrastructure’.

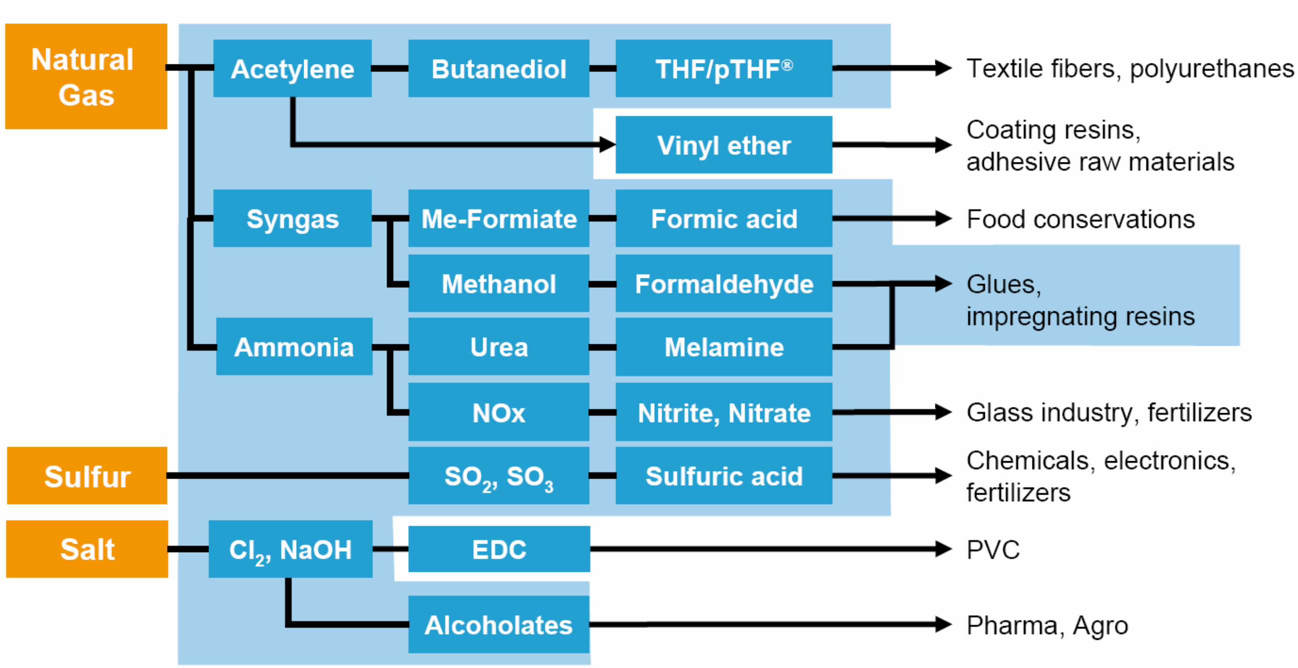
Examples of Materials Integration at Companies

The main value chains at two integrated sites are shown on the following pages.

Materials Integration at BASF

At BASF, approximately 200 types of basic products and intermediates are produced, from which approximately 8500 commercial products are produced (BASF, 2007). The key BASF value chains are shown below.





(BASF, 2007)

Figure 3.13 Examples of Materials Integration at BASF

Materials Integration at Marl

The Marl site consists of many firms and integrated materials flows. The raw materials available by pipeline are: ethylene, propylene, hydrogen, and methanol (ChemSite Inititative, 2006). The following graphic provided by ChemSite shows some of the materials flows at the site.

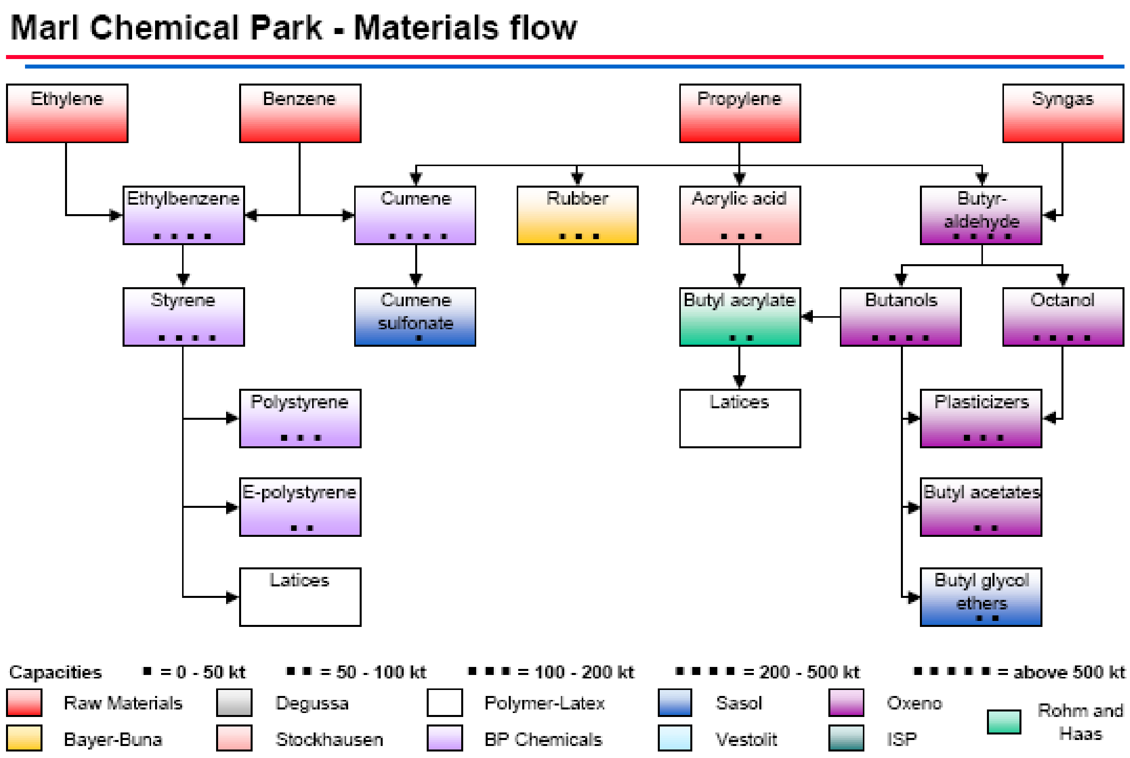


Figure 3.14. Examples of Materials Integration at Marl

Examples of Different Types of Materials Integration

Vertical Materials Integration

In the polystyrene value chain, the cracker products ethylene and benzene are converted to ethylbenzene. From this, styrene is formed and polymerised into polystyrene. Polystyrene is then processed as a thermal insulation material.

Vertical and Horizontal Materials Integration

Natural gas is used to produce acetylene, which is reacted with formaldehyde to produce butadiene. During acetylene production, synthesis gas is produced which is used for methanol production. Methanol is used to produce formaldehyde. Hence, the production circle is closed, as formaldehyde is required to produce butadiene.

Horizontal Materials Integration

In the two examples below, co- or by-products are produced which are used as chemical feedstocks for further processes. For example, hydrogen chloride is produced as a by-product in methylene diphenylene isocyanate (MDI) production, which is used as a raw material in the production of vinyl chloride and polyvinyl chloride (PVC).

A second example is the production of styrene as a co-product in the production of propylene oxide by the ethylbenzene process (Ullmann, 2000). In this route, 2.2–2.5 kg styrene/kg of propylene oxide are produced. Styrene can then be further used at the ICPS in a multitude of chemical processes (see Table 6.1).

By-product as a Utility

In the above examples, by-products are used chemically. Also, by-products may be used at an ICPS as a fuel or a utility, shown by the following example. Carbon dioxide is produced as a by-product in the steam cracker at Lonza Chemicals in Visp, Switzerland. It is produced during the absorption step of gas stripping. Of the 70 kt/a of technical grade carbon dioxide produced, 20 kt/a is accounted for by losses, heating gas, and preheating, 15 kt/a is used in various plants for inertisation or cooling, and the remaining 35 kt/a undergoes a further process step, purification to food grade carbon dioxide (Gerritzen, 2005). This example shows how a by-product stream can be used internally as a utility, as well as further processed to be sold offsite.

3.7.2 Logistics Integration

One unique aspect of the ICPS is that materials exiting one plant may enter another onsite plant as a feedstock. Logistics integration describes this transport of integrated products, generally through pipeline linkages between plants. Pipes in an ICPS may transport not only raw materials between plants, but also utilities, wastes, and products in the form of gases, liquids, or solids. As a result, materials only need to travel short distances. Also, logistics integration describes the shared logistics facilities between plants in an ICPS, such as for storage.

The onsite use of materials which exit one plant to be used as a feedstock in another plant is an economical advantage for the ICPS, as these materials do not need to be transported to offsite customers. Whereas in a stand-alone site, these would need to be transported by sea, rail, or truck, incurring various logistics-related costs. Also, the environmental and safety aspects related to transporting dangerous raw materials are avoided for materials transferred within an ICPS.

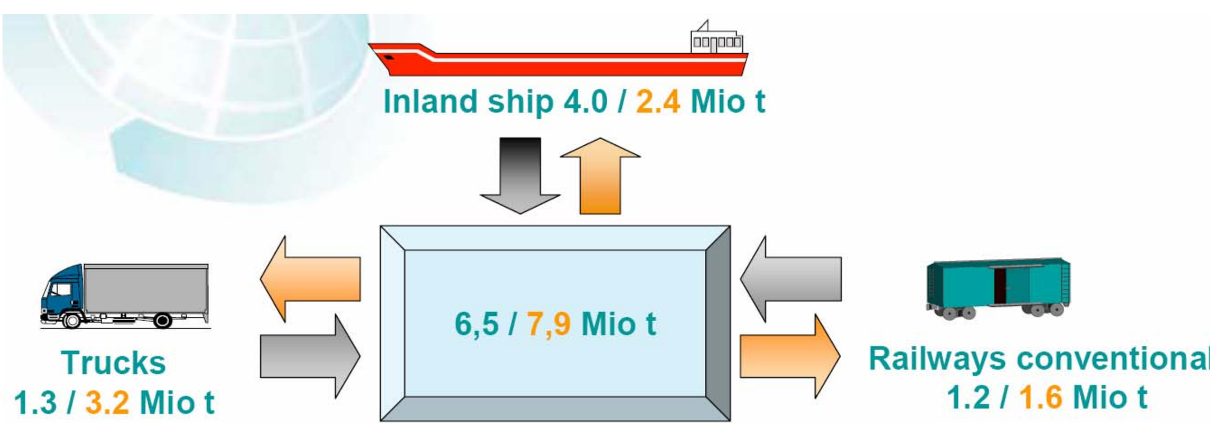
Examples of Logistics Integration at Companies

Logistics Integration at the Lonza Site

At the Lonza site in Visp Switzerland, 500 kt/a of raw materials and intermediates are transported via pipeline within the integrated site (Gerritzen, 2005).

Logistics Integration at the BASF Ludwigshafen Site

According to BASF, over 2000 km of aboveground piping provide short transport distances for products, energy, and utilities. Additionally, 211 km of rail track and 115 km of roads link the production plants. The below graphic shows the amount of goods transported in and out of the Ludwigshafen site in 2003. For outbound goods, the distribution was 44% by road, 33% by ship, and 22% by rail. Overall, for in and outbound transport, the distribution was: 47% ship, 33% road, and 20% rail. For Germany as a whole, the distribution was 65% road, 19% rail, and 16% by ship in ton·km (Verkehr in Zahlen, 2003). Thus, road transport is still a common mode of transport, as it provides the greatest flexibility in terms of transport route. On the other hand, ship or barge may be favoured if the site has a port, such as the BASF site, as it is the most economical for longer distances.



(Prengel, 2004)

Figure 3.15 Inbound/Outbound Transport at BASF Ludwigshafen

An integrated site may also participate in transport provision. For example, at BASF Ludwigshafen, the operative handling of trains is by Rail4Chem and the integrated logistic control is by BASF. The operating benefits for BASF are: daily whole-train transports, optimisation of rolling stock by rapid rail car turnover, and transport guarantee for BASF rail cars. Commercial benefits are realised through the purchase of whole trains at production costs, the maximisation of train utilisation by third-party freight, and ultimately freight cost savings.

3.7.3 Energy Integration

Energy is of fundamental importance in the chemicals industry, as it is needed inter alia to control the pressure and temperature of chemical processes. It is through the control of these two variables that the breaking down and formation of molecules from the elements occurs. Steam is a commonly used heat carrier in the chemical industry and is distributed via a pipeline network in an ICPS in order to provide the energy requirements of individual plants.

Energy Provision

As an integrated site has several plants to provide steam and electricity for, the energy requirements are much greater compared with a smaller stand-alone site. Due to these greater requirements, integrated sites may generate steam and electricity through a combined heat and power principle via cogeneration power plants, currently the most cost-effective and eco-efficient way to generate energy. This technology becomes more economically advantageous as a site’s energy requirements increase; thus economies of scale lead to reduced energy costs for larger sites. Small stand-alone plants may only require a steam boiler and source their electricity from the public grid. Hence, a comparison of energy provision costs for integrated and stand-alone sites must take economies of scale as well as technology type into consideration, as a site’s requirements will determine whether the use of cogeneration technology is warranted.

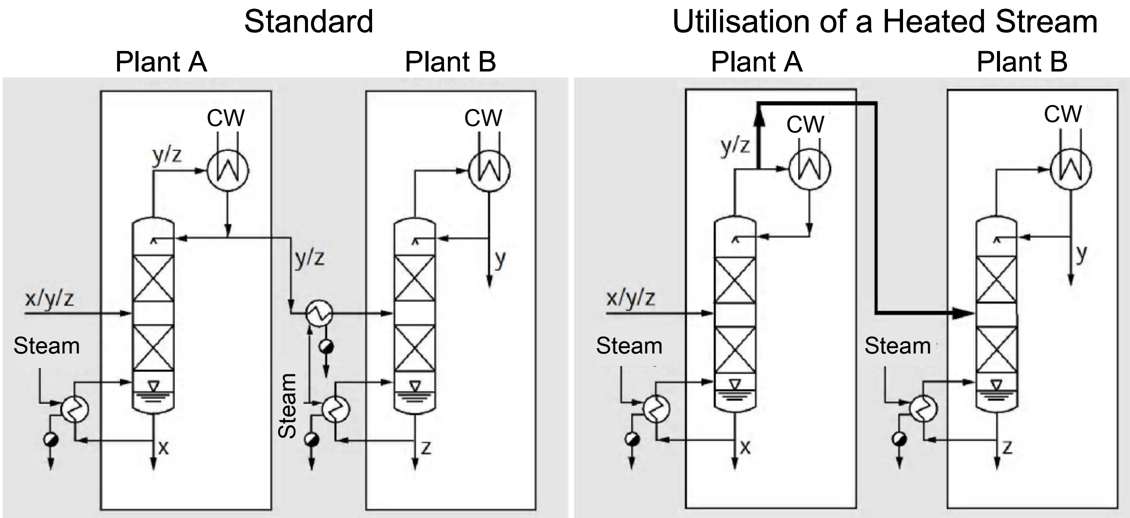
Heat Recovery and Incineration

The goal of energy integration is to minimise the overall energy requirements of the site. This may be done by balancing energy requirements and surpluses among plants within a site. For example, the energy released by processes involving exothermic reactions may be used to convert water to steam, which may be fed to the steam network. The steam network acts as a carrier for this energy and allows it to be applied as a heat source in processes requiring heat. Thus, optimal energy integration is a balance between energy inputs and outputs. The potential benefits of energy integration arise, for example, from two sources in an ICPS: excess heat recovery and energy generation by waste incineration. Due to these energy sources, the use of fossil fuels like oil and natural gas is reduced.

Pinch Analysis has been applied routinely to individual processes since the 1980's (Linnhoff, 1982). Here, heating and cooling demands are reviewed to identify the most appropriate types and temperatures for heating and cooling utilities in a particular process. The company Linnhoff March developed a Total Site^{TM} analysis in the 1990's to extend the technique and software from the single plant to an entire site. The software enables the optimal site utility structure to be identified for several individual processes. Minimum energy demands for the whole site can be determined and the user can choose between individual process optimisation and site infrastructure improvements. Using this method, inter-process or inter-plant integration opportunities may be identified.

Excess Heat Recovery

Excess heat recovery is the recovery of heat from one process to be applied in another process. For example, an exothermic reaction conducted in a reaction vessel containing an internal heat exchanger may be used to convert water into steam, which is then fed into the site's steam network. Another example is the transfer of heated streams between processes. In an ICPS, chemical streams are passed from one process to another as feedstocks. The transfer of a warm rather than cooled down product from one plant to another plant can yield a few benefits, as shown in the schematic below: reduction of cooling water required in plant A, reduction of steam required in plant B, and reduction of one heat exchanger in plant B.



CW = cooling water
(based on BASF, 1995, p.19)

Figure 3.16 Energy Integration: Example of Utilising a Heated Stream

Waste Incineration and Substitute Fuels

Another source of energy savings in an ICPS is the incineration of certain wastes from chemical processes. The heat provided by waste incineration is converted into steam via a waste heat boiler and fed into the steam network. A stand-alone production site may also have an incinerator. However, as for heat recovery, the steam generated by an individual plant's incinerator may not be in balance with the plant's steam requirements. An ICPS is expected to benefit more from onsite waste incineration compared to a stand-alone site, as a larger amount of waste is generated by several plants. This provides economies of scale warranting an onsite incinerator. Also, a steam network allows the steam to be transferred to other processes. Therefore, a better balance of energy requirements can be achieved. Offsite incineration facilities, due to their location, may not produce steam from the heat generated, but rather provide district heating for residential areas. This is the case for the sludge incinerator at BASF Ludwigshafen, which provides district heating for the Pfingstweide residential area (BASF, 2002, p.13). Also, by substituting fuels with certain chemical wastes, costs are reduced. For example, certain wastes may replace natural gas as a fuel in a power plant. Further, substitute fuels may be used as a fuel in production plants.

These concepts are illustrated through examples from industry, as follows.

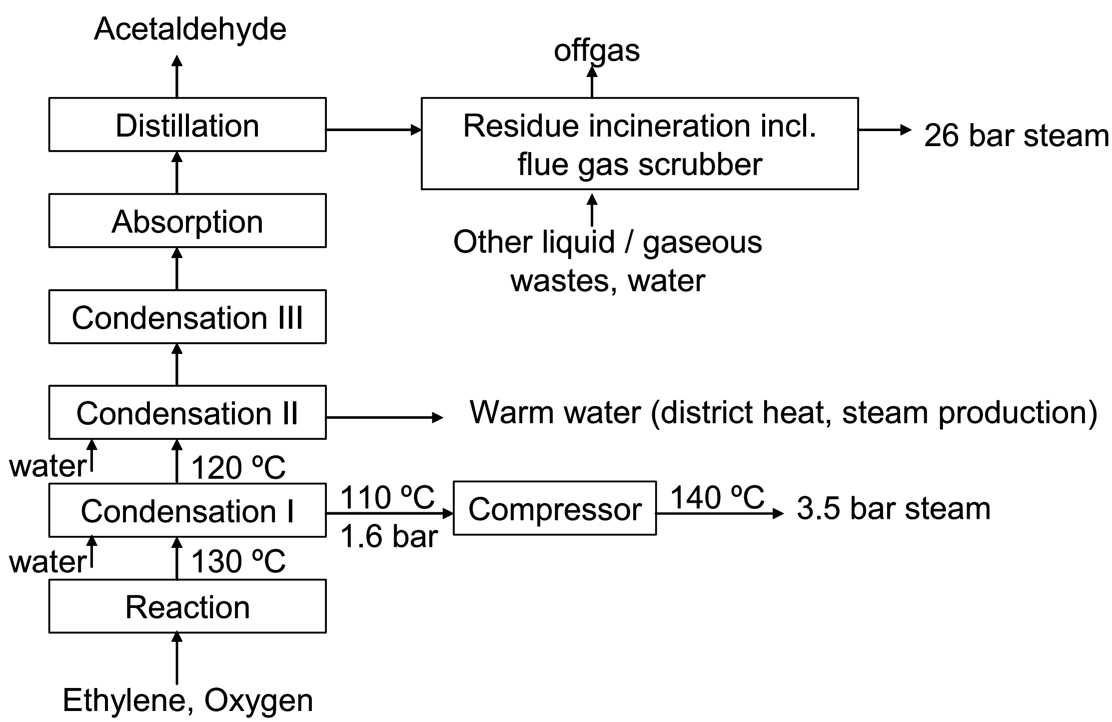
Examples of Energy Integration at Companies

Energy Integration at Marl

Three cogeneration plants at the Marl site provide 300 MW_{el} and over 1 kt/h of steam. Gas pipeline systems are provided for waste gas used as heating gas. Also, residues from the site's chemical plants are incinerated to provide energy for the site (ChemSite Initiative, 2006).

Heat Recovery at Lonza

At the Lonza site in Visp, Switzerland, excess heat is produced in the production of acetaldehyde from ethylene during various process steps. This benefits the site in an amount of 20 GWh (Gerritzen, 2005).



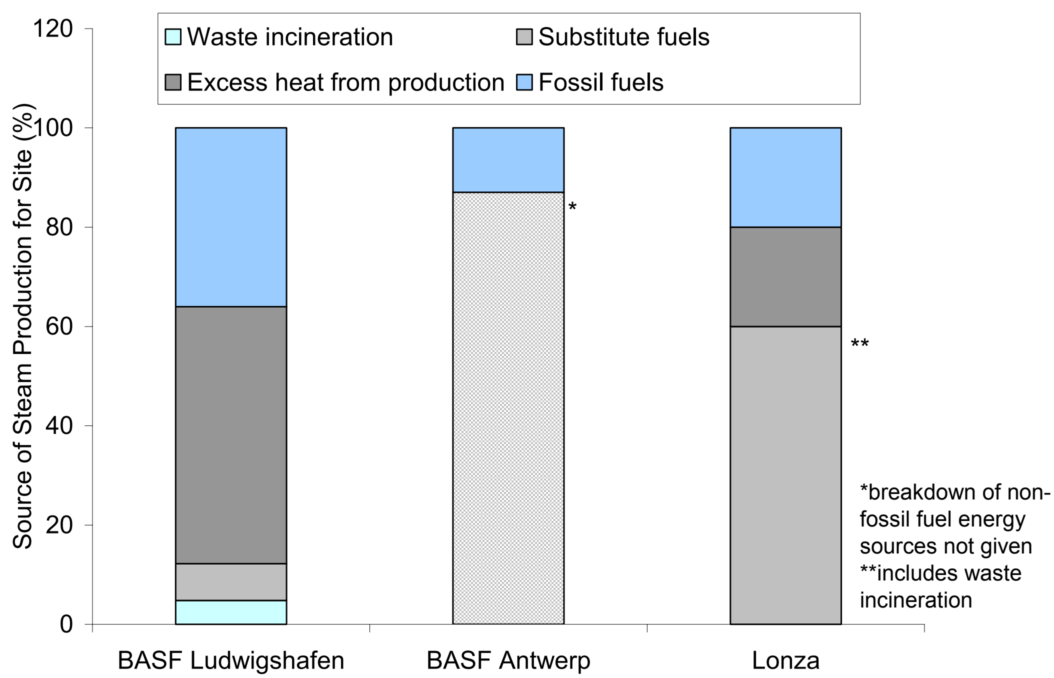
(based on Gerritzen, 2005)

Figure 3.17 Excess Heat Recovery in the Acetaldehyde Process at Lonza

Energy Integration at BASF and Lonza

The BASF Ludwigshafen site requires approximately 18 million tons of steam annually. Therefore, efficiencies provided through process integration may have significant effects. Steam production via exothermic processes and waste by-product incineration provide over half of BASF's steam requirements. Also, the use of fossil fuels for electrical power and steam generation has been reduced by about 52% since 1976 while the production output has increased by 50%. BASF attributes these reductions to continuous improvements in energy integration. For the BASF Ludwigshafen production site, the steam demand of 2160 t/h (in 2003) was provided as follows: 43% by two power plants (one using 33% substitute fuels) and 57% by production sources, where 52% was supplied by excess heat from production and 5% by waste incineration (BASF, 2002).

In Visp, Switzerland, 80% of the energy required for steam production comes from incineration or waste heat, which translates to a savings of 65 kt/a of heating oil. The graphic below shows the use of various sources for the generation of steam at the Lonza Visp site and two BASF sites.



(based on BASF 2002, 2007, and Gerritzen, 2005)

Figure 3.18 Steam Production Sources for BASF and Lonza Sites

Examples of Waste Incineration and Substitute Fuels at BASF

In 2006, the BASF Ludwigshafen polystyrene plant was the first plant onsite to successfully switch to substitute fuels (BASF, 2006, p.71). Other examples of the use of chemical wastes as fuels are given below. In the production of isophytol, by-product streams are separated into a high-value and a lower-value product stream. The high-value portion is much larger and allows residue-free incineration as a high calorific substitute fuel.

Another example is in the Citral plant, which is the production platform for Vitamins A and E, carotinoids, and aroma chemicals. Here vinylionol is produced, which requires highly concentrated sulphuric acid from the sulphuric acid plant. Contaminated sulphuric acid remains after the reaction. This acid is cleaved to sulphur dioxide in the splitting unit of the sulphuric acid plant. The organic residues are incinerated during this process, creating a source of energy.

In the production of tanning agents, aqueous solutions are dried to fine powders in a heated air stream. The required energy is usually supplied by natural gas. During manufacture of another product in a neighbouring plant, a liquid, non-recyclable hydrocarbon mixture is created. This waste is used in place of natural gas to heat the drying air. Therefore, the hydrocarbon mixture is used as fuel and waste disposal is not necessary. In the spray drying of dispersants and tanning agents, the plant saves more than 200 km^3/a of natural gas (BASF, 2006).

3.7.4 Shared Infrastructure

The extent of infrastructure required at a chemical site may vary depending on the specific site requirements. However, there are certain facilities required by all chemical sites. According to Hauthal (2003, p.37), the mandatory and optional services an infrastructure provider of a chemical site should offer are as follows:

- Mandatory services:
  - Availability of industrially zoned land
  - Energy (electrical, steam, natural gas)
  - Utilities
  - Waste water treatment and disposal
  - Infrastructure (roads and pipe bridge network)
  - Site planning

  - Permission and clearance management
  - Safety and environmental protection (fire brigade, site security, environmental protection, coordination of safety management)
- Optional services:
  - Logistics (rail service, vehicle services, freight forwarding)
  - Analytical laboratory services
  - Engineering services
  - Maintenance services
  - IT and communication services
  - On-site medical and occupational services, accident prevention
  - Material testing
  - Human resources, training, and education

Examples of Shared Infrastructure at Companies

Shared Infrastructure at Synia Chemical

The below schematic shows the layout of the Synia chemical production site, located outside of Shanghai. Networks for the distribution or collection of electricity, waste water, raw water, steam (not shown), and nitrogen (not shown) ensure that each production plant benefits from site-wide utilities provision (Synia Fine Chemical, 2005).

(Synia Fine Chemical, 2005)

Figure 3.19 Site wide Distribution Network for Electricity and Water

Shared Infrastructure at Marl

There are 140 km of rail and roads, highway access, a cogeneration power plant, gases, waste water treatment and various plant-related services at the Marl site. There is a port (connected to the Rhine River and the North Sea ports) with an inland waterway and a railway station connected to the European railway network. Tank farms, laboratories, warehouses, and a container terminal are provided. Various utilities are provided: nitrogen, oxygen, hydrogen, pressurised air, and various types of water including a hot water grid. The Marl site offers waste disposal, including hazardous waste incineration and sludge incineration plants, and waste water treatment consisting of two biological treatment plants with sludge incineration. Further, facility management, purchasing, telecommunication, safety and environment, emergency response, security, fire brigade, maintenance, workshops, project and plant engineering, plant construction, communications, and human resources are provided (ChemSite Initiative, 2006).

3.7.5 Environmental Aspect of Integration

Sustainable chemical production requires both economical and ecological efficiency. An ICPS allows economic and environmental requirements to be reconciled by minimising the use of resources and energy. This is done through reutilising by-products which would otherwise be disposed of and avoiding the transport of sales products through onsite use. Through the efficient large-scale provision of electricity and steam, fossil fuel usage and costs are reduced. Additionally, through heat recovery, overall energy requirements are reduced.

Chemical wastes may arise from: incomplete chemical conversion, off-spec products, impurities in raw materials, by-product formation, catalyst waste, the reaction medium, or emissions from energy provision. Some wastes or residues can be reduced through process alteration, such as a new synthesis route or improved selectivity. Other wastes, which cannot be avoided even under optimum operation conditions, may potentially be reused within a process or as a raw material in a separate process, possibly requiring further physical or chemical processing. Reutilising residues by linking processes through horizontal material integration in an ICPS allows resources to be used more effectively. This decreases the use of solutions such as waste treatment, disposal, or incineration, which result in further costs, emissions, and resource use.

The table below shows how economic and ecological aspects are reconciled in an ICPS.

Table 3.4 Economic and Ecological Efficiency through Integration

	Economic efficiency	Ecological efficiency
Goal	Turnover	Sustainability
Factors	Costs (eg. materials, utilities, waste treatment)	Environmental impact Use of resources
Economic & Ecological efficiency via reductions in:	Resources → utilise chemical residues Energy → efficient utilities provision, heat recovery Emissions → onsite transport, etc.	

For example, the BASF and Bayer integrated sites utilise significant amounts of residues. At Bayer Leverkusen in 1989, 1,200 kt/a of production residues were utilised: 80% directly, 15% recycled to production after chemical conversion, and 5% incinerated for steam production. This is more than the amount of waste produced in the same year of 875 kt. For BASF in 1987, 750 kt/a of residues were utilised in chemical production: 380 kt/a in product manufacture and 110 kt/a by outside companies. These quantities are very large with respect to the quantity of products sold at 8,300 kt/a and the amount of waste at 897 kt/a in the same year (Ullmann, 2000).

3.7.6 Organisational Integration

Lastly, there is integration of an organisational nature, which can be described as intangible or conceptual, such as the sharing of information or knowledge. Examples are given below:

- Product innovation: finding new uses or value in waste products
- Purchasing: centrally coordinated purchasing of goods and services
- Corporate functions: human resources, strategy, administration
- Safety and environment: safety concepts, transport safety, wastes, emissions
- Knowledge management: databases, patents, coordinated research, IT systems, interdisciplinary cooperation (research, engineering, logistics systems, sales and marketing)

The communication and knowledge sharing which arises from organisational integration is certain to benefit a site. Various information flows or organisational systems which support production, marketing, and sales and distribution may help to standardise and increase transparency in the information flow regarding production planning, stocks, market situations, price developments, customer service, and invoicing and result in cost savings. Easier communication between R&D and production and marketing may shorten the time required for innovations to be realised. These more streamlined processes may lead to higher economic efficiencies. Additionally, it may be that these types of integration are even stronger if the site consists of only one or a few companies, as there are no additional barriers created by cross-company communication. This type of integration is not easily quantified and is of a more qualitative nature. Organisational integration is mentioned here for completeness, however, will not be addressed in this work.

4 Methodology for Quantifying Integration Aspects

This work proposes a methodology as an approach for determining the economic and environmental benefits of integrated sites relative to less integrated sites based on different types of integration. First, site types are defined for the methodology. This is followed by an introduction of the nomenclature employed for tracking flows. Then the components of the methodology according to integration types are given. Finally, how the methodology is applied on the plant level is proposed.

4.1 Definition of Site Types

As discussed earlier, chemical production sites range from stand-alone sites consisting of a single production plant and basic facilities to large-scale integrated sites. An ICPS was defined as having several production plants, value chains, and facilities linked through various types of integration. In order to make the results of this work more plausible, an intermediate form of integrated site is introduced, the semi-integrated chemical production site or semi-ICPS.

The difference between the ICPS and semi-ICPS is that the semi-ICPS has much fewer plants and less materials integration. The minimum number of plants in an ICPS is difficult to define, however, an approximation based on sites reviewed is 5-10 plants. As a result of the few plants in a semi-ICPS, vertical materials integration through value chains (or forward/backward integration) is either absent or limited to one or few linkages. Also, the semi-ICPS is defined as having no horizontal materials integration or chemical utilisation of by-products, again due to the small number of plants.

Key infrastructure facilities (security, utilities, emergency response, fire fighting capabilities) are present in all three site types to varying extents. The ICPS and semi-ICPS have additional infrastructure, such as an incinerator, power plant, biological waste water treatment, etc. Whereas, stand-alone sites rely on external providers, such as the public power grid or external waste treatment. The site types are summarised as well as shown schematically on the following pages.

Table 4.1 Facilities and Integration at Site Types for Methodology

Difference	ICPS	Semi-ICPS	Stand-alone
# of Plants	Several (> 5-10)	Few (< 5-10)	One
Value Chains	Value chains consisting of several plants (backward/forward integration)	Incomplete value chains	No value chains
Provision of power and steam	Onsite power plant for electricity and steam production, steam network	Same as ICPS	Steam boiler, electricity from public grid
Energy integration	Steam production via onsite incineration and heat recovery, transfer of heated streams	Same as ICPS (plus incineration of some by-product wastes)	n/a
Materials integration	Vertical integration (captive-use products), horizontal integration (use of by-products as feedstocks)	Limited vertical integration, no horizontal integration due to few plants	n/a
Logistics integration	Onsite transport of captive-use products and useable by-products	Less transfer of captive-use products	n/a

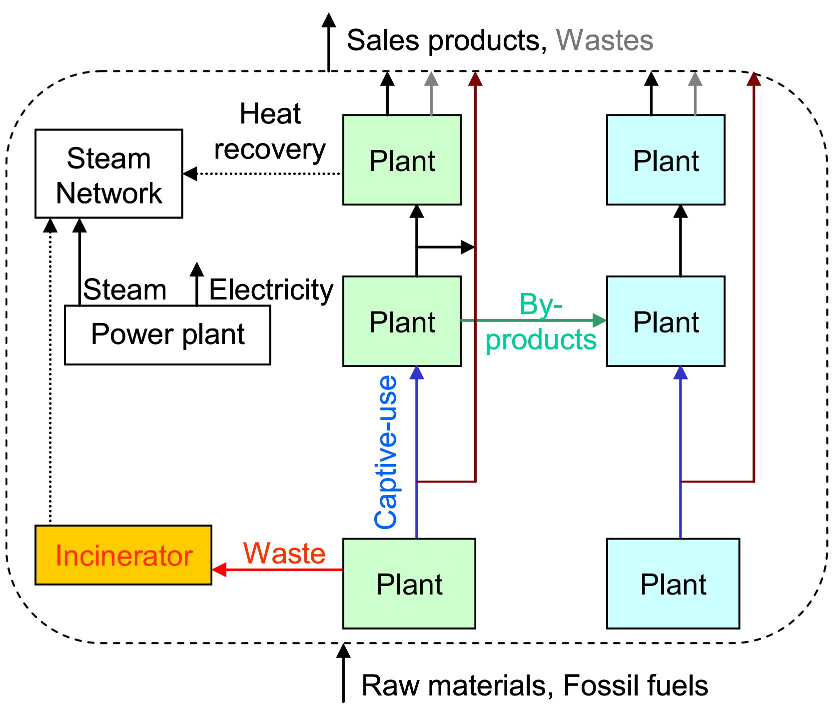


Figure 4.1 Site Types for Methodology: ICPS

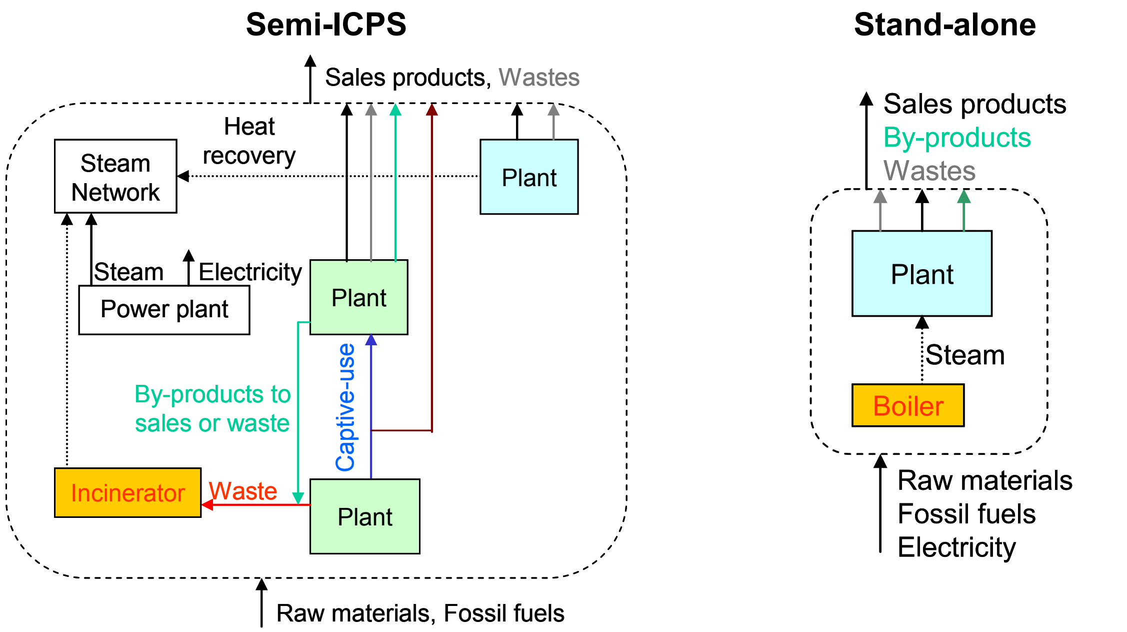


Figure 4.2 Site Types for Methodology: Semi-ICPS and Stand-alone Sites

4.2 Mapping the Site

The methodology has its conceptual foundation in Industrial Ecology and Material Flow Analysis. The term mapping is used to describe the process of identifying value chains, material flows, and energy flows at a site. First, the main value chains at the site are identified. Second, the main production plants are identified and categorised according to the value chain they belong to. Third, the product and energy streams connecting various parts of the site are accounted for.

4.2.1 Nomenclature

Material flows are designated by an ‘M’ and energy flows by an ‘E’. The letter following the M or E designates the group to which the stream belongs to. For example, M_v is a material belonging to a value chain (see Abbreviations List, p.vii). Furthermore, subscripts denote where the streams arise from and enter. The exiting and entering locations are designated by value chain and plant. For example, plant B in value chain 2 is designated as 2B. If the location is the incinerator or power plant, this is denoted by in or pp. As there may be more than one flow connecting two locations, a flow number is assigned. Thus, the streams are denoted as follows: $M_{\text{group, exiting location, entering location, flow number}}$. The figures below exemplify the use of this nomenclature.

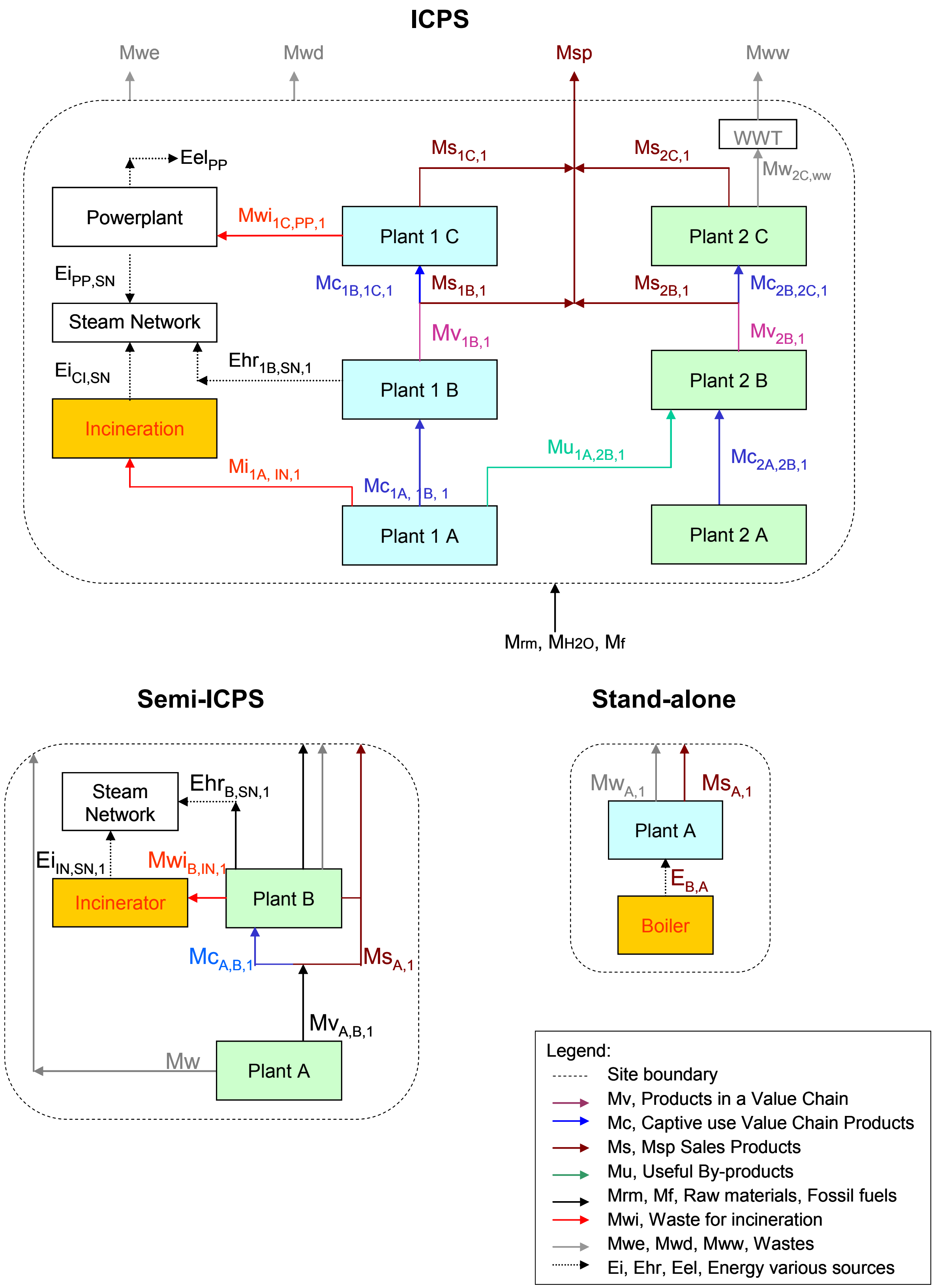


Figure 4.3 Site Schematics exemplifying Nomenclature for Methodology

4.3 Assumptions

The assumptions and exclusions of the methodology are summarised below.

- Integration advantages in terms of procurement costs are not addressed.
- The raw material and fossil fuel supplies are ample.
- Products transferred between plants in an integrated site sell the products according to transfer prices which reflect market prices.
- Selling cost, royalties, freight insurance, and the cost of inventory are not considered.
- Costs for additional process steps to separate or refine a by-product for onsite use or sales are neglected and part of the plant from which it arises.
- Streams categorised as waste in the ICPS are also wastes in a semi-ICPS or a stand-alone site. Only wastes exiting a plant are considered, not wastes such as fuel used directly in a plant.
- The types of processes are similar at all sites.
- The cost of waste heat boilers for processes with heat recovery and steam export is neglected and assumed to be part of the production plant.
- Lowered emissions due to economies of scale within the chemical production plant are not considered.
- Heat recovery is only considered for streams exiting a plant and not used within a plant.
- Heat recovery is only used for steam production or the heating of materials streams and not for electricity production or district heating.
- The costs of pipelines between integrated plants, between plants and utilities, between the power plant and plants (eg. steam network), and for tie-ins to olefins pipelines are not considered.
- Storage, handling, packaging, transport, and materials management costs for waste streams disposed of or incinerated are neglected.
- Country specific issues, such as incentives, taxes, or legal implications are not within the scope of this work. Import tariffs are included.
- Benefits from organisational integration are not addressed, as these are outside of the scope of the work.

4.4 Materials Integration

4.4.1 Material Types in the ICPS

Materials in an ICPS are mapped according to the following eight categories:

- Materials in Input System:
  - External raw materials for the entire site, including water
  - Fossil fuels for the site
- Materials in the Core System:
  - Value chain products for captive use as onsite feedstocks
  - Internally used by-products not sold offsite
  - Materials incinerated to provide energy for the site
- Materials in the Output System:
  - Sales products
  - Emissions to the atmosphere or waste remaining in treated waste water
  - Wastes transported offsite for land-filling

Conservation of Mass

The sum of all mass flows entering the core system should equal the sum of all mass flows leaving the core system according to the first law of thermodynamics.

$$M_f + M_{rm} + M_{H2O} = M_{sp} + M_{we} + M_{wd} + M_{ww}$$

Materials in the Value Chain

First, value chains at a particular site are mapped. A material stream in a value chain, M_v, can be partly sold to offsite customers in an amount M_s. The sum of sales materials from all value chains at a particular site is referred to as M_{sp}. A material in a value chain which is used internally for captive use as a feedstock to another plant in the same value chain is designated M_c. Therefore, the following holds true:

$$M_v = M_s + M_c \qquad \textit{for a particular value chain}$$

$$M_{sp} = \sum_{i,j=1}^{I,J} M_s\,(i,j) \qquad \textit{for I sales streams in J value chains}$$

Wastes

All materials exiting a plant in an ICPS which are not fed to another plant on the site as a chemical feedstock or sold are considered as wastes. If they can be used as fuel either in an incinerator or power plant, they are termed 'incineration wastes', M_{wi}. If they cannot be used for fuel, they must be disposed of offsite and are designated M_{wd}. Other types of waste may be emitted either as emissions, M_{we}, or in treated waste water, M_{ww}. The following schematic shows how materials exiting a plant in an ICPS can be either: a captive use product, sales product, internally used by-product, or waste.

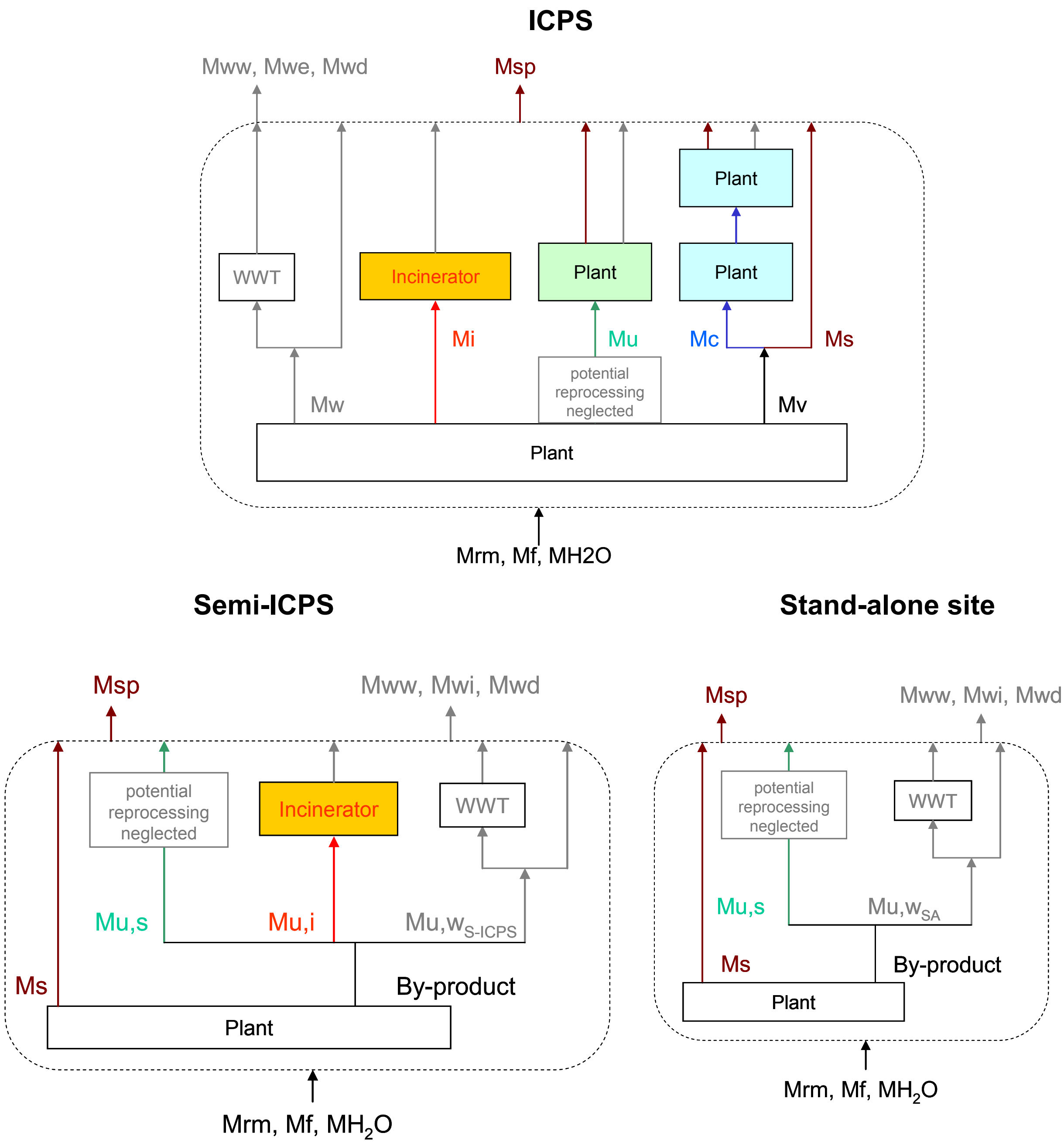


Figure 4.4 Materials Mapping for the Different Site Types

Sales Products and Captive use Products

Sales product streams are not considered in the methodology on the site level, as for both an ICPS and a stand-alone site, they must be transported offsite to customers. Captive use products only travel a short distance by pipeline in an ICPS (or potentially in a semi-ICPS) compared to a stand-alone site. Therefore, they represent an economic benefit for the ICPS, as they do not need to be transported offsite. This benefit is covered later under the logistics section.

Useable By-products

Once all materials for the value chains are mapped out as either M_v, M_c, or M_s, the remaining chemical feedstocks used within the ICPS can be identified. These are by-products or intermediates which arise in one plant to be used as feedstocks in another plant of a different value chain (horizontal integration). These materials are referred to as 'useable by-products' and designated as M_u.

If these streams arise in a stand-alone site, they may be either sold offsite, used as fuel, or disposed of. Therefore, it must be determined for each by-product stream, which of the three options is most appropriate.

The decision chart below shows the process in determining the fate of a by-product. It is assumed that the product is sold as a first choice. Thus, first it is determined if the product is sellable. A by-product may not be sellable if there is no customer nearby requiring the product, such as if the by-product has little value or a low volume. Or else it may be sellable once further processed, in which case, the useable by-product is considered a sales product. Then, if there is a recipient of the material within an ICPS, logistics costs are reduced for the ICPS compared to a semi-ICPS or stand-alone site from which the material would be transported offsite, incurring further logistics costs.

If the by-product cannot be sold or it is uneconomical to further process the material, it is categorised as a waste and incineration or disposal costs are incurred. If the material can be incinerated in a residue incinerator in a semi-ICPS, steam can be produced for onsite use. The final choice is to dispose of the waste via waste water treatment, incineration (without steam production), or land-filling at an expense.

Thus, horizontal materials integration in an ICPS may result in either logistics integration or energy integration through waste incineration, depending on how the particular stream is categorised.

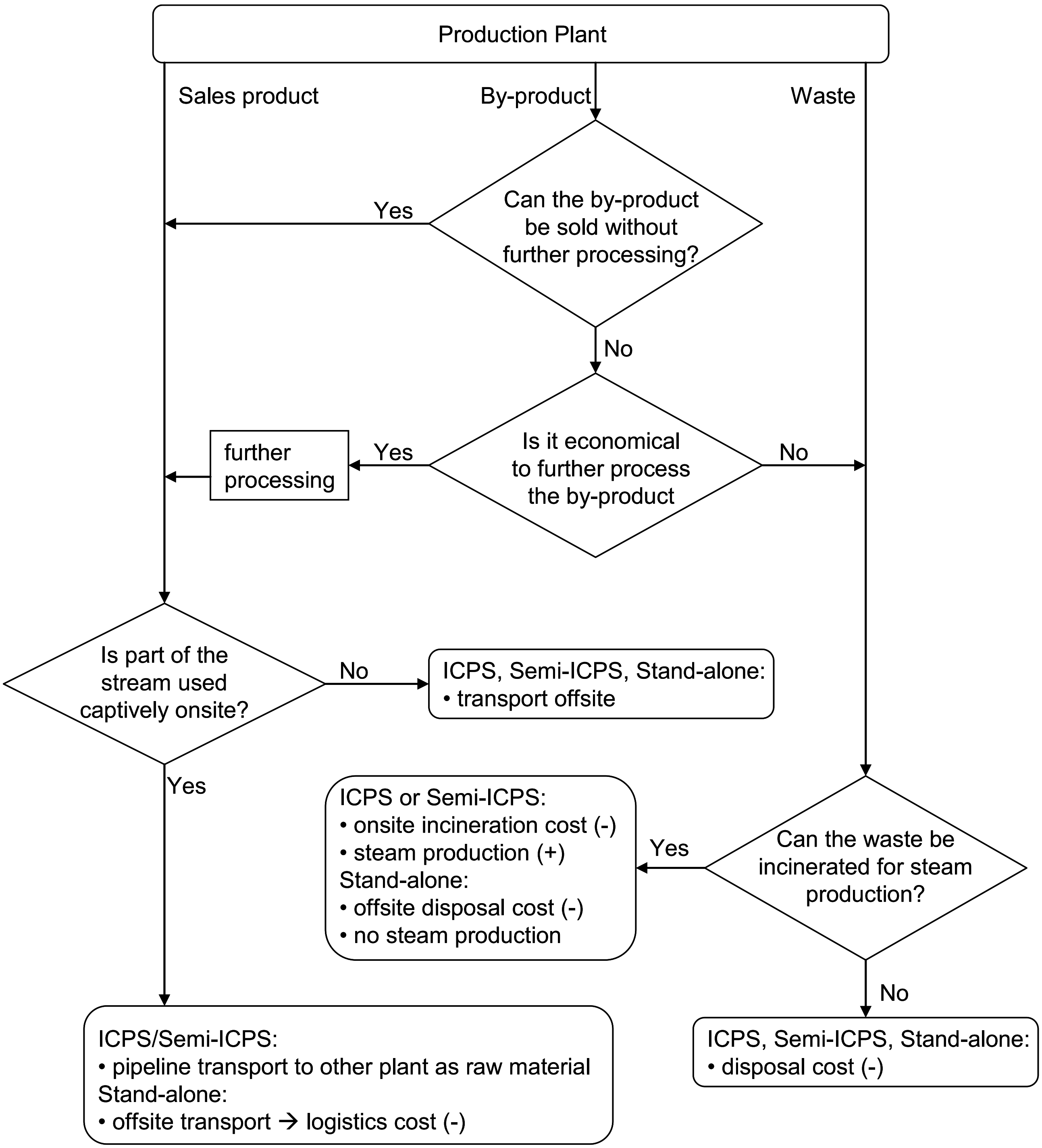


Figure 4.5 Decision Flow Chart for By-products

4.4.2 Economic Benefit of Materials Integration

As the whole site is considered, material streams passing between two plants within the ICPS are only accounted for once; only product and not raw material streams are accounted for. The boundary is set around the production plants, from the first plant in the vertical chain (normally the first plant following the cracker) to the last.

Economic Benefit of Useable By-Products

In the methodology, a useable by-product in an ICPS, M_u, becomes either a sales product, $M_{u,s,SA}$, or a waste to be disposed of, $M_{u.d,SA}$, in a stand-alone site. In a semi-ICPS, this stream becomes either a sales product, $M_{u,s,S\text{-}ICPS}$, a waste to be incinerated, $M_{u,i,S\text{-}ICPS}$, or a waste to be disposed of, $M_{u.d,S\text{-}ICPS}$. Therefore, the following holds:

$$M_{u,ICPS} = M_{u,s,SA} + M_{u,d,SA} \qquad \textit{for a stand-alone site}$$

$$M_{u,ICPS} = M_{u,s,S-ICPS} + M_{u,i,S-ICPS} + M_{u,d,S-ICPS} \qquad \textit{for a semi-ICPS}$$

Thus, if $M_{u,i,S\text{-}ICPS} > 0$, then $M_{u.d,S\text{-}ICPS} < M_{u,d,SA}$

and $M_{u,s,SA} = M_{u.s,S\text{-}ICPS}$

The different options for the categorisation of an integrated by-product stream in an ICPS versus in a semi-ICPS or stand-alone site are shown below.

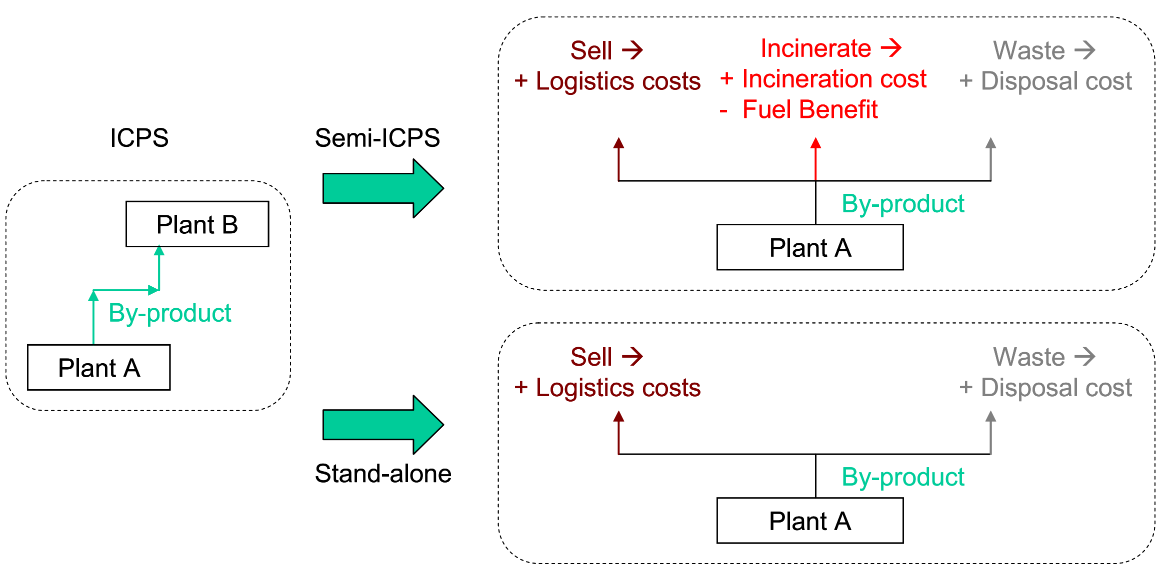


Figure 4.6 Fates of Useable By-products in Semi-ICPS or Stand-alone Site

If the useable by-product can be sold in a semi-ICPS or stand-alone site, then logistics costs are saved in the ICPS (covered under logistics integration). If it is possible to incinerate it for steam production in the semi-ICPS, then the semi-ICPS gains the value of steam (covered under energy integration), however, similar to the stand-alone site, incurrs costs for incineration (covered under materials integration). Otherwise, it is a waste stream and the ICPS saves the disposal cost (under materials integration).

Additionally, the loss of the chemical value of the material must be considered in the semi-ICPS or stand-alone plant. For this, the chemical value of the stream must be determined. This may be difficult if the stream is a mixture of components, which is often the case. The chemical value of the stream represents a savings in the ICPS relative to both a semi-ICPS and a stand-alone site. If the material can be used as a fuel or as a utility (as shown by the Lonza example for carbon dioxide in Section 3.7.1), then this is a benefit in the semi-ICPS, where the fuel or utility value of the stream is determined and deducted from the chemical value of the material. Hence, the material-related cost savings of the ICPS relative to the stand-alone site and semi-ICPS are determined as follows:

$$S_{M,ICSPS,SA} = M_{u,wd,SA} \cdot c_{wd} + M_{u,SA} \cdot v_u$$

$$S_{M,ICPS,S-ICPS} = M_{u,i,S-ICPS} \cdot c_i + M_{u,wd,S-ICPS} \cdot c_{wd} + M_{u,S-ICPS} \cdot \left(v_u - v_{f,ut}\right)$$

4.5 Energy Integration

Below, the energy provision for the different site types is briefly described. Benefits derived from shared energy provision are described more fully under ‘shared infrastructure’ in the next section. This is followed by a schematic showing how excess heat is recovered in integrated sites.

4.5.1 Energy Provision

Power and Steam

Electricity and steam are provided for the ICPS and semi-ICPS by an onsite power plant, whereas, electricity for the stand-alone site is provided by the public grid. An ICPS and a semi-ICPS have a steam network which provides high pressure steam in a centralised form by pipeline to the individual plants. From the power plant, a steam network runs through the site to distribute steam to various plants and facilities. A stand-alone site does not have a steam network and steam is provided through individual boilers. Thus, an ICPS has the following:

- Power plant which produces steam and electricity for the site
- Steam network pipeline
- Plants which take steam from the network
- Plants which donate steam to the network

Incineration

Waste materials may be incinerated in lieu of fossil fuels to generate energy. An ICPS and a semi-ICPS have one or more central incinerators in which wastes are incinerated to provide steam to the site via a steam network. Also, wastes may be incinerated in a power plant for both steam and electricity production. Whereas, a stand-alone site provides steam through a boiler and sends wastes offsite for disposal.

4.5.2 Excess Heat Recovery

An integrated site can implement the concept of excess heat recovery better than a stand-alone plant because of the following two main reasons. First, the transfer of heated liquid streams or steam requires production plants to be in close proximity. Second, the presence of several processes may allow a better balance of heating requirements and surpluses for the overall site to be achieved.

Heat recovery in an ICPS is assumed to only be used for the heating of chemical streams or steam production and not for electricity or district heating. Heat recovery is an advantage to the ICPS and semi-ICPS, as less steam needs to be produced for the site via the power plant. However, the extent to which a particular integrated site can benefit from this concept depends on the number of suitable processes providing heat to neighbouring plants via either heated streams or steam export to the network. Thus, the advantages of excess heat recovery depend on the balance of energy requirements, which is more likely to improve as the number of different processes at a site increases.

The following schematics compare the energy flows in an ICPS or semi-ICPS to a stand-alone site.

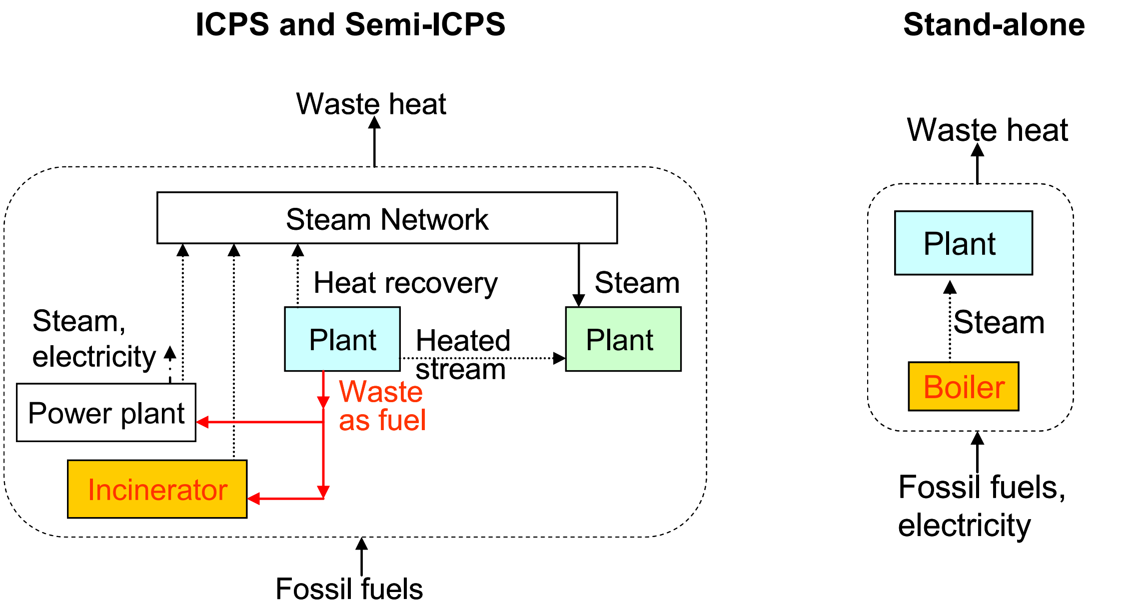


Figure 4.7 Energy Mapping for the Different Site Types

4.5.3 Economic Benefit of Energy Integration

Energy integration provides economic benefits to the ICPS relative to a stand-alone site through the following processes, which also reduce fossil fuel consumption:

- Incineration and heat recovery → steam production
- Transfer of heated streams → reduction of cooling water, steam, or equipment

In the determination of cost savings, the site-specific cost of steam and cooling water are used, including costs for water, fuel, capital, and operation. The cost savings for additional equipment, such as a heat exchanger, required to cool a heated stream if it is not integrated, is taken as the annual operating cost including the cost of capital.

$$S_{E,ICPS,SA} = \left(c_{St} \cdot \left(M_{St,i} + M_{St,hr} + M_{St,hs}\right) + \left(M_{cw,hs} \cdot c_{cw}\right) + C_{eq,hs}\right)$$

In a semi-ICPS, as in an ICPS, waste incineration and heat recovery are practiced. The savings associated with the transfer of heated streams may also apply, as a semi-ICPS has more than one plant. Additionally, the semi-ICPS incinerates by-products which are used chemically in an ICPS, but cannot be sold in a semi-ICPS. This represents an energy benefit for the semi-ICPS and is deducted from the ICPS savings. The additional cost for incinerating this stream is covered under materials integration.

$$S_{E,ICPS,S-ICPS} = -c_{St} \cdot \left(M_{St,ui}\right)$$

4.6 Logistics Integration

Pipes transport raw materials, utilities, and products among plants and utilities providers within an ICPS. In the methodology, the logistics cost savings for an ICPS relative to a stand-alone site arise from the onsite transport of: captive use materials, M_c, and useable by-products which are sellable, $M_{u,s}$, as both of these streams would otherwise require transport to offsite customers. Compared with a semi-ICPS, the logistics cost savings in an ICPS result from the onsite transport of useable by-products. Although the semi-ICPS may also benefit from the onsite transport of captive-use products, the volume is expected to be greater in the ICPS due to the presence of value chains. Logistics integration is shown schematically below. Through the onsite use of raw materials and products, transport and different logistics steps are reduced.

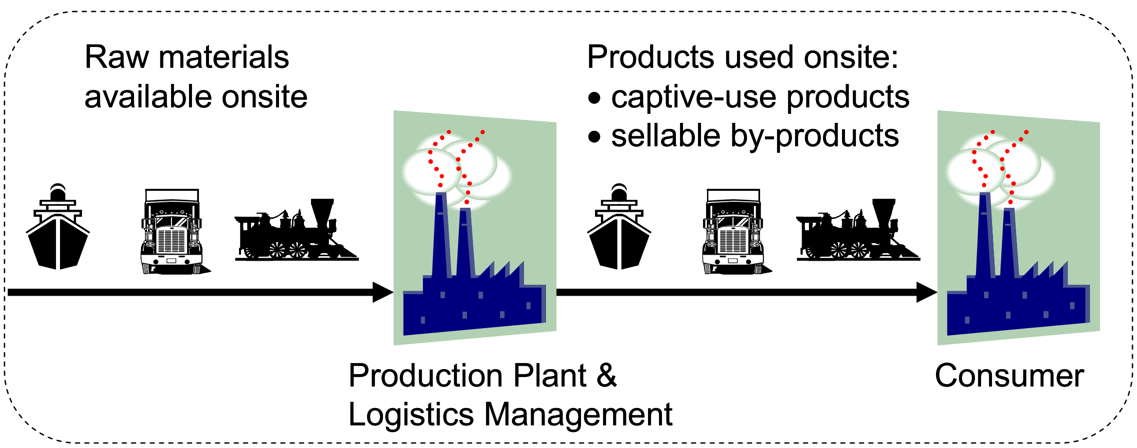


Figure 4.8 Logistics-related Costs in a Stand-alone Site and Semi- ICPS

4.6.1 Logistics Management

The steps in the logistics chain for chemical products are shown in the following schematic provided by BASF AG. Administrative processes which support the physical processes are described as logistics management. Costs are associated with these processes, as they require personnel, information systems, office space, etc.

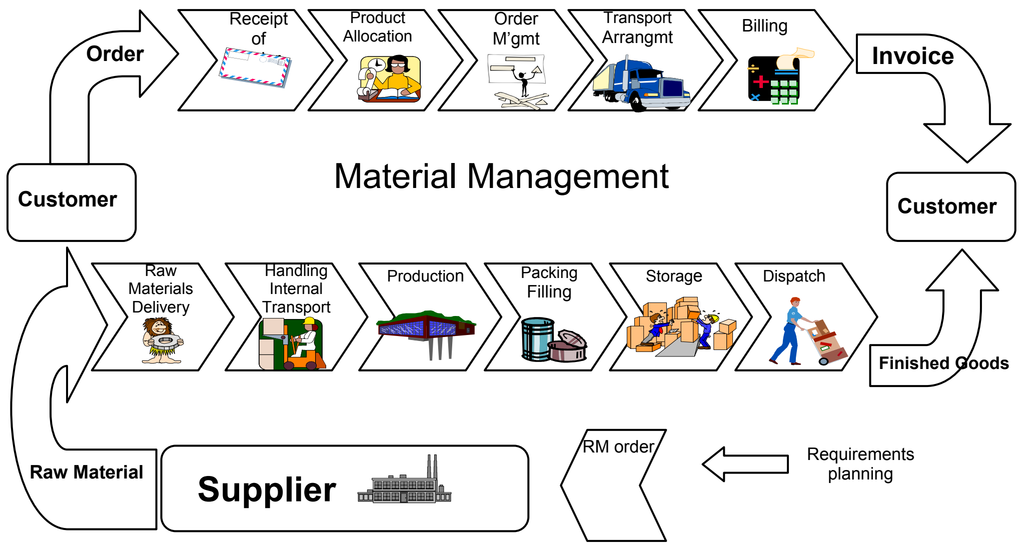


Figure 4.9 Logistics Chain for Chemical Production

The main cost blocks associated with logistics processes for chemical production sites are:

- Filling and packaging
- Storing/warehousing: packed goods in warehouses, bulk goods in tank terminals, eg. at a port before containers are loaded onto ships
- Dispatch: commissioning, site transportation, labelling for shipping
- Freight: outbound freight, transportation to distribution centres, inbound freights for returned goods, rental cost for cars and containers
- Order-/material-management: management of orders and materials, management of all transportation modes

The costs for logistics-related management processes and warehousing used in this work are based on results from an internal company study[2]. The costs varied little among the regions of America, Europe, and Asia and were on average in 2004 per ton of product:

- Dispatch costs = 1 €/t
- Order and materials management = 4.6 €/t
- Filling of liquid bulk materials = 4 €/t

[2] The company is not named in order to maintain confidentiality.

- Offsite warehousing = 10 €/t

For materials transferred between plants within a site, management-related activities are required, such as monitoring inventory and communication between the two plants, at a cost of 1 €/t.

4.6.2 Transport

Chemical products may be transported by truck, rail, inland waterway, sea, or air. The transport mode or combination of modes selected depends on the location of producer and consumer, cost considerations, and other constraints such as availability and urgency. A study by Börjesson and Gustavson (1996) found the most cost effective mode of transport to depend on distance: below 100 km, road transport is the most economical, after which rail becomes most economical up to 110 km, followed by ship. In general, costs are highest for air, followed by road, rail, barge/inland waterway, and sea freight. However, as costs cited by different authors vary (see below), transport costs are determined by inquiry for this work.

Table 4.2 Transport Costs per Mode of Travel from Different Studies

Author , Transport cost (€/ton·km)	Air	Road	Rail	Barge	Sea
Knell [3]	0.102	0.036	0.025	0.015	0.001
SCI Verkehr GmbH [4]			0.035	0.016	
Prognos AG [5]			0.086	0.012	

The specific cost for road transport was found to decrease with distance, as shown in Figure 4.10, based on data from the BASF AG logistics department in 2005. However other factors (supply/demand, transport supplier, etc.) also influence the cost, which is shown by the specific cost for transport to Montpellier and Rome, which deviate slightly from the trend.

[3] Knell, 2003, p.96
[4] Alles et al., 2000, p.74
[5] Hobohm et al., 2006, p.40-41

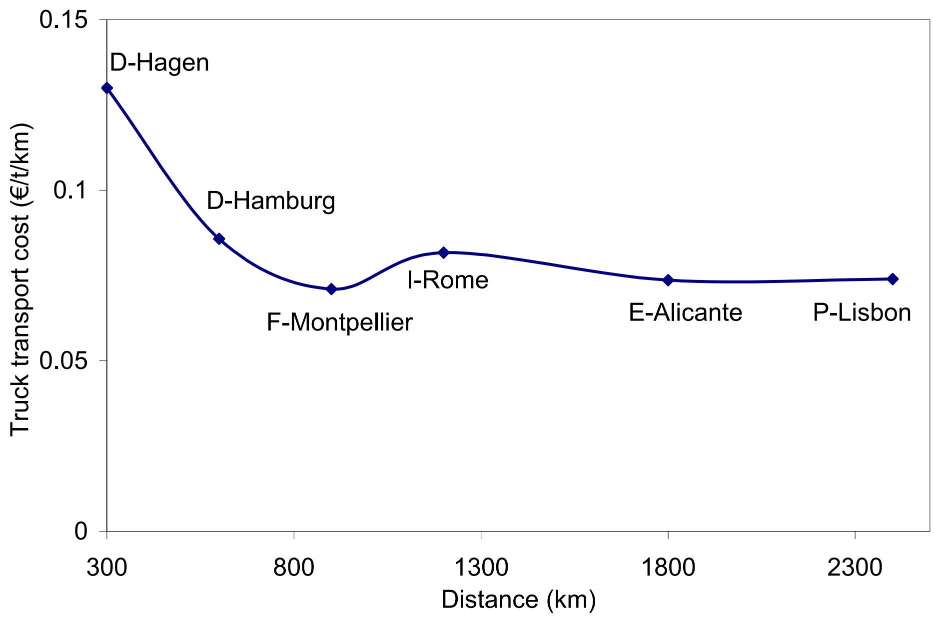


Figure 4.10 Specific Road Transport Cost versus Distance travelled

External Costs for Transport

It may be noted that transport of products or raw materials between production sites carries not only the costs associated with the actual transport (vehicle, personnel, fuel), but also has external effects. In a study by Schreyer et al. (2004, p.14), the external costs for the transport of goods were determined within Europe. These consist of the costs related to: accidents, air pollution, noise, nature, urban effects, climate change, up- and downstream processes and are given as follows (in €/t/km): 0.0878 for road, 0.0179 for rail, and 0.0225 for waterway. These external costs which society pays for transport are in some cases higher than those of the actual transport. Also, it should be noted that transport by rail poses the lowest cost to society compared to road to waterway transport. Additionally, the safety aspect of the transport of dangerous goods has an even higher risk or potential cost associated with it.

4.6.3 Storage

The storage requirements are reduced for integrated plants. If a material is transferred between plants at different locations, each location will need a storage tank at its site. However, if a material links two plants in an integrated site, only one storage tank may be required to buffer any supply/demand differences between the two plants. Thus, the storage requirements are expected to be at least twice as high if the plants are separated due to storage at each location. In fact, if the plants are connected by pipeline within the ICPS, then storage requirements may even be less, as handling is not required.

Additionally, storage requirements for common raw materials are reduced at an ICPS as these can be centrally stored. Storage requirements are determined according to a balance of the frequency with which the tank must be refilled, tank investment costs, raw material/product inventory costs, and strategic factors, such as the necessity to hold inventory. For the methodology, the storage requirements for all materials requiring transport in non-integrated sites (captive use products and useable by-products) are determined on a case by case basis, as these depend on the product and process considered.

Economic Benefit of Logistics Integration

In applying the methodology, first the materials available onsite in the ICPS are determined. Then the relative amounts transported by road, rail, and ship are determined. Next specific costs for transport and other costs such as port charges are determined. As the semi-ICPS may have some captive use streams, the amount of captive use materials in the ICPS needs to be determined.

$$S_{L,ICPS,SA} = \left(\sum Mu,s + \sum Mc_{ICPS,SA}\right) \cdot \left(c_{lm} + \sum_{x=1}^{n} F_{t,x} \cdot D_x\right) + C_{Warehouse} + C_{Storage} + C_{other}$$

$$S_{L,ICPS,S-ICPS} = \left(\sum Mu,s + \sum Mc_{ICPS,S-ICPS}\right) \cdot \left(c_{lm} + \sum_{x=1}^{n} F_{t,x} \cdot D_x\right) + C_{Warehouse} + C_{Storage} + C_{other}$$

for n transport modes

4.7 Shared Infrastructure

This section investigates potential benefits in integrated sites for shared infrastructure. First, infrastructure is defined and what is involved in planning an integrated site is covered. Next, the costs for energy provision are reviewed, as this is normally one of the most costly aspects of infrastructure. This is followed by a review of the costs for utilities provision.

Some facilities are not investigated, as they tend to only exist in larger sites and not in stand-alone sites due to the high capital investment required. A stand-alone site will utilise these services offsite; examples are waste incineration and biological waste water treatment. The external operating costs for such services may be comparable with those in the ICPS, as both may achieve similar economies of scale. However, costs may differ due to transport to the service provider or lower performance in the ICPS, as the service is not a core competence of the site. Also, it should be noted that such services, even if they are located within the ICPS, may be operated independently, such as a canteen or site security. Thus, infrastructure not included here are: a canteen, port or train station, fire-fighting facility, safety/environment, security, roads, and piping.

Facilities included in the methodology are those which exist at both a stand-alone site and an ICPS, such as utilities and buildings. Facilities which normally exist for each plant, but may be partly centralised in an ICPS, such as laboratories, a maintenance workshop, or storage facilities are considered if applicable to the case study. Costs for waste incineration and waste water treatment are also investigated if deemed appropriate for the case study.

4.7.1 Definition of Infrastructure

When a chemical production site is conceived, its facilities and areas are assigned to one of three categories: inside boundary limits (ISBL), outside boundary limits (OSBL), or infrastructure, defined below:

Table 4.3 Definitions of ISBL, OSBL and Infrastructure

	ISBL	OSBL	Infrastructure
Definition	Installations required to operate the plant regardless of site location	Site-dependent installations, mainly to connect the plant to the infrastructure	General installations for the whole site
Examples	- Process equipment - Production building/control room - Motor control centres - Instrumentation/ controls - Process tanks - Laboratory - Process safety	- Tank farms for raw materials/products - Production-related power supply, switch gear, transformers - Connection of production unit to site (roads, channels, railroads, pipe racks, product/utility pipelines)	- Site preparation - Central tank farms/ warehouses - General pipe racks - Roads/access ways - Utilities and power - Central waste disposal - Fire-fighting facilities - Telecommunications - Weigh bridge

4.7.2 Investment Cost

The costs involved in site development can vary greatly depending on the scope of the project and the surrounding conditions. To determine how infrastructure costs relate to the total project costs, eight chemical production sites constructed for a chemical company were reviewed. The investment amount allocated to infrastructure relative to the total project cost was approximately 30% based on projects of varying size and production process type, as shown below. Although economies of scale exist for many aspects of infrastructure (as will be shown in the following sections), the investment cost increases with increasing site size. A review of the projects showed that as the site size increases, the scope and type of onsite facilities changes, such as onsite biological waste water treatment or incineration facilities in a large site.

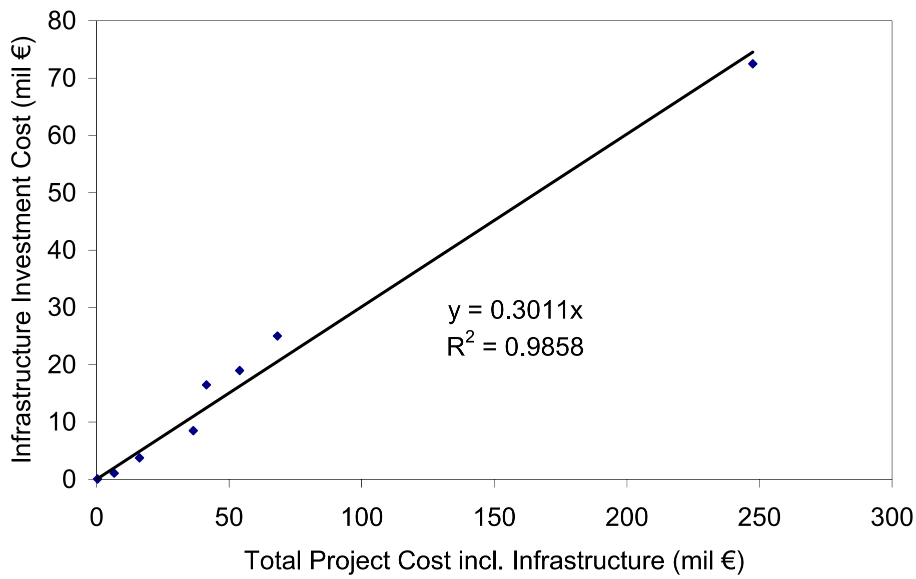


Figure 4.11 Infrastructure Investment Costs versus Project Costs

4.7.3 Operating Costs

In this section, the costs of utilities are reviewed in more detail. Utilities are an essential component of process plants. They include electricity, water, steam, inert gas, refrigeration, high temperature heating oil, and compressed air. They are generally part of the infrastructure of the site, however, may be integrated within the process plant in some cases. For example, the steam and refrigeration systems in an ethylene plant are thoroughly integrated into the ethylene production process (PEP report 136A, 1995, p.2-1). First, energy facilities are investigated, as this generally represents the greatest cost of all the utilities.

4.7.4 Steam and Power Provision

The requirements for steam and power are provided for differently according to site type. This research compares the costs for energy provision based on the most commonly found technologies in the chemical industry. The overview of boilers and electricity costs is based on PEP report 136A (1995, updated for inflation).

Electricity from the Public Grid

The price of electricity obtained from a public grid varies greatly depending on location and sales conditions. For example, within the United States, the average electricity sales price varied by approximately 50% depending on location (3.9 cents/KWh in south central U.S. versus 8.5 cents/KWh in New England, compared with the U.S. average of 4.7 cents/KWh in 1994, PEP report 136A 1995). Additionally, many factors affect the cost, such as hours of use, transmission voltage, distribution voltage, and load factor. Also, other charges come into play: demand charge, energy charge, fuel cost adjustment factor, etc. Thus, the exact electricity cost for a particular plant built either within an integrated site or as a stand-alone plant will depend very much on the location of the plant. However, there is a general trend that the greater the electrical consumption, the lower the price. Also, if the customer can accept an interruptible power service, significant cost advantages can be achieved. The below table is indicative of the trends in electricity prices.

Table 4.4 U.S. Electricity Prices for Different Conditions

Electricity service	Operating cost including capital charges (US cent/kWh)
2,000 KVA	4.33
20,000 KVA standard rate	4.19
20,000 KVA 30 minute interruptible rate	2.73

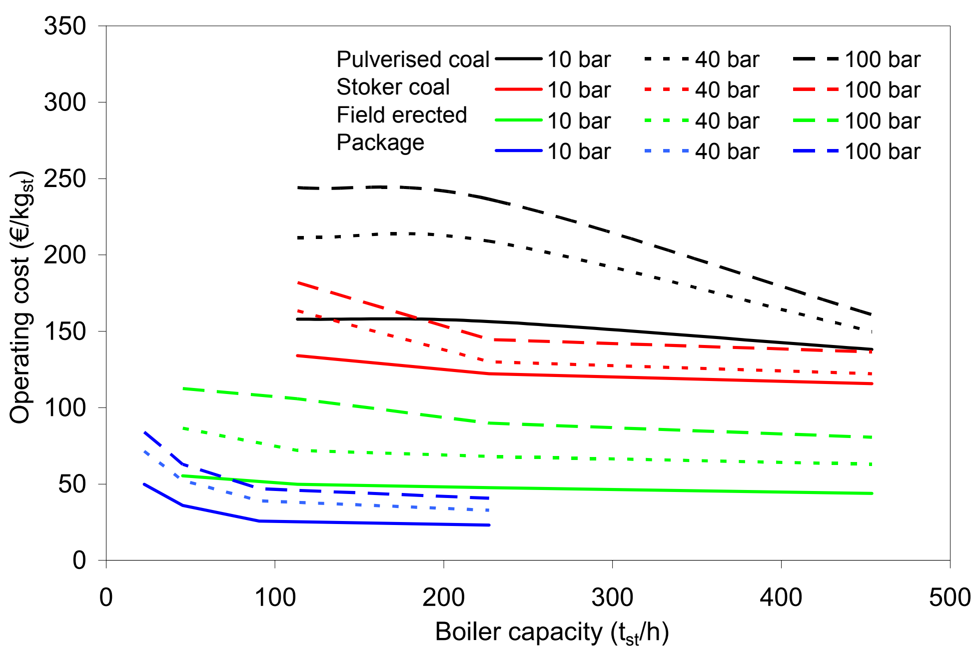
(PEP report 136A, 1995, pp.5-5, 5-8)

Since the case of electricity is so specific to location, the table is only given as an indication of price differences according to demand and conditions. In this work, electricity prices are determined for specific locations and conditions.

Steam Preparation

Steam is prepared in industrial facilities using either a boiler or a cogeneration system. Industrial steam boilers exist in either fire-tube or water-tube configurations. For fire-tube boilers, combustion gas passes through tubes surrounded by boiling water and for water-tube boilers, water is inside the tubes which are surrounded by hot gas. Fire-tube boilers are uneconomical beyond approximately 13 t/h of steam. Water-tuber boilers can be built much larger, up to about 450 t/h and 125 bar for chemical applications. The main types of boilers and costs relative to capacity are given below:

- Package boilers: shop-assembled units that require field erection, offering compactness, short delivery times and low costs. Their physical size is limited, so they have a limited practical capacity of approximately 160 t/h of steam and 100 bar.
- Field-erected oil/gas-fired boilers: offer higher steam and pressure capacity (450 t/h steam at 125 bar) than package boilers, but are more expensive.
- Coal-fired boilers: come in a few variations. Stoker boilers have a coal-feeding device in the firing zone and are generally sized below 135 t/h steam due to economics and coal handling. Pulverised coal-fired burners have larger capacities, above 100 t/h steam.



(based on PEP report 136A, 1995, pp. 6-23,29,35,41)

Figure 4.12 Operating Cost including Capital Costs for Steam Boilers

Cogeneration

The following section is based on PEP report 181A (2001). Cogeneration refers to systems which sequentially produce both steam and electricity from the same energy source. Compared to the production of steam and electricity in separate facilities, cogeneration can reduce fuel consumption by 25 to 35%. Gas Turbine Combined Cycle (GTCC) cogeneration is the most popular and efficient cogeneration system in commercial use today, as it offers high thermal efficiency, short installation time, quick start-up and low installed costs. Natural gas or liquid fuel is burned with compressed air in a turbine combustor. The hot combustion gas (up to 1288ºC) drives a gas turbine to generate electricity. The exhaust gas from the gas turbine (up to 566ºC and containing 10-12 volume% oxygen) passes through an unfired heat recovery steam generator to produce steam. The steam may be produced at two pressures, lower pressure steam is passed directly to the processes, whereas the higher pressure steam can move on to an extraction steam turbine to generate additional electricity and extract lower pressure steam.

These systems are also available in various configurations. Power can be co-generated from steam via either a topping cycle (where electricity is generated from the high temperature source and the lower temperature level is used to produce low pressure steam) or a bottoming cycle (where power is recovered from a low temperature energy source, which would normally be rejected to a heat sink). Bottoming cycles are generally process-oriented and site-specific and are small in number. Topping cycles are the predominant form of cogeneration and may use a gas turbine to generate electricity followed by heat recovery from the hot exhaust gas to produce steam (either for processes or the generation of additional electricity). Another form is using non-condensing steam turbines in which high pressure steam passes through a turbine to produce electricity, the low pressure steam which exits is used for processes.

Cost Comparison of Different Energy Provision Configurations

In this section, the costs for different configurations for energy provision are calculated. The following three cases are shown schematically below:

Case 1: Steam Boiler, using power from the public grid

Case 2: CHP (combined heat and power) Boiler

Case 3: CHP Boiler + Gas Turbine

In case 2, a combined cycle system is used to produce both steam and power in one operation. In case 3, natural gas is burned in a gas turbine to generate power. The residual thermal energy from the gas turbine exhaust gases at 542ºC is recovered in a heat recovery steam generator.

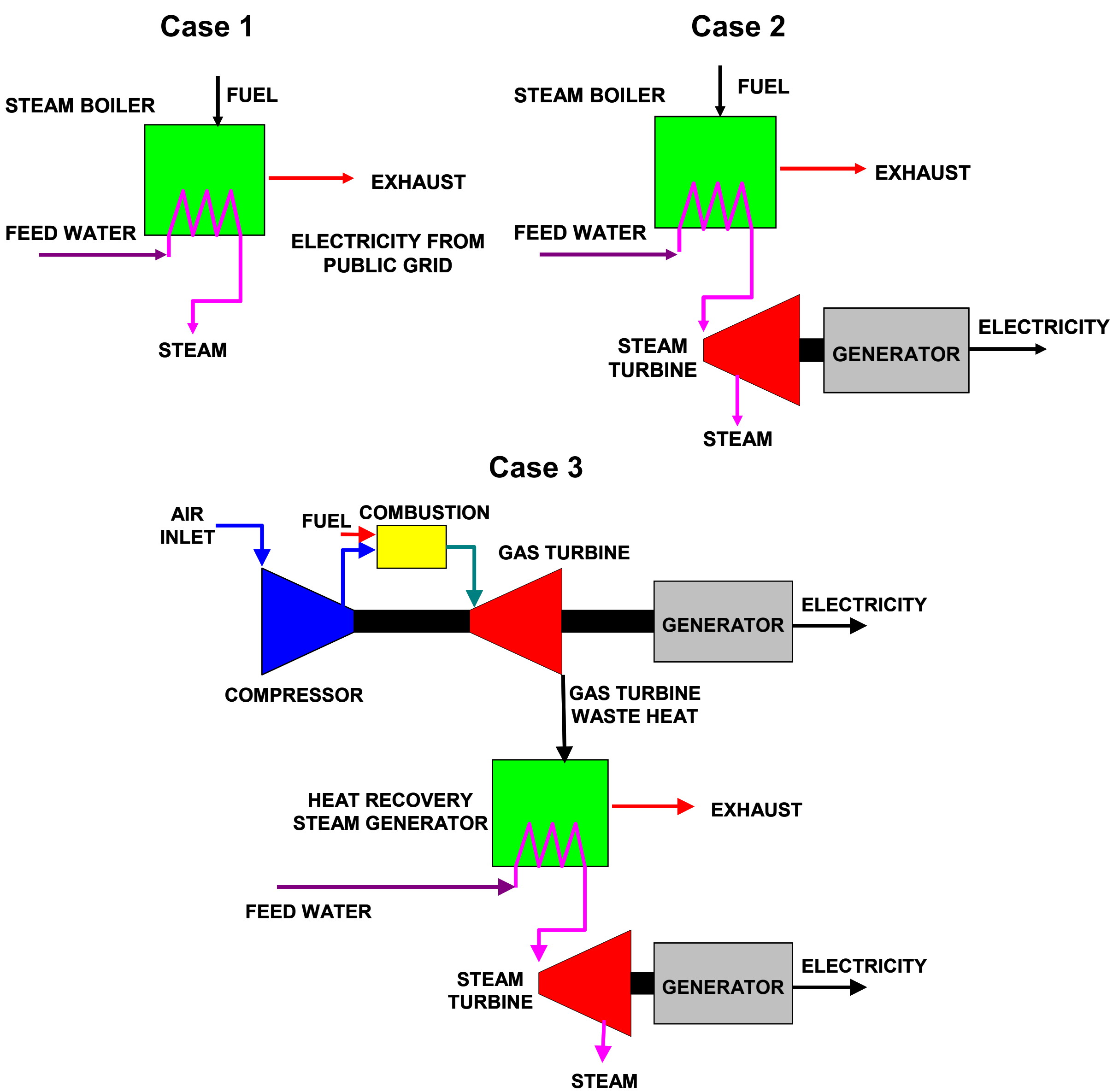


Figure 4.13 Comparison of Steam and Power Provision Configurations

The variables used in the calculation and steam demand profile are given in Appendix B. The following parameters were selected for the base case:

- Steam pressure: varied from 4 to 125 bar, base case 16 bar
- Steam demand: varied from 10 to 650 t/h, base case 250 t/h

- Electricity demand: varied from 10 to 400 MW, base case 200 MW

The range for steam demand and electricity demand are representative of the lower and upper ranges for chemical production sites: a small stand-alone site at the bottom range and an ICPS at the top range. In each case the boiler efficiency is set at 90%.

Case 1. Boiler with Electricity from Grid

In this case, the site has 3 boilers. Boiler 3 is the reserve and the demand is split between boilers 1 and 2 (boiler 1 at 50% of maximum demand and boiler 2 at current demand – steam production of boiler 1). The number of personnel is 6.

Case 2. CHP Boiler

In this case, the steam demand is higher than for case 1 (280 t/h): steam demand for the site (250 t/h as in case 1) plus the steam demand for the power plant (34 t/h for base case) minus the steam generated by injection water (4 t/h). Again, there are 3 boilers, where boiler 3 is the reserve and the demand is split between boilers 1 and 2 (boiler 1 at 50% of the maximum demand and boiler 2 at current demand – steam production of boiler 1). Live steam at 120 bar and 520°C is used for the auxiliary steam demand in an amount of 14% of the total steam demand. Also, injection water in an amount of 3% of the steam demand for the site and power plant is required for cooling the turbine. For the base case, the steam turbine generates 34 MW of the 200 MW required. Also, the auxiliary steam demand required by the power plant is 1 MW. Thus, 167 MW must be taken from the outside grid. Again the number of personnel is 6.

Case 3. CHP Boiler with Gas Turbine

In this case, one boiler is equipped with a gas turbine, the other two are CHP boilers. Boiler 1 is sized to meet the average steam demand. Boiler 2 fulfils excess steam requirements over the average demand and boiler 3 is again the reserve boiler. The boilers are sized at 75% of the total demand, compared to 50% in cases 1 and 2 to safeguard against failures, more common in gas turbines. The number of personnel is set at 12. For the base case, the gas turbine/steam turbine configuration generates 161 MW of the 200 MW required. The auxiliary electrical demand was set at 2% (3 MW). Thus, the electricity required from the grid is 42 MW.

The overall operating costs are a function of:

- Fixed costs: capital costs (boilers and turbines), maintenance, capacity charge, back up electricity, personnel
- Variable costs: fuel, demineralised water, variable charge for electricity, (minus credit for electricity)

The specific capital costs for the steam boilers (€/t_{st}) and turbines (€/kW) are based on the following functions, generated from fitting actual cost data:

$$c_{Boiler} = 2.2 \cdot 10^5 \cdot \left(M_{St} \cdot \frac{a}{7500h} \right)^{0.3}$$

$$c_{Turbine} = -101.7 \cdot \ln\left(El_{ST+GT}\right) + 1211.7$$

Electricity generation for both the steam and gas turbines (MW) was determined as:

$$E = \left(h_{ST,in} - h_{H2O}\right) \cdot M_{St} \cdot \left(\frac{a}{7500h}\right) \cdot \left(\frac{h}{3600s}\right) \cdot \left(\frac{1000kg}{t}\right) \cdot \left(\frac{MW_{el}}{MW_{th}}\right)$$

where the electricity to steam ratio is based on the following function:

$$\left(\frac{MW_{el}}{MW_{th}}\right) = 0.0732 \ln\left(M_{St} \cdot \left(\frac{a}{7500h}\right)\right) + 0.454$$

The fuel demand is determined based on the following efficiency function:

$$\left(\frac{MW_f}{MW_{el}}\right) = 0.0348 \ln\left(MW_{el}\right) + 0.2142$$

Below, the total efficiency of the system is shown relative to capacity:

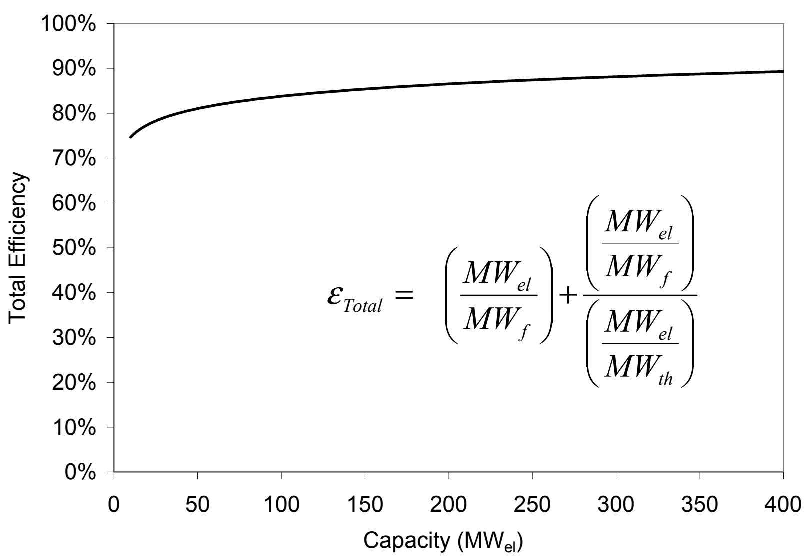


Figure 4.14 Efficiency of CHP Plant versus Capacity

Below a summary of the costs for the three cases is given.

Table 4.5 Cost for Steam and Power Generation

Item	unit	Case 1	Case 2	Case 3
Electricity demand	MW	200	200	200
Steam demand	t/h	250	250	250
Generation:				
Steam GT+ST	t/h	0	0	222
Steam Boiler	t/h	250	282	28
Electricity	MW	0	33	141
Fuel Demand	MW	209	252	367
Investment	mil €	18.632	48.648	128.093
Fixed Costs	mil €/a	3.887	9.807	27.286
Fuel Costs	mil €/a	27.469	33.089	51.281
Electricity Costs	mil €/a	74.097	62.061	21.159
Total Costs	**mil €/a**	**105.453**	**104.957**	**99.726**

Sensitivity Analysis

A sensitivity analysis for the base case was carried out in order to see how the variance of certain cost assumptions affects the overall costs. The costs for fuel, electricity, steam demand, and electricity demand are varied. The sensitivity analysis shows that case 3 is more dependent on changing fuel prices due to its higher fuel consumption compared to cases 1 and 2. However, cases 1 and 2 are more dependent on changing electricity prices. The overall operating cost in all cases depends highly on the electricity demand and less strongly on the steam demand. The results of the sensitivity analysis are given in Appendix B.

Variation without Electricity Export

If a site has high steam requirements, which when produced via a GTCC, provides electricity in excess of its own requirements, then this excess electricity can be exported (case 3). Below, the calculation was made for a steam requirement of 400 t/h in order to meet the criterion that excess electricity is produced. However, it may be more desirable to meet the excess steam requirement using a boiler without a gas turbine (boiler 2) and build a smaller boiler with gas turbine (boiler 1) if electricity export is not economically attractive versus the higher investment costs for a larger gas turbine. This is represented by case 4, where the steam production in boiler 1 is limited. A summary of the results of this calculation are given below. Which case is most economically attractive depends on the particular conditions, such as the cost of electricity.

Table 4.6 Cost for Steam and Power Generation without Electricity Export

Item	unit	Case 1	Case 2	Case 3	Case 4
Electricity demand	MW	200	200	200	200
Steam demand	t/h	400	400	400	400
Generation:					
Steam GT+ST	t/h	0	0	356	290
Steam Boiler	t/h	400	452	44	110
Electricity	MW	0	53	234	187
Fuel Demand	MW	335	403	585	477
Investment	mil €	24.791	72.378	193.776	156.898
Fixed Costs	mil €/a	5.099	14.474	41.276	33.359
Fuel Costs	mil €/a	43.950	52.943	81.665	74.842
Electricity Costs	mil €/a	74.096	54.850	-11.118	4.797
Total Costs	**mil €/a**	**123.145**	**122.267**	**111.823**	**112.998**

Investment Cost Compared with Other Sources

The results of the calculation are compared with the calculation based on Boeddicker as given in Frank (2003, pp.41-43), the PEP report 181A (2001, pp.6-9 to 6-17), and existing cogeneration plants, summarised below.

Table 4.7 Examples of Cogeneration Plants and Investment Costs

Location	MW	Start-up year	Investment Cost (mil €)	€/KW
BASF Ludwigshafen[6]	440	2005	240	545
BASF Antwerp[6]	400	2005	230	575
Muenster[7]	170	2006	75	441
Duisburg, Germany[7]	240	2006	110	458
Electrabel / Solvay, Italy[8]	400	2006	200	500

The cost estimate used in this work lies between those in PEP report 181A (2001) and Frank (2003) and shows a lesser dependence on capacity than the other functions. The actual cases were found to have lower costs than the estimates and were independent of capacity.

[6] BASF corporate communications, 2006
[7] Reuters, 09.12.2002
[8] Electrabel press release, 18.10.2004

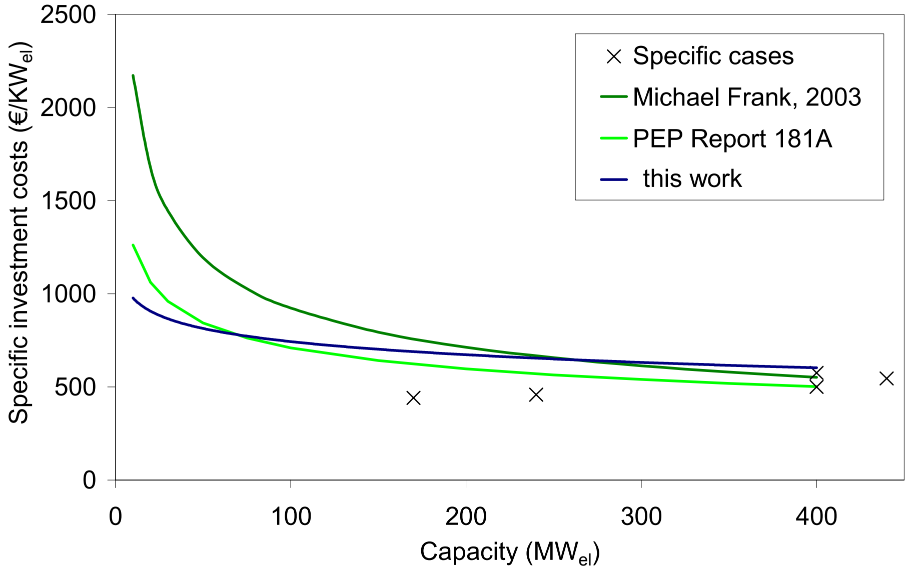


Figure 4.15 Comparison of Costs for Cogeneration

Below, the operating costs for different levels of steam generation are determined with increasing CHP capacity.

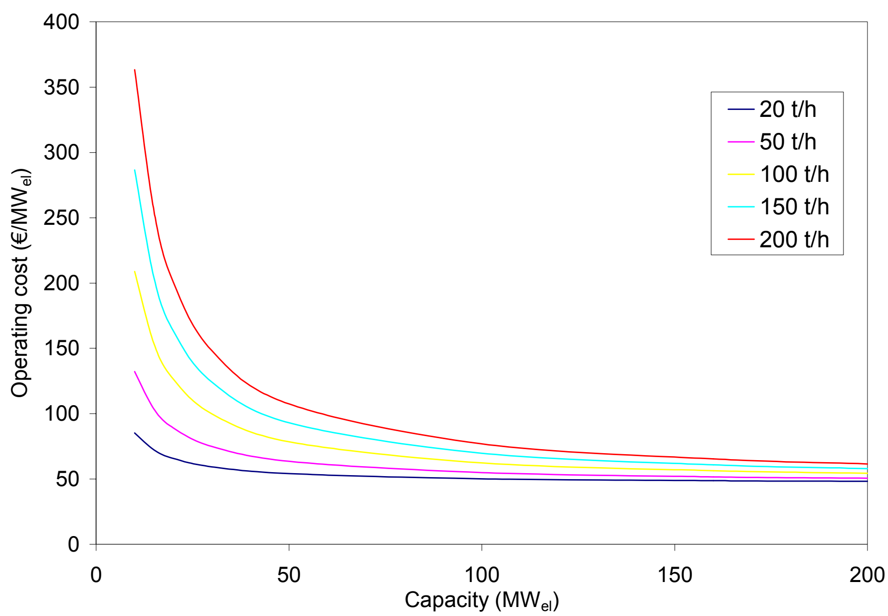


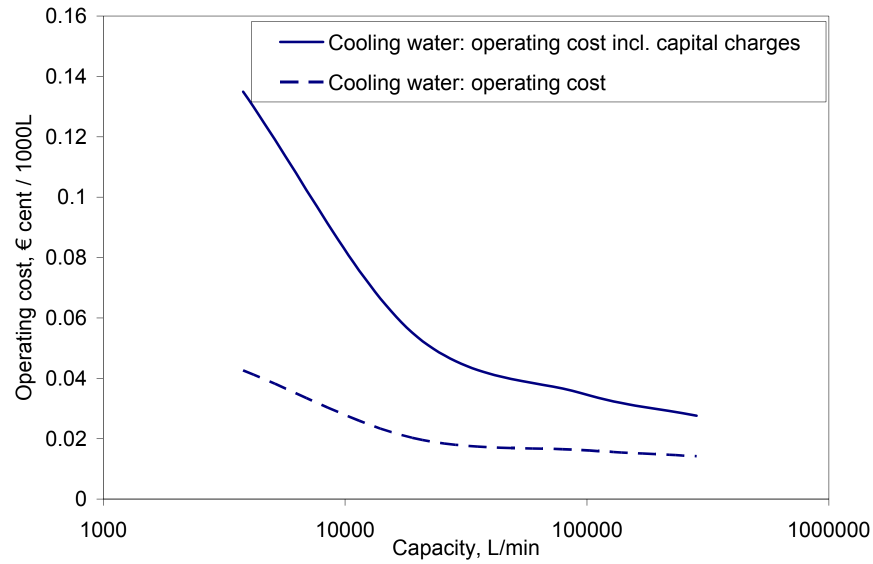
Figure 4.16 Operating Cost of CHP Plant relative to Capacity

4.7.5 Utilities Provision

Primary utilities such as water, steam, and electricity are distributed through an ICPS to enable each production plant easy access. Here, the costs for water and nitrogen are reviewed based on PEP report 136A (1995) and adjusted according to currency and inflation. For details regarding the cost determination or the processes, please refer to the PEP report.

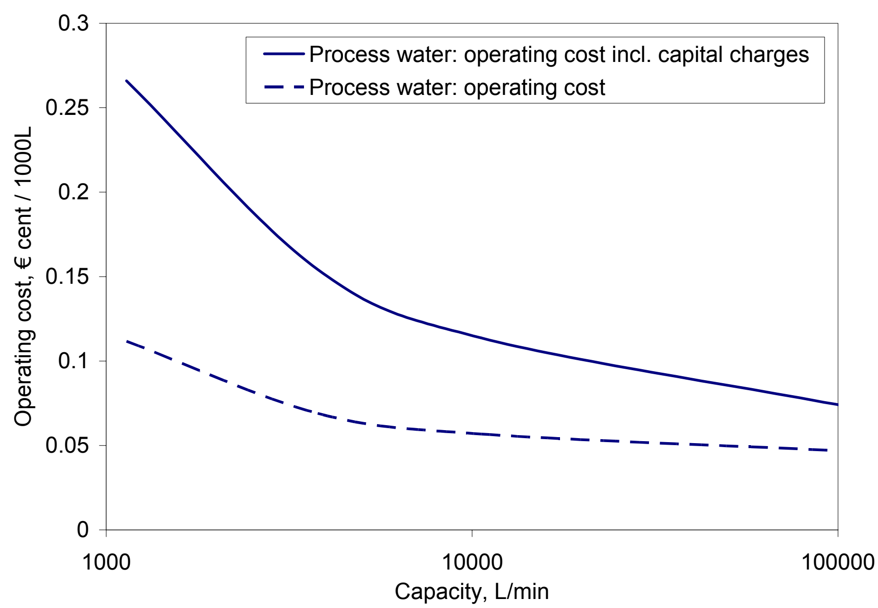
Water Provision

Based on the PEP report, the costs for cooling and process water exemplify economies of scale, shown in the graphs below.



(based on PEP report 136A, 1995, p.4-34)

Figure 4.17 Operating Cost of Cooling Water Preparation versus Capacity

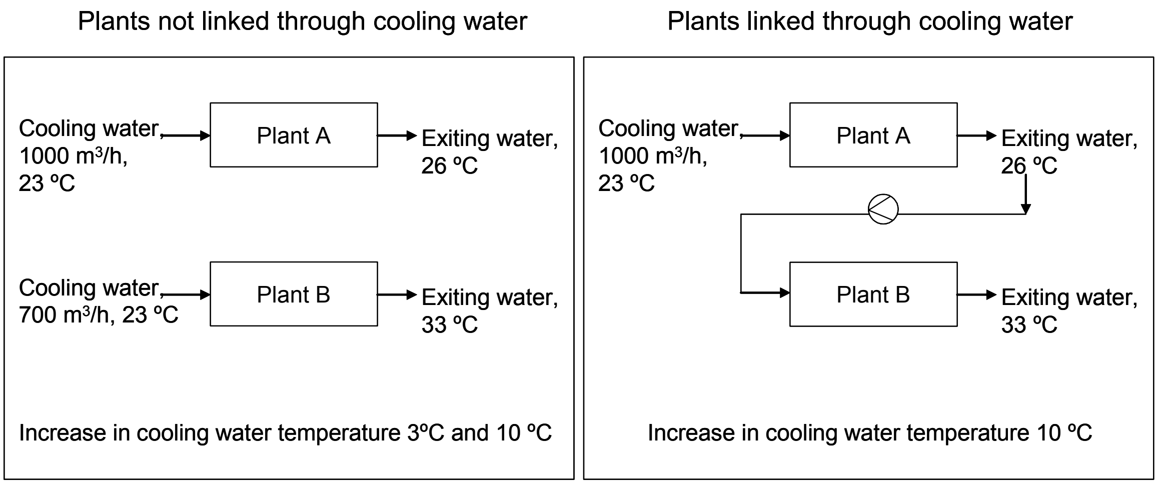


(based on PEP report 136A, 1995, p.4-23)

Figure 4.18 Operating Cost of Process Water Preparation versus Capacity

Potential Savings of Cooling Water in an ICPS

The transfer of cooling water between plants is another benefit of integration. For example, if one plant has a small increase in cooling water temperature, a neighbouring plant may be able to further use this water for cooling, as shown below.



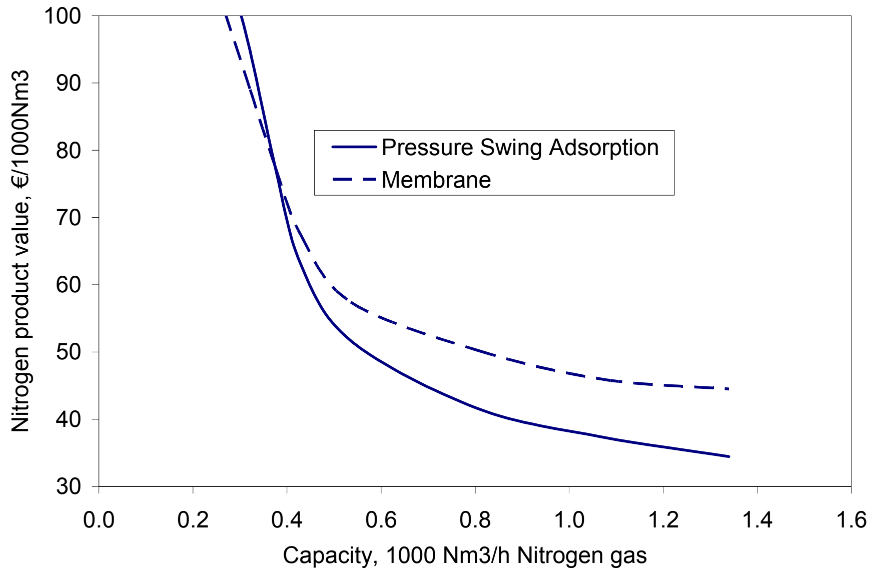
(based on BASF, 1995, p.7)

Figure 4.19 Example of Energy Integration through Cooling Water

Through the secondary use of cooling water from plant A, plant B is able to reduce its cooling water requirement. Higher process temperatures in the coolers in plant B allow the use of warmer cooling water from plant A. This concept is applied in various plants at the BASF Ludwigshafen site: butanediol, hydrosulfide, styrene, and ethylbenzene plants (BASF, 1995, p.7).

Nitrogen Provision

Nitrogen preparation costs for pressure swing adsorption and membrane separation methods also show economies of scale, as shown in the following figure.



(based on PEP report 136A, 1995, p.8-6)

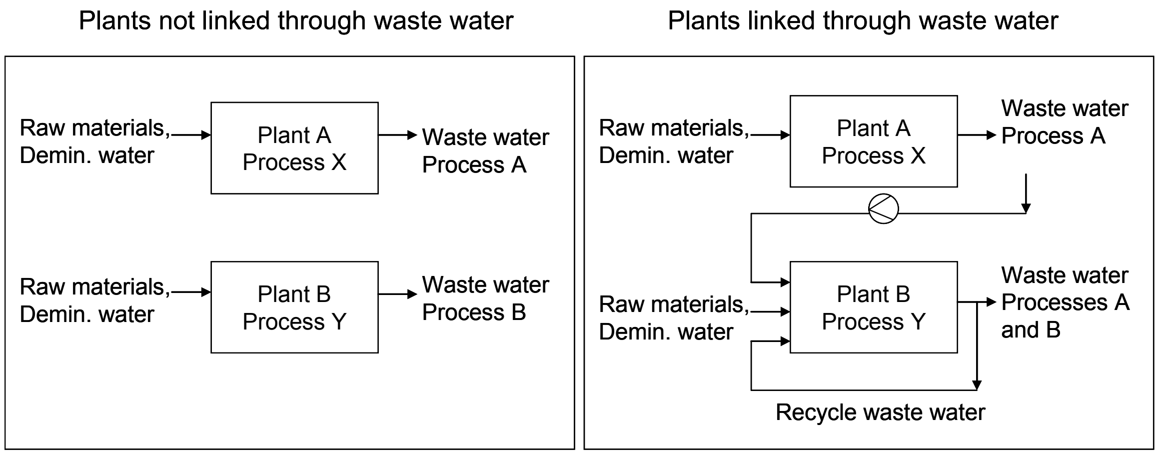
Figure 4.20 Nitrogen Product Value relative to Capacity

Waste Water Treatment

The costs for waste water treatment within a group of companies were investigated. As the capacity of the treatment facility increased, the specific cost decreased exponentially. The same trend was found for the costs related to sludge treatment.

Waste Water Reduction through Integration

The amount of waste water production may be reduced through integration. For example, waste water from a process containing product A is sent to an offsite waste water treatment plant in a stand-alone plant. However, in an ICPS, a nearby process may be able to use the waste water as process water. Then plant A saves costs for waste water treatment and plant B saves costs for demineralised water. Furthermore, the product yield may be increased in plant B. This concept is shown schematically in the following figure and is used at the BASF Ludwigshafen site in the formaldehyde, formol, and propylene oxide plants (BASF, 1995, p.18).



(based on BASF, 1995, p.18)

Figure 4.21 Reduction of Waste Water use through Integration

Incinerator

Wastes formed through chemical production may be disposed of via an incineration plant. Incineration plants may be specifically designed to handle certain kinds of waste, such as chemical residues, household waste, waste water, hazardous waste, or sewage sludge. Types of chemical waste which may be incinerated are:

- By-product gases and vapours
- Organic liquid streams
- Aqueous wastes containing dissolved organics and salts
- Distillation bottom tars
- Organic sludge and semi-solids
- Slurries and sludge with high moisture
- Granular solids or filter cakes

The following chemical residue incinerators within integrated chemical production sites use rotary kiln incinerators and waste heat boilers:

- BASF Ludwigshafen (BASF, 2002): of the total amount of waste produced (621 kt/a), 538 kt/a are incinerated, but only 139 kt/a were used to produce 104 t/h of steam (5.6 t_{st}/t_{wi}).
- Bayer operates two residue incinerators (Bayer Industry Services, 2004).
  - Bayer Dormagen: 50 kt/a residue incinerator with a thermal output of 32.8 MW or 4.9 MWh per ton of residue to produce 36.8 t/h of 39 bar steam (5.5 t_{st}/t_{wi}).

– Bayer Krefeld-Ürdingen: 25 kt/a residue incinerator with a thermal output of 13.8 MW or 4.14 MWh per ton of residue to produce 13.5 t/h of 16 bar steam (4 t_{st}/t_{wi}).

The specific costs per ton of waste for a residue incinerator with a capacity of 100 kt/a is approximately 135 €/t including operating costs for personnel, maintenance, electricity, ash disposal, and capital (Stubenvoll et al., 2002, p.144). Of this, the firing system and boiler are estimated at 36 €/t and the water-steam cycle to generate steam at 8 €/t. Stubenvoll et al. (2002, p.144) determine economies of scale as: 135 €/t for 100 kt/a, 111 €/t for 200 kt/a, and 100 €/t for 300 kt/a. The economics of an onsite incinerator relative to sending waste offsite needs to be addressed for an individual integrated site. It is interesting to note that some integrated sites which operate incinerators (BASF, Bayer) accept waste from outside companies in order to better utilise their own onsite waste incinerators (BASF, 2002; Bayer Industry Services, 2004).

There are more aspects of plant utilities which may be investigated, such as refrigeration systems and hot oil heating systems, however, these are often integrated into the process and are not reviewed here.

4.7.6 Economic Benefit of Shared Infrastructure and Utilities

Infrastructure costs are difficult to compare between small stand-alone sites and large integrated sites, as the types of infrastructure change with increasing size. Economies of scale have been shown for power and steam provision as well as for other utilities. To determine the cost savings for infrastructure in an ICPS, the difference between the costs for facilities in an ICPS and those in a semi-ICPS or stand-alone site are determined on a case by case basis. These generally consist of power, steam, cooling water, production water, nitrogen, waste water treatment, and incineration. Additionally, savings achieved in the ICPS in terms of waste water reduction, cooling water reduction, and demineralised water reduction are included.

$$S_{Infras,ICPS,SA} = \sum_{x=1}^{n}\left(C_{Fac,x,ICPS} - C_{Fac,x,SA}\right) + S_{cw,ICPS} + S_{ww,ICPS} + S_{dw,ICPS}$$

$$S_{Infras,ICPS,S-ICPS} = \sum_{x=1}^{n}\left(C_{Fac,x,ICPS} - C_{Facx,S-ICPS}\right) + S_{cw,ICPS} + S_{ww,ICPS} + S_{dw,ICPS}$$

for n facilities

4.8 Environmental Aspects

Energy and logistics integration in an ICPS lead to environmental benefits relative to less integrated sites. Lower fuel requirements for site steam production, the avoidance of offsite transport of integrated products, and efficient production of power and steam lessen the depletion rate of non-renewable resources and reduce emissions created by the combustion of fossil fuels.

4.8.1 Fossil Fuels

Fossil fuel savings in an ICPS result from heat recovery and incineration as well as the onsite transport of sellable by-products and captive use products, determined as follows:

$$M_{F,ICPS,SA} \quad = \quad \left[\left(\sum Mu,s + \sum Mc \right) \cdot F_f \cdot D \right] + \left[\left(Mst_i + Mst_{hr} \right) \cdot h_{st} \cdot \left(\frac{1}{\varepsilon_b} \right) \cdot \left(\frac{1}{e_f} \right) \right]$$

In a semi-ICPS, the additional transport of sellable by-products and potentially some additional captive-use materials in the ICPS result in additional fossil fuel requirements. Additionally, greater efficiencies for larger scale facilities such as a power plant may result in further fossil fuels reductions.

$$M_{F,ICPS,S-ICPS} \quad = \quad \left(\sum Mu,s + \sum Mc_{ICPS,S-ICPS} \right) \cdot F_f \cdot D$$

The reduction in natural gas consumption due to steam production through heat recovery and incineration is based on a heating value of 44 MJ/kg and boiler efficiency of 90%. The reduction in diesel fuel consumption for transport is based on the following factors (in MJ diesel fuel / ton product·km): 1.8 for truck (28 ton loading), 0.47 for train, 0.46 for inland waterway, and 0.088 for sea freight (Frischknecht and Jungbluth, 2004, p.13). These data correspond well with data from other sources (Knörr and Reuter, 2005, p.35). The combustion energy for diesel fuel is taken as 43 MJ/kg. It should be noted that fuel consumption depends on transporter size and loading. Gilbert (2002, p.8) shows this by giving a range of factors for the different transport modes. In this work, the factors are assumed to be the same for different geographical regions.

4.8.2 Emissions

Since the combustion of fossil fuels for an ICPS is lower due to heat recovery and reduced transport, the amount of related emissions caused by these fossil fuels, M_{es}, is avoided. As waste incineration also creates emissions (the type and amount depend on the material incinerated and are not considered here), it does not provide a benefit for the ICPS.

Emissions from Transport

The emissions generated through transport have been calculated by various institutes[9] and found to vary significantly (Schmidt et al., 1998, p.284). Emissions factors used for this study were provided by the following sources: for truck transport by Schmidt et al. (1998, p.284), for train, sea, inland waterway and air transport (not including SO_2) by Borken et al. (1999) as cited by the Umweltbundesamt Berlin (1999, p.24), and for SO_2 emissions for train, sea, and inland waterway by Hobohm et al. (2006, pp.50-52).

Table 4.8 Emissions Factors for Different Transport Modes

Emission Factors g/ton·km	Truck	Train	Sea	Inland waterway	Air
CO_2	83	32	17.5	35.4	903
SO_2	0.024	0.013	0.0929	0.0214	n/a
CO	0.140	0.040	0.046	0.11	0.97
NO_x	0.890	0.120	0.42	0.61	4.24
NMVOC	0.072	0.010	0.02	0.05	0.5
Dust	0.036	0.005	0.03	0.017	0.13

Emissions from Steam Generation

Less emissions are generated in an ICPS compared with a non-integrated site through the lowering of steam requirements through heat recovery and the reduction of fuel requirements through greater efficiencies via economies of scale for larger power plants. In this work, the reduction in emissions related to these benefits from integration are determined based on emissions levels measured for natural gas powered CHP power plants cited by the Fraunhofer Institute (2005), given in Table 4.9.

[9] GEMIS or Gesamt-Emissions-Model Integrierter Systeme by Hessisches Ministerium, Ecoinvent by ETH Zürich, Umberto by Institut für Umweltinformatik Hamburg.

Table 4.9 Emissions Factors for CHP Power Plants

Emission type	Emissions (kg/MWh)
CO_2	380
SO_2	0.01
CO	0.27
NO_x	0.23
NMVOC	0.004
Dust	0.004
CH_4	0.004
N_2O	0.012

Thus, the emissions reduction through integration is determined as follows:

$$M_{em,ICPS,SA} = \sum_{x=1}^{n} \left[\left(\sum Mu,s + \sum Mc_{ICPS,SA} \right) \cdot D_x \cdot F_{em,t,x} \right] + M_f \cdot e_f \cdot F_{em,pp}$$

$$M_{em,ICPS,S-ICPS} = \sum_{x=1}^{n} \left[\left(\sum Mu,s + \sum Mc_{ICPS,S-ICPS} \right) \cdot D_x \cdot F_{em,t,x} \right]$$

for n transport modes

4.9 Economic and Environmental Benefits of Integration

A summary of the functions for determining the economic and environmental benefits of an ICPS relative to a semi-ICPS or stand-alone site are given below.

Total

$$S_{ICSPS,SA} = S_{M,ICSPS,SA} + S_{E,ICSPS,SA} + S_{L,SA} + S_{Infras}$$

$$S_{ICSPS,S-ICPS} = S_{M,ICSPS,S-ICPS} + S_{E,ICSPS,S-ICPS} + S_{L,ICSPS,S-ICPS} + S_{Infras}$$

Materials

$$S_{M,ICSPS,SA} = M_{u,wd,SA} \cdot c_{wd} + M_{u,SA} \cdot v_u$$

$$S_{M,ICPS,S-ICPS} = M_{u,i,S-ICPS} \cdot c_i + M_{u,wd,S-ICPS} \cdot c_{wd} + M_{u,S-ICPS} \cdot \left(v_u - v_{f,ut} \right)$$

Energy

$$S_{E,ICPS,SA} = \left(c_{St} \cdot \left(M_{St,i} + M_{St,hr} + M_{St,hs} \right) + \left(M_{cw,hs} \cdot c_{cw} \right) + C_{eq,hs} \right)$$

$$S_{E,ICPS,S-ICPS} = -c_{St} \cdot \left(M_{St,ui} \right)$$

Logistics

$$S_{L,ICPS,SA} = \left(\sum Mu,s + \sum Mc_{ICPS,SA}\right)\cdot\left(c_{lm} + \sum_{x=1}^{n} F_{t,x}\cdot D_x\right) + C_{Warehouse} + C_{Storage} + C_{other}$$

$$S_{L,ICPS,S-ICPS} = \left(\sum Mu,s + \sum Mc_{ICPS,S-ICPS}\right)\cdot\left(c_{lm} + \sum_{x=1}^{n} F_{t,x}\cdot D_x\right) + C_{Warehouse} + C_{Storage} + C_{other}$$

for n transport modes

Infrastructure

$$S_{Infras,ICPS,SA} = \sum_{x=1}^{n}\left(C_{Fac,x,ICPS} - C_{Fac,x,SA}\right) + S_{cw,ICPS} + S_{ww,ICPS} + S_{dw,ICPS}$$

$$S_{Infras,ICPS,S-ICPS} = \sum_{x=1}^{n}\left(C_{Fac,x,ICPS} - C_{Facx,S-ICPS}\right) + S_{cw,ICPS} + S_{ww,ICPS} + S_{dw,ICPS}$$

for n facilities

Fossil Fuels

$$M_{F,ICPS,SA} = \left[\left(\sum Mu,s + \sum Mc\right)\cdot F_f\cdot D\right] + \left[\left(Mst_i + Mst_{hr}\right)\cdot h_{st}\cdot\left(\frac{1}{\varepsilon_b}\right)\cdot\left(\frac{1}{e_f}\right)\right]$$

$$M_{F,ICPS,S-ICPS} = \left(\sum Mu,s + \sum Mc_{ICPS,S-ICPS}\right)\cdot F_f\cdot D$$

Emissions

$$M_{em,ICPS,SA} = \sum_{x=1}^{n}\left[\left(\sum Mu,s + \sum Mc_{ICPS,SA}\right)\cdot D_x\cdot F_{em,t,x}\right] + M_f\cdot e_f\cdot F_{em,pp}$$

$$M_{em,ICPS,S-ICPS} = \sum_{x=1}^{n}\left[\left(\sum Mu,s + \sum Mc_{ICPS,S-ICPS}\right)\cdot D_x\cdot F_{em,t,x}\right]$$

for n transport modes

4.10 Application of the Methodology on the Plant Level

In applying the methodology on the plant level, scenarios are defined and compared in which the plant exists as a stand-alone plant and in an integrated site. Applying the methodology on the plant level allows the effects of integration on a specific process to be investigated. Different from applying the methodology on the site level, in the application on the plant level, both entering and exiting streams need to be considered. The boundaries are given in the figure below.

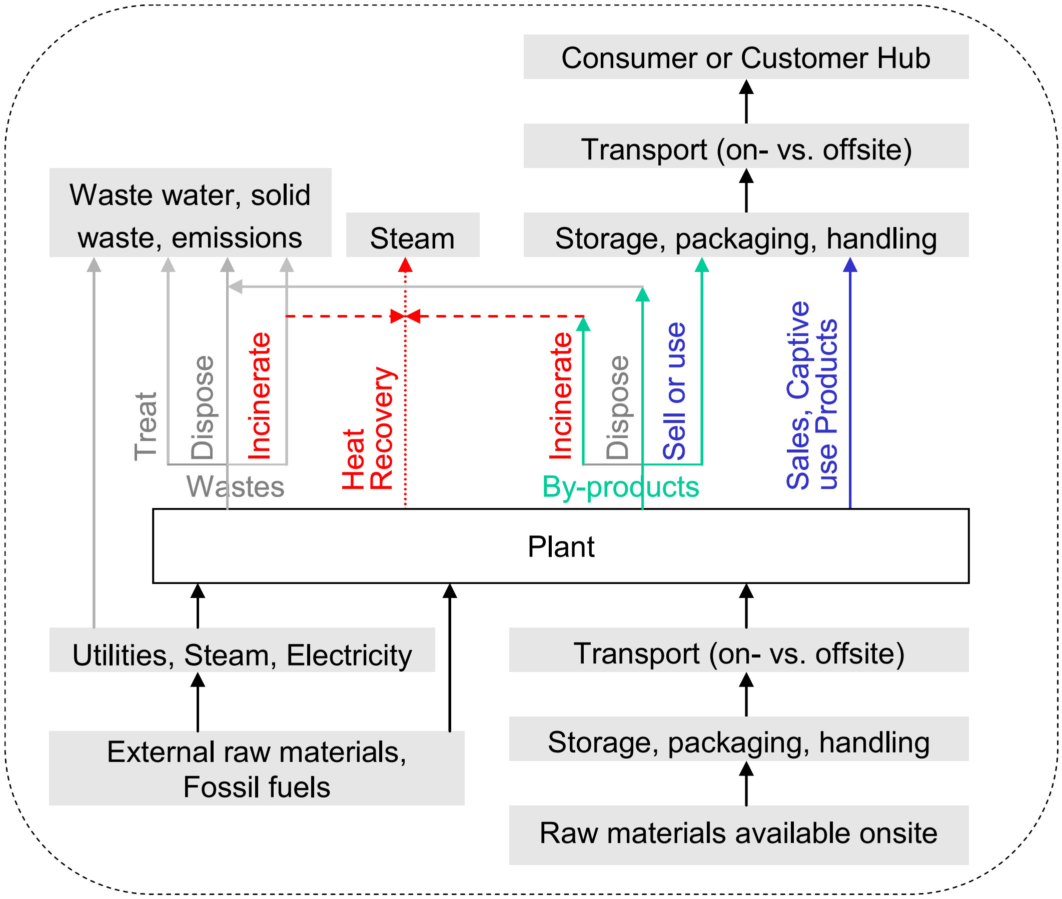


Figure 4.22 Boundaries for Application of Methodology on Plant Level

4.10.1 Integration Types for Methodology on the Plant Level

Materials Integration

A plant in an ICPS may be part of a value chain and linked to either upstream or downstream processes. Therefore, raw materials entering the process as well as products leaving the process must be taken into consideration. Raw materials are classified as either externally sourced or available onsite for each particular scenario. A raw material is considered ‘available onsite’ if it is provided by another process within the ICPS and does not require transport from another site.

As in the application of the methodology on the site level, products leaving the process are categorised as either sales products, captive use products, or wastes for disposal or incineration. Again, the fate of by-products is determined based on their use in a non-integrated site.

Energy Integration

The benefits derived from heat recovery and waste incineration for the particular plant inside an integrated site are determined.

Shared Infrastructure

Infrastructure and utilities requirements are determined for the individual plant and the costs are determined for the plant as a stand-alone plant versus in an integrated site.

Logistics Integration

For each scenario, it is determined which logistics measures are necessary for both raw materials available onsite and products sent offsite. For example, for a scenario in which the process is in an ICPS, the logistics requirements for raw materials onsite may consist of simply an intermediate tank and piping connecting the two linked processes. Whereas, for the same process in a stand-alone plant, the same raw material is stored, packaged, and transported offsite. Product transport costs are considered up to the location of the consumer, customer hub, or port. This is done in order to address the effects of having an onsite downstream consumer versus an external consumer.

4.10.2 Production and Logistics Costs

As application of the methodology on the plant level investigates specific scenarios which may influence production cost, both the production and logistics costs related to integration are determined per scenario. Production costs include the costs related to materials and energy integration as well as shared infrastructure. Logistics costs refer only to costs related to logistics integration.

- Production costs include:
  - Fixed costs: personnel, fixed utilities, depreciation (infrastructure and economies of scale reflected), laboratory, maintenance
  - Variable costs: variable utilities, raw materials, packaging, energy
  - Overhead: administration, safety and environment, etc.
  - Deducting any credits for energy provision through integration
- Logistics costs include:
  - Raw materials storage, packaging, and transport to production site
  - Product transport from production site to consumer, customer hub, or port

Aspects which are equivalent in both scenarios are not included in the system boundary. For example, raw materials externally purchased are not considered, as they are neutral in the model. Also, if the plant size and design are equivalent for both scenarios, the investment costs and thus depreciation are considered to be equivalent.

4.10.3 Allocation

The topic of allocation is introduced here, as an integrated flow benefits more than just the plant from which the flow arises. According to Ullmann (2000), when processes generate more than one product or receive more than one input, there is more than one process reference. The allocation of material and energy streams up to this process is split among all products through allocation. Process products in addition to the main product may be useable by-products, wastes for incineration, or steam generated by the process. Allocation can be carried out by mass, volume, energy content, or another physical quantity (Feuerherd, 1993).

Examples are as follows:

- By-products: if a useable by-product is produced by process A and transferred for use as a raw material in process B within the same site, then both processes A and B are allocated a credit. For example, the sales price of the by-product is allocated equally between the two plants. For example, styrene is produced as a co-product with propylene oxide in the ethylbenzene process. As the process produces both styrene and propylene oxide, the production costs, environmental burdens, or integration benefits may be allocated to each product according to their mass flow.
- Steam export from heat recovery: an exothermic process A produces a main chemical product as well as steam which is exported to the site’s steam network. This benefit is credited to process A and the steam network. This may be a monetary credit or based on energy input, which is discussed in more detail below.
- Incineration of waste to produce steam: a process produces waste which is incinerated in an onsite incinerator to produce steam for the site. The benefit is credited to the process and to the incinerator, as the waste represents a raw material input for the incinerator.

Example Steam Export

A process produces 1 kg of product A with an energy input of 100 MJ/kg. At the same time, 15 kg steam are produced from the process' heat of reaction and exported to the site steam network. This exported steam has an energy content of 3 MJ/kg. The steam network carries an additional 100 kg of steam which is produced by boilers with an efficiency of 90%. The amount of energy supplied by the exported steam, E_{St}, is calculated as:

$$E_{St} = M_{St} \cdot e_{St} \cdot \frac{1}{\eta}$$

where: M_{St} = 15 kg, e_{St} = 3 MJ/kg, η = 90% → E_{St} = 50 MJ

This benefit is allocated equally to the plant producing A and the steam supply system ($a_A = a_{St}$ = 50%).

Allocation to Production Plant

The energy input normally required to produce product A, e_A, 100 MJ/kgA, is now reduced to 75 MJ/kgA due to the allocation of the steam benefit:

$$e_{A,allocation} = \frac{M_A \cdot e_A - E_{St} \cdot a_A}{M_A}$$

where: M_A = 1 kg, a_A = 50%

Allocation to Steam Provider

The amount of energy required for the steam network, e_{St}, is now reduced from 3.3 to 3.1 MJ/kg steam:

$$e_{St,allocation} = \frac{M_{St} \cdot e_{St} \cdot \frac{1}{\eta} - E_{St} \cdot a_{St}}{M_{St}}$$

where: M_{St} = 115 kg, a_{St} = 50%

5 Case Study on the Site Level

The methodology is applied to an actual integrated site. The site selected is suitable, as several types of integration are present yet manageable in its scope as a case study. It is located on approximately 22 km^2 of land with road, rail, and water access and consists of the following plants:

Table 5.1 Capacities of Plants for Site Level Case Study

Plant	Capacity (kt/a)
Steam cracker: ethylene, propylene	600 / 300
EO/EG (Ethylene Oxide, Ethylene Glycol)	600 / 300
LDPE (Low Density Polyethylene)	400
Oxo-alcohols	250
AA/AE (Acrylic Acid / Acrylic Esters): Crude AA, butylacrylate, methyl-/ethylacrylate, 2-ethylhexylacrylate	160 / 100 / 60 / 60
C1 complex: formic acid, methylamines, propionic acid, dimethylformamide	50 / 30 / 30 / 30

Additionally, a synthesis gas (syngas) plant and an Air Separation Unit (ASU) are part of the site. Below, the feedstocks, raw materials, fuels, products, and waste streams are described. A schematic of the site including these flows follows.

5.1 Material and Energy Mapping of the Site

Feedstocks

- Naphtha: feedstock for cracker, received by ship
- Ethylene (gas): from cracker is used by the EO/EG, Oxo-C3 and LDPE plants (liquid ethylene stored at cracker)
- Propylene (liquid): used in the AA/AE and Oxo-C4 plants
- Methane: from cracker is used in the EO/EG plant
- Oxogas, CO, and hydrogen: from syngas unit to C1 and Oxo-C3/C4
- Oxygen: from ASU used in EO/EG and WWT
- Propane (gas): from Oxo-C4 is transferred back as feedstock to cracker

Other Raw Materials

- Methanol and caustic soda for several plants, ethanol for AE plant stored centrally

- Ammonia (for methylamine plant), sulphuric acid (for AE plant) stored locally

Products

- Aromatic extraction products: benzene, xylene (centrally stored), toluene (stored at cracker)
- EO/EG products: stored locally prior to transport by truck and train
- Oxo and AA/AE products: stored in central tank farm prior to transport by ship
- Cracker co-products: C9 stream and Pyrolysis Fuel Oil (PFO) are stored at cracker and PFO is pumped to the jetties

Fuels and Alternate Fuels

- Natural gas: supplied by pipeline with a heating value of 34 (min) to 37 MJ/Nm^3 (max) is used in cracker, power plant, AA/AE, Oxo-C3/C4
- Light fuel oil: from C9 stream of cracker used as backup fuel for power plant
- Combustible off-gases: collected from several plants in a fuel gas header, heating value of 25 (min) to 35 MJ/Nm^3 (max)

Wastes

- Waste treatment: all wastes are treated onsite via WWT or incineration. Solid wastes, mainly sludge from WWT, and organic liquid chemical wastes are incinerated.
- Waste discharge: a waste water stream is discharged to the river after WWT, some wastes sent to landfill, and emissions
- Waste gas system: gases not fed to the fuel gas header or burned in the incinerator are flared or used as combustion air

5.2 Infrastructure for the Site

Steam and Power

A gas turbine combined cycle (GTCC) power plant designed at 160 MW_{el} and steam output of 200 t/h serves the site. It is designed to operate on a continuous basis to provide electricity at 110 kV and steam at 48, 40, 16, and 4 bar. It consists of three 40 MW_{el} gas turbines, supplementally fired heat recovery steam generators, an extraction condensing steam turbine rated at 40-60 MW_{el}, associated electrical generators, an air-cooled condensing system, switchgear, and other associated equipment. A diesel generator is available in case start-up power from the grid is not available and as a back-up for safe shut down of the power plant in case of a sudden power failure.

In addition to steam provided by the power plant, steam is provided through heat recovery from the following processes:

- Steam cracker: 40 t_{st}/h at 16 bar
- AA/AE: 40 t_{st}/h at 16 bar
- LDPE: 50 t_{st}/h at 40 bar

Water, Gases, WWT, Incineration

- Water systems: production water, cooling water, demineralised water, and potable water. Low silica water is supplied to the site which is then used to produce demineralised and potable water. Production water is used for fire water. There is a condensate recovery and supply system and boiler feed water treatment.
- Utility gases: nitrogen and compressed air (for instrument and plant air)
- WWT: waste water is collected and treated in the WWT plant and consists of domestic, production, and clean waste water and rain water
- Incinerator: with chemical waste containment facilities has a throughput of approximately 600 kg/h

Other Infrastructure

- Tank farms: one per plant plus one central tank farm
- Safety: fire fighting, gas fighting, rescue services
- Common facilities: telecom, lab, first aid, canteen, administration, training, management information systems, security, car garage, forklift garage, warehouses, substations
- Passages: rail/truck tanker loading/unloading stations, pipelines, roads
- Other: environmental monitoring station, maintenance shop, cleaning station, weigh bridge

5.3 Methodology Application

Step 1. Division of ICPS into Production Blocks

Rather than completely separating each production plant, such as EO and EG, a grouping was carried out to separate the site into realistic plant blocks, as they actually occur within an ICPS. For example, EO/EG and AA/AE exist as production blocks within an ICPS and therefore are not separated. Also, the plants associated with the C1 complex are grouped together along with a syngas plant to provide their feedstocks. As the Oxo C3-C4 complex relies on both an air separation unit and syngas unit, these are also grouped with this production block. A nearby cracker provides feedstocks to the separated sites. Thus, the site was divided into five production areas:

1. AA/AE
2. EO/EG
3. LDPE
4. Oxo C3-C4 + ASU + syngas
5. C1 Complex + syngas

Step 2. Allocation of Utilities Requirements to Production Blocks

The requirements for electricity, steam, water, gases, etc. are allocated to each production block. The electricity and steam requirements include those for both the production processes and their utilities.

Step 3. Material Streams Relevant to Integration

The material and energy streams relevant to integration are investigated: useable by-products, captively used products, and incineration wastes.

Step 4: Energy Streams Relevant to Integration

Here, the processes are reviewed for their production of excess heat as either steam production for the steam network or heated streams which can be used in neighbouring plants.

The separation of production blocks is shown in the following schematic. Sales products, raw materials, and infrastructure are excluded from the schematic showing the separated production blocks for presentation purposes.

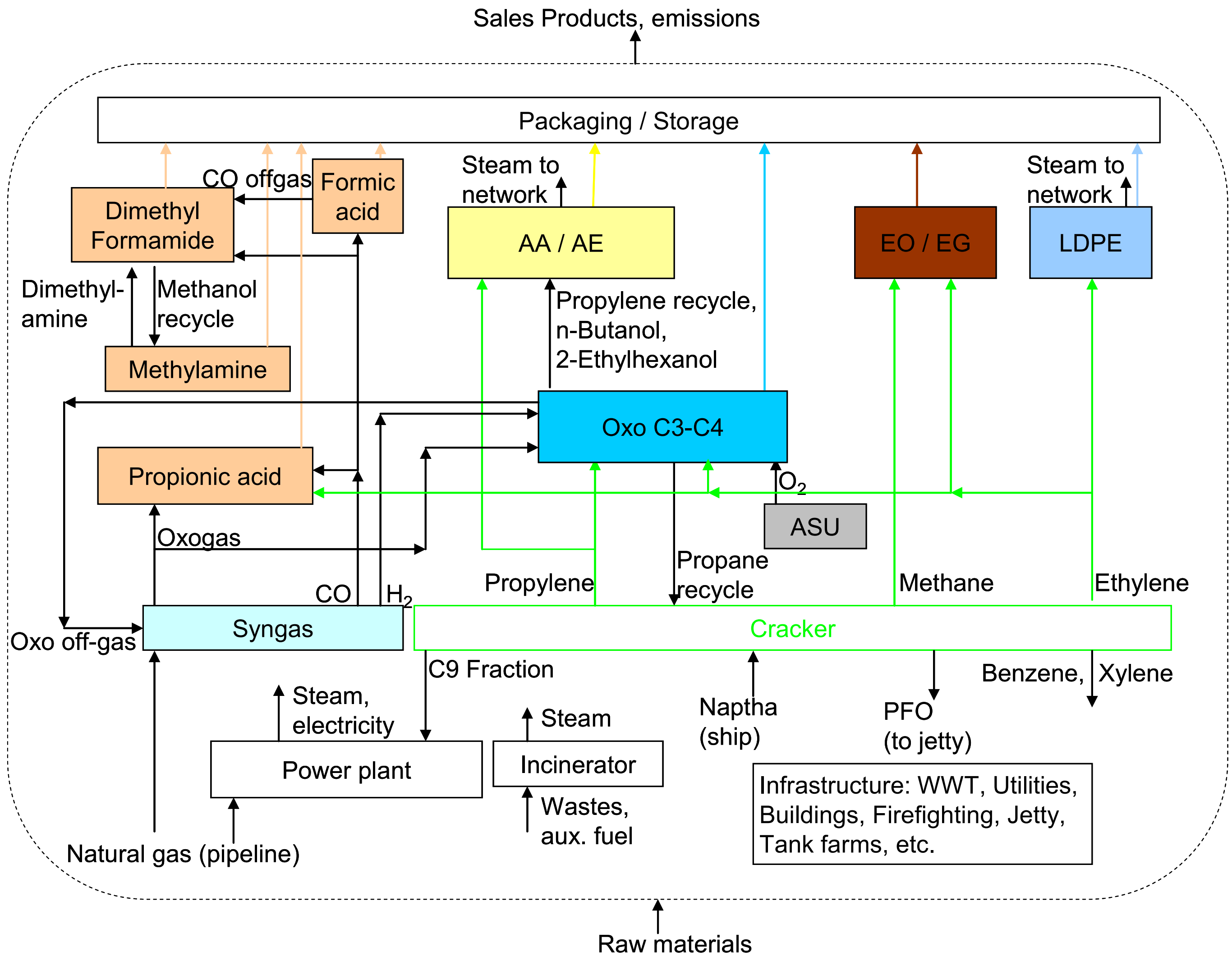


Figure 5.1 Schematic of Flows in Site Case Study

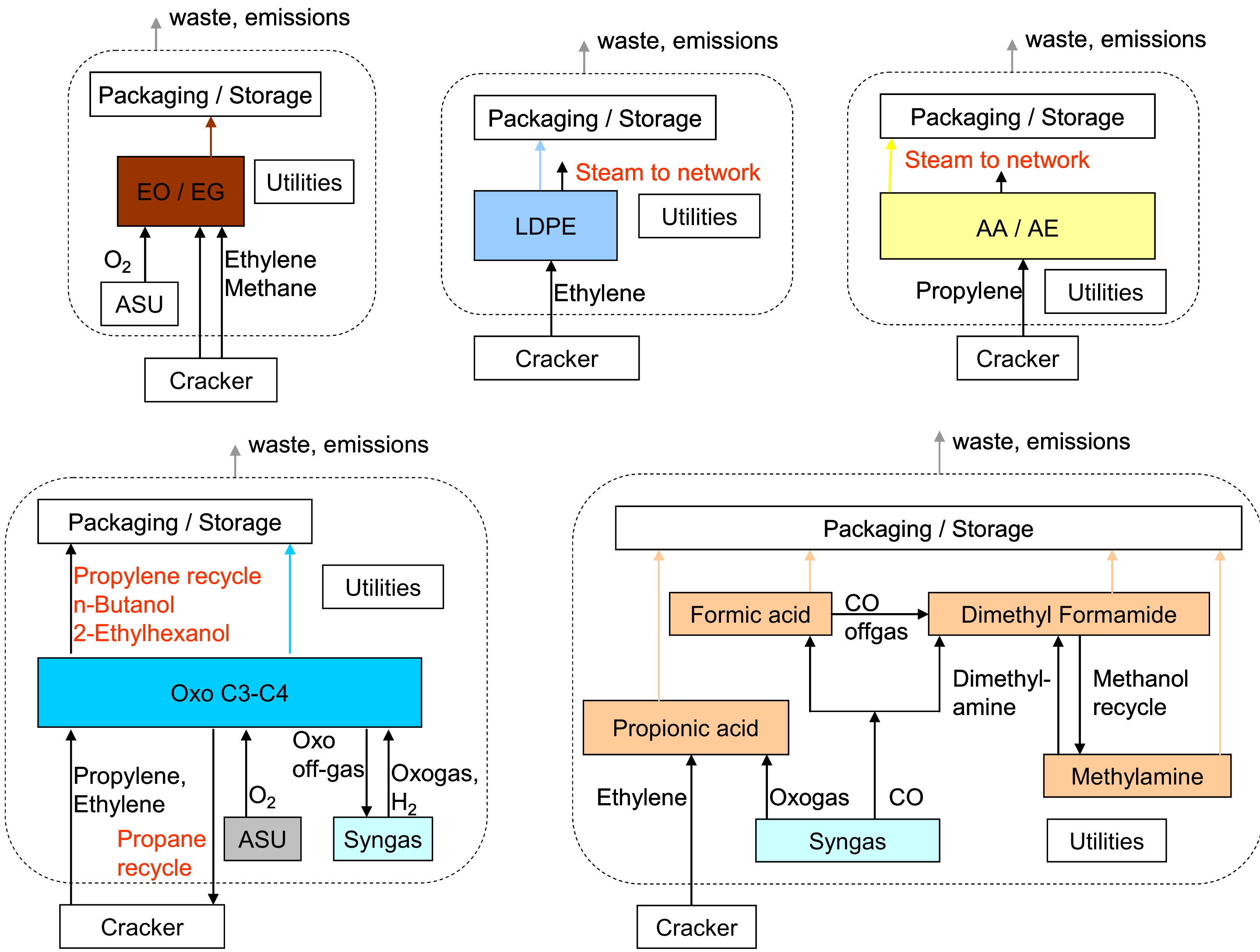


Figure 5.2 Separated Production Blocks for Site Case Study

5.4 Analysis

5.4.1 Materials / Logistics integration:

Horizontal Materials Integration / Useable By-products

Products from the Oxo alcohols plant are transferred to the AA/AE process as feedstocks, shown below. The linkage of these plants is considered to be horizontal materials integration, as the plants are not part of a vertical value chain. If the processes are separated, these raw materials would require transport.

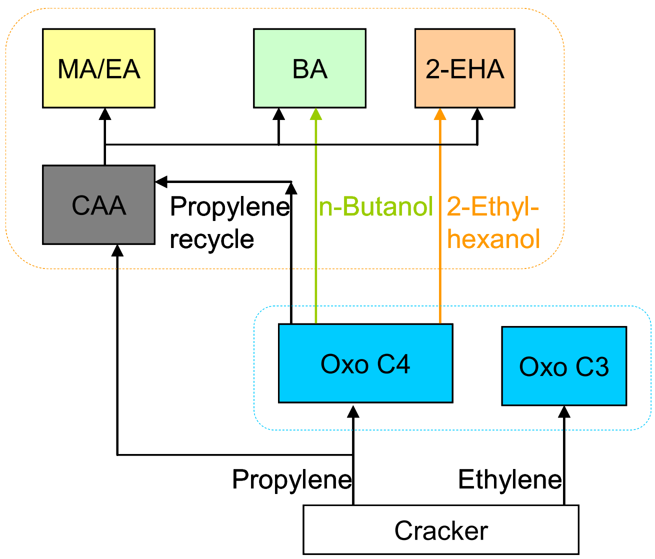


Figure 5.3 Materials Integration between AA/AE and Oxo Plants in ICPS

Also, light fuel oil, a useable by-product from the steam cracker, is used in the power plant as backup fuel (9 kt/a, assumed at 1% of cracker output, based on European Commission 2003, p.154). The logistics benefit of having these raw materials available onsite is determined as follows. A transport distance of 100 km by truck is taken (cost of 25 €/t based on inquiry). The specific costs for filling, dispatch, and order- and materials management are based on those given in the methodology. Storage costs are for four 1,000 m^3 tanks based on actual cost data. The logistics-related savings due to the product transfer between the Oxo and AA/AE production blocks as well as the light fuel oil used in the power plant are estimated at 4.1 million €/a. The transport distance selected has an effect on the overall costs. Increasing the distance to 200 km increases the transport cost to 33 €/t, resulting in overall costs of 5.1 million €/a; thus doubling the distance increases the costs by 24%. The cost breakdown is given in the following table.

Table 5.2 Cost Benefit of Useable By-products for Site Case Study

Materials available at ICPS (t/a):	
Propylene recycle	24,000
n-Butanol	62,400
2-Ethylhexanol	22,640
Light fuel oil from cracker	9,000
Total Materials available at ICPS (t/a)	118,040
Distance (km)	100
Transport cost (€/a)	2,951,000
Storage (€/a)	56,354
Filling (€/a)	472,160
Dispatch (€/a)	118,040
Materials management (€/a)	542,984
Logistics Costs for By-products available at ICPS (mil €/a)	**4.14**

Captive-use Raw Materials

The only captive-use products at the site are the cracker products: ethylene (600 kt/a), propylene (300 kt/a), and methane (<1 kt/a). Depending on the location of the nearest cracker, logistics costs for these feedstocks are incurred. Logistics costs for these feedstocks are based on transport and storage costs. For this study, the separated sites are assumed to be located close to a refinery, which provides cracker products. Transport of ethylene from local refineries in western Europe is estimated by the European Commission (2003, p.147) to be 17.2 €/t, which represents 9% of the ethylene production cost. This results in an overall transport cost of 15.5 million €/a. Storage requirement costs are estimated based on storage tanks for propylene and ethylene per site at 0.34 million €/a for 5,000 m^3 (for 2 weeks of inventory). Thus, the costs for transport and storage of olefins are estimated at approximately 16 million €/a. Logistics management for raw materials entering the site are part of the input system and thus not considered for cracker products.

For completeness, the costs for pipeline transport and international ship transport are given below. If a pipeline must be constructed, the cost will be approximately 68 €/t for 25 km and 102 €/t for 100 km, including the cost of the pipeline, capital, compression, electricity (based on a natural gas pipeline, Amos, 1998, p.E-32, updated for currency and inflation). However, normally a site's location is based on proximity to an olefins pipeline already constructed by a petrochemicals producer. Thus, these costs are normally not directly incurred by the chemicals producer. Also, olefins are transported internationally by sea tanker by firms such as GasChem and Camillo Eitzen. A cost of 100 €/t is estimated for long haul international sea freight (Braemar Seascope Ltd., 19.07.2007), 50 €/t for intra-America transport, and 85 €/t for intra-Asia freight (Platts, 19.07.2007). For transport by sea tanker as opposed to pipeline, additional logistics management costs must be added. However, these are part of the input system, as these processes are carried out on the side of the olefins supplier. Applying these costs to the case study, the cost for olefins transport would be approximately 61 million €/a for pipeline transport (25 km) or 76 million €/a for sea freight (for intra-Asia).

Sales products produced at the site and other cracker products (PFO, aromatics) are sold offsite and therefore considered neutral in the calculation. In the site studied here, there are no vertical production chains. If, for example, a polyacrylic acid or superabsorber (SAP) plant would be located downstream of the AA/AE plant within the ICPS, then its main feedstock, glacial acrylic acid (70 kt/a), could be transferred by pipeline. The logistics savings, based on the logistics calculation for useable by-products (Table 5.2) for 70 kt/a of AA transport (and 2,000 m^3 storage tank) is 2.5 million €/a. Thus, the amount of logistics savings would increase as more downstream plants are added.

By-products which can be Incinerated

In the ICPS, the Oxo process produces propane as a by-product which is recycled back to the cracker as a raw material. If the Oxo plant is located outside of the ICPS, there is no onsite recipient for the propane. The propane can be either sold offsite if the purity is high enough or, if no customer is available, is incinerated. As this gaseous stream is estimated at only 1,200 t/a (1% of the Oxo-C4 production) and its purity is unknown, it is assumed to be uneconomical to (potentially) reprocess, compress, store, and transport the stream for offsite sales. Thus, for the separated Oxo plant, this stream may be flared or incinerated. If it is flared, the stream’s value as a raw material is lost: this is estimated at 547 thousand €/a, assuming pure propane valued at 456 Euro/t (Terasengas, 06.08.2007).

If the stream is used as fuel, then its value is lower than if it is used as a raw material, as propane represents a higher level of chemical refinement compared to a fuel. If the value of the propane incinerated is set at that for natural gas, 262 €/t (Intelligence Press, Inc., 08.08.2007), since the heating value is similar (46 MJ/kg for pure propane relative to 44 MJ/kg for natural gas), the fuel value is 329 thousand €/a. Thus, the economic loss of using propane as a fuel in compared to as a raw material in the ICPS is thus reduced to 218 thousand €/a.

Table 5.3 By-product as Fuel in Site Case Study

By-product	Propane
Source	Oxo-C4 plant
Amount (t/h)	0.15
Amount (t/a)	1,200
Energy of combustion (MJ/kg)	46
Value as a raw material (€/t)	456
Cost of natural gas (€/t)	262
Loss of raw material value (€/a)	547,200
Value as a fuel (€/a)	328,691
Raw material value – fuel value (€/a)	218,509

Fuel Waste Gases

Additionally, offgases which may be incinerated are collected from various plants via a fuel gas header in the ICPS. The value of the stream will be lower than for natural gas due to its lower heating value. Also, it may not be possible to use it interchangeably with natural gas due to technical reasons, as the stream may have coke forming components which may cause a problem in certain apparatus or may not be appropriate due to its lower heating value. Most likely this stream may be used as fuel for the power plant. As the stream may also be used as fuel in the separated production blocks, it is considered neutral in the calculation.

5.4.2 Energy Integration

Heat Recovery

Steam is produced by the steam cracker, the AA plant, and the LDPE plant. The value of the steam produced based on the site-specific steam price represents a benefit of 7.0 million €/a.

Waste Incineration and WWT

In the ICPS, organic liquid and solid wastes are collected for central incineration. The liquid wastes arise primarily from chemical production and the solid waste primarily from waste water treatment sludge and residues from separation processes. For the five separated sites, the waste is assumed to be sent for offsite incineration. Also biological waste water treatment is carried out offsite. Waste incinerated at the ICPS amounts to 6,322 kg/h or 51 thousand t/a to produce 28 t/h of 16 bar steam valued at 1.7 million €/a for the site. Over 15 kt/a of natural gas would normally be required to produce the same amount of steam. The operating costs for incineration and WWT are considered equivalent for the ICPS and offsite treatment, as both are considered to be large-scale facilities where economies of scale are achieved.

5.4.3 Utilities and Infrastructure

Power Plant

Using the calculation method described in the methodology, the operating costs for a power plant for each individual process block were determined, including utilities, syngas, and ASU requirements. The sum of these requirements is equal to the requirements for the actual site, not including the requirements for the cracker and aromatics plants, as these are not under investigation. For each production block, the costs for the three cases were calculated:

Case 1. boiler and public grid

Case 2. boiler and steam turbine

Case 3. boiler, steam turbine and gas turbine

For each of the separated production blocks, case 2, a boiler and steam turbine was the most economical option, and for an ICPS, case 3, inclusion of a gas turbine was the most economical. A summary of the costs and steam and power requirements for each process block and the additional requirements for utilities and associated processes (such as ASU and syngas) is given in Table 5.4. All costs and variables used for the calculation may be found in Appendix C. Economies of scale for one onsite power plant in the ICPS compared to five individual power plants results in reduced operating costs including capital costs of approximately 4.3 million €/a. This represents a savings of 6.4%. If the five production blocks each have a system with a gas turbine (case 3 rather than case 2), then operating costs of 11.0 million €/a are saved, representing a reduction of 15% compared to individual power plants. Ultimately, the option which is most economical depends on the local conditions.

Table 5.4 Steam and Power Requirements for Site Case Study

Production block	Steam (t/h)		Power input (MW)		Total cost (mil €/a)
	process	Process + utilities + associated processes	process	process + utilities + associated processes	
AA/AE		3	18	22	8.9
Oxo	49	53	3.5	10	10.8
LDPE	8	11	43	47	19.3
EO/EG	32	37	6.5	33	17.5
C1 complex	56	58	4	7	10.4
Total for separate CHP	**145**	**162**	**75**	**119**	**67.0**
One CHP		**162**		**119**	**62.7**

The costs for main utilities are summarised in the table below. The source for the costs is PEP report 136A (1995), except for that of incineration, which is estimated by Stubenvoll (2002, p.144). The greatest difference is found in the cost of cooling water, due to economies of scale. According to PEP report 136A (1995), nitrogen production costs are independent of economies of scale beyond approximately 1,400 Nm^3/h, where the cost curve flattens out (see Figure 4.32). As the requirements for the separated sites and the ICPS (10,000 Nm^3/h) are above this, the nitrogen costs are considered to be comparable for both cases.

Table 5.5 Utilities Requirements for Site Case Study

Utilities	Amount	Cost, Sum of 5 SA (mil €/a)	Cost, ICPS (mil €/a)	Cost Difference (mil €/a)	% Dif
Process water	3,000 m^3/h	2.8	2.3	0.5	17
Demin. Water	300 m^3/h	0.6	0.4	0.3	44
Cooling water	35,000 m^3/h	9.5	3.2	6.3	66
Compressed air	15,000 Nm^3/h	1.2	0.7	0.5	40
Waste water	170 m^3/h	3.1	3.1	0.0	0
Incineration[10]	6,322 m^3/h	7.3	7.3	0.0	0
Total		**24.7**	**17.1**	**7.5**	

Other Infrastructure

Some facilities are part of the production units and are thus relatively unaffected by the separation of the production blocks: plant management and control

[10] Estimated at 145 €/t based on data from Stubenvoll et al., 2002, p.144.

buildings, piping, loading stations, roads, environmental monitoring, plant laboratories, and tank farms (the potential benefit of an additional central tank farm at the ICPS is not investigated). Other shared facilities are not investigated as they are associated with a large scale site and assumed to not be required at the separated sites, such as a port, extensive safety facilities, a site administration building, a car garage, or a forklift garage. Other facilities which may exist on a smaller scale at the separated sites may have an influence on the operating costs, however are not addressed here: a canteen, warehouses, security, loading stations, cleaning stations, and weigh bridge.

5.4.4 Overall Cost Differences

Below, the overall cost benefits of the ICPS studied are summarised.

Table 5.6 Summary of Economic Benefits for Site Case Study

Integration Type	Amount	Unit	Cost, Sum of 5 SA (mil €/a)	Cost, ICPS (mil €/a)	Cost Difference (mil €/a)	% of total
Logistics for useable by-products	118	kt/a	4.1		4.1	10.2
Logistics for cracker products	900	kt/a	15.5		15.5	38.0
Steam via heat recovery	1,040	kt/a		-7.3	7.3	17.9
Steam via waste incineration	208	kt/a		-1.7	1.7	4.3
Use of by-products	1.2	kt/a		-0.2	0.2	0.5
Shared power plant	160	MW	67.0	62.7	4.3	10.6
Shared utilities			24.7	17.1	7.5	18.5
Total			**111.3**	**70.6**	**40.7**	100

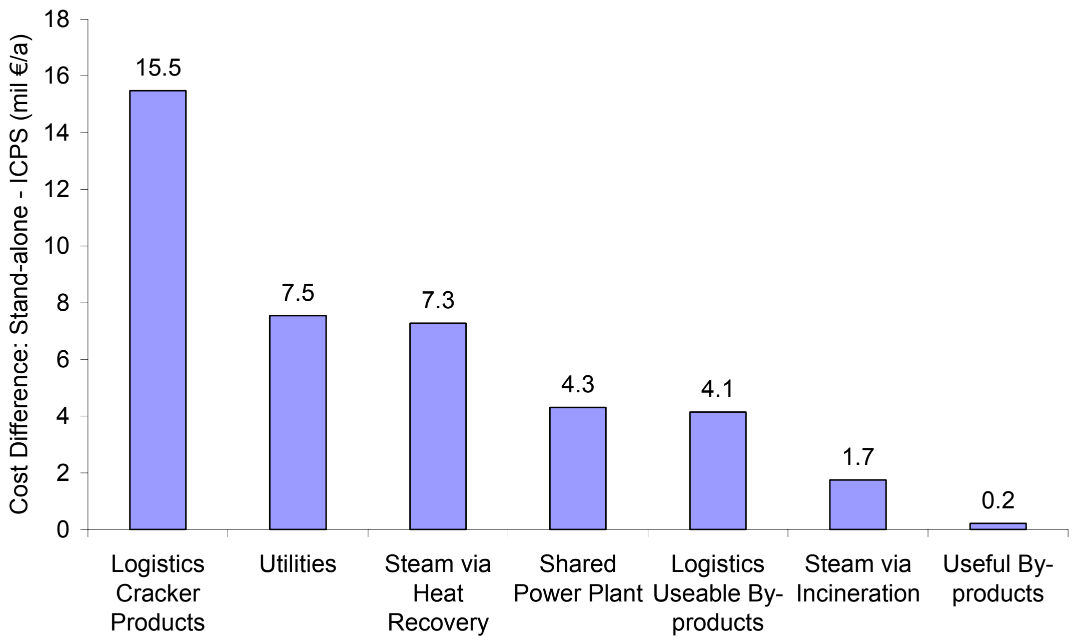


Figure 5.4 Economic Benefits for Site Case Study

Thus, the total cost benefit of integration for this particular case study is approximately 41 million €/a. Logistics savings for the use of by-products and onsite transport of cracker products results in 48% of the cost savings. Logistics savings are limited to these two aspects, as no vertical value chains exist at this particular site. Energy integration from steam export and waste incineration accounts for 22% of the savings. Shared utilities and a single power plant are a very significant cost factor accounting for 29% of the savings. Materials integration from the chemical use of the propane by-product stream represents less than 1% of the savings.

5.4.5 Reduction in Fossil Fuels and Emissions due to Integration

Reductions in fossil fuels are determined based on methodology section 4.8.

Fossil Fuels

Fossil fuels consumption is reduced through the following types of integration. The amounts of fossil fuels are given below. The economic value of these fuels is included in the cost savings for each integration type (eg. as operating costs).

- Energy: the amount of natural gas required to produce the same amount of steam provided in the ICPS is as follows
  - Heat recovery: 130 t/h of steam via steam boilers requires 77 kt/a
  - Incineration: 28 t/h of steam via steam boilers requires 15 kt/a

- Shared infrastructure: if the five production blocks are equipped with individual power plants[11], the energy consumption is reduced by 10 MW (231 MW versus 241 MW or 4%), equating to savings of 6,262 t/a of natural gas.
- Logistics: for the transport of oxo products and light fuel oil (118 kt/a, Table 5.2), 494 t/a of diesel fuel are required and for the transport of olefins from a nearby refinery (distance of 50 km assumed), 1,884 t/a of diesel fuel are required. Thus a total of 2,378 t/a of fuel are saved through integration.

Table 5.7 Fossil Fuels Reduction for Site Case Study

Source		Amount
Heat recovery	Steam produced by heat recovery (t/a)	1,040,000
	Natural gas equivalent (t/a)	76,582
	Energy equivalent (MWh)	933,925
Incineration	Amount of waste incinerated (t/a)	50,576
	Steam produced by incineration (t/a)	208,132
	Natural gas equivalent (t/a)	15,326
	Energy equivalent (MWh)	186,903
Single PP vs 5 individual PP	Natural gas equivalent (t/a)	6,262
	Energy equivalent (MWh)	76,537
Transport	Diesel Fuel (t/a)	2,378

Emissions

The overall emissions reduction due to integration compared to the five separated sites is estimated based on the methodology.

Table 5.8 Emissions Reduction due to Integration for Site Case Study

Emission	Steam from heat recovery (t/a)	Single Power Plant (t/a)[12]	Transport (t/a)
CO_2	354,891	29,084	4,715
SO_2	9	1	1
CO	252	21	50
NOx	215	18	8
NMVOC	4	0	2
Dust	4	0	4
CH_4	4	0	
N_2O	11	1	

[11] The determination of fossil fuel reduction due to economies of scale is based on the same power plant concept, cogeneration utilising steam and gas turbines.
[12] Based on emissions data from Fraunhofer Institute (2005, pp.250-251).

5.4.6 Summary

To summarise, the ICPS investigated possesses the following types of integration:

- Materials/Logistics integration: the use of products from the Oxo plants as feeds for the AA/AE plants, light fuel oil from the cracker as power plant backup fuel, and onsite cracker products
- Energy integration: waste incineration and steam export from processes providing steam (cracker, AA, LDPE) for processes requiring steam (C1 Complex, Oxo C3-C4, EO/EG)
- Infrastructure: economies of scale for a shared power plant and facilities for the preparation of different types of water and compressed air.

Logistics benefits are limited due to the absence of value chains. As a site becomes more forward integrated, a greater number of downstream plants and volume of captive use materials will lead to greater logistics cost savings. These savings are expected to increase in proportion to the other types of integration. For example, at Bayer, significant amounts of residues are used chemically onsite (see Section 3.7.5). If these are assumed to be used in different processes from which they arise, the resulting logistics cost savings based on the calculation for useable by-products employed for the case study is 40.2 million €/a (based on liquid materials). Further, additional reductions through economies of scale in processes which belong to the 'input system' (cracker and syngas plants), not investigated here, are expected.

The reductions in costs, fossil fuels, and emissions for the site case study are summarised below.

Table 5.9 Cost, Fossil Fuel, and Emissions Reduction for Site Case Study

Integration type	Cost savings (mil €/a)	Fossil fuel savings (t/a)	CO_2 reduction (t/a)
Material	0.2	[13]	[14]
Energy	9.0	91,908	355,891
Logistics	19.6	2,378	4,715
Infrastructure	11.9	6,262	29,084
Total	**40.7**	**100,548**	**389,690**

[13] Materials are used chemically in an ICPS, but as fuel or waste in stand-alone site.
[14] Emissions result whether the material is used chemically or as a fuel.

6 Case Studies on the Plant Level

The suitability of a particular chemical production plant to be integrated in an ICPS depends on various aspects. This chapter investigates these aspects through case studies on the plant level. The chapter begins with a summary of processes with characteristics favoured for integration:

- the production of useable by-products, or
- the ability to export excess process heat as steam

This is followed by the selection of two case studies, each based on a different chemical production process which vary in process and product type as well as the forms of integration possible. The first case study investigates the polyacrylate dispersions process and the second investigates the aniline process. Following the case studies, the concept of integration potential is proposed to investigate a plant's suitability for integration in an ICPS.

6.1 Processes which Produce Useable By-products and/or Steam

All chemical production processes described in Ullmann (2000) were reviewed to determine if they possess the key integration aspects of useable by-product formation or excess process energy which may be exported as steam[15]. It should be noted that the production of co- or by-products may also be a disadvantage for a process if the demands of the main and co-product are not properly balanced. Whereas, the production of excess energy is advantageous for an integrated process as long as there is a net steam requirement at the site. The tables below summarise the findings of this review.

[15] Only processes with steam export and not heated liquid streams are reviewed here.

Table 6.1 Chemical Processes with Useable By-product Formation

Main Product	By-product	Process	Comments	Uses of Co-product
Apatite	Phlogopite	Co-product of apatite mining		
Barium Peroxide	Barium sulphate	$BaO_2 + H_2SO_4 \rightarrow BaSO_4 + H_2O_2$	Sales opportunities for the co-product barium sulphate have a decisive effect on the profitability of the barium peroxide process. The other co-product, 3% concentrated H_2O_2, has a limited market because of high production cost and impurities.	Starting material for the production of barium compounds, filler in paints and plastics
Caprolactam	Ammonium sulphate	Hydroxylamine → Caprolactam + Ammonium sulphate	From synthetic-fiber intermediates, such as caprolactam, acrylonitrile and methyl methacrylate and in the production of formic acid and acryalamide. The most important source is the production of caprolactam. Per ton of caprolactam, 2.5-2.4 tons of Ammonium sulphate are produced.	Fertilizer, however must compete with more concentrated nitrogen fertilizers
Chromium (III) Sulphate	Iron (II) Sulphate	Ferrochromium + Sulphuric acid → Iron (II) Sulphate + Chromium (III) Sulphate	Economical preparation of a pure product has been only partially successful.	Nutrition, dyes, agriculture
Copper or Scheelite	Molybdenum	Co-product of Copper and Scheelite mining	55% of world's production via this route	Metal production
Cracker	Isobutene	Butadiene from steam cracker C4 fractions		Feedstock for MTBE process
Cresol	Sodium Chloride	Chlorotoluene + NaOH → Cresol + NaCl		Can be returned for use as an electrolyte to the chlor-alkali electrolysis
Ethanol	Di-ethylether	Synthetic ethanol production	In countries where ethanol is produced synthetically, di-ethylether is produced in sufficient quantities as a by-product to make its synthesis unnecessary. Normally, ether is produced from ethanol by dehydration.	Oxygenates

Main Product	By-product	Process	Comments	Uses of Co-product
Ethylene	Various	Ethylene by thermal cracking	**Acetylenes** (C2 and C3) are hydrogenated to ethane, ethylene, propane, and propene; or they may be recovered and sold as products **Aromatics** (various fractions) can be recovered or they may remain in the hydrotreated pyrolysis gasoline **C4 olefins** can be refined for butadiene, butylene, isobutylene, or mixtures thereof **C5 olefins** can be either recovered and refined to give isoprene, piperylene, and cyclopentadiene, or hydrotreated in the pyrolysis gasoline fraction **Ethane** is recycled as cracking feedstock or used as fuel **Fuel oil** is used as fuel or to produce coke or carbon black **Hydrogen** is purified and used for hydrogenation steps in the plant; excess hydrogen is sold or used as fuel in the plant **Methane** is used chemically, as fuel, or sold **Naphthalene** is recovered for sale or left in the pyrolysis fuel oil fraction **Propane** is recycled as a cracking feedstock, used as fuel, or sold **Propene** is sold in various grades **Raw pyrolysis gasoline** is sold **Carbon dioxide** is used or sold	Various, mainly as feedstock for several processes
Ethylene oxide	CO_2	Oxidation of Ethylene → Ethylene Oxide + CO_2	About 60 % of the ethylene feedstock is converted to the desired product. About 40 % of the feed is converted to CO_2.	Various
Feldspar or Kaolin	Mica	Co-product of feldspar mining and kaolin extraction		Pigments

Main Product	By-product	Process	Comments	Uses of Co-product
Furfural	Diacetin (glyceryl diacetate)	Wood chips + Steam + Acetic Acid (produced in situ) → Diacetin + Furfural + cellulose residue	Diacetin is produced as a co-product. Also, cellulose residue is produced, which can be burned as fuel to support energy requirements in the furfural plant.	Various for diacetin: solvent for flavouring agents, cement additive, etc.
5-Inandol	4-tert-butylphenol	Isobutene with bisphenol → 5-indanol + 4-tert-butylphenol	The 5-inandol yield for the process is 80% and 4-tert-butylphenol as co-product.	Stabilizers
Isobutene	Methanol	Cracking of MTBE to form Isobutene	Methanol obtained as a co-product is recycled to methyl tert-butyl ether (MTBE) synthesis.	Feedstock for MTBE process
Melamine	Ammonia	Melamine production from Urea	Integration of urea and melamine production processes is beneficial.	Fertilizer, chemical feedstocks
Methylene Diphenylene Isocyanate (MDI)	Hydrogen chloride	Condensation of aniline with formaldehyde in the presence of HCl		Various
MnO_2 battery active	$MnSO_4$	Oxidic Manganese ore (80% MnO_2) + H_2SO_4 → battery active MnO_2 + $MnSO_4$	Co-product $MnSO_4$ is separated by leaching with water.	Fertilizer
P_2O_5	H_2SiF_6	Concentration of wet phosphoric acid	Apart from water vapour, a mixture of SiF_4 and HF is generated during the concentration of wet phosphoric acid. About 50 – 60 % of the fluorine content of wet phosphoric acid is volatilized on concentration from 30 to 55 % P_2O_5.	Glass, ceramics, catalysts, etc.
Phenol	Acetone	Isopropylbenzene (cumene) → Phenol + Acetone	83% of acetone is produced via this route. Phenol demand determines availability of acetone to large extent.	Automotive, housing, similar to phenol
Propylene Oxide	Tert-butanol	Epoxidation of propene with tert-butyl hydroperoxide (TBHP) → Propylene oxide and Tert-butanol (TBA)	In the case of high methyl tert-butyl ether (MTBE) demand in the market, TBA is sometimes dehydrated to isobutene which is then fed to the MTBE process.	Octane enhancers

Main Product	By-product	Process	Comments	Uses of Co-product
Propylene oxide	Tert-butanol (TBA)	Epoxidation of propene with tert-butyl hydroperoxide (TBHP) → Propylene oxide and Tert-butanol (TBA)	In the case of high MTBE demand in the market, TBA is sometimes dehydrated to isobutene which is then fed to the MTBE (methyl-tert-butyl-ether) process.	MTBE process
Propylene oxide	Acetic acid	Epoxidation of Propene with Peroxycarboxylic Acids	The required peroxy acids can be prepared by different routes. If acetaldehyde is used, the co-product acetic acid must be removed. The yield of PO is 90 % and typically 1.3 kg of acetic acid is produced per kg of PO.	Various
Propylene oxide	Tert-butyl alcohol or alpha-phylethanol	Indirect oxidation with organic hydroperoxides	The tert-butyl alcohol or a-phenylethanol co-products formed in parallel with PO are of considerable economic value, because they can be converted to methyl tert-butyl ether (MTBE) or styrene in subsequent reaction steps. When styrene or MTBE is in great demand, co-product process economics are competitive with those of the alternative chlorohydrin production routes. The co-products are always formed in larger amounts than PO itself. In the case of the process with tert-butyl hydroperoxide, 2.5 – 3.5 kg of tert-butyl alcohol are formed per kg PO. A regional limitation of the co-product processes results from raw material logistics. Especially for the tert-butyl hydroperoxide process, economic operation requires integration into a refinery complex, where mixed butanes and ethylbenzene are readily available.	MTBE: as a fuel component in motor gasoline, Styrene: see below
Propylene oxide	Styrene	Ethylbenzene process	15% of total production is via this route, where 2.2 – 2.5 kg of styrene are produced per kilogram of PO.	Polystyrene, Acyrlonitrile-butadiene/styrene resins, styrene-butadiene elastomers or co-polymer latexes, styrene-acrylonitrile resins, cross-linking agent in polyester manufacturing

Main Product	By-product	Process	Comments	Uses of Co-product
Sodium hydroxide	Chlorine	Sodium carbonate to sodium hydroxide by causticisation	The growth rate of co-product chlorine is estimated to be in the same range or higher than NaOH.	Vinyl chlorine, solvents, pulp and paper, water treatment, etc.
Sulphuric acid	Cinder	Sulphuric acid from pyrite	Depending on chemical composition and market conditions, cinder may have positive or negative influence on total costs. If the cinder can be utilized nearby, the credit may cover up to 15 % of the pyrite costs.	Cement
Synthetic Fatty Alcohols	Hydrated alumina	Alfol process	Hydrolysis with water gives high-purity hydrated alumina as a co-product.	Aluminum oxide in catalytic applications, ceramics
Synthetic Fatty Alcohols	Aluminum sulphate	Epal process	Hydrolysis with hot sulphuric acid leads to high-purity aluminum sulphate as a co-product.	Used for treating water or for the paper industry (paper sizing, pH adjustment, waste water purification)
Synthetic Fatty Alcohols	Isobutanol	Via alpha-olefins with hydroperoxides and transition-metal catalyst	If tert-butyl hydroperoxide is used, the co-product isobutanol can be readily separated from the epoxide.	As a solvent, diluent, additive for resins, wetting agent, cleaner additive and component of printing inks
Urea	Ammonium nitrate (and other ammonium salts)	NH_3 and $CO_2 \rightarrow$ Urea (once-through process)	Nonconverted NH_3 neutralised with acids to produce ammonium salts (such as ammonium nitrate) as co-products of urea production. Large quantity of ammonium salt formed as co-product and the limited amount of CO_2 conversion. Combined urea – ammonium nitrate production facilities. Since an ammonia plant is a net heat (steam) producer and a urea plant is a net heat (steam) consumer, it is normal practice to integrate the steam systems of both plants.	Fertilizer

Table 6.2 Chemical Processes with Steam Export

Product	Process	Energy production
Acetaldehyde	Oxidation of ethanol	Reaction heat used for steam production in waste-heat recovery system immediately following reaction zone. Also, waste gas is burned as lean gas with low calorific value in steam generators.
Acetylene	Thermal cracking via Advanced cracking reactor process	120 bar steam production possible, this particular boiler design developed for high heat transfer rate without coke formation.
Acryl acid	Propylene oxidation	In BASF's process, 3 to 4 times the amount of heat is produced as steam compared to the amount of the main product acrylic acid (BASF).
Acrylonitrile	Sohio process (propene, oxygen and ammonia catalytically converted to acrylonitrile)	The heat of reaction can be recovered as high pressure steam using an internal heat exchanger within the fluidized bed reactor.
Ammonia	Single-train steam reforming Ammonia production	Highly efficient use of energy within the plant - process steps in surplus supply energy to those in deficit. Surplus energy available from the flue gas of the reformer and process gas streams, while heat is needed for the reforming reaction and in the CO2 removal system. Use of steam turbine drives, as 100 bar steam is generated from the waste heat.
Aniline	Catalytic vapor phase hydrogenation of benzene	Reaction heat used for steam production via heat exchanger within reactor.
Copper	Reverbatory furnace smelting	The off-gas (1200 – 1300 °C) flows through a waste-heat boiler for steam generation and then a gas purification plant.
Exhaust from gas turbines	Ammonia production	Used for preheating duties or as combustion air in primary reformer.
Exit gas	Coal gasification	Waste heat boilers use exit gas for steam production, which is essential for improveed process efficiency because 15-20% of energy is contained in the sensible heat of the exit gas.
Formeldahyde	Formox process for production of Formeldahyde from methanol	Here, 1.5 to 3 tons of steam are produced per ton of CH_2O (depending on if with or without methanol recovery).
Gas production	Entrained-flow processes	A waste heat boiler is mounted on top to recover heat from hot effluent gases to produce high pressure steam.
Gas production	Methane synthesis	The waste-heat recovery system is normally designed to generate saturated steam up to 10.0 MPa, but superheated steam may also be withdrawn.

Product	Process	Energy production
Gas production	Partial oxidation - Shell process	The process is equipped with a waste heat boiler for steam generation.
Hydrogen	Partial oxidation	Process gas from the partial oxidation reactor is cooled in a waste-heat boiler to produce high pressure steam.
Hydrogen	Gasification of coal and hydrocarbons	The process gas from the partial oxidation reactor is cooled in a waste-heat boiler thus producing high pressure steam.
Iron	Dry coke quenching	The heat is removed from the coke with the help of recirculating gas and used for steam generation in a waste-heat boiler.
Lead	Outokumpu Process	The process generates steam via a waste heat boiler (3 t/h steam).
Maleic anhydride	Oxidation of butane to maleic anhydride	If a fluidized bed is used for the reaction (rather than a multitube reactor), then steam can be produced using an internal heat exchanger within the fluidized bed.
Nickel	Primary smelting	Off-gases leave the flash furnace through the uptake shaft and enter a waste-heat boiler where the heat content of the gas is recovered as high-pressure steam.
Nitric acid	Ostwald process at medium pressure	The reaction is exothermic and proceeds at ca. 890 °C. The nitrous gas stream is cooled in the waste-heat boiler, raising steam. Waste-heat boilers can be designed for pressures up to 10 MPa and temperatures up to 550 °C in the superheater.
Oil refining	Catalytic cracking	The heat of the flue gas is utilized in a waste-heat boiler for steam generation.
Sludge from waste water	Incineration section of a waste water treatment plant	The coal introduced into the clarifier sludge as a filter aid provides fuel for subsequent incineration. Five fluidized-bed furnaces are capable of burning up to 1000 t of filter cake daily to carbon dioxide and ash. Organic constituents of the sludge decompose completely at a furnace temperature of ca. 1000°C. The heat generated during incineration is used in waste-heat boilers for steam production, air preheating, and boiler-feed preheating. At BASF Ludwigshafen, the steam supplies a two-stage turbine which generates 14 MW of electric power, provides heat for the waste water-treatment plant, and also supplies a portion of Ludwigshafen with domestic heat.
Steel		The hot waste gas formed in an oxygen converter is used to produce steam in a waste heat boiler in the primary dedusting installation.
Sulphur	Recovery via Claus process	Cooling of the process gas from the combustion chamber occurs in the waste-heat boiler. For each ton of sulphur produced, more than 2 t of steam is coproduced.

Product	Process	Energy production
Sulphur dioxide	Pyrite roasting	The BASF – Lurgi fluid bed furnace roaster was developed for dry pyrite feeding and designed to recover the maximum amount of heat for steam production. The temperature of the fluid bed is kept constant by indirect cooling; the surplus heat of reaction is removed in the fluid bed by immersed cooling elements which form part of a waste heat system for the production of high-pressure steam. Approximately 70 % of the total energy is recovered from the fluid bed and roaster gas in the form of high-pressure steam. This corresponds to the production of about 1.5 t of steam of 40 bar and 400 °C per t of 48 % S pyrite. The remaining 30 % of the total energy is represented by the heat content of the roaster gases at an exit temperature of 350 °C, the heat content of the cinder, and radiation losses.
Sulphur dioxide	Combustion of liquid sulphur	Here 3.8 to 4.0 tons of steam at 40 bar and 400 °C can be produced per ton of liquid sulphur.
Sulphuric acid	Contact process - double absorption process	Of the total energy input, 97 % is accounted for as energy released in the conversion of sulphur to sulphuric acid and 3 % of the energy is consumed in driving the gas through the plant. Up to about 70 % of the total energy is normally utilized for the generation of ca. 1.35 t of high-pressure steam (40 bar, 400 °C) per t sulphuric acid; the remaining 30 % is usually lost as waste heat. The high-pressure steam is generated with high-temperature heat recovered by indirect exchange with gases from the converter system and the sulphur furnace.
Synthetic cresol (o-creson and xylenol)	Methylation of phenol with methanol to form cresol	The heat of reaction is dissipated by the generation of high pressure steam (or boiling organic high temperature media or circulating salt melts).
Vinyl chloride monomer (VCM)	Conventional process (ethylene, chlorine, oxygen and possibly HCl from other chlorination processes to VCM)	Most of the waste heat of the flue gas is utilised to generate 20 bar steam by a waste-heat boiler. Despite steam credit for the integrated heat recovery in the central vent gas incineration plant and for recovery of reaction heat from the exothermic oxychlorination reaction (generation of 20 bar steam) and exothermic chlorination of oxychlorination vent gas (generation of 1.5 bar steam), the specific steam consumption amounts to 1.74 t per ton of VCM with 55 % conversion rate at EDC cracking.
Vinyl propionate	BASF: acetylene and propionic acid in gas phase	The heat of reaction is removed via a cooling medium by means of evaporative cooling and is used for steam production.
Waste, household and hazardous	Waste incineration	Steam generators or hot-water boilers are used: natural-circulation, forced-circulation, and once-through.

6.2 Case Study Selection

The two case studies which follow investigate the influence of integration on particular processes. For each case study, scenarios are defined in which the process exists as either part of an ICPS, semi-ICPS, or stand-alone site. The processes have been selected as they vary in key aspects: product/process type and types of integration possible. Also, they are based on actual cases from industry.

Plant Case Study 1 – Polyacrylate (PA) Dispersions

The polyacrylate dispersions process is the final process in the acrylic acid value chain in an ICPS producing basic chemicals. These functional chemicals are represented by a wide range of products and sold to different industries for diverse applications, discussed later in more detail. In practice, these plants exist as both stand-alone plants and within an ICPS. This case study is selected due to its end position in the value chain. Two scenarios are investigated, one in which a single large-scale polyacrylates plant in an ICPS exports products to different countries, and another in which several smaller stand-alone plants are located in different countries, close to customers. Thus, this case study focuses on logistics integration for products at the end of the value chain and on the effect of integration on production costs.

Plant Case Study 2 – Aniline

This process is an integral part of the polyurethane value chain and is mainly used in the production of methylene diphenylene isocyanate or MDI. Through its heat of reaction, high pressure steam can be produced and exported into a steam network in an ICPS for use by other plants. This process has been selected, as the benefit of energy integration from exported steam can be investigated, which does not exist in the polyacrylates case study. Also, as an intermediate plant within a value chain, integration in terms of both raw materials and products may be investigated. This case study investigates three alternate scenarios. In one scenario, based on a real case, the process' main raw material is not available onsite; as a result, the plant is not upward integrated and the value chain is incomplete. Thus, for this scenario, the site is considered a semi-ICPS. This scenario is compared with two other scenarios; the process in an ICPS and as a stand-alone plant, each with the same capacity. Thus, this case study investigates energy integration as well as logistics integration for an intermediate plant. The schematic below shows where the processes selected for the case studies are located within their value chains in an ICPS with respect to the cracker and customers.

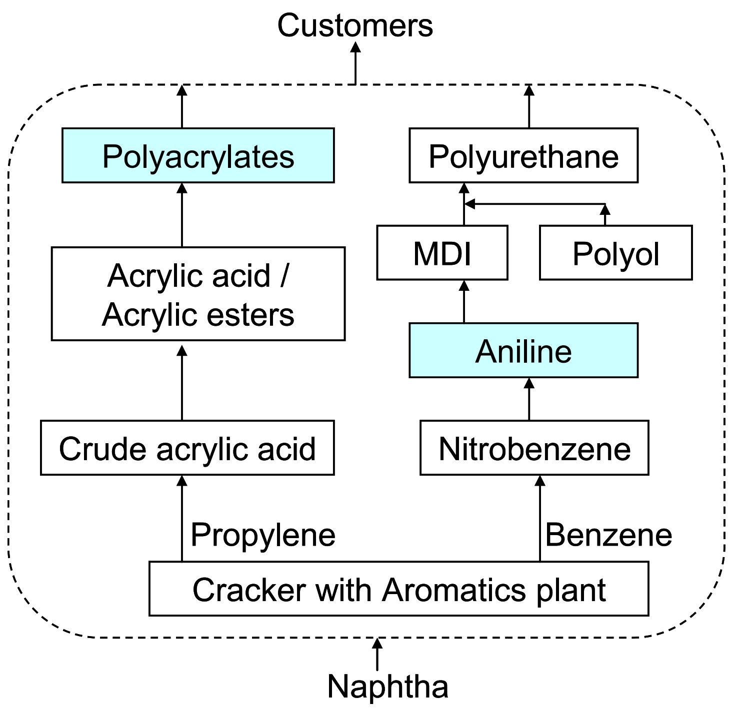


Figure 6.1 Location of Plant Case Studies in ICPS Value Chains

6.3 Plant Case Study 1: Polyacrylate Dispersions

6.3.1 Background on the Process

Co-polymers based on acrylic esters are important raw materials in a wide variety of applications, such as paints and coatings, adhesives and sealants, concrete, and fibre bonding. Integrated into finished products, they endow products with certain properties. For example, they may impart a paint with stain resistance, improve the effectiveness of adhesives, or reduce the development of cracks in concrete due to harsh weather. Polyacrylates are normally formulated for specific applications. Hence, a particular plant will produce several products according to different recipes in order to serve various applications. Some of the main global producers of polyacrylates are Rohm & Haas, DuPont, BASF, Johnson SC & Sons, Celanese, National Starch, Mitsubishi Rayon, Sumitomo Chemical, and Asahi Chemical (PEP report 65A, 1991, p.3-6).

These products are produced by polymerising acrylic esters with co-monomers, such as methacrylates (particularly methyl methacrylate), styrene, acrylonitrile, vinyl acetate, vinyl chloride, vinylidene chloride, and butadiene. The choice of co-monomer will determine the co-polymer's properties. In addition, auxiliary monomers are frequently incorporated into polyacrylates to obtain specific technical properties in dispersions. Although these auxiliary monomers are only present in low concentrations in the polymer, they have a substantial influence on the colloid chemistry and other properties of polymer dispersions. Commonly used auxiliary monomers include acrylic acid, methacrylic acid, acrylamide, methacrylamide, and other monomers with functional groups (Ullmann, 2000).

Polyacrylates can be produced by various processes, emulsion polymerisation being the most important industrial method, followed by solution polymerisation. In both processes, the final product is a polymer dispersion suspended in a liquid phase. In emulsion polymerisation, monomer droplets are dispersed to a size of 0.1 to 5 microns and polymerised in an aqueous solution, which has the added benefit of efficient removal of reaction heat, thus providing a safe medium for the reaction of monomers and enabling polymers of high molecular weight (PEP report 65A, 1991, p.6-1). The water is retained in the product through to the product's delivery to the customer. This allows for easier handling throughout the production process, as the viscosity of the polymer is reduced as a dispersion. It is only at the customer side, when the polymer is integrated into the finished product, where the water may be removed through evaporation in the subsequent production process.

The acrylic acid/polyacrylate value chain is shown in the following figure. As the greatest portion of raw materials for the process is represented by acrylic monomers, the polyacrylates process is located downstream of the acrylic acid/acrylic esters process in the value chain. Thus, in an ICPS based on the production of basic and intermediate chemicals, the polyacrylates plant is located at the end of the value chain, as the consumers of polyacrylates are producers of end products, such as paints and adhesives, or construction companies.

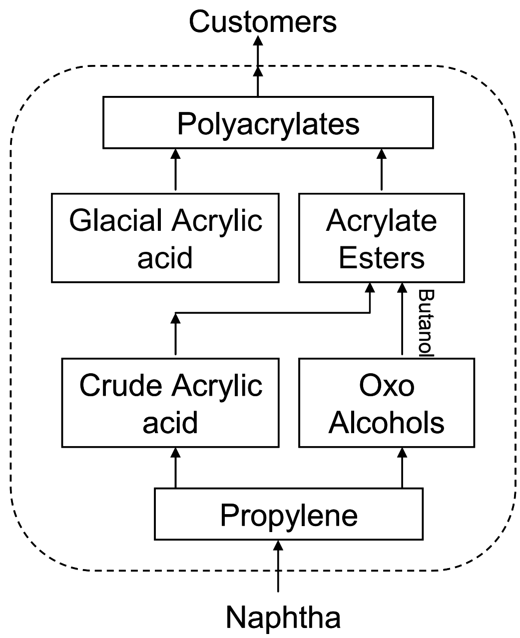
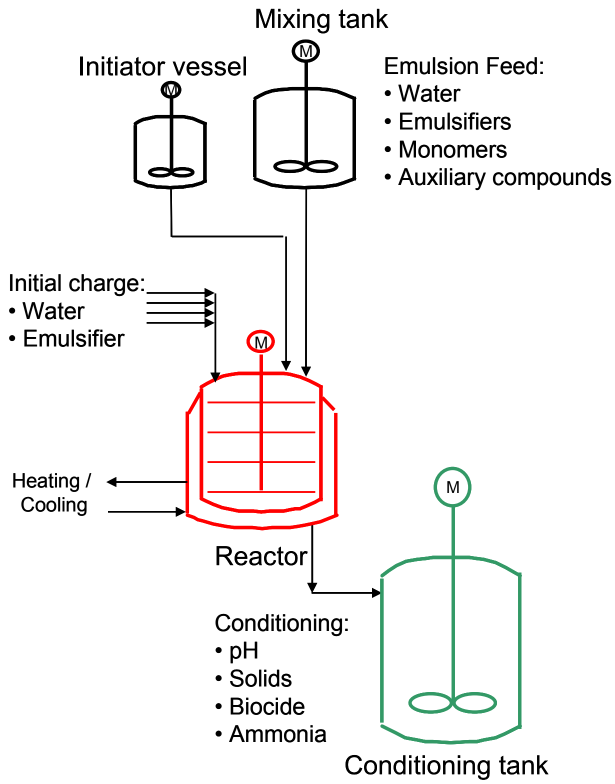


Figure 6.2 Value Chain for Polyacrylates within an ICPS

6.3.2 Process Description

Ullmann (2000) describes the production system as follows. Water, monomers, emulsifiers, and additives are contained in storage tanks and fed via metering devices to a mixing tank or fed directly to the reactor via an in-line mixer. The monomer emulsion is usually added to the polymerisation reactor batchwise or continuously over a period of minutes or hours. The reactor may be connected to further feed vessels to supply initiator and other additives. The internal reactor temperature may be regulated by wall cooling or evaporative cooling. The reactor may have a capacity of 30 m^3 or more. The design, size, and power of the stirrer depend on the batch size and viscosity of the dispersion. Following the feeding stage, the dispersion is maintained at the reaction temperature for a further 1 to 2 hours to reduce the residual monomer content before being cooled. The dispersion is discharged through a filter and pumped to a conditioning tank where the solids content and pH value are often adjusted and stabilizers and biocides are added. Dispersions typically have solids contents ranging from 40 to 60%, the rest being an aqueous phase. The main raw materials used in the production of polymer dispersions are: water, monomers, emulsifiers, and auxiliary compounds, which are added to the reactor. Other raw materials are added later during the conditioning phase, such as biocides, defoaming agents, and ammonia to correct pH. A typical recipe may have 15 raw materials. Auxiliary components account for a very small portion of the raw materials, most (over 90%) of the emulsion consists of water and main monomers. The dispersions are transported to the consumer in polyethylene-lined metal drums, polyethylene vessels, or tank cars. Below is a schematic showing the typical production process.



(based on Ullmann, 2000)

Figure 6.3 Production Process for Polyacrylate Dispersions

6.3.3 Scenarios for Polyacrylate Case Study

In this work, two scenarios are selected in order to compare a polyacrylate plant as a stand-alone plant with a polyacrylate plant within an ICPS. To make this evaluation, the locations must be specified. The ICPS is located in Shanghai, China, where many chemical clusters are currently located (please refer to Figure 3.9). For the stand-alone case, five plants are located in different countries, based on an actual case.

Information for the execution of this case study is derived from actual operations. The data is based on polyacrylate dispersions plants in Asia which are either stand-alone plants or in small sites consisting of few production plants. Where necessary, actual figures have been omitted to maintain confidentiality.

Table 6.3 Scenario Description for Polyacrylates Case Study

	Scenario 1 Five stand-alone plants	Scenario 2 One plant in ICPS
Description	Local polyacrylate production, transport of monomers from Shanghai ICPS to countries	Integrated monomer / polyacrylate production in ICPS, transport of products from Shanghai ICPS to local countries
Location of AA/AE production	Shanghai ICPS	Shanghai ICPS
Location of Polyacrylate production	5 plants in: • Shanghai, China • Manila, Philippines • Osaka, Japan • Jakarta, Indonesia • Melbourne, Australia	1 plant in Shanghai
Polyacrylate Capacity	100 kt/a (20 kt/a at each location)	100 kt/a as two production trains of 50 kt/a each

The following conditions are defined for both scenarios:

- Output for each plant is based on 75% capacity utilisation
- Product spectrum is the same for each site and consists of 20 grades of polyacrylate dispersions (both pure acrylic and co-acrylic emulsion polymers)
- Based on the product spectrum:
    - 85% of the raw materials are monomers
    - 66% of the raw materials are monomers produced in the ICPS
- The weighted average solids content for all products is 50%

The flow of the acrylic monomers/esters and polyacrylate products for the two scenarios is shown in the following graphic. In both scenarios, acrylic monomers /esters are produced in the ICPS in Shanghai. In scenario 1, they are transported to five stand-alone polyacrylate production sites in Asia, four requiring export and transport by sea freight and one at a separate site in Shanghai. In scenario 2, a single large-scale polyacrylate production plant is located within the ICPS and acrylic acid/esters produced at the same site are transported to the polyacrylates plant by pipeline.

The following schematic shows the flow of acrylic acid/esters and polyacrylates for the two scenarios. Products are sold ex works for scenario 1 and from country ports (or ex works for domestic sales in China) for scenario 2. The plant locations in scenario 1 are close to the port, thus the customer does not pay more for sourcing from the plant compared to the country port.

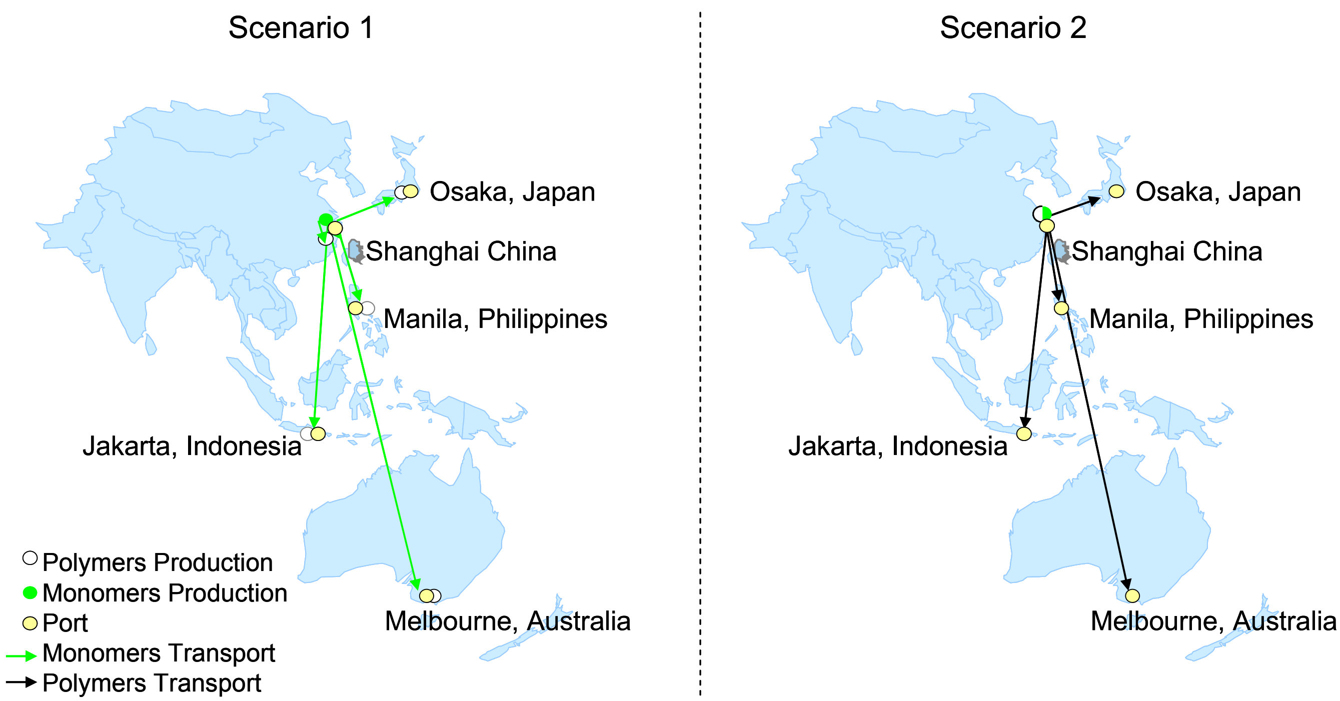


Figure 6.4 Schematic of Scenarios for PA Case Study

The main aspects of integration for the two scenarios are given below.

Table 6.4 Comparison of Scenarios for Polyacrylates Case Study

Aspect	Scenario 1 Five stand-alone plants	Scenario 2 One plant in ICPS
Logistics	Storage tanks for AA/AE at both sites, transport of AA/AE from ICPS to sites	Smaller intermediate tanks for AA/AE, pipeline transfer of AA/AE, transfer of products to countries
Energy	n/a	Incineration of waste for the production of steam
Materials	No useable by-products , off-gases incinerated	As for scenario 1
Infrastructure	Stand-alone infrastructure	ICPS infrastructure

6.3.4 Production Costs

The main cost items in the determination of production cost are reviewed below. This is followed by a table summarising the results of the calculation.

Raw Materials

The total raw material consumption for the site is 7,482 t/a, comprising of 85% monomers. A total of 45 raw materials are required, of these 10 are monomers. Of the monomers, six are basic monomers: butylacrylate, styrene, 2-ethylhexylacrylate, glacial acrylic acid, ethylacrylate, and methylacrylate and the remaining four are specialty monomers. All basic monomers except for styrene are sourced from the ICPS in Shanghai. Styrene and the specialty monomers are sourced externally.

Table 6.5 Raw Materials for a 20 kt/a Stand-alone Polyacrylates Plant

Raw Materials	All	Monomers	Available at ICPS	Purchased locally	Purchased as imports
Number	45	10	5 (monomers)	8	32
Amount required (t/a)	7,482	6,365	4,909	1,215 (85% styrene)	2,367
% of total	100	85	66	16	18

Site-specific raw materials costs are determined for: six basic monomers, specialty monomers, and other raw materials (imported emulsifiers, additives etc.). Raw materials are the highest cost component, at 63 % of the production cost for scenario 1 and 87 % for scenario 2. The highest cost of raw materials is in Shanghai, which may be due to a limited supply resulting from China's booming chemical industry.

Utilities

The utilities considered are: electricity, steam, demineralised water, raw water, and nitrogen. The per unit utilities costs are site-specific based on actual data and the utilities consumption is determined as an average on a per ton basis and applied to each site. Steam and electricity are produced via an onsite power plant in scenario 2 and via a steam boiler and public electricity grid in scenario 1. In the ICPS, the unit cost for steam is 12% lower and for electricity 14% lower compared with the stand-alone site in Shanghai. The analysis shows the cost of electricity to be the largest cost component under utilities, followed by steam and water. The cost of electricity is highest in Japan, followed by Philippines. The below chart shows the utility costs for each scenario.

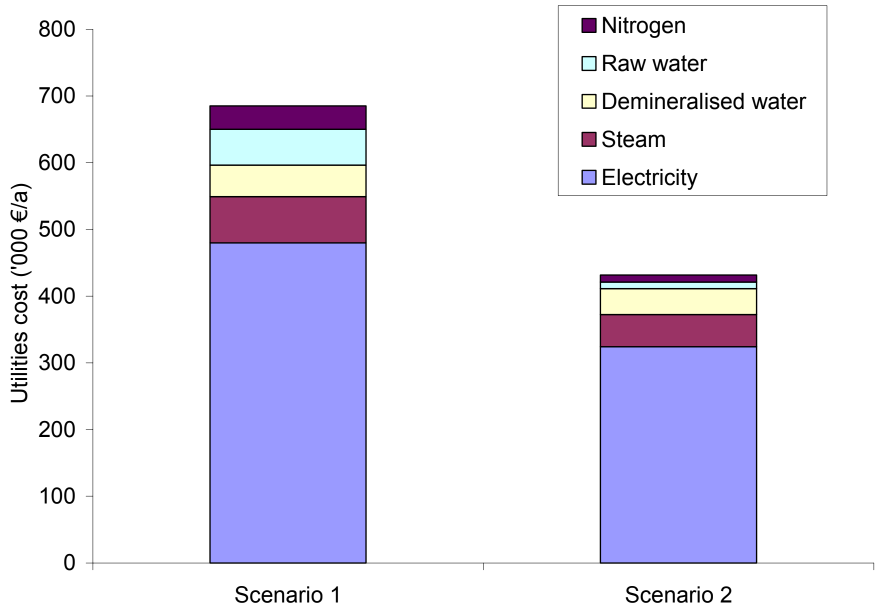


Figure 6.5 Utilities Cost for Scenarios for PA Case Study

Waste

Waste water

Waste water is generated primarily through the rinsing of the reactor in an amount of approximately 6,000 m^3/a per stand-alone site. The polymer in this waste water is flocculated out by coagulating it with alum and calcium hydroxide at an onsite waste water pre-treatment facility which is part of the production process. Then the waste water is put through a filter press and the decanted slurry is left to dry in a sludge drying bed. Biological treatment of waste water is conducted offsite for the stand-alone sites and onsite for the ICPS. The cost of waste water treatment varies significantly among the sites and is the most reasonable in the ICPS. The waste water treatment costs are 60 thousand €/a less in scenario 2 compared with scenario 1.

Solid waste

The amount of waste is assumed as constant at 2% of the product solid fraction. This equates to 200 t/a for the stand-alone sites and 1,000 t/a for the ICPS. For scenario 1, wastes are sent offsite for incineration and actual disposal costs at are used. Scenario 2 employs an onsite incinerator. The specific costs for waste disposal however vary considerably for the different sites in scenario 1. Overall, the costs for onsite incineration are 80 thousand €/a less in scenario 2 compared with scenario 1.

Waste for incineration preferably has a calorific value of from 13-25 MJ/kg and the waste fraction from polymer chemistry typically has a calorific value of over 25 MJ/kg, preferably of 28 to 32 MJ/kg (Kohler et al., 2000). For this case study, the calorific value of the polymer sludge is set at 28 MJ/kg. This is in the upper range for wastes which are incinerated, which normally fall between 6.5 and 29 MJ/kg (Stubenvoll et al., 2002, p.104). Thus, for 1,000 t/a of polymer waste, a residue incinerator operating at an efficiency of 80% and 7,500 h/a provides a thermal output of 0.8 MW and contributes 0.8 t/h of 16 bar steam. Based on the value of steam at Shanghai ICPS of 10.4 €/t, this equates to 63 thousand €/a.

Personnel

Actual personnel numbers and salaries were used as a basis for the calculations. This was done for the two main groups of employees, operations and laboratory personnel. In order to determine the number of personnel required for scenario 2, regression analysis was performed on personnel data from six actual sites ranging in capacity and number of production lines. The number of operations personnel was found to be strongly related the number of production lines (r^2 = 0.99), but not to capacity (r^2 = 0.36). The resulting trend is: $y = 30 \cdot x + 12$ *(for* $x \geq 1$*)* where: y = number of operations personnel, x = number of production lines. Thus, for Scenario 2, the number of operations personnel is calculated as 72 for two production lines. No trend was found for the number of laboratory personnel with increasing capacity or increasing number of production trains. For scenario 2, the same number of laboratory personnel is assigned as for scenario 1 in Shanghai. For scenario 2, the salaries for laboratory and operations personnel were taken as those for scenario 1 in Shanghai. Personnel overhead costs are calculated at 35% of the personnel cost.

The overall costs for scenario 2 are significantly lower than for scenario 1 due to the lower number of personnel required for a single production plant. Also, the personnel costs in China, although higher than in Indonesia and Philippines, are significantly lower compared to Japan and Australia. Within scenario 1, Japan was found to have the highest personnel costs, followed by Australia.

Maintenance

The costs for maintenance are assumed to be the same for each plant, at 5% of the cost of fixed capital.

Interest on Working Capital

This is fixed at 5%.

Indirect Plant Overhead

This is set at 60% of the cost of labour and maintenance.

Depreciation

For scenario 1, the investment cost for battery limits equipment and utilities provision are taken from actual project cost data. The costs per site for different countries are assumed to be equivalent, as the same production technology and sourcing for major equipment is assumed. For scenario 2, the investment costs for scenario 1 were scaled up based on capacity exponents. A capacity exponent of 0.60 was determined using actual investment data for all equipment (battery limits and utilities provision), which corresponded well to the factor given in the PEP report of 0.59 (PEP report 65A, 1991, Table 7.12). The capacity exponents used were: 0.55 for battery limits equipment and 0.61 for utilities provision, based on the PEP report. As the base case for scenario 2 has two production lines, the investment cost for the battery limits equipment was determined per line and summed for the two lines.

For scenario 2, the cost of buildings was calculated by scaling up the cost of buildings for scenario 1 according to the capacity exponent of 0.94, which was determined from actual investment data. This corresponded well to the exponent of 0.95 given for in PEP report 65A (1991, Table 7.12). Linear depreciation over 10 years for equipment and 20 years for buildings was determined.

Overall, the production cost for scenario 1 was calculated at 56.3 million €/a compared to scenario 2 at 47.2 million €/a. This is an annual difference of 9.1 million € in favour of scenario 2. The main cost components can be seen in the following table and graphic.

Table 6.6 Production Costs for the Polyacrylates Case Study

Scenario	1 - Stand-alone Sites						2 - Plant within ICPS	Cost Scenario 1 - Cost Scenario 2
Amount in '000 €/a	Shanghai, China	Manila, Philippines	Melbourne, Australia	Jakarta, Indonesia	Osaka, Japan	Sum Scenario 1	Shanghai, China	
Raw Materials	8,181	6,927	6,902	6,671	7,027	35,708	40,904	-5,196
Utilities	88	201	96	121	181	685	431	254
Waste	40	63	120	36	70	329	189	140
Personnel	638	229	3,070	973	3,518	8,428	1,057	7,370
Maintenance	243	243	243	243	243	1,216	775	441
Interest on Working Capital	292	292	292	292	292	1,460	1,000	460
Indirect Plant Overhead	529	284	1,988	730	2,257	5,786	1,099	4,687
Depreciation	535	535	535	535	535	2,677	1,775	902
Total Production Cost	10,547	8,774	13,246	9,600	14,123	56,289	47,231	9,058
Total Production Cost (mil €/a)						**56.3**	**47.2**	**9.1**

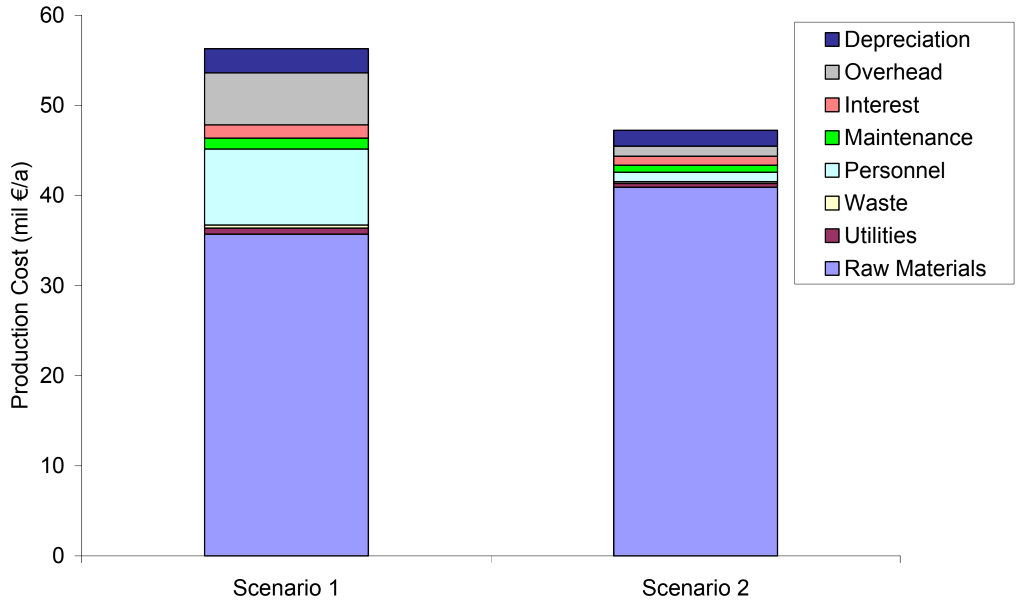


Figure 6.6 Production Cost Breakdown for PA Case Study

The following graph shows the breakdown of the production cost for scenario 2 (20 kt/a), scenario 1 (100 kt/a), and PEP report 65A (1991, Table 6.7) for a 23 kt/a emulsion polymerisation plant. It is evident that as the capacity increases, overhead and personnel costs become less important and raw materials costs become more prominent.

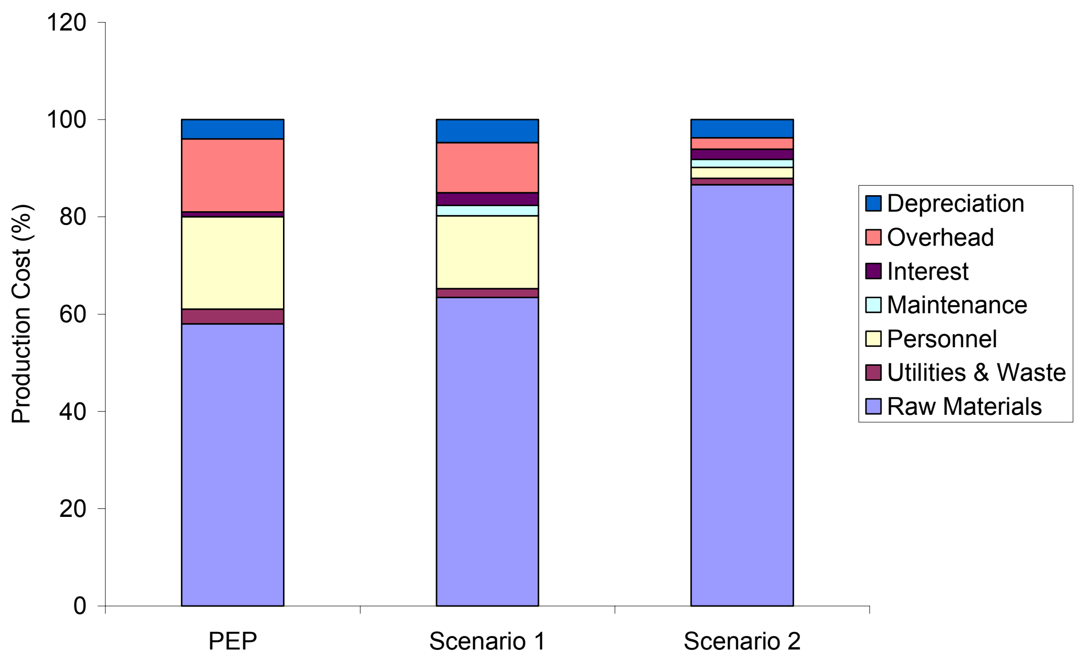


Figure 6.7 Comparison of Production Cost Breakdown for PA Case Study

The graphic below shows the cost difference between the two scenarios.

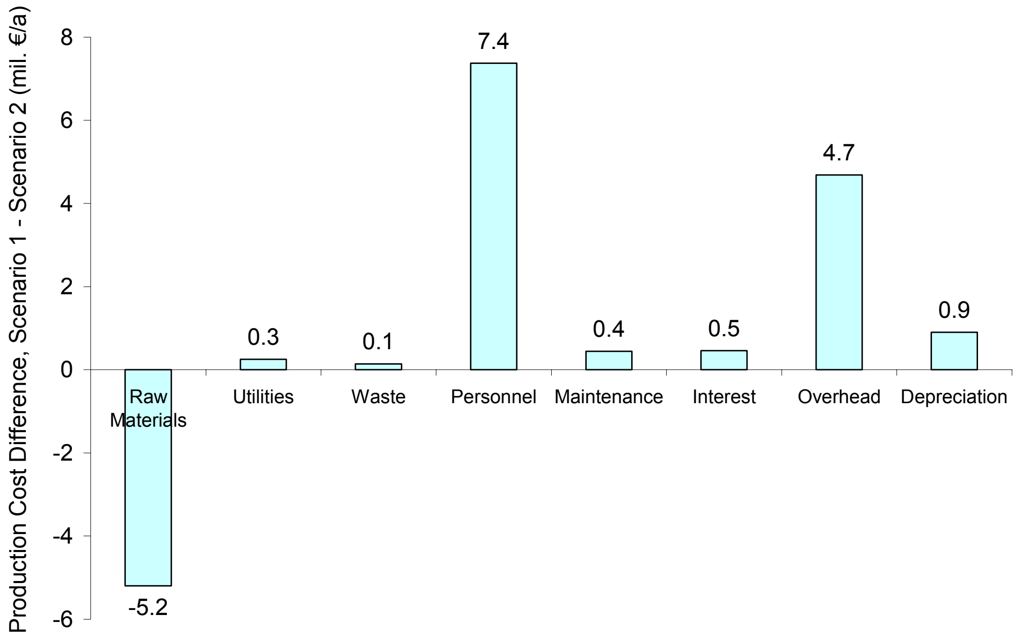


Figure 6.8 Production Cost Differences for PA Case Study

The only cost item which is higher for scenario 2 compared with scenario 1 is the raw materials cost; all other cost components are higher for scenario 1. The greatest difference in cost components between the two scenarios is for personnel, which comprises 52% of the increased cost for scenario 1, followed by overhead at 33%, depreciation at 6%, maintenance and interest at 3% each, utilities at 2%, and waste at 1%.

Variation of Major Parameters

In order to test the influence of certain parameters in the calculation, the following test scenarios are investigated. A graph showing the results of the tests follows.

Test A: Reduced Raw Materials Cost for Scenario 2

As raw materials costs are one of the predominant cost factors, this should be critically reviewed. The costs of raw materials are 19% higher than the average of the other sites. Perhaps if a larger volume of raw materials is purchased at a single site in China for scenario 2, lower costs may be negotiated. If the raw materials cost is held constant between the two scenarios, then the production costs for scenario 2 are further reduced to 42.0 million €/a.

Tests B and C: Change in Solids Content

Since raw materials are such a substantial cost, the % solids is also critical to the production cost. For test B, the % solids is reduced from 50% to 40%; thus, the raw materials cost decreases by 20% and the production cost becomes 49.2 million/a for scenario 1 and 39.1 million €/a for scenario 2. For test C, the % solids is increased from 50% to 60%; thus, the raw materials costs increase by 20% and the production cost becomes 63.4 million €/a for scenario 1 and 55.4 million €/a for scenario 2.

Test D: Reduced Personnel Cost for Scenario 1

The greatest cost difference between the two scenarios is for personnel, followed by overhead, which is calculated as a percentage of personnel costs. This is due to the larger number of personnel required for five sites compared to one large site as well as the higher salaries in Japan and Australia. To test the influence of salaries on the calculation, the salaries are assumed to be equivalent among the five stand-alone plants and set at the level of Shanghai. Then, the difference in the personnel cost between the two scenarios is 2.7 million €/a rather than 8.4 million €/a. Therefore, the additional personnel costs due to higher salaries in Japan and Australia account for an additional 5.7 million €/a.

Test E: Effect of One Plant Train for Scenario 2

The costs for maintenance, interest on working capital, and depreciation are all related to investment costs and reduced in scenario 2. This is due to economies of scale, as the investment costs for a single large plant with two production trains are lower than for the sum of five smaller plants. These costs can be even further reduced for scenario 2 if it is possible to construct a 100 kt/a plant with a single production train. Also, for one production train, the number of operations personnel is reduced to 42. For this test scenario, the depreciation is reduced by 347 thousand €/a, maintenance and interest on working capital by 174 thousand €/a, overhead by 365 thousand €/a, and personnel by 434 thousand €/a compared to the base case. The overall production cost for scenario 2 becomes 45.7 million €/a.

Other cost components are not investigated via test scenarios. The higher costs of waste removal for scenario 1 result from less expensive incineration due to an onsite incinerator in scenario 2. The higher costs for utilities in scenario 1 result from higher utilities costs in Philippines and Japan. As costs for waste incineration and utilities represent such a small fraction of the production costs, these are not further investigated.

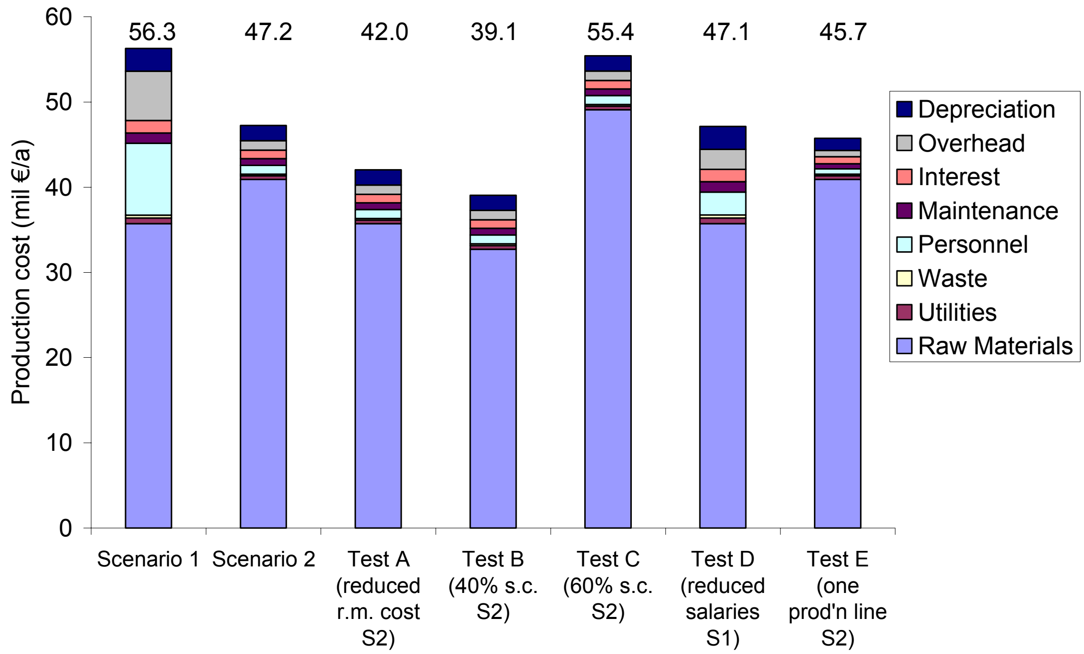


Figure 6.9 Production Cost Test Scenarios for PA Case Study

6.3.5 Logistics Costs

The comparison of logistics costs between scenarios investigates the costs for the logistics process chain only for raw materials which are available at the ICPS for scenario 2 and products for both scenarios. Raw materials available onsite in scenario 2 due to the plant's location in an ICPS are not available in scenario 1 and undergo various logistics steps in their transport from the ICPS to the different stand-alone sites. For scenario 2, these raw materials are transferred via pipeline within the ICPS. Products, on the other hand, undergo filling, packaging, storage, and dispatch for both scenarios, as products leave the site in both scenarios, however, only scenario 1 incurs freight costs for products.

Logistics costs for the eight locally sourced raw materials and the 32 imported raw materials are not considered, as these are considered equivalent and neutral in the calculation. For example, one of the locally sourced raw materials is styrene monomer, for which the transport costs within each country depends on the location of the provider.

The required logistics steps for raw materials and products are as follows:

- Storage, filling, packaging at the plant
- Inland transport and freight
- Port charges at both exporting and importing ports
- Import duty and taxes
- Storage/warehousing enroute
- Logistics management: dispatch, order- and materials management

Explanations and outcomes regarding the logistics cost items are given below, followed by tables summarising the logistics costs.

Storage

For raw materials available at the ICPS, the storage requirements per site for scenario 1 are three tanks, one each for butylacrylate (100 m^3), 2-ethylhexyl-acrylate (80 m^3), and glacial acrylic acid (20 m^3); for scenario 2, tanks are only located at the acrylic acid/esters plant as the raw materials are transferred by pipeline. For products, the storage requirements per site for scenario 1 are four products storage tanks: two at 100 m^3 and two at 200 m^3 and for scenario 2 the requirements are four tanks at 100 m^3 and six tanks at 200 m^3 (based on inquiry).

Filling

Filling costs for bulk shipments are set at 4 €/t for bulk and 13 €/t for drums for all locations (Stolt-Nielsen Transportation Group). For raw materials available at the ICPS, filling costs are incurred, as they need to be transferred from storage tanks to either containers or bulk tank trucks. At the polyacrylates plant they are again transferred from the tank truck to storage or kept in containers until they are required by production. Unloading costs are set equal to filling costs.

Packaging

For raw materials available at the ICPS, no packaging costs are incurred for butylacrylate, 2-ethylhexylacrylate, and glacial acrylic acid as they are transported by bulk. For ethylacrylate and methylacrylate, 1 ton containers are used. The polymer products are shipped as either bulk or packaged in drums or 1 ton containers. Each site has a different ratio of bulk/container/drum packaging. The packaging requirements for scenario 2 reflect the mix of packaging requirements in scenario 1 and the costs per packaging type are those for the Shanghai stand-alone site.

Inland Transport

Inland transport of raw materials in China is required for scenario 1 from the ICPS to the China stand-alone plant (50 km) by road at a cost of 4 €/t, but not for the other stand-alone sites, as their raw materials are shipped directly from the ICPS port via the Shanghai port (included in the freight cost). Once at the country port, they are transported by road to the stand-alone site, 100 km from the port. The inland transport costs are: Philippines 9 €/t, Australia 28 €/t, Indonesia 7 €/t, and Japan 83 €/t. No inland transport is required for products, as these are sold from the site or port.

Port Handling and Import Costs

Costs for raw materials or products leaving or entering a country include: customs clearance, import handling fees, broker costs, wharfage/port charges, tax and duty. These costs are incurred for raw materials in scenario 1 and for products in scenario 2. The port handling and clearance costs at disembarkation in China are 178 €/container for either raw materials or products per 20 foot container. The port costs for the materials arriving at each country is given below.

Table 6.7 Port Handling and Clearance Costs per 20 foot Container

Country	€ / transfer
Japan	321
Philippines	233
Australia	484
Indonesia	130
China	178

Import Tariff

These costs result for the import of raw materials and products. The total cost is based on different product categories and determined based on the product value. The product value is the CIF price, or cost, insurance and freight price, which is "*the price of a good delivered at the frontier of the importing country, including any insurance and freight charges incurred to that point, before the payment of any import duties or other taxes on imports or trade and transport margins within the country*" (OECD Glossary of Statistical Terms). The CIF price is set at 0.7 €/kg for products and 0.8 €/kg for raw materials available at the ICPS for this study based on actual data. Australia taxes polymers but not monomers, as there are no facilities in Australia for the manufacture of acrylic acid/esters. Whereas, Japan imposes a higher tariff on the raw material than on the polymer, as shown in the table below.

Table 6.8 Tariff Rates for AA/AE and Acrylic Polymers

Tariff (%)[16]	China	Philippines	Australia	Indonesia	Japan
Acrylic acid/ester (Tariff 2916)	6.5	3	0	10	6.4
Acrylic polymer (Tariff 3906)	8.4	7	5	17.5	4.6

It is important to note that the ASEAN (Association of Southeast Asian Nations) Free Trade Agreement (AFTA) has reduced tariffs among its Southeast Asian members by up to 5% and will eliminate duties entirely by 2010. China will join AFTA in 2010 and potentially Australia, Japan, and India may join (Graff, 2005).

Freight

Freight costs were acquired between various ports in Asia. The costs varied on average ±32% based on different carriers. Cost data were sourced from various carriers: Maersk, Cosco, PIL, CMA-CGM, Hanjin, NYK, Evergreen, OOCL, HL, KMTC, and RCL. The container transport costs are summarised below and shown graphically as specific costs per distance travelled in Figure 6.10.

Table 6.9 Freight Rates from Shanghai to Different Ports in Asia

	€ / 20' Container	€ / 40' Container
Shanghai -> Melbourne	904	1,761
Shanghai -> Osaka	640	1,083
Shanghai -> Jakarta	492	897
Shanghai -> Manila	650	1,093

However, it is important to note that the prices for sea freight are not only a function of distance, but also depend very much on the supply and demand for different routes. For this study, all shipments are transported by 20 foot

[16] Based on the Asia Pacific Economic Cooperation Tariff Database.

container. The loading per container is adjusted according to packaging type (eg. 20 tons for bulk, 17.7 tons for drums, 18 tons for containers).

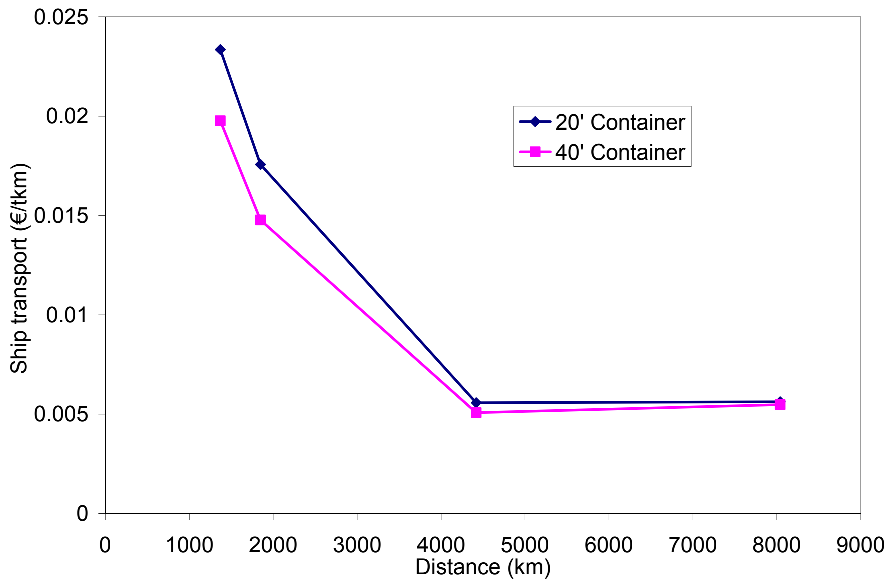


Figure 6.10 Freight Costs as a Function of Distance

In the below table, freight rates among the different locations are provided. On average, freight rates out of Jakarta are the least expensive, followed by Shanghai.

Table 6.10 Freight Rates within Asia for 20 foot Container

Freight cost (€/container), From/To	Melbourne Australia	Jakarta Indonesia	Manila Philippines	Shanghai China	Osaka Japan	Mean
Jakarta Indonesia	840	X	348	227	671	522
Manila Philippines	1,217	467	X	325	917	732
Shanghai China	904	492	650	X	640	672
Osaka Japan	1,725	433	588	620	X	842

Storing / Warehousing

This is required for raw materials available at the ICPS for scenario 1 and for products for scenario 2. For scenario 1, enroute storing/warehousing is not considered to be required for the stand-alone plant in Shanghai.

Handling, Dispatch, Order & Materials Management

Handling, dispatch, and order- and materials management costs are incurred for both raw materials and products transported offsite. Also, there is a minimal cost for the management of flows between integrated plants in scenario 2.

Raw Materials Available at the ICPS

The graphic below shows the logistics costs for raw materials at the ICPS. The largest components are import tariff, freight, inland transport, and port costs.

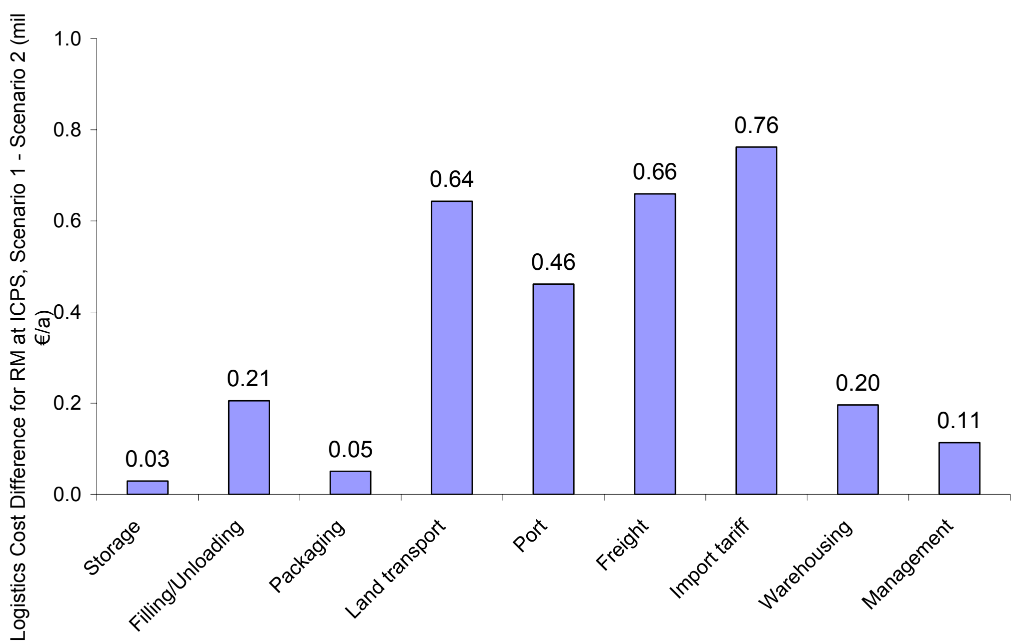


Figure 6.11 Logistics Cost Differences for Raw Materials in PA Case Study

Products

Scenario 2 incurs much greater logistics costs due to the transport of products to the countries. For scenario 1, logistics costs are highest in Shanghai due to high packaging costs. The only item which is greater in scenario 1 than scenario 2 is the cost of storage tanks, due to greater requirements for five stand-alone sites. The import tariff is the highest logistic cost, followed by freight and port costs.

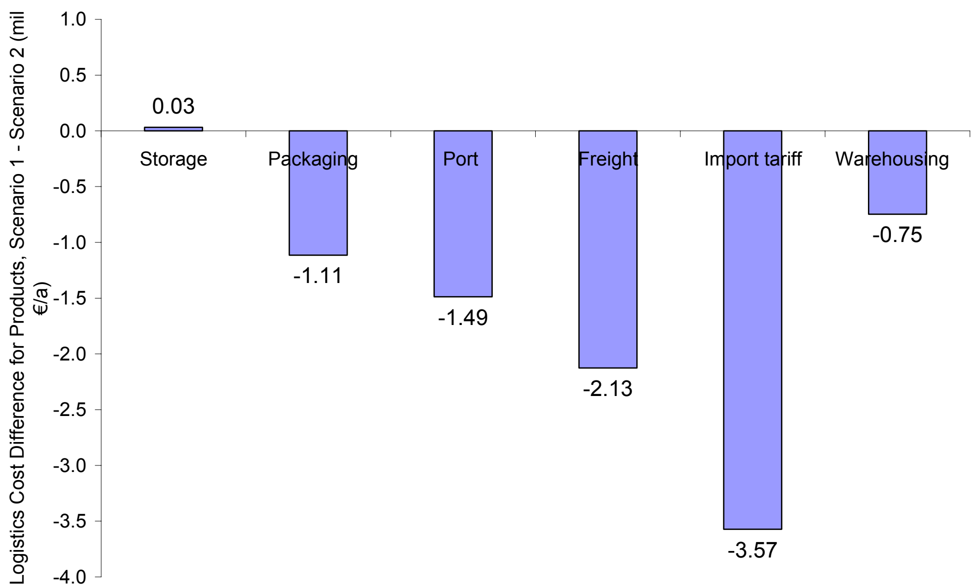


Figure 6.12 Logistics Cost Differences for Products for PA Case Study

The graphic below shows the distribution of logistics-related costs for the two scenarios for raw materials available at the ICPS and products. In scenario 1, raw materials are transported from the ICPS to the countries, thus incurring costs from various logistics steps, whereas products only incur logistics costs in the country where they are produced, mainly due to packaging. In scenario 2, the products incur costs for all logistics steps, as raw materials never leave the site.

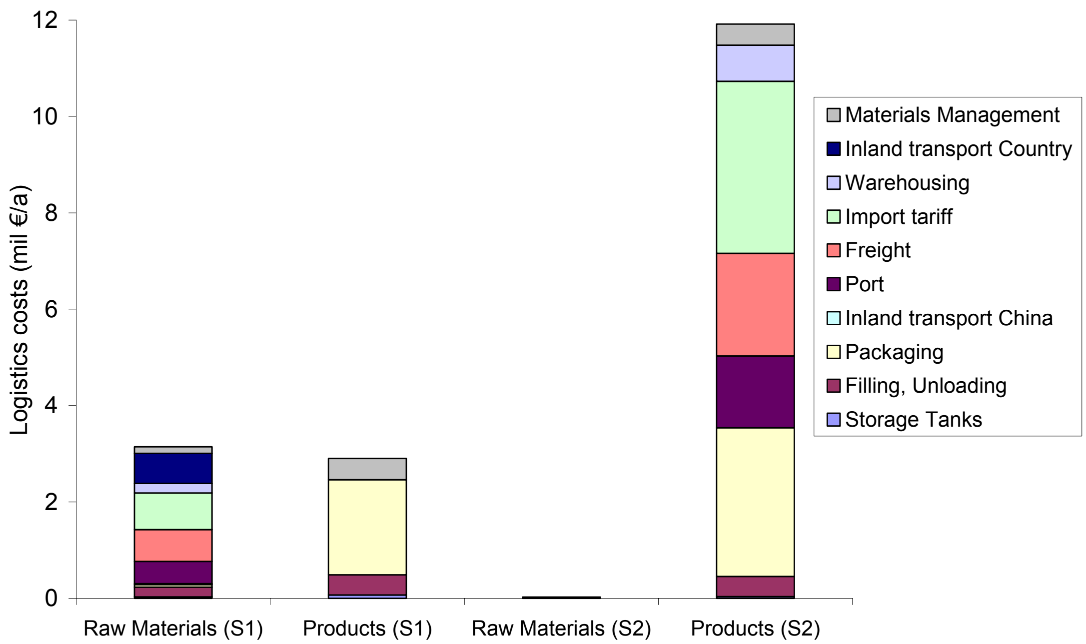


Figure 6.13 Logistics Costs for Raw Materials & Products for PA Case Study

Table 6.11 Logistics Costs for Raw Materials in PA Case Study

Scenario	1 - Stand-alone Site						2 - Plant within ICPS	Cost Scenario 1 – Cost Scenario 2
Amount ('000 €/a)	Shanghai, China	Manila, Philippines	Melbourne, Australia	Jakarta, Indonesia	Osaka, Japan	Sum Scenario 1	Shanghai, China	
Storage Tanks	6	6	6	6	6	29	0	29
Filling	21	21	21	21	21	103	0	103
Packaging	10	10	10	10	10	51	0	51
Inland transport China	20	0	0	0	0	20	0	20
Port	0	101	162	76	122	461	0	461
Freight	0	160	222	121	157	659	0	659
Import tariff	0	118	0	393	251	762	0	762
Warehousing	0	49	49	49	49	196	0	196
Inland transport Country	0	44	137	34	407	643	0	623
Unloading	21	21	21	21	21	103	0	103
Dispatch, Order & Materials Management	27	27	27	27	27	137	25	113
Total Logistics Costs for Raw Materials available at ICPS	98	576	675	777	1,092	3,242	25	3,091
Total Logistics Costs for Raw Materials available at ICPS (mil €/a)						**3.1**	**0.02**	**3.1**

Table 6.12 Logistics Costs for Products in PA Case Study

Scenario	1 - Stand-alone Site						2 - Plant within ICPS	Cost Scenario 1 – Cost Scenario 2
Amount (‘000 €/a)	Shanghai, China	Manila, Philippines	Melbourne, Australia	Jakarta, Indonesia	Osaka, Japan	Sum Scenario 1	Shanghai, China	
Storage Tanks	14	14	14	14	14	68	35	33
Filling	162	105	15	79	58	419	419	0
Packaging	895	373	181	299	224	1,973	3,087	-1,115
Port	0	0	0	0	0	0	1,489	-1,489
Freight	0	0	0	0	0	0	2,127	-2,127
Import tariff	0	0	0	0	0	0	3,572	-3,572
Warehousing	0	0	0	0	0	0	748	-748
Dispatch, Order & Materials Management	88	88	88	88	88	441	441	0
Total Logistics Costs for Products	1,159	580	298	480	384	2,901	11,919	-9,018
Total Logistics Costs for Products (mil €/a)						**2.9**	**11.9**	**-9.0**

Table 6.13 Logistics Costs for Raw Materials & Products in PA Case Study

Scenario	1 - Stand-alone Site						2 - Plant within ICPS	Cost Difference: Scenario 1 - Scenario 2
Amount (mil €/a)	Shanghai, China	Manila, Philippines	Melbourne, Australia	Jakarta, Indonesia	Osaka, Japan	Sum Scenario 1	Shanghai, China	
Total Logistics Costs for Raw Materials available at ICPS	0.10	0.55	0.65	0.75	1.07	3.12	0.02	3.09
Total Logistics Costs for Products	1.16	0.58	0.30	0.48	0.38	2.90	11.92	-9.02
Total Logistics Costs for Raw materials avail. at ICPS and Products	**1.26**	**1.13**	**0.95**	**1.23**	**1.45**	**6.02**	**11.94**	**-5.93**

6.3.6 Variation of Major Parameters

The previous test scenarios are revisited with respect to logistics costs. Tests A (reduced raw materials cost for scenario 2), D (reduced personnel cost for scenario 1), and E (one plant train for scenario 2) all have no influence on the logistics costs. However, tests B and C (changes in solids content), do. For these, the amount of raw materials changes, so the logistics costs change. The logistics costs for scenario 1 then become 5.3 and 6.5 million €/a for solids contents of 40% and 60%, respectively, compared to the base case at 6.0 million €/a. For scenario 2, the same amount of emulsion is transported, however, a change in raw materials costs is expected to be reflected in product price and thus in product tariff, which is estimated to increase or decrease by 80 thousand €/a, representing less than 1% of the logistics costs.

The schematics below compare the overall costs for the tests. Since raw material costs are such a significant component of the production costs, changing the solids content has a large impact on the total costs. Also, personnel costs changes strongly effect the overall cost.

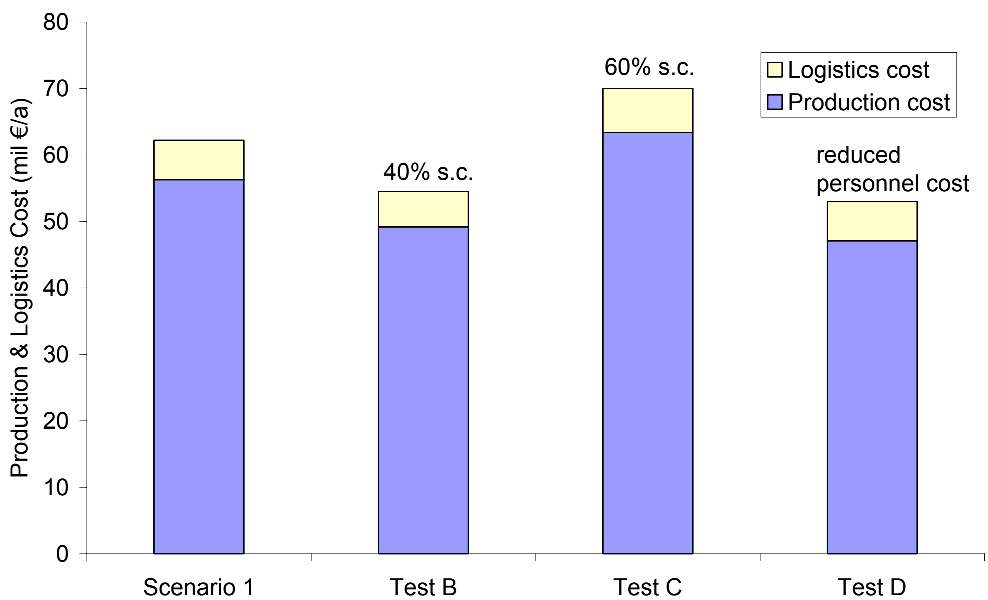


Figure 6.14 Costs for PA Case Study Scenario 1 and Test Scenarios

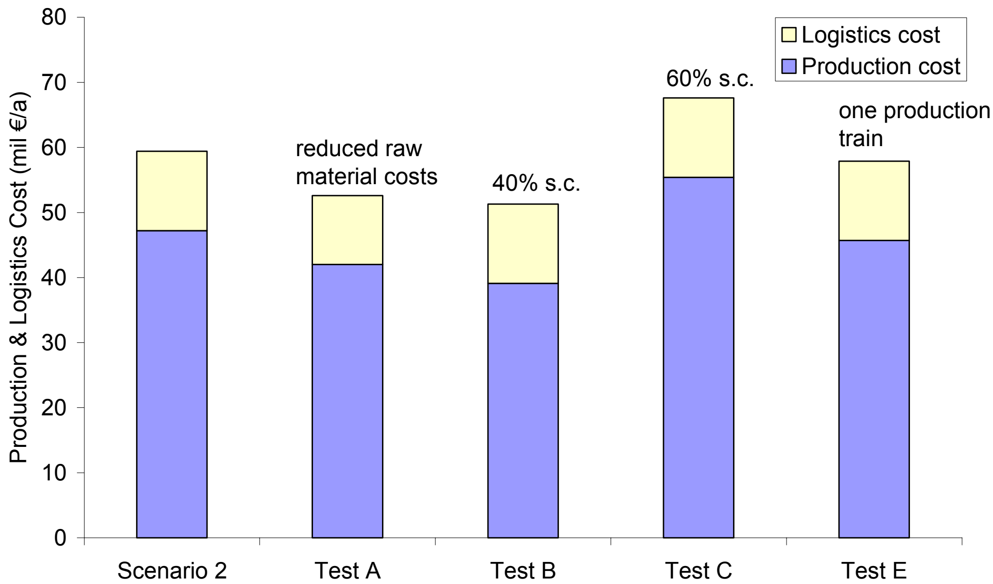


Figure 6.15 Costs for PA Case Study Scenario 2 and Test Scenarios

Variation Spraydried Polyacrylates

Polyacrylate dispersions have a high water content for ease of reaction and handling. This water is added during the production process and remains in the product through to its delivery to the customer. This water may be removed when the customer processes the product in the manufacture of a paint, adhesive, or construction material. Thus, in most cases, the transport of water in the product is required. However, it may be possible to spraydry some polyacrylates so that the product is transported as a powder. In this case, the additional costs for the transport of water in the product are saved. The tariff is assumed to be unchanged. Then the total logistics cost becomes 4.5 and 6.1 million €/a for scenarios 1 and 2, respectively; a difference of 1.6 million €/a.

Table 6.14 Costs for PA Case Study with Spraydried Product

Total Logistics Cost (mil €/a)	Scenario 1	Scenario 2	Difference S1 – S2
Base case cost	6.0	11.9	-5.9
Cost if product spraydried	4.5	6.1	-1.6

6.3.7 Discussion of the results

The difference in the sum of production and logistics-related costs for the two scenarios is 3.3 million €/a in favour of scenario 2. This is a reduction of 5% in the combined production and integration-related logistics costs relative to scenario 1.

Table 6.15 Summary of Costs for PA Case Study

	Scenario 1	Scenario 2	Cost Difference S1 - S2
Production cost (mil. €/a)	56.3	47.2	9.1
Steam benefit through waste incineration (mil. €/a)		-0.06	0.06
Logistics cost (mil. €/a)	6.0	11.9	-5.9
Total cost (mil. €/a)	**62.3**	**59.0**	**3.3**
% Logistics cost relative to Production cost	10	26.0	
% Steam benefit from Incineration relative to Production cost		-0.1	

The production of steam through onsite waste incineration provides a negligible advantage for scenario 2. The costs are shown graphically below.

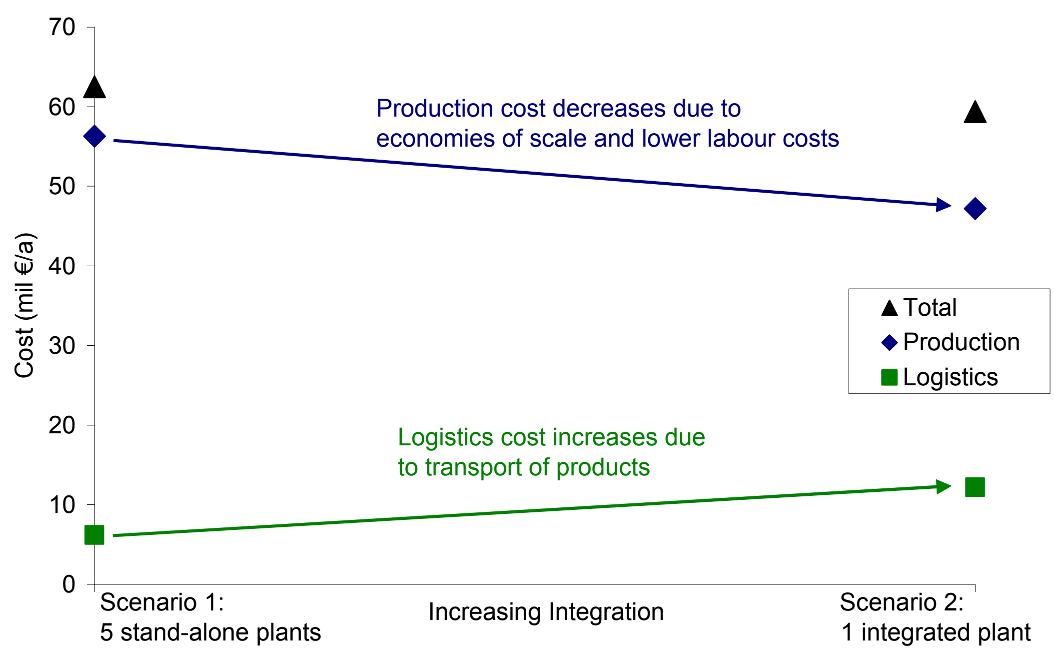


Figure 6.16 Total Costs for PA Case Study

As one scenario does not present a clear cost advantage over the other, additional advantages or disadvantages of the two scenarios are considered.

Advantages and Disadvantages of the two Scenarios

Advantages of Scenario 1

- Local production may be able to better cater to customers' local needs. The product spectrum and packaging requirements may be adjusted locally to suit specific needs in a country.
- Local production allows the product to be delivered to the customer more quickly compared to shipping from Shanghai. The additional delivery time for products arriving from Shanghai may be up two additional weeks, as this depends on several logistics steps and freight schedules. A customer may appreciate short delivery times, particularly for urgent orders. Shipping time is not a concern for the product shelf-life (on average 6 months).
- Local production may allow for better partnership with local customers. By having a plant in the same country as the customer, closer communication between the producer and customer is expected. Language barriers are avoided and the customer may be able to visit the production site more easily. Also, there may be customer loyalty to locally produced products.
- It may be difficult to export products to certain countries where tariff barriers exist. For example, importing products to India may be very costly due to tariffs, thus local production may be favoured.
- Possibly more input regarding production improvements may result due to an increased number and diversity of employees as well as variations in production practices at the different locations.

Advantages of Scenario 2

- The handling of monomers, an explosive raw material, is contained at only at one site, limiting risk.
- Better product consistency may be achieved through the use of one production plant.
- Procurement costs for packaging and raw materials may be reduced due to the ability to negotiate better prices for larger quantities.
- Product volumes per country can be adjusted to meet local sales demands.
- All knowledge is pooled at one location.

Disadvantages of Scenario 1

- Plant size is fixed per country, making it difficult to adjust volumes according to market needs.
- Greater coordination is required among plants and headquarters regarding production issues.

Disadvantages of Scenario 2

- A greater transport volume due to product transport to the countries leads to increased fuel consumption and emissions (shown in detail in Section 6.6).
- Higher risk of loss if a production batch is off-specification due to the larger batch size.
- Potentially higher dependency on raw materials suppliers in terms of supply and price.

Concluding Remarks and Comparison with Actual Cases

The polyacrylates case study was conceived based around the actual production configuration of a particular chemical company. In Asia, the company has several stand-alone polyacrylate plants in different countries, whereas in Europe, one large-scale plant located within an ICPS serves primarily European countries. For the polyacrylates plant in Europe, the favourability of being located within an ICPS may depend on where primary customers are located. The scenario of production within an ICPS in Asia evaluated in this work shows that significant production cost reductions can be achieved through economies of scale by having only one production site. However, the costs associated with port and tariffs/duties are very high; these are anticipated to be reduced due to new free trade regulations in Asia in the future. This aspect, however, is not a current concern within Europe. Transport costs associated with the increased volume of products compared with raw materials due to the high fraction of water in the product may be reduced if products are spraydried and sold in powder form. This is not expected to be possible for all products due to technical/chemical limitations, as this not common in the polyacrylate industry. This case study shows that the benefits of integration depend on the location (port, tariffs, distance) of raw materials and customers, as the plant is located at the end of the value chain and all products require offsite transport.

6.4 Plant Case Study 2: Aniline

The aniline process is selected as the second case study, as it provides one important aspect which is advantageous for integration which the previous case study does not. For aniline production based on the fluidised-bed process, the heat of reaction may be utilised for steam production for the steam network in an ICPS. As for the previous study, this study investigates an actual case. The aspects of steam export and logistics in this case study allow the relative significance of these two aspects to be investigated.

6.4.1 Background on the Process

Aniline is an aromatic amine and has, over the last 145 years, become one of the hundred most important building blocks in chemistry. It is used as an intermediate in many different fields of application: MDI, rubber processing chemicals, dyes and pigments, agricultural chemicals, and pharmaceuticals (Ullmann, 2000). Nearly 80% of the world's aniline is used in the production of MDI (PEP report 76C, 1993, p.1-1), which is the main isocyanate reacted with alcohols to produce polyurethanes used in construction, furniture, automotives, and insulation. The polyurethane value chain in which aniline is an intermediate process, is shown below.

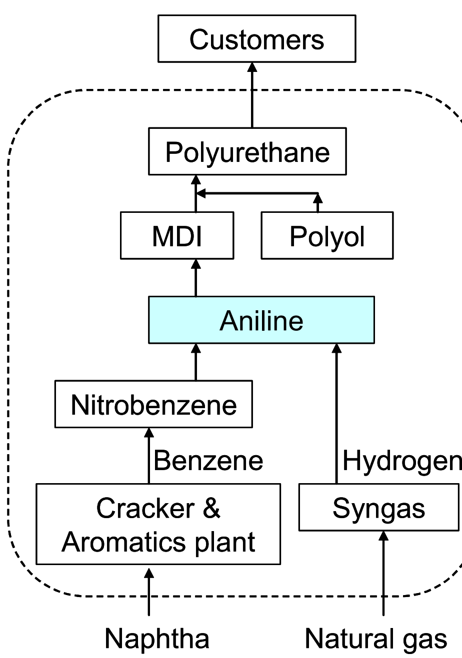
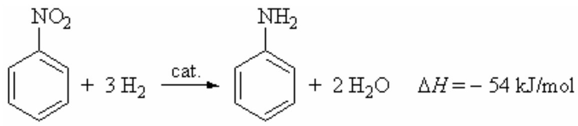


Figure 6.17 Location of the Aniline Process in Polyurethane Value Chain

The highly exothermic catalytic hydrogenation (△H=–544 kJ/mol at 200°C) of nitrobenzene with hydrogen, shown below, is performed commercially in either the vapour or liquid phase (Ullmann, 2000).



More than 95% of all nitrobenzene produced globally is used for the production of aniline (PEP report 76C, 1993, p.2-1).

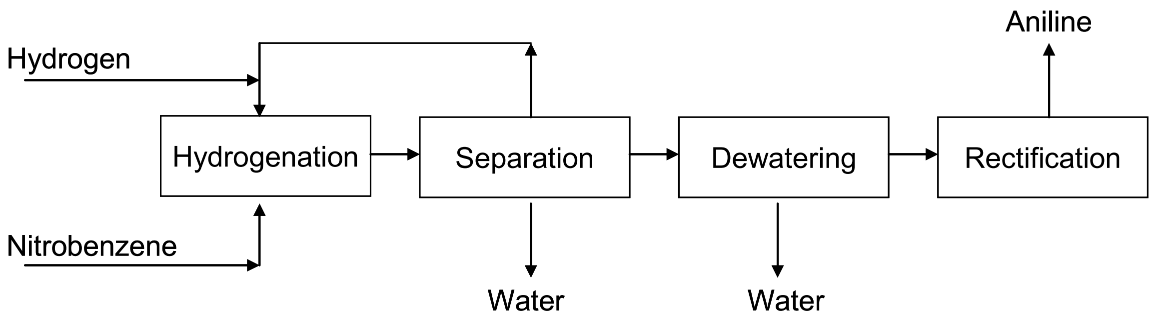
6.4.2 Process Description

The following is summarised from Ullmann (2000). In the catalytic vapour-phase hydrogenation process, nitrobenzene is hydrogenated to aniline with over 99% yield via a fixed-bed or fluidised-bed reactor. A copper or palladium catalyst on an activated carbon or an oxidic support in combination with other metals as modifiers or promoters is used in order to achieve high activity and selectivity.

In the vapour-phase, fluidised-bed process, the focus of this case study, nitrobenzene is injected through nozzles located at several heights in the fluidised bed and the hydrogenation is carried out at 250 to 300°C and 400 to 1000 kPa in the presence of excess hydrogen. A stream of gas is circulated in the presence of a fluidised catalyst, the reaction products are condensed, and aniline is separated from the isolated crude reaction products. The catalyst is copper on a silica support promoted with chromium, zinc, and barium. The hot product gas is cooled by passing it through a heat exchanger, and aniline is isolated in a liquid–gas separator. The reaction heat is used for steam production.

For catalyst regeneration, after flushing the whole system with nitrogen, the organic material deposited on the catalyst surface is burned off with air. After the regeneration, the air is replaced with nitrogen and the catalyst is activated again by reducing the copper oxide to copper with hydrogen at 200 to 300 °C.

A general schematic of the production process is given below. A detailed process flow diagram can be found in Appendix D.



(based on Ullmann, 2000)

Figure 6.18 Simplified Aniline Process

6.4.3 Scenarios for Aniline Case Study

For all scenarios, the plant has a capacity of 100 kt/a of aniline and is fully utilised, producing at 7,500 h/a.

Three scenarios are defined:
Scenario 1: a stand-alone plant in Antwerp, Belgium
Scenario 2: as a semi-integrated plant in Ludwigshafen, Germany
Scenario 3: fully integrated in an ICPS in Antwerp, Belgium

As for the polyacrylates case study, scenario 1 represents the stand-alone case. However, in reality, aniline plants, are not known to exist as stand-alone plants, thus a second scenario is defined where one of the two main raw materials, nitrobenzene, is not available onsite. This scenario (scenario 2) is based on an actual case in which nitrobenzene required transport from an ICPS in Antwerp, Belgium to an aniline plant in Ludwigshafen, Germany. For scenario 2, the nitrobenzene plant capacity is sufficient to supply the aniline requirements in both Antwerp and Ludwigshafen. For scenario 3, the aniline plant is located within an ICPS in Antwerp, Belgium.

For scenario 2, both the Ludwigshafen and Antwerp sites are, on the whole, integrated sites. However, for the case of the polyurethane value chain, the Ludwigshafen site is considered to be a semi-ICPS, as the value chain is incomplete, since nitrobenzene is not available onsite and must be purchased externally and transported to the site. The scenarios are described in the following table as well as shown schematically.

Table 6.16 Scenario Description for Aniline Case Study

	Scenario 1 one stand-alone plant	Scenario 2 one plant in semi-ICPS	Scenario 3 one plant in ICPS
Description	No onsite nitrobenzene and hydrogen supply, no steam export, aniline transport offsite	No onsite nitrobenzene, steam exported to site network, 80% of aniline used onsite by MDI plant	Nitrobenzene and hydrogen onsite, steam exported to site network, 80% of aniline used onsite by MDI plant
Nitrobenzene production	Antwerp ICPS	Antwerp ICPS	Antwerp ICPS
Hydrogen production	Antwerp ICPS	Ludwigshafen, Germany	Antwerp ICPS
Aniline Location	100 kt/a plant 50 km from Antwerp ICPS, 50 km from port	100 kt/a plant in Ludwigshafen, Germany, 400 km from Antwerp	100 kt/a plant in Antwerp ICPS

For scenario 1, all aniline is shipped offsite, as it is a stand-alone plant. In scenarios 2 and 3, the aniline is further processed along the polyurethane value chain to produce MDI and then polyurethane, which is sold to offsite customers. In scenarios 2 and 3, 80% of the aniline is used for onsite MDI production. This is consistent with other producers, as 80% of the world's aniline goes into MDI production (PEP report 76C, 1993, p.1-1).

Below, a schematic showing the locations and transport routes for the three scenarios is shown. This is followed by a discussion of the production and logistics costs related to integration.

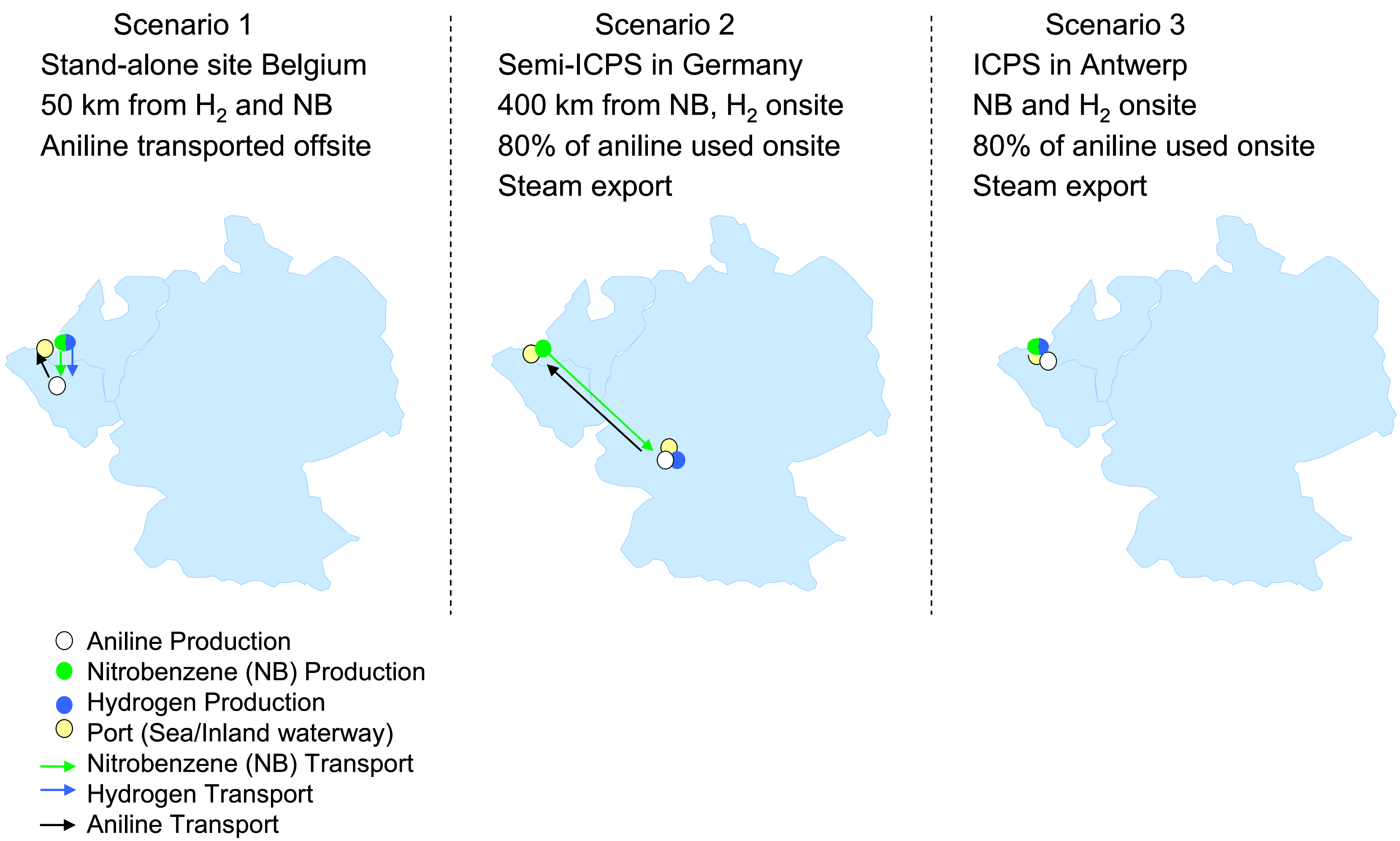


Figure 6.19 Locations and Transport Routes for Aniline Case Study

6.4.4 Production Costs

Production costs given in PEP report 76C (1993, p.5-15) for a comparable plant (capacity and process) are 815 €/t, or 81.5 million €/a for the vapour phase aniline production process, where raw material costs account for over 75% of the product cost. Production costs are assumed to be equivalent for the three scenarios for this case study, as the plants are identical in capacity and design. Personnel costs between Antwerp and Ludwigshafen are assumed to be similar. Cooling water and electricity are the main utilities requirements. These costs, as well as the costs for other utilities and infrastructure may be lower for scenarios 2 and 3, as they are located in integrated sites. However, the costs for utilities are assumed to be the equivalent at both Antwerp sites. Also, the costs for water and electricity are less than half the value of the benefit derived from steam export, thus the overall utilities costs for the process are negative (PEP report 76C, 1993, p.5-14). Thus, any differences in utilities cost for electricity or cooling water due to economies of scale in an integrated site are expected to not be significant for the case study. The only aspects related to production considered in the case study are the energy benefits related to heat recovery and waste incineration, but not costs related to equipment or infrastructure, as this is not the main focus of this case study.

Table 6.17 Comparison of Scenarios for Aniline Case Study

Aspect	Scenario 1 one stand-alone plant	Scenario 2 one plant in semi-ICPS	Scenario 3 one plant in ICPS
Logistics	Handling, transport, storage of NB, H_2 and AN (50 km).	Handling, transport, storage of NB (400 km). Pipeline transfer of 80% of AN.	Pipeline transfer of NB and 80% of AN.
Materials	No useable by-products, wastes incinerated offsite, off-gases flared, waste water sent offsite for treatment	No useable by-products, wastes and off-gases incinerated onsite for steam production, waste water treated onsite	Same as scenario 2
Energy	No heat recovery or steam from waste incineration	Steam from heat recovery and waste incineration exported to steam network	Same as scenario 2
Infra-structure	SA infrastructure	ICPS infrastructure	Same as scenario 2

Waste Treatment and Incineration

According to PEP report 76C (1993, p.5-12), an incinerator and waste treatment are part of the production plant comprising 14% of the total capital investment. The incinerator is integrated in the purification section of the plant and is used to treat both the organic streams (heavy and light ends from distillation) and waste water streams (PEP report 76C, 1993, p.7-13). Thus, the operating costs for waste treatment are included in the production costs for each of the scenarios. However, in an ICPS, perhaps the residue streams would be centrally incinerated for steam production. Potentially the heavy and light ends, hydrogen purge stream, and uncondensed vapours, totalling 3,211 t/a, may be incinerated in a residue incinerator. The amount of steam produced, based on a calorific value of 15 MJ/kg (consistent with Bayer's chemical residue incinerator) is 13,214 t/a of 16 bar steam. Based on the value of steam at Ludwigshafen and Antwerp, this is a benefit of: 96 and 71 thousand €/a, respectively.

6.4.5 Logistics Costs

The required logistics steps for raw materials and products are as follows:

- Storage and filling at the plant
- Inland transport
- Logistics management: dispatch, order- and materials management

Compared to case study 1, there are no costs associated with ports, import, or packaging, as the materials are transported in bulk and within the EU. Also, external warehouse costs are not considered due to the direct inter-company transport. Explanations and outcomes regarding the cost items under production cost are given below, followed by tables summarising the logistics costs.

Storage of Nitrobenzene and Aniline

In scenarios 1 and 2, nitrobenzene storage at the aniline plant is required consisting of one 3,000 m^3 tank to hold an inventory of one week. In scenario 3, no nitrobenzene storage is considered at the aniline plant. Aniline storage for scenario 1 is one 2,200 m^3 storage tank, representing a one week inventory, as there is no onsite recipient of the aniline. For scenarios 2 and 3, as 80% of the aniline is consumed onsite, a 600 m^3 storage tank is assumed, representing two days of inventory. For all cases, nitrobenzene storage at the nitrobenzene plant is not considered, as this is outside of the system boundary.

Transport of Nitrobenzene and Aniline

For scenario 1, aniline and nitrobenzene are transported by tank truck (as the stand-alone plant is assumed to not have access to a rail line) at a cost of 18 €/t for the 50 km distance. For scenario 2, nitrobenzene transport is estimated at 44 €/t for tank truck and 31 €/t for rail for the 400 km distance between Antwerp and Ludwigshafen. Thus, the transport cost is reduced by 30% for rail versus road transport. In this case, rail transport is chosen as it is used in the actual case. In scenario 2, there are costs associated with the transport of 20 kt/a of aniline to the nearest international port or customer hub, which is Antwerp. In scenario 3, 20 kt/a of aniline undergo logistics management costs, as they are sold offsite, however, transport is not considered due to the location of the ICPS at a major chemicals hub. The costs for dispatch, filling, and order- and material management are determined according to the methodology.

Storage and Transport of Hydrogen

Hydrogen transport and storage are considered separately from aniline and nitrobenzene storage due to greater technical requirements and costs. The costs of various transport and storage modes according to the required amount and distance were reviewed by Amos (1998). The most suitable combination for this case, based on the amount (8 kt/a) and distance (50 km) is transport by either pipeline (without storage) or transport as liquid hydrogen by metal hydride tank truck and storage in underground tanks. Process costs for the liquification of the hydrogen at the Antwerp ICPS are assumed to be part of the hydrogen production process.

The cost for transport by metal hydride tank truck is 308 €/t and 100 €/t for underground storage (Amos, 1998, pp.H-2-H-5). This is consistent with transport costs cited by other sources (Barry and Acevez, 2005). The annualised cost for pipeline transport, at 292 €/t, is slightly less than the cost of transport by metal hydride truck (Amos, 1998). However, in this case, in addition to avoiding emissions from road transport, storage is not required, reducing the overall logistics costs from 9.7 to 8.9 million €/a, or 9%. For this study, as the plant is considered to be truly stand-alone, transport by tank truck rather than by pipeline is selected. For scenarios 2 and 3, hydrogen is supplied onsite via pipeline from an onsite synthesis gas plant.

Table 6.18 Logistics Costs for Aniline Case Study

Scenario	1 - Stand-alone plant	2 - Semi-ICPS	3 - Plant within ICPS	Difference: Scenario 1 - Scenario 3	Difference: Scenario 2 - Scenario 3
Location	50 km from Antwerp ICPS and port	Ludwigshafen, Germany	Antwerp, Belgium		
Amounts for logistics calculation:					
Aniline (kt/a)	100	20	20		
Nitrobenzene (kt/a)	135	135			
Hydrogen (kt/a)	8				
Transport H2 ('000 €/a)	2,382				
Transport NB, An ('000 €/a)	4,230	4,860		4,230	4,860
Storage H2 ('000 €/a)	774				
Storage NB, An ('000 €/a)	59	34	0.9	58	33
Filling (NB, An) ('000 €/a)	940	620	80	860	540
Dispatch ('000 €/a)	243	155	20	223	135
Materials management ('000 €/a)	1,118	713	92	1,026	621
Total Logistics Costs for RM ICPS per Site ('000 €/a)	**9,746**	**6,382**	**193**	**9,553**	**6,189**

Below, the logistics costs for both raw materials and products are shown as well as the difference in costs between scenarios.

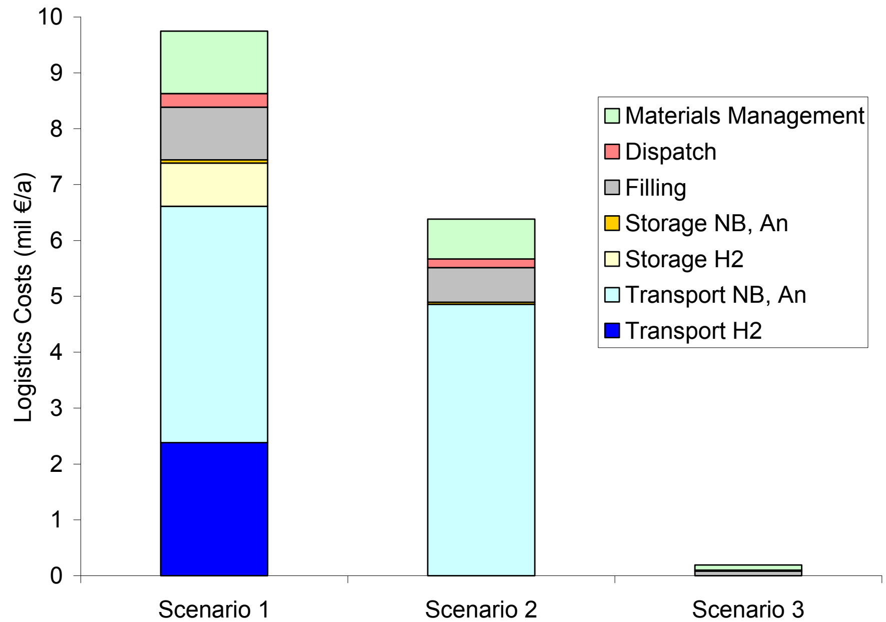


Figure 6.20 Logistics Costs for Aniline Case Study

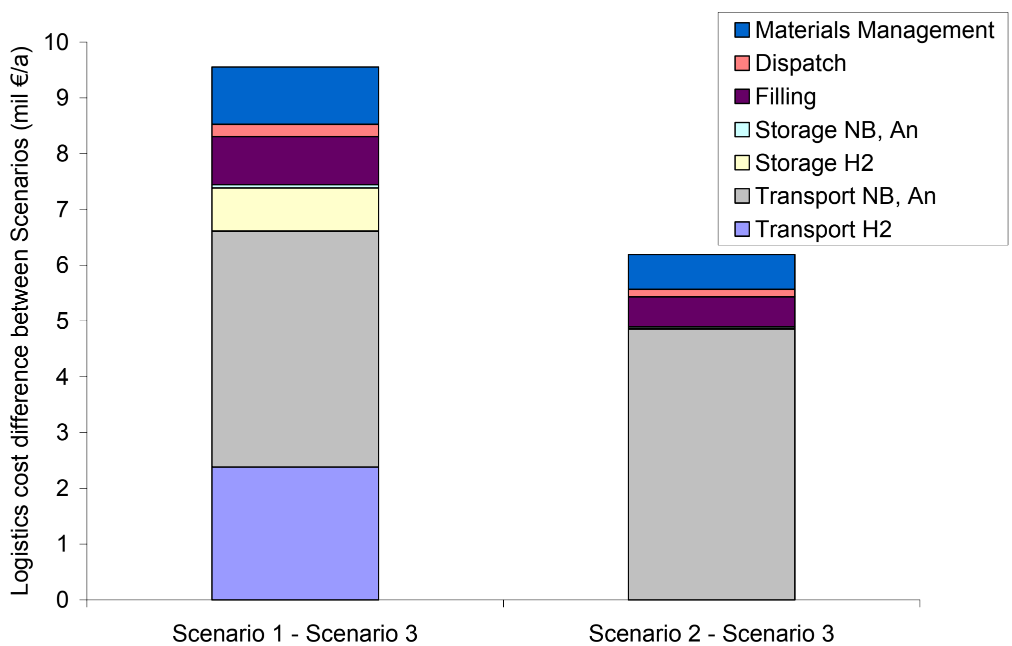


Figure 6.21 Logistics Cost Differences for Aniline Case Study

The cost of hydrogen transport and storage are very substantial for scenario 1. Also, the cost of transport is high for both scenarios 1 and 2 on account of nitrobenzene transport. In scenario 1, although both hydrogen and nitrobenzene require transport, the distance that the nitrobenzene is transported is much higher for scenario 2.

6.4.6 Energy

For the vapour-phase fluidised-bed process, the heat of reaction is removed via an internal heat exchanger which is used for the production of steam. For every ton of aniline produced, approximately 1.1 ton of steam is co-produced, as given in the table below (PEP report 76C, 1993, p.5-14). Due to the location of the aniline plant within an ICPS, this steam can be exported to a steam network for use by other onsite plants. The amount of steam produced from the process' heat of reaction is much more than that from incineration of wastes.

This exported steam is valued differently for the two sites based on the actual internal transfer prices. These are higher than the value of 4.6 €/t given for both pressure levels in the PEP report (PEP report 76C, 1993, p.5-14). The cost benefit is thus very dependent on how the value of steam is calculated at a particular site. For an ICPS, this value is moderate as it is based on the cost of producing steam in highly efficient cogeneration plants.

Table 6.19 Steam Export for Aniline Production by Fluidised-Bed Process

Steam Export	Scenario 2	Scenario 3
Amount of steam (t steam/t aniline)		
4 bar	0.47	0.47
16 bar	0.63	0.63
Value of steam (€/t)		
4 bar	6.3	5.4
16 bar	7.3	5.4
Benefit of steam (€/a)		
4 bar	297,990	255,420
16 bar	460,630	340,740
Benefit of steam from heat recovery (€/a)	758,620	596,160
Benefit of steam from waste incineration (€/a)	96,462	71,356
Total steam benefit (€/a)	**855,082**	**667,516**

Alternatively, a fixed bed reactor can be used for the production of aniline. It should be noted that only the vapour phase process enables steam export. Other processes have steam requirements as follows (PEP report 76C, 1993, pp.4-14,4-27,6-15) and therefore, do not provide an energy benefit to the ICPS:

- Conventional nitration process: 10 bar: 0.24 kg/kg AN, 40 bar: 0.026 kg/kg AN
- Adiabatic nitration process: 10 bar: 0.42 kg/kg AN, 40 bar: 0.158 kg/kg AN
- Ammonolysis of phenol: 10 bar: 0.39 kg/kg product, 40 bar: 1.301 kg/kg AN

6.4.7 Discussion of the Results

The logistics costs and energy savings are summarised below and calculated as a percentage of production cost for comparison purposes. The logistics costs relative to the production costs for scenarios 1 and 2, at 9.7% and 6.4%, respectively, are very substantial. The steam benefit for scenarios 2 and 3 is minimal, representing less than 1% relative to the production cost.

Table 6.20 Logistics and Steam Costs Relative to Aniline Sales Value

	S1	S2	S3	**Difference S1 – S3**	**Difference S2 – S3**
Production cost (mil €/a)	81.5	81.5	81.5		
Logistics cost for RM avail. onsite (mil €/a)	9.7	6.4	0.19	**9.6**	**6.2**
Steam cost (mil €/a)		-0.9	-0.7	**0.7**	**-0.2**
Logistics cost relative to production cost (%)	12.0	7.8	0.2		
Steam cost relative to production cost (%)	0	-1.0	-0.8		

These findings are shown graphically in terms of total costs and cost differences.

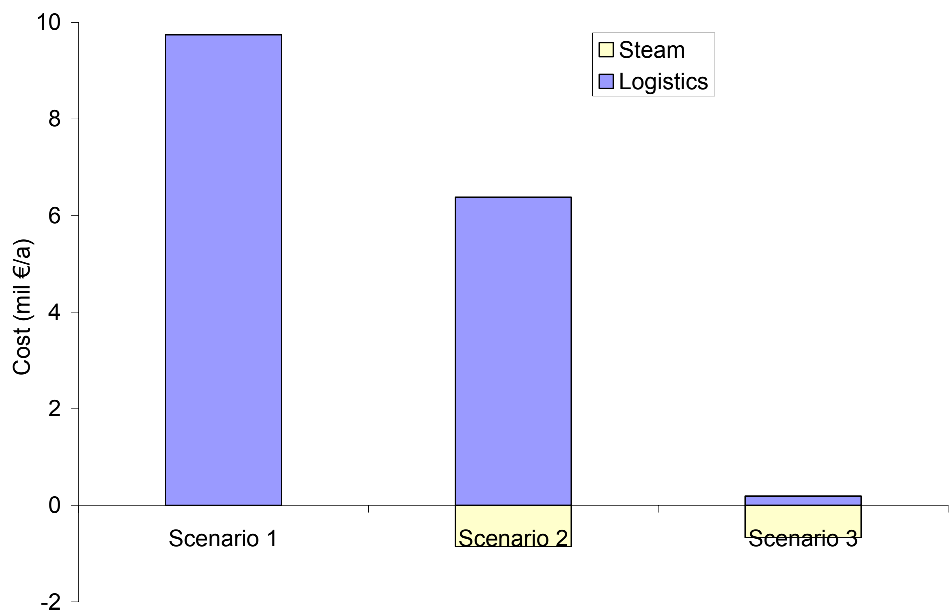


Figure 6.22 Logistics and Steam Costs for Aniline Case Study

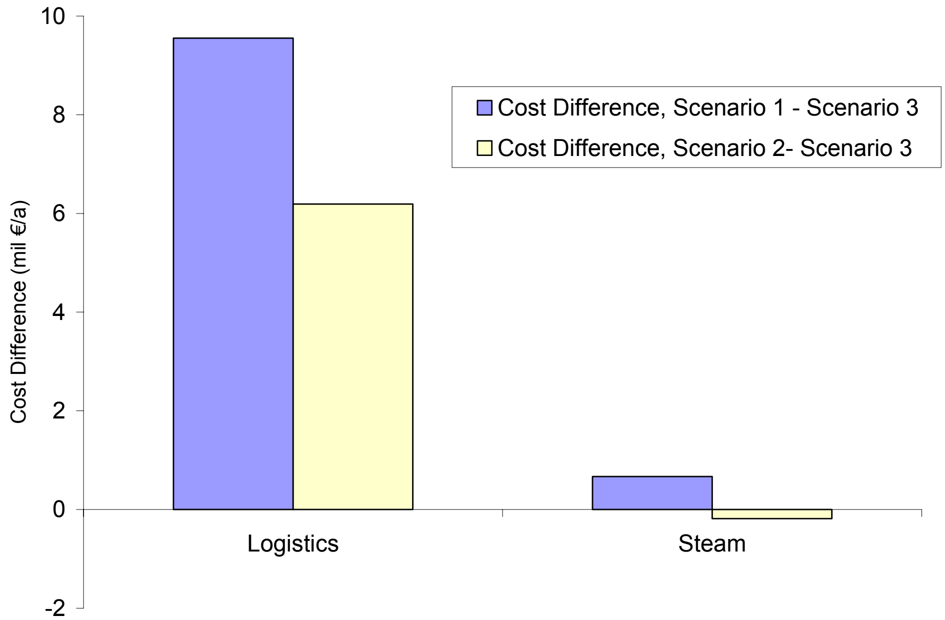


Figure 6.23 Cost Differences between Scenarios for Aniline Case Study

Concluding Remarks

This case study exemplifies how a plant which is located firmly within a value chain in an ICPS depends strongly on the availability of onsite raw materials. If one or more main raw materials are not available onsite, logistics costs can be prohibitive. Also, the case study shows that steam produced through the utilisation of reaction heat provides savings of 1 million €/a. However, relative to the production cost, this is less than 1%. This case study shows that processes which produce intermediates within a value chain and depend on few raw materials achieve significant logistics savings if located within an ICPS.

Advantages and Disadvantages of the Scenarios

Advantages of Scenario 1

This scenario is not economically attractive.

Advantages of Scenario 2

Scenario 2 shows that the transport of gaseous feedstocks within an ICPS is a significant advantage.

Advantages of Scenario 3

The aniline process, due to its dependence on few raw materials, one of which is gaseous, is best suited as part of an ICPS. Also, steam export through its heat of reaction has a small added benefit.

Disadvantages of Scenario 1

Scenario 1 shows that if a stand-alone plant is located close to an ICPS which is the source of its raw materials, unless it is physically linked through pipeline, even short transport distances lead to high logistics costs. Particularly, the very high logistics costs for hydrogen put this scenario at a strong disadvantage compared to the other scenarios.

Disadvantages of Scenario 2

Scenario 2 shows that if even only one key raw material is not available, significant logistics costs arise, even in an otherwise integrated site. Also, this scenario shows that the location of an ICPS is important, exemplified by the inland location of the Ludwigshafen site. The further an ICPS is from other important raw materials producers, the more dependent the ICPS becomes on itself as the main provider of main raw materials.

Disadvantages of Scenario 3

The main disadvantage of scenario 3 is that integration and interdependencies between plants create inflexibilities. If an integrated site is to divest in one plant which is part of a value chain, the economics of the whole value chain are affected.

6.5 Summary of Economic Benefits for Plant Case Studies

The below tables summarise the economic benefits determined for the plant case studies. Clearly logistics is the integration aspect which leads to the greatest cost differences between integrated and stand-alone or semi-integrated plants.

Table 6.21 Summary of Economic Benefits for Case Studies

Amount (mil €/a)	Polyacrylates ICPS vs. SA	Aniline ICPS vs. SA	Aniline ICPS vs. Semi-ICPS
Production benefit	9.1		
Logistics benefit	-5.9	9.6	6.2
Steam benefit via heat recovery		0.7	-0.2
Steam benefit via incineration	0.06	0.07	
Overall Benefit	**3.3**	**10.3**	**6.0**

Table 6.22 Economic Benefits as % Production Costs for Case Studies

	Polyacrylates ICPS vs. SA	Aniline ICPS vs. SA	Aniline ICPS vs. Semi-ICPS
Production benefit	16%		
Logistics benefit	-11%	12%	8%
Steam benefit via heat recovery		1%	[17]
Steam benefit via incineration	0.1%	0.1%	[17]

Below, the benefits resulting from integration are shown for the two case studies.

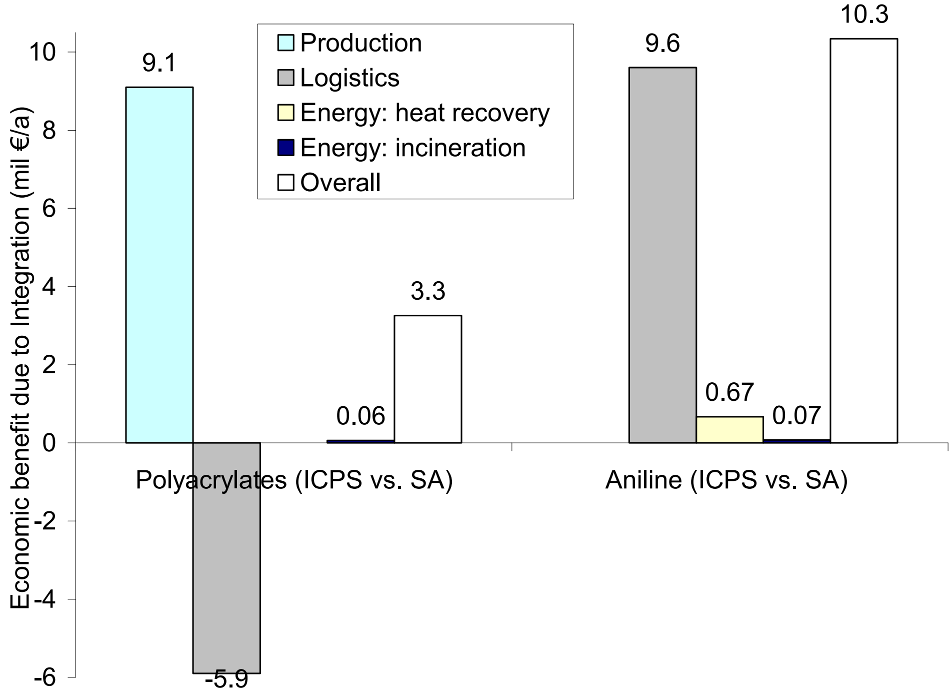


Figure 6.24 Economic Benefit of Integration for Plant Case Studies

6.6 Environmental Aspect of Integration for Plant Case Studies

Reductions in fossil fuels are determined based on methodology section 4.8.

6.6.1 Logistics-related Environmental Aspects

Emissions Polyacrylates Case Study

The transport distances are as follows. For scenario 1, a portion of the raw materials (4,909 t/a) are transported to the Shanghai polyacrylates plant (50 km).

[17] Differences in the steam value between an ICPS and semi-ICPS are not shown.

The raw materials requiring shipping (19,636 t/a) are freighted from Shanghai to Manila (1,850 km), Osaka (1,370 km), Melbourne (8,040 km) and Jakarta (4,420 km). Once at the port, they are transported by road to each polyacrylates plant (100 km). For scenario 2, the products requiring export (59,060 t/a) are shipped to the ports (according to above distances) and then sold from the port location. The total emissions are greater for scenario 2 due to the much greater volume transported. The transport emissions determined according to the methodology are given in the below table.

Table 6.23 Emissions for Transport for PA Case Study

	Scenario 1			Scenario 2
Amount (t/a)	Monomers by land	Monomers by sea	Monomers total	Products by sea
CO_2	183	1,347	1,530	4,106
SO_2	0.1	7.1	7.2	21.8
CO	0.3	3.5	3.9	10.8
NO_x	2.0	32.3	34.3	98.6
NMVOC	0.2	1.5	1.7	4.7
Dust	0.1	2.3	2.4	7.0

Emissions Aniline Case Study

For scenario 1, 135 kt/a of nitrobenzene and 8 kt/a of hydrogen from the Antwerp ICPS to the Antwerp stand-alone site (50 km) and 100 kt/a of aniline from the Antwerp stand-alone site to the port (50 km) are transported. For scenario 2, 135 kt/a of nitrobenzene are transported from Antwerp to Ludwigshafen (400 km) and 20 kt/a of aniline are transported to the port (400 km).

Table 6.24 Emissions for Transport for Aniline Case Study

Emission type, t/a	Scenario 1		Scenario 2	
	AN, NB, H_2 by truck	AN, NB, H_2 by train	NB and AN by truck	NB and AN by train
CO_2	1,058	411	5,146	1,996
SO_2	0.3	0.2	1.5	0.8
CO	1.8	0.5	8.7	2.5
NO_x	11.3	1.5	55.2	7.4
NMVOC	0.9	0.1	4.5	0.6
Dust	0.5	0.1	2.2	0.3

The following table shows the reduction in emissions due to integration for the two case studies. For the polyacrylates case study, higher emissions result with integration due to the higher transport volume resulting from water in the product. Whereas, for the aniline case study, emissions are reduced through integration.

Table 6.25 Transport Emissions Reduction for Plant Case Studies

Emissions (t/a)	Polyacrylates SA - ICPS	Aniline SA (truck)	Aniline Semi-ICPS (train)
CO_2	-2,576	1,058	1,996
SO_2	-14.6	0.3	0.8
CO	-6.9	1.8	2.5
NOx	-64.3	11.3	7.4
NMVOC	-3.0	0.9	0.6
Dust	-4.7	0.5	0.3

Fuel Consumption

The below table shows the amount of diesel fuel consumed for transport in each case study and scenario. The diesel fuel consumption calculation for aniline and nitrobenzene is based on a truck loading of 28 tons (see methodology, Section 4.8.1). However, for hydrogen transport, the fuel requirements are determined separately as there is a greatly reduced loading of only 454 kg/truck for the metal hydride truck compared the transport of bulk liquids. This results in significantly higher costs, based on Amos (1998, p.E-23).

Table 6.26 Fuel Consumption for Transport for Plant Case Studies

Fuel (t/a)	Polyacrylates		Aniline	
Transport mode	SA	ICPS	SA	Semi-ICPS
Truck	92		1,580[18]	
Rail				681
Ship	158	480		
Total	**250**	**480**	**1,580**	**681**

The reductions in fossil fuel consumption resulting from integration based on the differences in consumption between the different scenarios are shown in the following figure.

[18] For nitrobenzene and aniline 492 t/a are required and for hydrogen 1088 t/a is required.

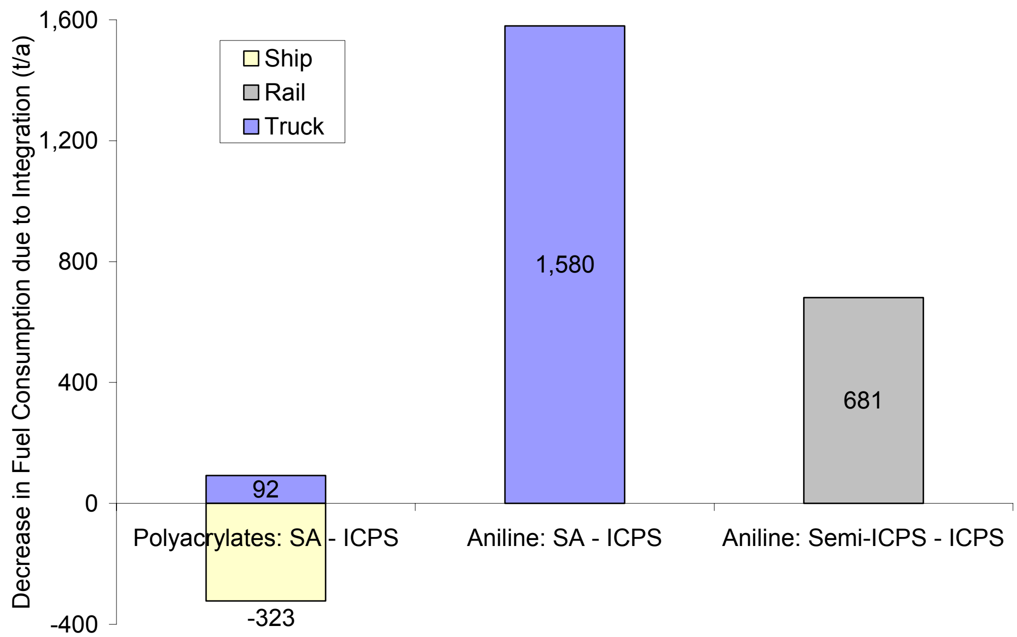


Figure 6.25 Reduction in Fuel Consumption for Transport

For the polyacrylates case study, fuel consumption is moderate although the transport quantity and distance are high. This is because the products are primarily transported by ship, a fuel efficient transport mode.

For the aniline case study, high fuel requirements result from the transport of hydrogen and nitrobenzene for the stand-alone plant. In particular, the lower loading in the case of hydrogen transport by metal hydride truck results in substantial fuel requirements. The more frequent hydrogen transport should be associated with higher emissions, however this is not captured through the methodology, as the emissions factors do not take loading into consideration.

6.6.2 Energy-related Environmental Aspects

Energy integration in the form heat recovery or waste incineration results in a reduction in the amount of natural gas required. The below table gives the amount of natural gas which would be required to produce the same amount of steam provided through integration for the case studies.

Table 6.27 Reduction in Natural Gas Consumption for Plant Case Studies

Energy Integration aspect	Amount	Polyacrylates	Aniline
Heat recovery	Steam produced by heat recovery (t/a)	n/a	110,000
	Natural gas equivalent (t/a)	n/a	8,174
	Energy equivalent (MWh)	n/a	99,900
Incineration	Amount of waste incinerated (t/a)	1,000	3,211
	Steam produced by incineration (t/a)	6,048	13,214
	Natural gas equivalent (t/a)	636	899
	Energy equivalent (MWh)	7,778	13,379

The amount of emissions saved by not using the above amounts of natural gas in a power plant for steam generation were determined only for heat recovery, as emissions are created during steam production through incineration. The emissions reductions, as shown below, are far greater for logistics than for steam generation.

Table 6.28 Emissions Reductions for Plant Case Studies

Emissions t/a	Polyacrylates SA - ICPS	Aniline SA (truck)	Aniline Semi-ICPS (train)	Aniline heat recovery SA-ICPS
CO_2	-2,576	1,058	1,996	37,962
SO_2	-14.6	0.3	0.8	1.0
CO	-6.9	1.8	2.5	27
NOx	-64.3	11.3	7.4	23
NMVOC	-3.0	0.9	0.6	0.4
Dust	-4.7	0.5	0.3	0.4
CH_4				0.4
N_2O				1.2

Below, a comparison of the reductions in emissions and fuel consumption with integration are shown for the plant level case studies. The amounts are greater for the aniline case study due to heat recovery for the integrated scenario. The amount of emissions related to hydrogen transport for the aniline stand-alone scenario is considered to be underestimated due to the use of general emissions factors per transport mode which do not take transport loading into consideration.

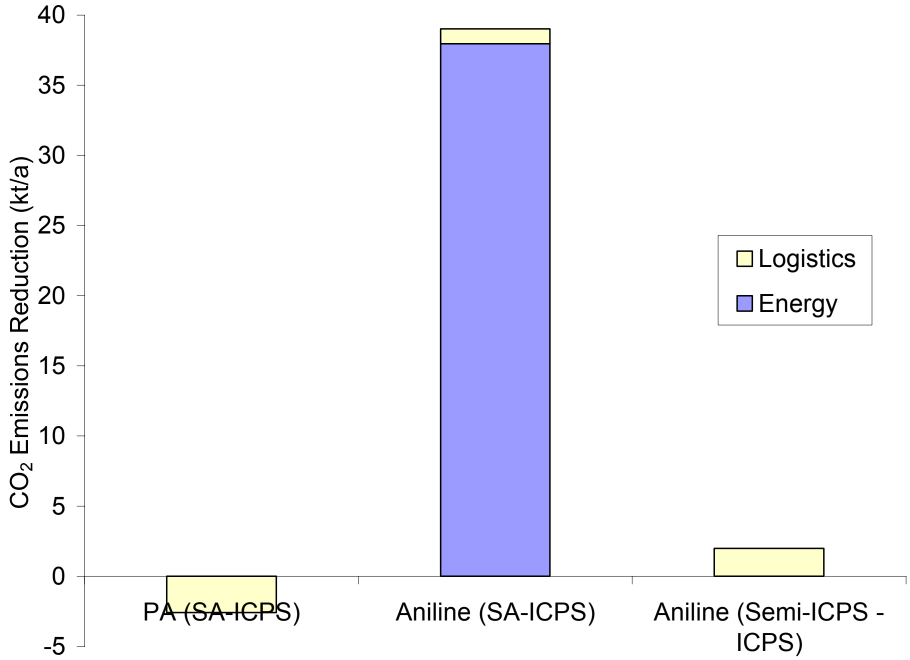


Figure 6.26 Reduction in CO_2 Emissions with Integration

The reduction in fuel consumption due to integration is much higher for energy integration than for logistics integration. This is due to the greater fuel requirements required in steam preparation.

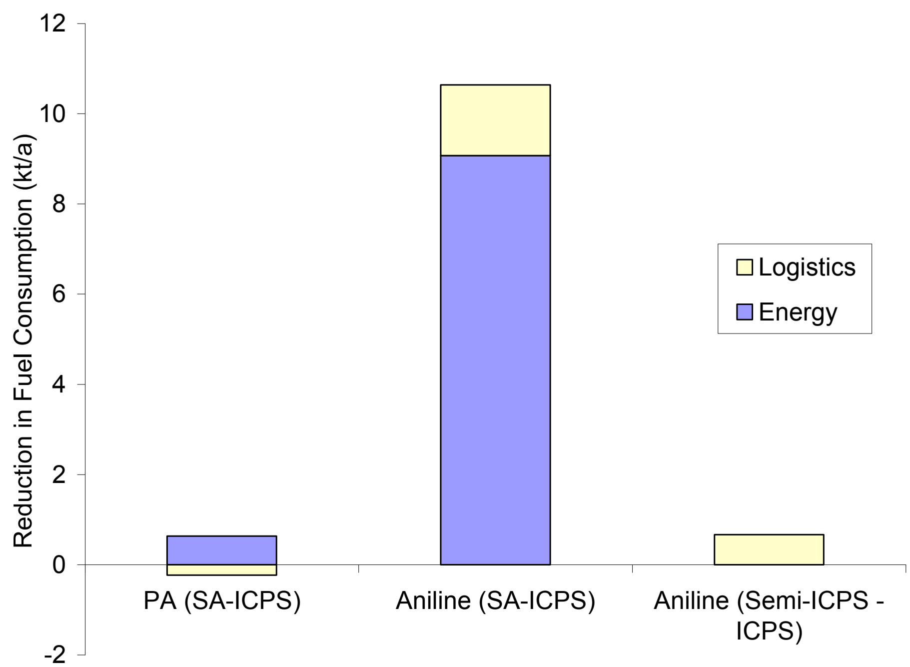


Figure 6.27 Reduction in Fuel Consumption with Integration

Savings for the plant case studies in costs, fossil fuels and CO_2 are given below.

Table 6.29 Cost, Material and Emissions Reduction for Plant Case Studies

Benefit	Difference	Production	Energy	Logistics	**Total**
Cost savings (mil €/a)	PA (SA-ICPS)	9.1	0.1	-5.9	**3.3**
	Aniline (SA)	n/a	0.7	9.6	**10.3**
	Aniline (Semi-ICPS)	n/a	-0.2	6.2	**6.0**
Fossil fuel savings (t/a)	PA (SA-ICPS)	[19]	636	-230	**406**
	Aniline (SA-ICPS)	n/a	9,073	1,569	**10,642**
	Aniline (Semi-ICPS - ICPS)	n/a	0	670	**670**
CO_2 reduction (t/a)	PA (SA-ICPS)	[19]	0	-2,576	**-2,576**
	Aniline (SA-ICPS)	n/a	37,962	1,058[20]	**39,020**
	Aniline (Semi-ICPS - ICPS)	n/a	0	1,996	**1,996**

6.6.3 Allocation and Case Studies on the Plant Level

In the above case studies, the advantages derived from energy integration, based on the value of steam at a site, are completely allocated to the production process under investigation. Actually, this steam also benefits the power plant as the steam requirements are reduced. In order to determine the relative benefit for the chemical plant and the power plant, allocation, covered in Chapter 4, is required. However, for this work, it is deemed acceptable to consider the total energy benefit, as the methodology aims to provide an indication of the overall benefit of integration for a particular process.

[19] Reductions in fossil fuels and emissions are expected due to economies of scale for a single polyacrylates plant compared to five smaller plants, however this aspect is not investigated here.
[20] The amount of emissions related to hydrogen transport is considered to be underestimated due to the use of general emissions factors per transport mode which do not take transport loading into consideration.

7 Integration Potential

In this chapter, the concept of integration potential is introduced to describe the suitability of a particular process to be located within an ICPS. Particular processes may be more suited for integration depending on their specific process characteristics. In the previous case studies, two chemical production processes, polyacrylate and aniline production, are investigated. The polyacrylate process benefits from the onsite availability of raw materials, but is disadvantaged in an ICPS due to the transport of products. Whereas, the aniline process benefits from the onsite transport of both raw materials and products, as well as from energy integration in an ICPS. Thus, different processes may derive benefits to varying degrees or even incur drawbacks when integrated in an ICPS.

Integration potential is defined here as the degree to which a particular process may benefit from integration in an ICPS. Its determination is based on characteristic factors identified from the case studies which are considered to influence a process' suitability for integration in an ICPS. These characteristics, defined in the following section, are related to the process: chemical pathway, raw material and product types and quantities, and process design. They are not related to a particular plant or scenario. Additionally, integration potential addresses the ability of a process to be forward or backward integrated in its value chain in an ICPS. Also, other considerations such as safety and environmental aspects are included. Plant integration potential is an elusive and subjective concept. In this work, a framework is suggested as a starting point as to how processes may be compared in their suitability for integration.

7.1 Process Characteristics Important for Integration

Below, key process characteristics are identified which may influence a process' suitability for integration. Based on the discussion below and the findings from the case studies, 14 integration factors are defined which are applied in the determination of an overall integration potential. These factors are grouped according to four categories: whether they relate to the process' main raw materials, its main products, the process (this includes by-products, wastes, and heat recovery), or if they are relevant to site strategy (this includes the aspects of safety/environment, economies of scale, and position in the value chain).

7.1.1 Main Raw Materials and Products

Amount and State of Raw Materials and Main Products

The greater the number of raw materials required by a process, the greater the likelihood that more raw materials need to be sourced from outside of the ICPS. Conversely, the fewer number of raw materials a process requires, the more likely these may be provided for onsite. This is exemplified by the case studies, as the polyacrylates process relies on a large number of raw materials, 45, of which only five are available at the ICPS studied, whereas for aniline, both main raw materials are provided at the ICPS. However, more important than the number of raw materials available at an ICPS is the required quantity, discussed below.

It is difficult to ascertain how the number of products influences a process' favourability for integration. A large number of products may be favoured in an ICPS, such as in ethylene production in a cracker, as an array of other raw materials for other processes is co-produced. On the other hand, numerous products produced in the polyacrylates process are not advantageous for integration, as the products are all sold offsite. Thus, what is important is the quantity of products used onsite. Further, the state of the raw materials or products is important, as shown by the aniline case study where the transport of gaseous hydrogen is much more costly than liquid raw materials due to compression requirements.

Thus, a process with few large volume raw materials or products may be better suited for integration in an ICPS than a process with many lower volume raw materials. Additionally, in order to derive logistics benefits, the likelihood of these large volume materials being present at the ICPS, or in other words, the likelihood of onsite forward or backward integration, should be high.

Based on the above discussion, the following factors are considered in the determination of integration potential:

- % Mass of top two raw materials relative to all raw materials
- % Mass of top one product relative to all products
- % Mass of gaseous raw material reactants (not including inert gas)
- % Mass of gaseous products (not including off-gases)

Thus, a process with few large volume raw materials or products in which the raw material provider or product recipient is located at the ICPS is more suited for integration. Next, it is determined if the provider of a process' main raw material or the recipient of a process' main product is likely to be located onsite. For this, the concept of captive use is addressed below.

Captive Use of Main Raw Materials and Main Products

Raw material captive use is based on a particular process' use of a key raw material from an immediately upstream process in the value chain. For example, in the acrylic polymers value chain, acrylic monomers are supplied to the polyacrylates process. For example, assuming 80% of acrylic monomers produced globally go into various value chains (47% into polyacrylate production) and 20% are used directly in non-integrated processes. Then, the degree of captive use for the determination of integration potential for the polyacrylates process is 47%.

Product captive use describes the amount of a particular product used for an immediately downstream process in the value chain. For example, if of all the aniline produced worldwide, 80% is used in the production of MDI and only 20% is used for other processes, then the captive use of the product aniline is 80%. The degree of captive use for a product may apply to more than one value chain. For example, ethylene, used as a starting block for several value chains, will have a high captive use due to the summed captive use for different value chains. If a process has a high degree of captive use products, then placing downstream processes at the same site has logistics advantages.

Thus, here the captive use for an upstream raw material is for the process in question and the captive use for a process' main product does not specify which value chain the product is fed to. The following factors are considered for the determination of integration potential:

- % Captive use of main raw material for process
- % Captive use of main product for various value chains

7.1.2 Process

Useable By-products

If a process generates useable by-products, then this may be an advantage in an ICPS, as logistics advantages may result. The factor considered for integration potential is the % mass of by-products which may possibly be used at an ICPS. Whether a process' by-product is able to be used depends on the requirements at the particular site. For this factor, a judgement must be made whether the useable by-product is commonly utilised at an ICPS. This is a process-related aspect, as the by-products generated depend on the process route selected.

Steam Production from Heat Recovery or Waste Incineration

The ability of a process to export reaction heat to produce steam for site use is an advantage in an ICPS. Also, processes in which waste is incinerated for steam generation are beneficial within an ICPS. For the determination of integration potential, the following factors are considered: steam production via heat recovery and via waste incineration relative to the process' main product.

Chemical vs. Mechanical Processes

Whether the process involves a chemical conversion or is simply a mechanical or mixing process is considered. If no chemistry is involved, then much of the ICPS infrastructure (process water, WWT, incinerator, etc.) may not be required and the process does not benefit from the shared infrastructure at the site. Examples are formulation plants, where mechanical / mixing processes are carried out.

7.1.3 Strategic Relevance

Position in Value Chain

A value chain is made up of chemical processes in which each downstream process further refines the product from the former process until a final process is reached from which all products are sold offsite. In an ICPS, the cracker may be the first process from which value chains branch off. Aniline, for example, is located within the polyurethanes value chain whereas polyacrylates is located at the end of its value chain; hence, no downstream plants in the ICPS depend on polyacrylate products. Thus, processes located at the end of the value chain do not benefit from the logistics advantages in an ICPS related to captive-use products. This is considered to be a strategic factor, as the degree of downstream integration is a strategic determination on the part of site planning.

Economies of Scale for the Integrated Process

One consideration may be whether further economies of scale can be realised if the process is built in an ICPS. Economies of scale may apply in an ICPS but not in a stand-alone plant if a plant's capacity is maximised in an ICPS to correspond with other processes in its value chain. This is true for the polyacrylates case study, where smaller stand-alone plants serve local markets, but the process is scaled up as a single plant in an ICPS. This may not apply for processes built as world-scale plants even in stand-alone sites. Also, processes which cannot be further scaled up in an ICPS which require several production trains may not fully utilise economy of scale advantages. Thus, whether further economies of scale are achieved in an ICPS is considered in the determination of integration potential.

It is important to note that economies of scale for upstream processes are also important. By locating a process which is part of a value chain in an ICPS, the scale of upstream process must be increased, which may lead to economy of scale advantages in these process. For example, if an acrylic acid/esters plant is additionally built in an ICPS, the cracker which supplies propylene to the process will need to be larger in capacity to serve the acrylic acid/esters plant, potentially leading to reduced production costs for the cracker. This aspect is mentioned here for completeness, however not applied in the determination of integration potential, as it relates more to upstream processes.

Strategic Reason for Integration

There may be strategically motivated reasons to locate a plant within a certain integrated site. For example, the plant may benefit from centralised services available at the ICPS, such as R&D. Or a process with very high energy requirements which influence its process' economics may benefit from potentially lower energy prices in an ICPS. A process may be located within an ICPS to secure the supply of a raw material for another process, thus avoiding fluctuations in raw materials availability and allowing for better production planning. A process may produce a waste which is not easily accepted by an external company. Another reason may be to co-locate at a site with a partner with which there is a strategic alliance.

Safety or Environmental Benefits with Integration

A process may be integrated due to safety considerations. For example, phosgene is used as a raw material in the production of isocyanates such as MDI which are used to produce polyurethanes. By producing this highly dangerous chemical within an ICPS, considerable transportation risk can be avoided (Isaac and Comer, 2000, p.60). Also, environmental benefits may be realised for a process by-product which may be considered a waste in a stand-alone site and incinerated compared to its chemical use in an ICPS, reducing chemical waste.

7.2 Determination of Integration Potential

Although the case studies show that some factors lead to greater integration benefits than others, the factors are not given weightings here, as the number of case studies is very few and the assignment of weightings would be somewhat arbitrary at this stage. It is recommended that as more case studies are investigated, the quantification of the relative importance of each factor may enable a weighting to be introduced. In total, 14 integration factors are defined, shown below.

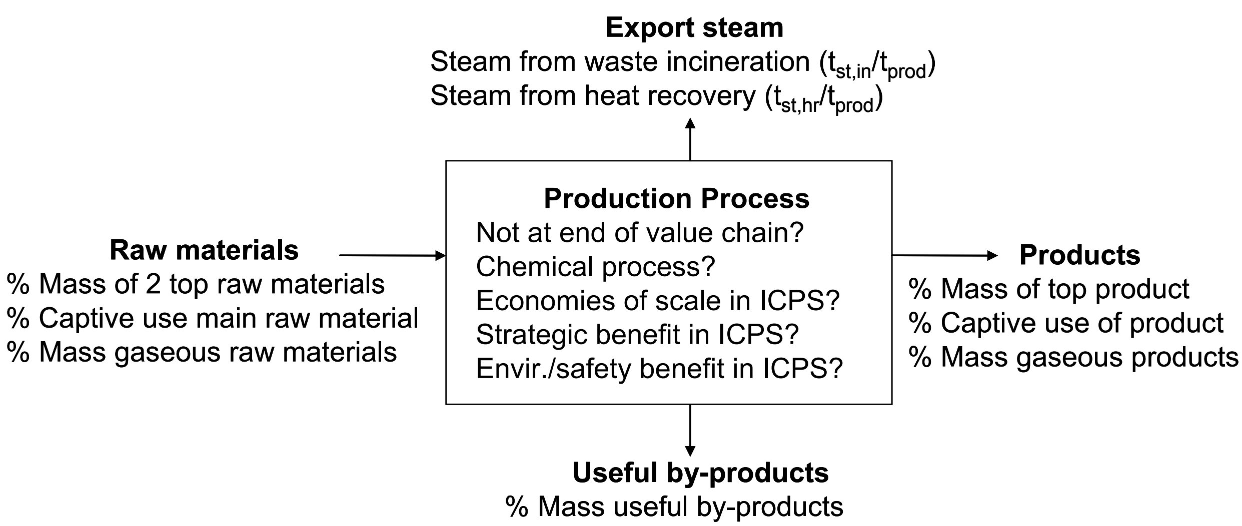


Figure 7.1 Factors for the Determination of Integration Potential

Values are determined for each integration factor for each process, for example, $X_{A,1}$ is the integration factor for process A and factor 1. Then each integration factor is normalised as a standard score, $x_{A,1}$, by mean shifting (subtracting from each value the mean for that factor over all processes) and then autoscaling by dividing each factor by the group's standard deviation, as follows:

$$x_{A,1} = \frac{X_{A,1} - \overline{X_1}}{\sigma_1}$$

This shifts the mean of the data to 0.0 and the standard deviation to 1.0 without disrupting the spread of the data, allowing factors with different ranges to be compared. Qualitative factors are assigned either a 0 or 1. The factors are further categorised according to: main raw materials, main products, process-related, or strategic. Capacities are assumed to be equivalent per process.

7.3 Application of the Integration Potential Concept

The characteristics identified above are utilised as factors in the determination of integration potential. In order to test this concept, it is applied to four cases: polyacrylates, aniline (fluidised-bed process), acrylic acid/esters and caprolactam. Background information for the first two processes is given in the case studies. In order to apply the concept of integration potential more widely, the processes for acrylic acid/esters and caprolactam are included. Background on these processes is given below. The location of the four processes in their value chains in an ICPS is shown below.

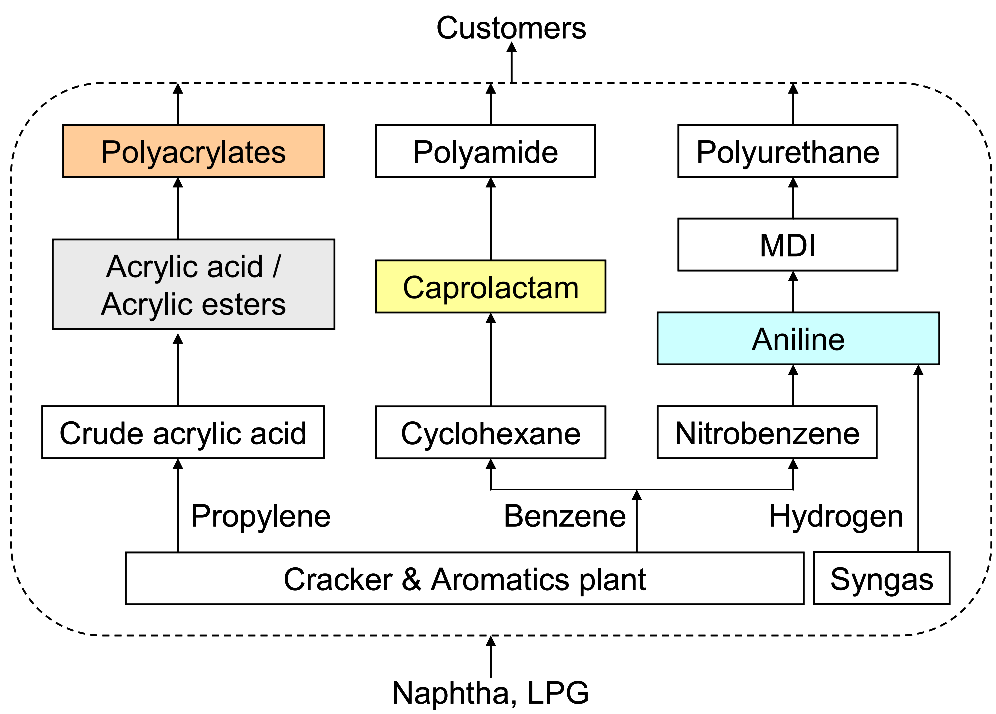


Figure 7.2 Processes Investigated for Integration Potential

7.3.1 Example Caprolactam

Large-scale industrial processes for the production of caprolactam are based on benzene or toluene as a starting material and involve multiple stages. About 90% of the world's caprolactam is produced via the cyclohexanone process based on the cyclohexanone oxime rearrangement (PEP report 7C, p.2-9). The main raw material for the process, cyclohexane (hexamethyleneimine), is produced from benzene and may be produced at the same site or purchased externally (PEP report 7C, pp.3-10, Isaac and Comer, 2000, p.83). Cyclohexane undergoes catalytic oxidation with air to form cyclohexanone (ketyohexamethylene). Tar from cyclohexanone production is incinerated (European Commission, 2003, p.53). The conversion of cyclohexanone to cyclohexanone oxime followed by Beckmann rearrangement gives caprolactam with a yield approaching 98%. In the conventional process, ammonium sulphate is formed as a co-product (2.5 kg of ammonium sulphate per kg caprolactam, PEP report 7C, 1998, p.2-11), which influences the cost-efficiency of the process. Hence, new processes have been developed which avoid the co-production of ammonia sulphate, such as Sumitomo's vapour-phase Beckmann rearrangement (Izumi et al., 2007). Approximately 90% of global caprolactam production is used in the production of polyamide nylon 6 for carpet manufacture or plastics and film, while 10% is used in nylon chips (Isaac and Comer, 2000, p.84).

The following useable by-products are produced in caprolactam production, which may be used onsite as raw materials or fuels, or sold.

- Organic wastes from distillation are produced during cyclohexane oxidation. Some light and heavy ends may be sold as fuel; others are incinerated (PEP report 7C, 1998, p.4-17).
- Useful organic acids may be separated from the organic layer of waste water: carboxylic acids and BVC (butyric, valeric, caproic) acids, used to produce lubricant base stocks. Nitric acid is formed and used in fertilizer production. Also, the heavy end residue may be combined with dicarboxylic and hydroxycarboxylic acids recovered from waste water and reacted with nitric acid to produce adipic acid and other dicarboxylic acids. Adipic acid is used to produce nylon 6.6 and dicarboxylic acids and may be converted to dimethyl esters for lubricant base stocks (PEP report 7C, 1998, p.4-17).
- Ammonium sulphate is produced as an undesirable co-product, which is sold externally for use as a fertilizer (Ullmann, 2000).

7.3.2 Example Acrylic acid / Acrylic esters (AA/AE)

Acrylic acid is a commonly used chemical intermediate, which because of its widespread use, is a valuable chemical commodity. Acrylic acid goes into the production of homopolymers such as Super Absorbent Polymers (SAP) for diapers and hygienic products or co-polymers and is also further reacted to acrylic esters such as butylacrylate, ethylacrylate, methylacrylate or 2-ethylhexyl-acrylate. Acrylic esters are used in the production of paints, adhesives and sealants, textiles, plastic additives, and paper. The most widely accepted process for making acrylic acid is the vapour phase oxidation of the cracker product propylene. In this process, oxygen is reacted with propylene to produce acrolein, an unsaturated aldehyde, which is further oxidized to acrylic acid. The most commonly used processes are based on those by the following multi-national companies: Nippon Shokobai, BASF, BP (Sohio) and Mitsubishi (Lacson et al, 2004, p.18).

Acrylic acid is then further reacted with alcohols in the production of acrylic esters. The most commonly used alcohols are n-butanol, ethanol, 2-ethyl-hexanol, and methanol. The governing reactions are given below.

$CH_2{=}CHCH_3$	+	O_2	→	$CH_2{=}CHCHO + H_2O$
propylene		*oxygen*		*acrolein*
2 $CH_2{=}CHCHO$	+	O_2	→	2 $CH_2{=}CHCO_2H$
acrolein		*oxygen*		*acrylic acid*
$CH_2{=}CHCO_2H$	+	ROH	→	$CH_2{=}CHCO2R + H_2O$
acrylic acid		*alcohol*		*acrylic ester*

Acrylic acid is highly reactive and not readily transported and thus generally supplied by local producers. Acrylic esters are more easily transported than acrylic acid, however, they may also polymerise and therefore require an inhibitor when transported (Lacson et al, 2004, p.14).

The conversion of propylene to acrylic acid generates heat, which is converted to steam. A small part is used for distillation in acrylic acid production, but in an ICPS, most of the steam can be fed into the steam network where it is made available to other plants. Waste streams are incinerated in a thermal oxidiser, also producing steam for the site network (PEP report 6C, 1987, p.31).

In the table below, the integration factors for each process are given.

Table 7.1 Factors for the Determination of Integration Potential

Integration Factor	Relevance factor	Poly-acrylates[21]	Aniline[22]	AA/AE[23]	Capro-lactam[24]
1. % Mass 2 top raw materials	Raw material	67	100	78	50
2. % Mass gaseous raw materials	Raw material	0	6	52	0
3. % Captive use main raw material	Raw material	47	95	29	93
4. % Mass 1 top product	Product	15	100	36	26
5. % Mass gaseous products in top 2 products	Product	0	0	0	0
6. % Captive use main product	Product	0	80	40	90
7. % Mass by-products used at ICPS	Process	0	0	0	7
8. Steam from waste incineration *($t_{st,wi}$/ $t_{product}$)*	Process	0.1	0.1	0.9	0.1
9. Steam from heat recovery *($t_{st,hr}$/ $t_{product}$)*	Process	0	1.1	1.1	0
10. Chemical process (yes=1, no=0)	Process	1	1	1	1
11. Plant not at end of value chain (yes=1, no=0)	Strategic	0	1	1	1
12. Economies of scale if in ICPS (yes=1, no=0)	Strategic	1	1	1	1
13. Environmental/ safety benefit in ICPS (yes=1,no=0)	Strategic	0	0	0	0
14. Strategic benefit in ICPS (yes=1,no=0)	Strategic	0	0	0	0

[21] *Pep report 65A, 1991, company data.*
[22] *Pep report 76C, 1998, p. 1-1, 4-16, 2-1, 5-10, 5-14, 5-15.*
[23] *Pep report 6C, 1987, p. 31, 34, 35, 47, BASF, 2007, Isaac and Comer (2000) p. 67. Note: AA/AE is considered to be two processes.*
[24] *Pep report 7C, 1998, pp. 4-5, 5-7, 5-11, 5-23, Isaac and Comer (2000) p. 82.*

For the determination of the integration factors, the following raw materials and products were identified for the processes.

Table 7.2 Raw Materials & Products for Determining Integration Factors

	Polyacrylates	Aniline	AA/AE	Caprolactam
Top 2 raw materials	butylacrylate, styrene	nitrobenzene, hydrogen	propylene, n-butanol	cyclohexane, oleum
Top 1 product	dispersion x	aniline	AA	caprolactam[25]
Main raw material	AA/AE	nitrobenzene	propylene	cyclohexane

The normalised integration factors per category and overall integration potentials are given below. This is followed by graphs showing the overall factors and factors per category for each process.

Table 7.3 Normalised Factors for the Determination of Integration Potential

Category	Polyacrylates	Aniline	AA/AE	Caprolactam
Raw material	-1.0	1.2	0.4	-0.6
Product	-1.2	1.2	-0.3	0.2
Process	-1.2	-0.1	1.2	0.1
Strategic	-1.5	0.5	0.5	0.5
Overall	**-1.4**	**0.9**	**0.5**	**0.04**

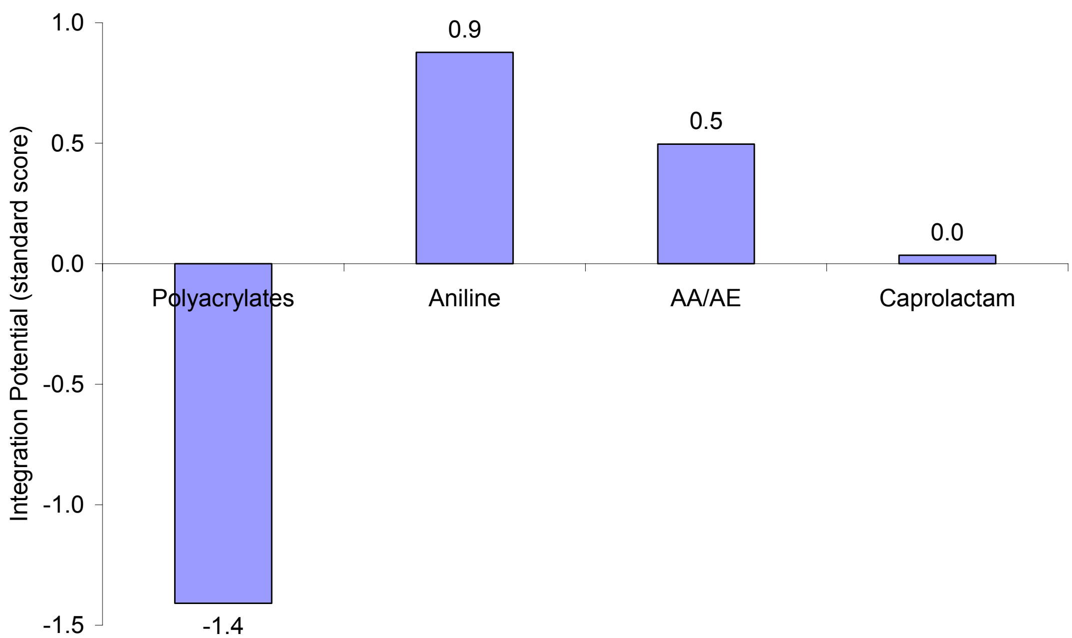


Figure 7.3 Integration Potential for Example Processes

[25] Caprolactam is designated as the desired product, although more AS is actually produced via the conventional Raschig process.

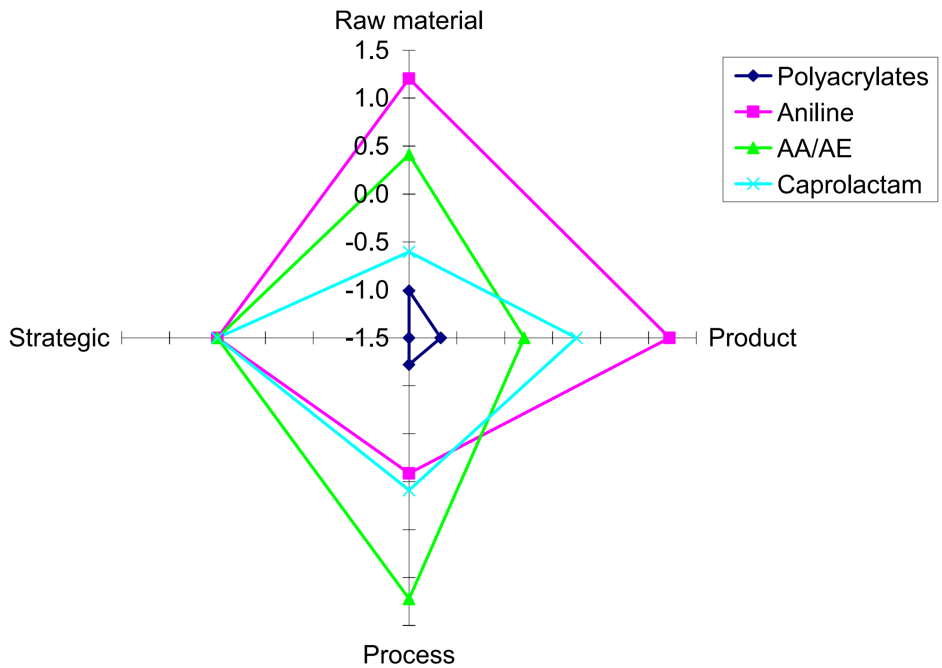


Figure 7.4 Integration Potential according to Categories

According to the integration potentials determined for the four processes, aniline is most suited for integration, followed by acrylic acid/esters. Polyacrylates has a negative integration potential and is least suited for integration and caprolactam has an integration potential close to zero. A possible interpretation of these values is that aniline and acrylic acid/esters are suitable for integration in an ICPS, polyacrylates, based on process characteristics alone, is not suited for integration, and caprolactam may be integrated, but possesses no key integration advantages.

The above graphic shows that for the aniline process, integration is important due to raw material and product related factors. This is a result of the high volume as well as high captive use of raw materials and products. The raw material factor is high for acrylic acid/esters as a key raw material, propylene, is gaseous, whereas the product related factor is lower due to a moderate % mass and captive use. The raw material related factor is even lower for caprolactam, followed by polyacrylates, as the number of raw materials increases and hence the % mass of top raw materials decreases. The product related factor is low for caprolactam due to the low amount of product produced (due to the large amount of co-product ammonium sulphate), even though the caprolactam product has a high captive use.

The acrylic acid/esters process has the highest process related factor due to the large amount of steam export. This is followed by caprolactam, which benefits from useable by-products and aniline due to its steam export. Polyacrylates is ranked lowest in process-related factors as there is no useful by-product formation or heat recovery. For strategic related factors, all processes are chemical, benefit from scale-up, and do not have a particular strategic, environmental, or safety[26] reason for integration. It is only the polyacrylates plant which is different from the others in that it is located at the end of the value chain, which is a disadvantage for integration.

The graphic below highlights key aspects of the processes which lead to different integration potentials.

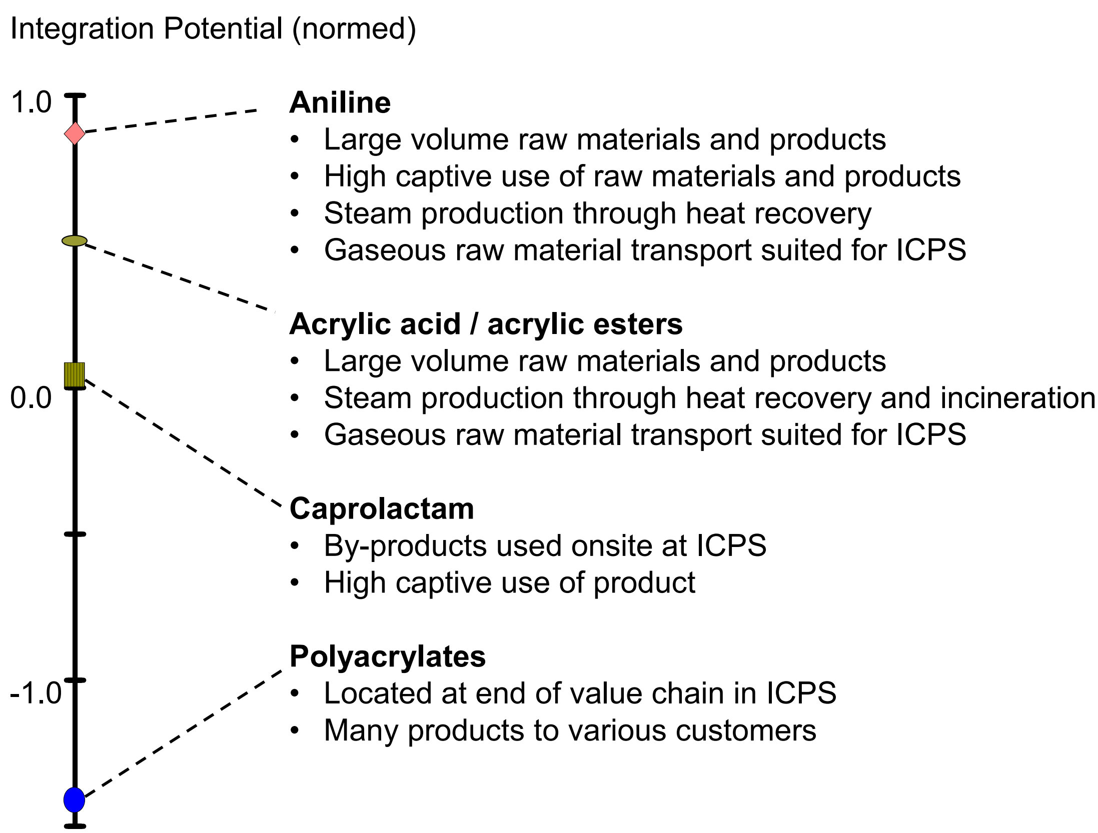


Figure 7.5 Key Process Differences relevant for Integration Potential

[26] The transport of monomers is not included as a safety reason for integration in the integration potential determination, as monomer transport is common.

7.3.3 Variation of Integration Factors

The selection of integration factors is subjective. Thus, the factors for raw materials and products are modified here to better understand their influence.

Test A: Mass % 1 Top Raw Material

Here, integration factor 1 is changed from *'% mass of 2 top raw materials*' to *'% mass of 1 top raw material*'. This results in: for polyacrylates 53% (butylacrylate), for aniline 95% (nitrobenzene), for acrylic acid/esters 52% (propylene), and for caprolactam 25% (cyclohexane).

Test B: % Mass Raw Material or Product · Captive Use

Rather than determining the % mass of raw materials (factor 1) and products (factor 4) and % captive use for top raw material (factor 3) and product (factor 6) separately, the factors are combined as multiples. The new factors represent the amounts of main raw material and product captively used:

- (% mass top 1 raw material) · (% captive use top raw material)
- (% mass top 1 product) · (% captive use top product)

The factor for % gaseous raw materials or products is unchanged.

Test C: Acrylic acid in place of Acrylic acid/esters

Before, acrylic acid and acrylic esters were taken as a single production block containing two linked processes, as they tend to be constructed as a single production complex. In this test, the integration potential of an acrylic acid plant, without including acrylic esters, is determined. The new factors become: % mass of top 2 raw materials = 100 % (propylene, oxygen), % mass of 1 top product = 100 % (acrylic acid) and % captive use of product = 66 %. The amount of steam produced is unchanged, as this is relative to acrylic acid.

Due to the normalisation procedure, the results for all processes are affected by a change for one process. The graphs below show the results for the raw material and product factors and the overall integration potential for the tests. For test A, the raw materials factor is reduced for AA/AE, since the amount of the second raw material, n-butanol, is large. For test B, caprolactam has the lowest raw material factor due to the low % mass for its main raw material. When only the AA plant is considered in test C, the raw material factors for AA and aniline are almost the same.

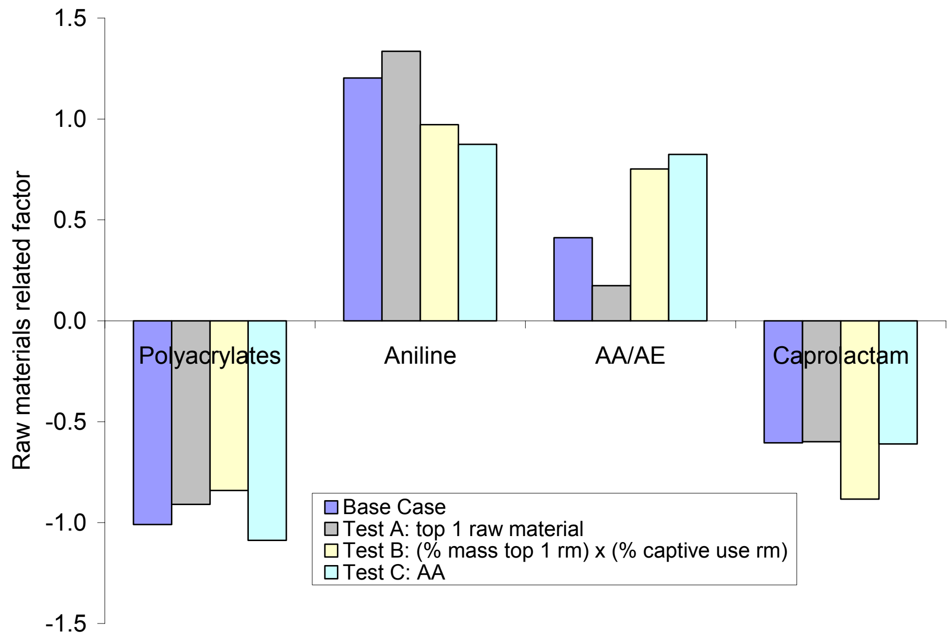


Figure 7.6 Raw Materials Factor for Base Case and Tests

For test B, the product factor is further increased for aniline, due to a high % mass and captive use of the product. For test C, the product factor becomes positive for the AA process as only one product is produced. Also, the % captive use is higher than for the AA/AE process.

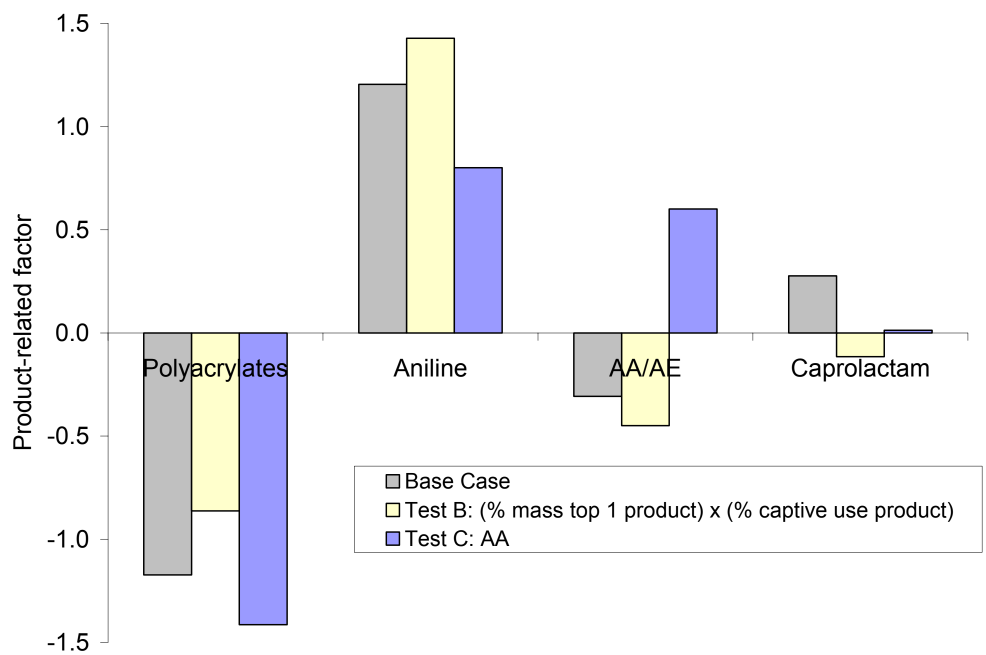


Figure 7.7 Product Factor for Base Case and Tests

The effect of test C on the integration potential is shown below. The overall integration potential for AA and AA/AE cannot be directly compared as the standard score is relative to the values for the other processes.

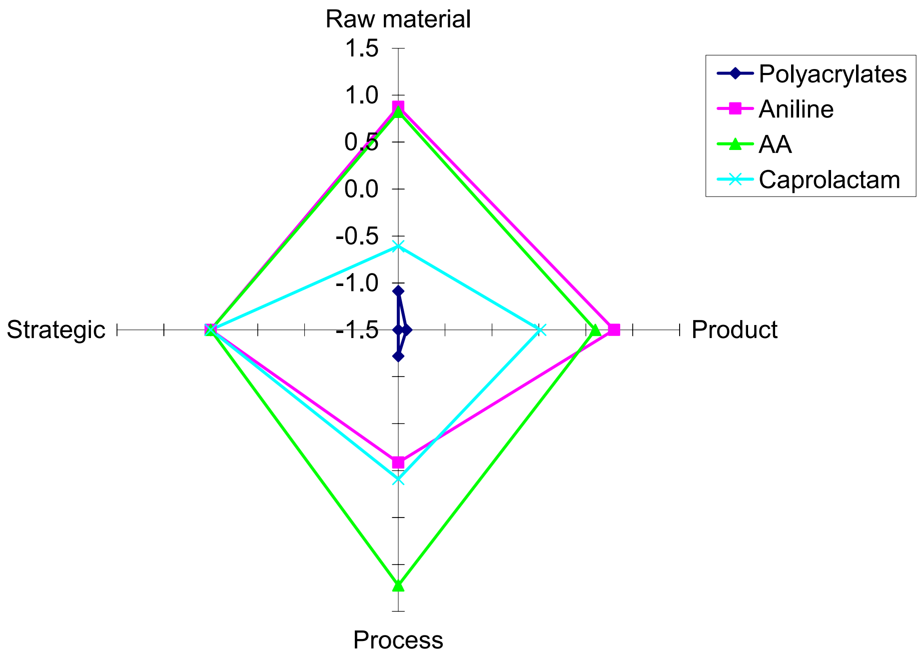


Figure 7.8 Results of Test C according to Categories

Due to the increase in raw material and product factors for test C, the AA process and not aniline has the highest overall integration potential.

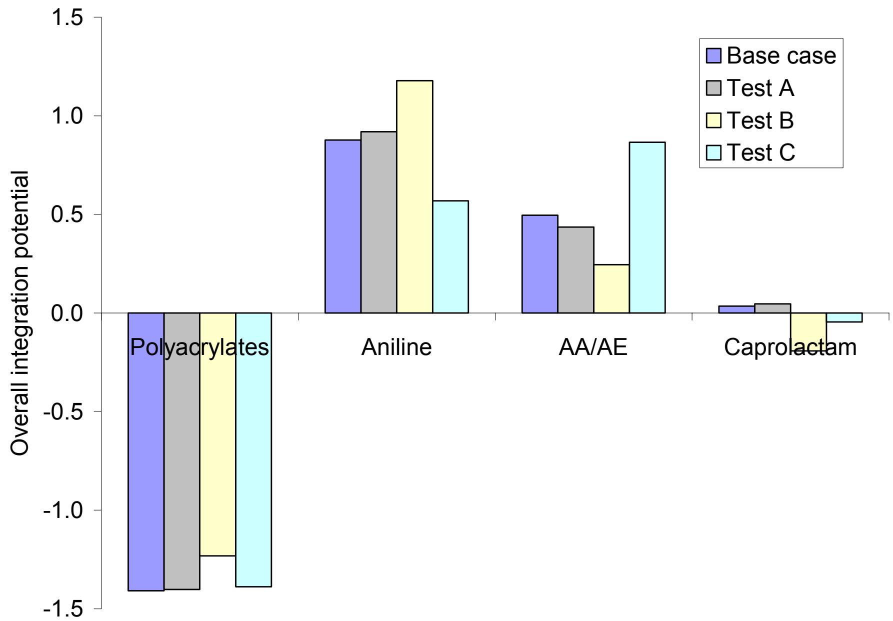


Figure 7.9 Overall Factors for Base Case and Tests

7.4 Concluding Remarks

One aim of this work is to introduce the concept of integration potential and to provide a perspective showing how factors important for integration may be applied in the comparison of processes. At this stage, based on few cases, it is difficult to define factors which can fully describe a process' suitability for integration. As more case studies are investigated, the factor definition may be modified or weightings introduced to reflect the importance of different aspects.

The determination of integration potential as defined in this work shows the intermediate processes aniline and acrylic acid/esters to have the highest integration potential of the processes reviewed. In comparison, the caprolactam process does not possess significant integration advantages, and the polyacrylates process is the least suited for integration. Modification of the factor definitions through the test cases has an effect on the integration potentials, however, the basic trend is unchanged. Test C, in which only the acrylic acid plant and not the acrylic acid/esters complex is investigated, shows the importance of where the boundary for a process is drawn.

Below, a comparison of the above findings is made with the actual locations of these processes for a particular chemical company. Polyacrylates plants are located in both integrated sites and as stand-alone plants. All others are only located in integrated or semi-integrated production sites:

- Polyacrylates: in ICPS in Europe, stand-alone in Asia, North America, and South America
- Aniline: in ICPS in Europe and Asia
- AA/AE: in ICPS in Europe, Asia and North America, in semi-ICPS in South America (always as an AA/AE production unit)
- Caprolactam: in ICPS in Europe and North America

This verifies to a certain degree the ability of the integration potential concept to determine a process' suitability for integration. The polyacrylates process, with the lowest integration potential, is almost always built as a stand-alone plant and aniline and AA/AE are always integrated. The integration potential of the caprolactam process is approximately zero, yet it is located in integrated sites. The reasons for locating a particular plant at a particular site involve many factors, such as space available at a location or possibly historical reasons, and are thus difficult to predict.

7.4.1 Plant Integration Potential According to Product Type

How plant integration potential is related to product type is discussed below. The concept of the pyramid of product types in the chemical industry was introduced in section 3.1. An onsite cracker generally represents the first product level in an ICPS, providing feedstocks to the next product level, basic chemicals. It is only reasonable to locate a basic chemicals production plant in an ICPS, as the cracker's sole purpose is to supply feedstocks to these processes. Therefore, basic chemicals production should represent the highest integration potential possible.

Intermediates and industrial chemicals are downstream of basic chemicals plants in an ICPS. They may receive their feedstocks from both within and outside of an ICPS. Three of the processes studied here (aniline, AA/AE, and caprolactam) belong to this category. Whether an intermediate or industrial chemicals plant has a high integration potential depends on the specific characteristics of the process, such as its ability to be forward and backward integrated or if it provides steam export. As shown by the case studies investigated, there is a wide range of integration potential in this category.

Specialties generally fall at the end of the value chain and thus cannot be forward integrated, limiting their integration potential. As shown by the widening of the production pyramid, a larger number of products are produced in such plants to serve many downstream customers. Due to the potentially higher number of raw materials required, less captive use through backward integration is expected. Thus, specialties are expected to have the lowest integration potential, exemplified by the polyacrylates case study. However, a specialties plant may have certain characteristics which favour integration, such as strategic considerations (the ICPS is located close to customers), or safety and environmental issues.

Based on the above explanations, the below figure shows the anticipated trend for integration potential with product type. As only a limited number of cases are investigated, further cases may validate this anticipated trend. In general, as a process' position in the value chain becomes further removed from the cracker, a lower integration potential is expected. However, in addition to value chain position, other factors, such as the amount of captive use raw materials and products, and whether these materials are readily transported must be considered.

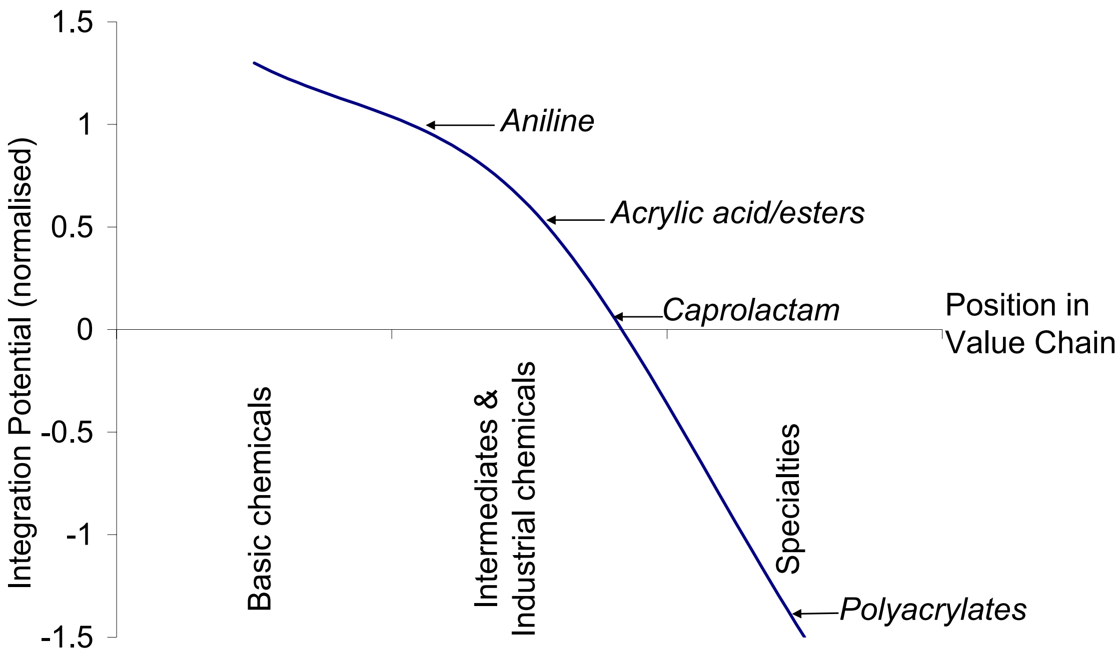


Figure 7.10 Anticipated Trend of Integration Potential with Product Type

The concept of integration potential, as defined in this work, relates only to the process. Capacity and factors related to geographic location are not considered, as the concept aims to compare process types. However, when determining whether to locate a specific plant in an ICPS, the proposed site location is known and thus, a deeper analysis may be made considering: distances from raw materials suppliers and customers, heat integration with neighbouring plants (heated water streams, etc.), and the use of by-products.

8 Conclusions and Outlook

In this work, the Integrated Chemical Production Site (ICPS) is defined and described, from which a methodology is developed to investigate the economic and environmental implications of integration. This work provides approaches to:

- Calculate the overall economic and environmental benefits of integration for an integrated chemical production site
- Investigate competing scenarios for a particular process to determine the economic and environmental effects related to integration
- Compare the integration potential or suitability of a process to be located within an integrated site for different processes

Through the application of these approaches, the importance and cost implications of different types of integration in chemical production sites are demonstrated. Further, the key process aspects important for the integration of particular processes are identified.

8.1 General Findings from the Case Studies

The significant impact of integration in both economic and environmental terms is exemplified by three case studies, one on a site and two on specific processes. These case studies allow the relative importance of the different types of integration to be assessed. Logistics-related integration is found to be the most significant of the integration types, in both economic and environmental terms. Integration advantages are present on a site level, as multiple plants derive benefits through co-location. However, whether a particular process benefits from integration depends on the suitability of that process for integration. Annual savings of millions of Euro and hundreds or thousands of tons of fossil fuels and emissions may be realised by locating a plant in an ICPS if the process is suited for integration. This is shown by the case study on the aniline process. Conversely, the integration of a process not as suited for integration may be accompanied by significant economic and environmental costs. This is shown by the case study on the polyacrylates process. Also, local determining factors, such as the geographical location, for example tariffs in Asia, may influence the results considerably.

8.2 Integration Potential

The concept of integration potential is proposed based on key process characteristics considered to be important for integration. These characteristics, identified through the case studies, are defined as factors, such as the ability to forward or backward integrate the process at an ICPS or the ability to recover process heat. By combining these factors, an integration potential is determined, which is an assessment of a process' suitability for integration. Four example processes which differ in key process characteristics are evaluated. The analysis shows that product type is an important determining factor in integration potential. Basic chemicals will have the highest integration potential. Intermediates may have a high integration potential depending on the particular process, and specialties are likely to have the lowest integration potential, primarily due to their end position in an ICPS value chain.

In addition to the above approaches developed in this work and their findings, which are summarised in greater detail in the Summary in Chapter 9, other conclusions related to site location and the general advantages and disadvantages of integration are discussed below.

8.3 Site Location

Site location is a vitally important consideration, both for the ICPS and the stand-alone site. An ICPS, in particular, benefits from proximity to a supply of natural resources to provide feedstocks to its chemical processes. If sites are located far from customer sites, logistics costs must be critically evaluated. On the other hand, sites located strategically close to customer sites rely on the customer remaining at that location.

In the polyacrylates case study, the location of the integrated plant in China resulted in very significant logistics costs for product transport due to port costs and tariffs. Whereas, if the integrated plant is located in Europe, perhaps it would not be disadvantaged, depending on the location of its customers. The larger-scale integrated plant is expected to benefit from lower production costs due to economies of scale and shared facilities and may be better able to accommodate shifts in sales among countries.

Ultimately, the decision of where to place a particular plant depends on an interplay of various factors. Also, the location selected may not be optimal in all respects. For example, if an integrated site concept is selected and located in China, this may be a benefit compared with local production in a country with high costs such as Japan, however be a disadvantage compared with local production in a country with import barriers such as India.

8.4 Advantages and Disadvantages of Integration

Through the case studies, the following advantages and disadvantages of integration are identified.

8.4.1 Advantages of Integration

The co-location and integration of plants in an ICPS may result in the following advantages:

- Logistics integration allows the costs, efforts, and risks for the transport, handling and storage of materials to be reduced. Networks for the distribution of materials ensure fast, safe, and environmentally friendly transport between plants compared to transport by truck, train, or ship. Also, there is a safety benefit related to the onsite handling and transport of dangerous goods.
- Excess heat recovery and the incineration of wastes reduce the use of fossil fuels for steam production. Greater efficiency in power and steam production is achieved through larger scale power plants.
- Economies of scale may be achieved through increased capacities for production processes.
- Shared infrastructure may lead to reduced costs through economies of scale in waste treatment, incineration, and the provision of steam and other utilities.
- Materials integration in which by-products from one process become the raw materials for other processes reduces the amount of chemical waste and the additional costs associated with externally purchased raw materials.
- Through the bundling of demands for external raw materials and other requirements such as packaging, procurement costs may be reduced.
- Lowered raw material dependency is achieved through backward integration. The utilisation of internal raw materials and the reduction of externally purchased raw materials allows the site to be more self-reliant.

- Centralised functions may lead to organisational integration and potentially greater know-how in areas such as R&D, process engineering, logistics, and safety and environment. This may lead to:
  - greater expertise due to dedicated personnel with specialised functions
  - more systematic processes resulting in efficiencies
  - greater implicit knowledge due to the exchange of information and experiences among personnel at the same site
  - process improvements through knowledge sharing via informal networks; eg. the transfer of a process improvement from one plant to another plant
  - better documentation of experiences and knowledge through centralised functions
  - greater opportunity for innovation through greater onsite knowledge

8.4.2 Disadvantages of Integration

Integration also brings disadvantages with it, as integration necessarily leads to inflexibility. The following disadvantages are identified:

- Risks are associated with the large investment required, in particular if one company dominates the site. This large investment also means that there is a higher barrier to divest.
- Inflexibility is created through the interdependencies among plants and linked production capacities. Thus, if one process has technical difficulties or a raw material shortage and cannot produce to full capacity, the downstream plants which rely on the process are affected. In particular, there is a dependence on key plants to produce at full capacity, eg. cracker.
- The ability to divest in a certain process is reduced for processes which are part of a value chain.
- A greater dependence on key raw materials at one location is created through the large quantities required.
- A high degree of complexity results from various inter-connections in materials and energy streams between processes.
- Location risk may be considered to be higher due to the greater concentration of plants at a certain location.
- The total amount of emissions at one geographical location is very high.
- Public relations issues due to the site size and concentration of plants at one location may arise from public concerns related to safety and environment.

Furthermore, there are limits to integration. As a site becomes more integrated and its complexity increases, the whole site becomes more difficult to manage. Problems may arise due to interdependencies, such as the accumulation of trace elements resulting in lowered process stability. Site-wide solutions may not always provide the optimal solution for each individual process, such as the type of technology selected for site waste treatment. Also, integration is limited by seasonal temperature differences which lead to variance in the amount of heat which can be recovered.

For some situations, a stand-alone plant has advantages over an integrated plant. For example, it may be able to respond more quickly to market changes, such as a plant closure or change in product range. Also, a stand-alone plant may introduce process changes without influencing onsite downstream processes. Thus, a stand-alone site may be favoured for processes in which market fluctuations or technological change is more rapid.

8.5 Outlook

In this work, the integrated chemical production site is defined and the key forms of integration it possesses are described. A novel approach for the quantification of economic and environmental benefits of an integrated chemical production site is developed and applied to case studies. Further, a new concept is proposed, that of integration potential.

The investigation of integration in a chemical production site brings some difficulties with it. First, the system is very complex. An integrated site may have thousands of material and energy flows which are interrelated, making it difficult to capture all aspects related to integration for a site. Also, the selection of various parameters is critical and may influence the overall results. Thus, it is important that all assumptions are critically reviewed. The methodology provides a snapshot view of the benefits of integration. However, industrial chemical processes are dynamic. Changes may result from the implementation of process improvements or changes in materials; thus, the methodology should be applied repeatedly to ensure the results are current.

The topic of the integrated chemical production site is a very broad one. Through this work, aspects are identified which may be addressed in future studies. For example, an ICPS may derive benefits in input and output systems, not addressed here, such as reduced costs in the procurement of raw materials or packaging, economies of scale for a cracker, or reduced costs for transport provision, such as BASF's train system described in section 3.7.2. Also, the costs for additional process steps to separate or refine a by-product for onsite use or sales may be investigated. Additionally, the evaluation of further case studies may allow the approach developed here, particularly for the determination of integration potential and the definition of its factors, to be further refined. Organisational integration, thought to bring considerable advantages to an ICPS, but which are difficult to quantify, is a worthy topic of further study. Also, a question which arises through the work is how integration and innovation relate; that is, whether the proximity of plants leads to process modification or innovation.

By applying the methodology to planned or existing sites, greater integration efficiencies may be identified in order to maximise potential savings. In conjunction with other tools, such as pinch analysis described in section 3.7.3 or process design software, the methodology may provide support in the selection of process types and technologies to optimise integration advantages.

In light of increasing costs of depleting natural resources and the importance of environmental concerns, efficiencies in chemicals production are expected to become increasingly important. Integration in chemicals production may result in reductions of fossil fuels consumption and the production of chemical waste. Further, reductions in green house gases may be realised, particularly CO_2 from transport, an important aspect in light of restrictions imposed by the Kyoto protocol or EU emissions trading. Safety benefits result from the onsite containment of dangerous goods. Further, how companies are viewed in terms of their commitment to the environment has important implications for corporate reputation and how companies are assessed, such as through the Dow Jones Sustainability Group Index and the balanced score card.

9 Summary

Large chemical production sites consisting of world-scale plants are generally oriented around the production of organic chemicals, from petrochemicals up to specialty products. These sites have grown over the last century in scale and number, beginning with sites which grew historically over time, such as the BASF Ludwigshafen site, to today's newly conceived green field sites. Due to increasing petrochemical feedstock prices and pressure on sales margins, maximising the returns in chemical production through efficiencies and economies of scale is more important than ever. The globalisation of chemical markets has seen the proliferation of large integrated chemical sites, particularly in developing regions, such as Asia. Further, over the last decades, the focus of the chemical industry on economic and process efficiency has widened to include the aspects of environment and social responsibility to ensure that chemical production is in line with the principles of sustainable development. Thus, large chemical production sites have become an important topic of public and political concern. These aspects highlight the importance of the subject of this work.

Despite the apparent importance of large chemical production sites, this topic is underrepresented in the literature. These world-scale sites possess significant advantages over smaller sites and are the state-of-the-art in chemicals production and thus a deserved focus of study. Through the review of existing sites and discussion of current trends, the most important aspects of such sites are highlighted. Examples of the integration forms which link members of these sites are provided to enable a better understanding of the advantages and complexities such sites possess. To examine and quantify these aspects is the focus of this work.

A conceptual foundation is established for this work through the definition and description of the Integrated Chemical Production Site or ICPS. The ICPS is defined as a site in which several chemical production plants are linked through various types of integration. A review of literature on industrial clusters and techniques used to describe linked systems provides a theoretical framework with which a novel methodology is developed for the quantification of economic and environmental advantages related to integration for an entire site or an individual process. This methodology may provide support in decision management, for example in the selection of a site location or competing process technologies. Also, the economic and environmental benefits determined for an existing or planned site may be utilised to endorse a site to shareholders or the public.

9.1 Methodology

This work proposes a methodology through which the economic and environmental implications arising from integration in chemical production sites may be quantified. The methodology is based on a comparison between three site types: an integrated, a semi-integrated, and a stand-alone site, which differ in the number of onsite plants, facilities, and types of integration present. A series of functions allows the differences in costs, fossil fuel consumption, and emissions to be quantified relative to defined integration types, outlined below. The methodology may be applied to a single site to determine overall benefits or on the plant level to investigate different scenarios.

Economic and environmental benefits result from the integration of materials, logistics, energy, and infrastructure in an ICPS. These forms of integration are shown below.

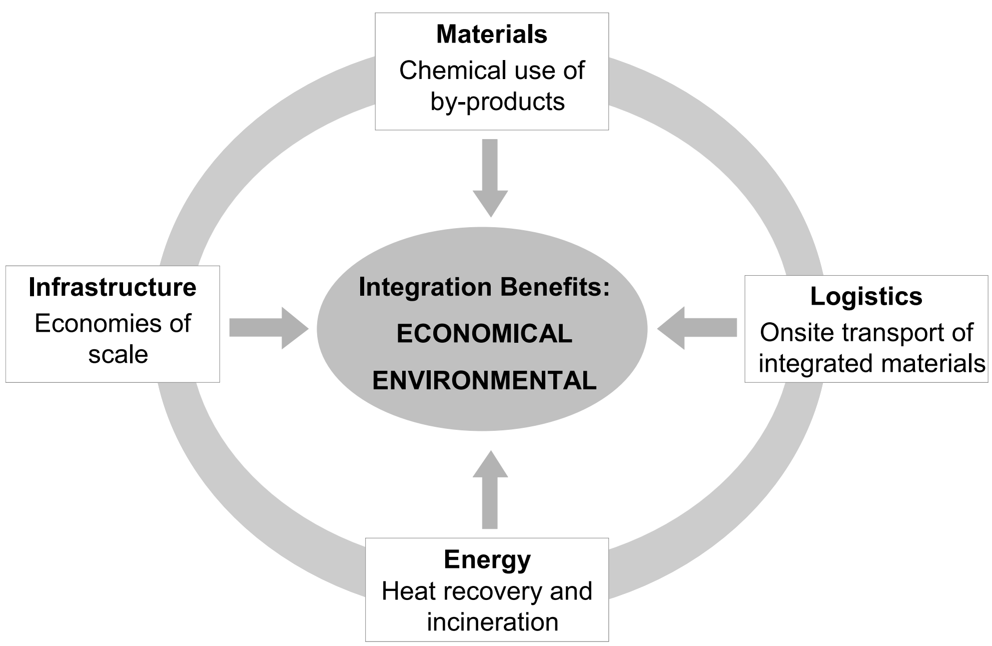


Figure 9.1 Aspects and Benefits of Integration

Materials integration describes the linkage of production plants through shared materials where a product from one plant becomes the feedstock for another. In this work, vertical integration and horizontal integration are differentiated. Vertical materials integration describes the flow of materials along a value chain linking production plants to produce chemical products with successively higher levels of refinement. Horizontal materials integration describes the less deliberate linkage of production plants within a site, such as the chemical use of a by-product from one process in a different process.

Materials integration is normally manifested as pipelines connecting various plants in an integrated site. This results in logistics-related advantages in terms of costs, fuel consumption, and emissions reductions due to the avoidance of offsite transport. Logistics costs related to transport, filling, packaging, storage, warehousing, dispatch, order- and materials management, and import tariffs are either completely avoided or reduced.

Another form of integration investigated in this work is energy integration, consisting of heat recovery, where energy from one process is exported to be provided to other onsite processes, and steam production through centralised waste incineration. The goal of energy integration is to fully utilise sources of excess energy in order to reduce the overall energy requirements of the site. Heat recovery and waste incineration reduce the use of fossil fuels, the generation of emissions, and the costs for equipment and resources associated with energy provision.

Integration through common infrastructure in an ICPS ranges from the provision of utilities to facilities such as a port. In this work, the benefits arising from the economies of scale in common utilities, power, and steam provision, as well as waste water treatment and incineration are investigated. Certain ICPS infrastructure, such as extensive fire-fighting facilities or a port, which do not exist in a stand-alone site, are not investigated in this work, as comparison of these requirements for stand-alone sites is difficult. Further, organisational integration, such as knowledge sharing or greater efficiencies in onsite processes are addressed in the work, but not investigated.

The methodology is applied to three case studies. First the methodology is applied to an actual integrated site to determine the overall integration benefits and relative importance of the different integration types. Next, the methodology is applied to two case studies on the plant level. These enable a more thorough investigation of how integration affects individual aspects of a production process. The two processes selected for the case studies differ in key process characteristics, allowing different aspects important for integration to be demonstrated.

9.2 Site Level Case Study

Applied on the site level, the methodology is used to determine the economic benefit of the co-location of plants and their associated infrastructure at a particular integrated site. An actual integrated site is investigated with world-scale production plants for ethylene oxide/glycol, low density polyethylene, oxo-alcohols, acrylic acid/esters, and C1 compounds, based around a cracker. Through the separation of the site into five production blocks, the benefits of integration are determined according to logistics, materials, energy, and shared infrastructure.

Horizontal materials integration exists through the linkage of the oxo-alcohols and acrylic acid/esters production blocks and the use of a cracker by-product stream as fuel. This results in logistics cost savings estimated at 4 million €/a. Vertical materials integration exists through the onsite provision of feedstocks from a cracker, represents savings estimated at 16 million €/a. Thus, the overall logistics savings are approximately 20 million €/a.

Propane is produced as a by-product in the oxo-alcohols production block and recycled back to the cracker as a feedstock, however due to its small volume, it would most likely be used as a fuel in a stand-alone site. The benefit of materials integration due to the chemical use of propane at the site results in savings of 0.2 million €/a.

Energy integration results in savings estimated at 9 million €/a: 7 million €/a from steam generated through heat recovery by three onsite processes, and 2 million €/a from steam generated through waste incineration.

Shared infrastructure at the site is extensive. Aspects of site infrastructure considered for this study are a common power plant for the provision of steam and power as well as the following utilities: production water, demineralised water, cooling water, and compressed air. The reductions in operating costs for these facilities at an integrated site are estimated at approximately 4 million €/a for steam and power generation and 8 million €/a for other utilities.

Thus, the overall savings for the site are estimated at 41 million €/a, where logistics represents the largest component (48%), followed by shared infrastructure (29%), and energy integration (22%). Materials integration from the chemical use of by-products is estimated at less than 1% of the cost savings. As the particular site studied has no value chains, the savings from logistics are limited. This component is expected to increase in proportion to the other types of savings as a site becomes more forward/backward integrated through onsite value chains.

Reductions in fossil fuel consumption result from a lower natural gas requirement for steam generation due to heat recovery, waste incineration, and economies of scale in the power plant, amounting to 101 kt/a. Additionally approximately 2.4 kt/a of diesel fuel is saved due to onsite transport of integrated products, mainly due to the transport of cracker products. Emissions are reduced through integration due to onsite transport, heat recovery, and economies of scale in the power plant, estimated at approximately 390 kt/a of carbon dioxide plus other emissions.

The case study on the site level demonstrates the importance of logistics as a key factor leading to economic and environmental benefits for an integrated site. Also, the reduction in operating costs for shared facilities in an integrated site is substantial.

9.3 Plant Level Case Studies

To apply the methodology on the plant level, two or more scenarios must be defined where one is represented by the ICPS and the other by a less integrated site. The polyacrylates and aniline processes are selected as case studies. These products are important raw materials for a variety of applications.

Polyacrylates are used in the production of finished products such as paints, adhesives and construction materials and aniline is an important intermediate in the production of polyurethanes, used in construction, automotives, and insulation. These two processes are selected as case studies, as they have different characteristics which influence their suitability for integration. Polyacrylates are categorised as specialties and typically located at the end of the value chain in an ICPS. Generally, a range of products is produced which are transported to offsite customers. On the other hand, Aniline is an intermediate product primarily used for the onsite production of MDI. For the fluidised-bed process, its reaction heat may be recovered as exported steam. Thus, the processes differ in various aspects, such as the types and number of raw materials required, the position in their value chain, and the ability to recover heat. Both case studies are based on actual cases from industry.

9.3.1 Polyacrylates Case Study

In the polyacrylates case study, one integrated production plant in China is compared with five separate stand-alone plants in different Asian countries in close proximity to customers. Below, the effects of integration on production cost and on logistics costs are discussed.

As the integrated plant possesses a five-fold capacity over the individual stand-alone sites, economies of scale in the production process result in cost savings, primarily due to lower personnel requirements. However, raw material prices are higher at the integrated site in China compared with the other countries, decreasing this advantage. Production cost savings for the integrated plant are estimated at 9 million €/a. This highlights the potential for cost savings through economies of scale for a single plant, but also the higher dependence on local conditions in an ICPS.

Although most of the monomers, the largest component of the raw materials, are transported onsite within the ICPS for the integrated polyacrylates plant, this plant is at a logistics disadvantage compared to the five stand-alone sites. This is due to the fact that the product is a 50% aqueous dispersion. Thus, transport of the product to various country ports is more costly than transporting the monomer to individual stand-alone plants in different countries. Costs in the logistics chain are associated with storage, filling, packaging, land transport, freight, port charges, import tariff, enroute warehousing, dispatch, order- and materials management. The largest component of the logistics costs is due to import tariffs[27], freight, and land transport. The additional logistics costs for the integrated plant are estimated at 6 million €/a, as 3 million €/a are saved due to the onsite transport of monomers, but 9 million €/a in costs are imposed due to product transport. Particularly the presence of water in the product results in high transport costs for the product. As a result, fuel consumption is increased by 230 t/a and CO_2 emissions by 2.6 kt/a for the integrated plant.

Thus the overall savings for a large integrated polyacrylates plant compared to five smaller sites is estimated at 3 million €/a. Advantages for local production include shorter delivery time, the ability to cater to local customer requirements, and reduced fuel consumption and emissions due to local production. The benefits of a single integrated plant, in addition to lower production costs and energy integration, include flexibility in adjusting product volumes according to country demands and consistency in production, but there is a disadvantage of higher risks associated with larger production batches. Thus, both advantages and disadvantages are identified with integration for this process.

9.3.2 Aniline Case Study

In this second case study on the plant level, an aniline plant in an integrated site in Belgium is compared with an aniline plant in another integrated site in Germany where one of the process' main raw materials, nitrobenzene, is not available onsite and provided by the ICPS in Belgium. This is based on an actual case. A third scenario is included, a stand-alone aniline plant, in order to highlight a key benefit of the aniline process in an integrated site: its ability to export steam to a site network. For the stand-alone plant, all aniline is transported offsite, whereas for the other cases, the aniline plant is forward integrated and 80% of the aniline is consumed by the MDI process.

The logistics costs for production in Germany, in which nitrobenzene and 20% of the aniline are transported are estimated at approximately 6 million €/a. For the stand-alone plant, located 50 km from the ICPS in Belgium, the transport of nitrobenzene, hydrogen, and aniline results in logistics costs estimated at

[27] Import tariffs are anticipated to be reduced in 2010 due to the ASEAN free trade agreement, see section 6.3.6.

approximately 10 million €/a. Of this 24% result from logistics costs related to hydrogen due to its more costly transport by metal hydride trucks. The logistics costs are substantial relative to the production costs for aniline: 12% for the stand-alone plant in Belgium and 8% for the semi-integrated plant in Germany.

Logistics integration results in significant environmental benefits through the reduction of diesel fuel consumption and emissions. For example, 0.7 kt/a of fuel and 1.9 kt/a of CO_2 are saved for the ICPS in Belgium relative to the site in Germany. A weakness of the model is highlighted in the transport of hydrogen. Fuel requirements for hydrogen transport with metal hydride trucks reflect the lower degree of loading. However, in the determination of transport emissions, a factor assumed to be constant per transport mode is used which does not reflect this decreased loading. Thus, emissions for hydrogen transport are underestimated in the methodology.

The benefit of the exported steam is valued at approximately 1 million €/a at the integrated sites in Belgium and Germany. The economic benefit of exported steam is low relative to the logistics benefits and represents only 1% of the production costs. Due to this heat recovery, 8 kt/a of natural gas are saved.

The aniline case study highlights why large scale intermediates plants, especially with gaseous raw materials which are costly to transport, are best located within an ICPS. The process' few, large volume raw materials and products can be efficiently transported by pipeline in an integrated site. The substantial logistics costs encountered for the stand-alone site located only 50 km from the source of raw materials and port highlight the fact that unless a process is physically linked via pipeline, even short transport distances lead to high logistics costs. Also, the scenario of the site in Germany highlights that if one key raw material is not available, significant logistics costs arise, even in an otherwise integrated site. Also, this scenario highlights the importance of location, as the further an ICPS is from other important raw materials producers, the more dependent the site becomes on itself as the main provider of raw materials.

9.4 Integration Potential

Findings from the plant level case studies enable process criteria important for integration to be identified. The concept of integration potential is proposed as a method for evaluating a process' suitability for integration in an ICPS. Fourteen quantitative and qualitative process characteristics are defined to describe integration potential. The concept is applied to four processes: aniline, polyacrylates, acrylic acid/esters, and caprolactam. The results are shown to correspond well to examples of actual locations of the processes.

The relevance of product type for integration potential is discussed. The specialties process investigated, polyacrylates, has the lowest integration potential of those studied. For the others, all intermediates processes, a range of integration potential is determined depending on process characteristics such as upward/downward integration, volume of raw materials and product streams, and heat recovery. In general, as a process' position in the value chain becomes further removed from the cracker, a lower integration potential is expected. However, other factors, such as the amount of captive use raw materials and products, and whether these materials are readily transported must be considered.

9.5 Closing Remarks

This work, through its definition, description, and economic and environmental analysis of the Integrated Chemical Production Site, is a novel addition to the literature on clusters, on industrial ecosystems, and on the chemicals industry in general. The different types of integration, how they are interrelated and their relative importance in economic and environmental terms are addressed. The methodology developed through this work may be used in the future to determine how effectively various sites are integrated or to assist in the comparison of competing value chain configurations or process technology types. This work provides a clearer picture of the ICPS and a foundation for the basis of future study.

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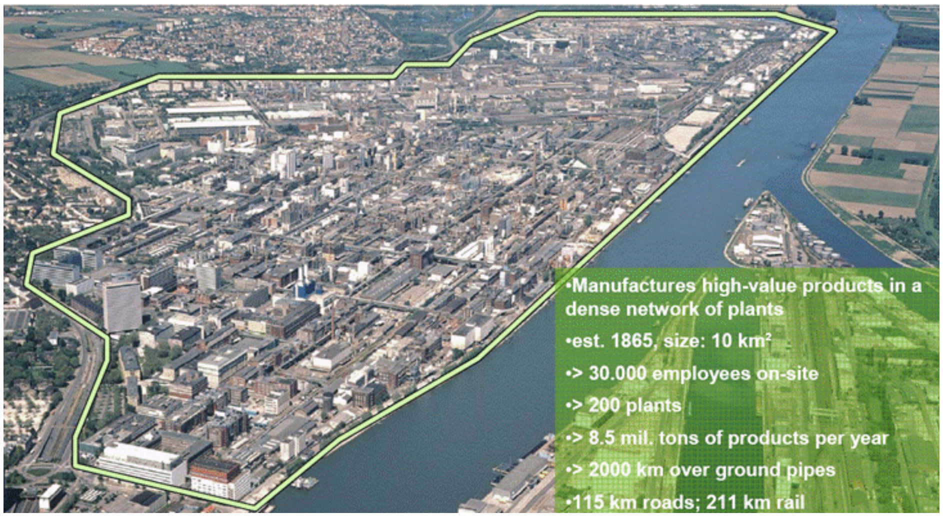
Appendix A. Photos of Integrated Chemical Production Sites

BASF site in Ludwigshafen, Germany (BASF)



BASF site in Antwerp, Belgium (BASF)

Lonza Site in Visp, Switzerland (Gerritzen, 2005)

Jurong Island Site, Singapore (Jurong Town Corporation, 2006)

Chemsite site in Marl, Germany (Chemsite Initiative, 2006)

Appendix B. Steam and Power Cost Calculation

Main design variables

- Steam pressure (typically 4, 16, 40, base case = 16 bar)
- Steam temperature (base case = 250 ºC)
- Boiler feed water (base case = 50 ºC)
- Steam demand (varied between 10 and 650 t/h, base case 250 t/h)
- Electricity demand (varied between 10 and 400 MW, base case 200 MW)

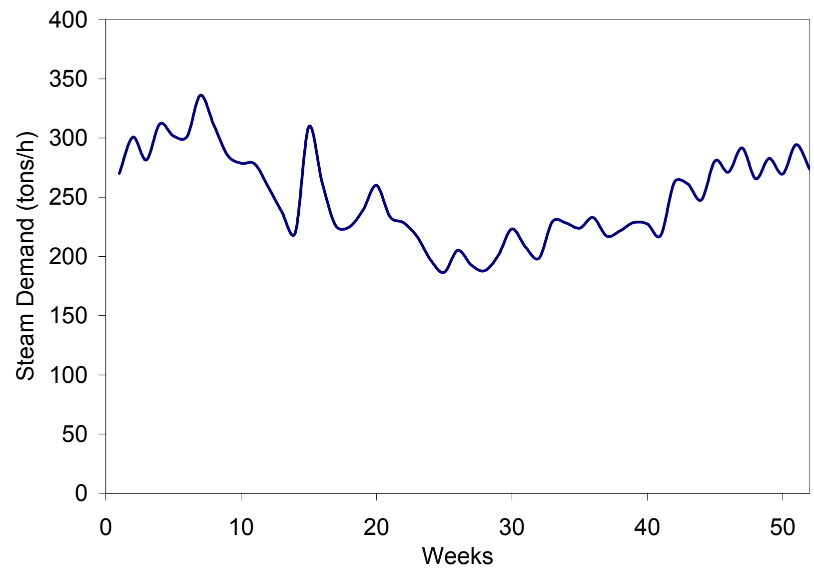
Electricity Price

Variable Charge	40 €/MWh
Capacity Charge	20,000 €/MW*a
Average with 8000h/a	42.5 €/MWh
Backup Electricity	10,000 €/MW * a
Price diff. Import/export	5 €/MWh
Electricity Credit	35 €/MWh
Investment Electricity	100,000 €

(transformers and hook-up to power grid)

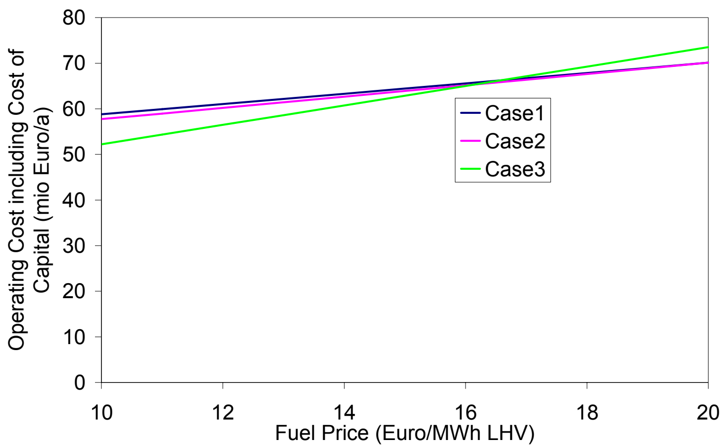
Capital Costs

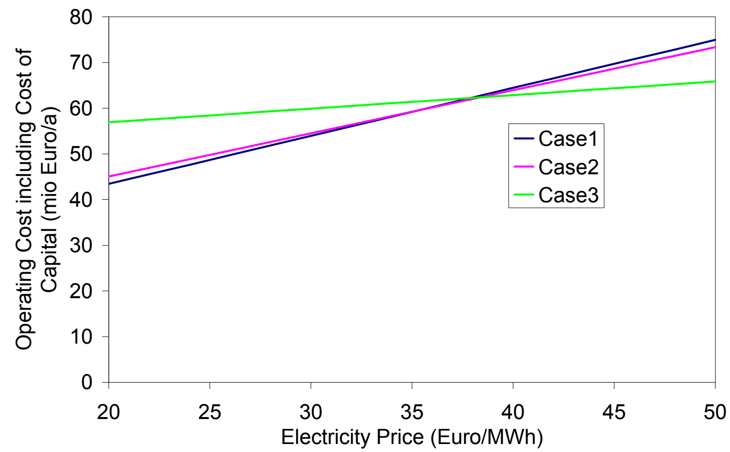
Depreciation	6.7 %
Interest	10 %
Maintenance	3 %
Staff costs	40,000 €/person/a
Hours/a	8,760 h/a
Fuel Price	15 €/MWh LHV

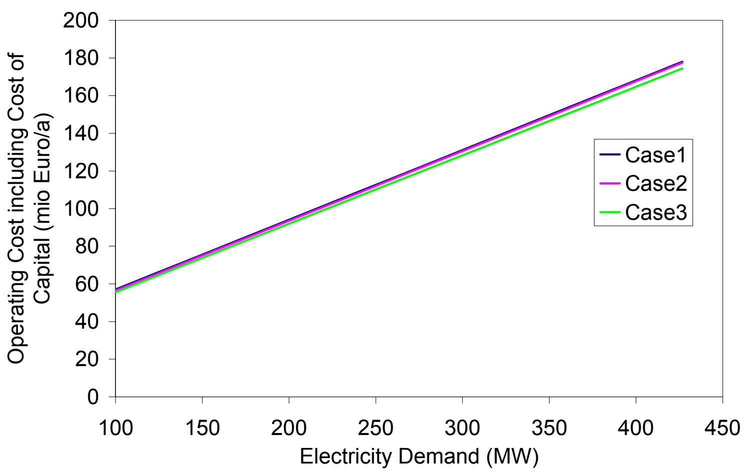


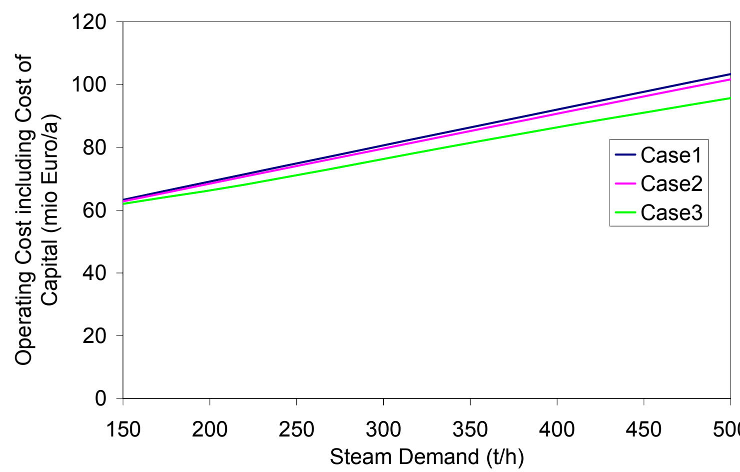
Annual Steam Demand Profile for 250 t/h

Results of Sensitivity Analysis for Steam and Power Cost Calculation









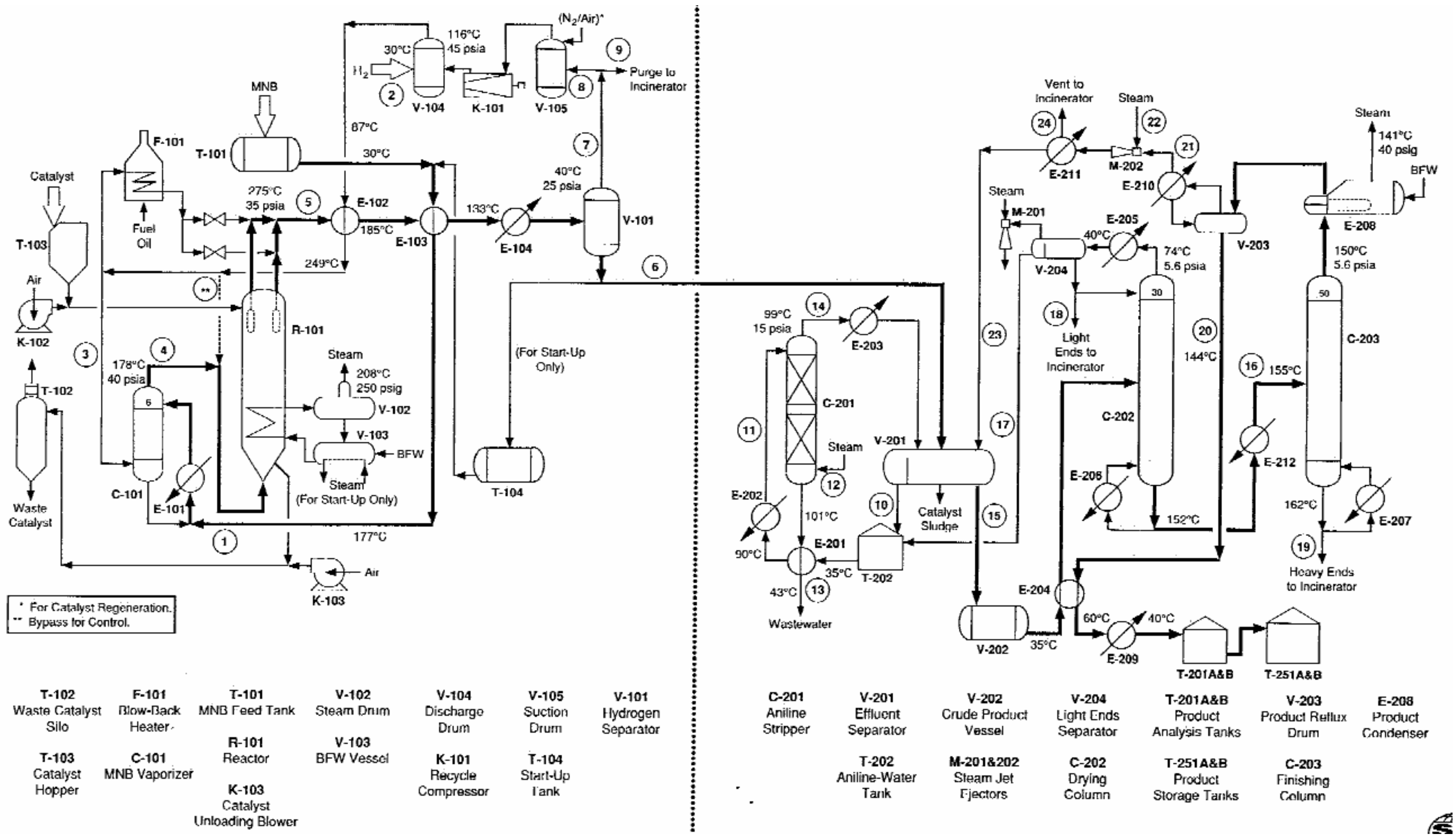
Appendix C. Steam and Power Cost Calculation for Site Case Study

Item		**EO/EG**			**LDPE**			**Oxo C3-C4**		
		Case1	Case2	Case3	Case1	Case2	Case3	Case1	Case2	Case3
Steam supply		Boiler	Boiler+ ST	GT+ST	Boiler	Boiler+ ST	GT+ST	Boiler	Boiler+ ST	GT+ST
Electricial supply		Grid			Grid			Grid		
Electricity demand	MW	33	33	33	47	47	47	10	10	10
Steam demand	t/h	37	37	37	11	11	11	53	53	53
Generation										
Steam GT+ST	t/h	0.0	0.0	32.9	0.0	0.0	9.8	0.0	0.0	47.1
Steam Boiler	t/h	37.0	41.8	4.1	11.0	12.4	1.2	53.0	55.2	5.9
Electricity	MW	0.0	4.9	17.4	0.0	1.4	4.5	0.0	4.7	25.3
Fuel Demand	MW	31	36	56	9	11	17	43	48	78
Investment	**mio €**	**5.54**	**10.22**	**22.98**	**2.53**	**3.99**	**7.66**	**6.99**	**11.58**	**31.28**
Fixed Costs	mio €/a	1.31	2.25	5.20	0.72	1.02	2.04	1.60	2.52	6.92
Fuel Costs	mio €/a	4.07	4.79	7.79	1.21	1.42	2.38	5.68	6.33	10.85
Electricity Costs	mio €/a	12.24	10.44	5.61	17.43	16.88	15.43	3.72	2.00	-4.72
Total Costs	mio €/a	**17.62**	**17.49**	**18.60**	**19.35**	**19.33**	**19.84**	**11.00**	**10.85**	**13.06**

Steam and Power Cost Calculation for Site Case Study, continued

Item		**C1 Complex**			**AA/AE**			**Single Power plant**		
		Case1	Case2	Case3	Case1	Case2	Case3	Case1	Case2	Case3
Steam supply		Boiler	Boiler+ ST	GT+ST	Boiler	Boiler+ ST	GT+ST	Boiler	Boiler+ ST	GT+ST
Electricial supply		Grid			Grid			Grid		
Electricity demand	MW	7	7	7	22	22	22	119	119	119
Steam demand	t/h	58	58	58	3	3	3	162	162	162
Generation										
Steam GT+ST	t/h	0.0	0.0	51.6	0.0	0.0	2.7	0.0	0.0	144.1
Steam Boiler	t/h	58.0	62.1	6.4	3.0	3.4	0.3	162.0	164.0	17.9
Electricity	MW	0.0	5.9	28.2	0.0	0.4	1.1	0.0	12.5	84.8
Fuel Demand	MW	48	54	86	3	3	5	131	143	232
Investment	**mil €**	**7.41**	**13.10**	**34.17**	**1.11**	**1.54**	**2.42**	**14.23**	**26.48**	**84.87**
Fixed Costs	mil €/a	1.68	2.82	7.52	0.44	0.54	0.97	3.02	5.45	18.14
Fuel Costs	mil €/a	6.28	7.13	11.96	0.33	0.39	0.68	17.20	18.82	32.36
Electricity Costs	mil €/a	2.61	0.45	-6.51	8.17	8.00	7.62	44.09	39.52	12.18
Total Costs	mil €/a	**10.57**	**10.40**	**12.97**	**8.94**	**8.93**	**9.26**	**64.31**	**63.79**	**62.69**

Appendix D. Schematic of the Aniline Production Process



(Pep report 76C, 1993, p.E-7)