BFE
OFEN
UFE
SFOE

Forschungsprogramm
Verfahrenstechnische Prozesse (VTP)

Analysis and Modelling of the Energy Consumption of Chemical Batch Plants

elaborated by
Patric S. Bieler
Laboratorium für Technische Chemie
Gruppe für Umwelt- & Sicherheitstechnologie, ETH Zürich
ETH Hönggerberg, HCI G138
8093 Zürich
pbieler@tech.chem.ethz.ch

by order of
Swiss Federal Office of Energy

March 2004 Final Report

Zusammenfassung

In dieser Studie wurden zwei verschiedene Arten der energetischen Analyse und Modellierung (ein top-down Modell und ein bottom-up Modell) von chemischen Batch Produktionsanlagen entwickelt. Sole, Dampf und Elektrizität waren die untersuchten Energien. Der vorliegende Bericht basiert auf einer Dissertation an der ETH Zürich (Bieler 2004). Ein top-down Modell (TODOMO), bestehend aus einer linearen Gleichung basierend auf dem spezifischen Energieverbrauch pro Tonne Produktionsausstoss und dem Grundverbrauch des Gebäudes wurde vorgeschlagen. Dieses TODOMO ermöglichte die energetische Modellierung von folgenden Typen von Batch Produktionsanlagen:

- Monoprodukt Batch Betriebe
- Mehrprodukt Batch Betriebe mit konstantem Produktemix
- Mehrzweck Batch Betriebe in denen ausschliesslich ähnliche Chemikalien produziert werden

Die Resultate zeigten, dass der Elektrizitätsverbrauch der Infrastrukturanlagen signifikant ist (ca. 50% des totalen Stromverbrauches). Der Grundverbrauch für Dampf und Sole war nur gering. Der spezifische Energieverbrauch der untersuchten Gebäude zeigte einen klaren Zusammenhang mit dem Automationsgrad der Produktionsgebäude und den produzierten Chemikalien.

Für den Heizdampfverbrauch des Gebäudes wurde ein Modell entwickelt, welches nur vom Luftwechsel innerhalb des Gebäudes und von den Heizgradtagen abhängig ist.

Für Mehrzweck Batch Betriebe mit stark wechselnden Produktionsprozessen und schwankendem Produktemix war das TODOMO nicht anwendbar und ergab ungenaue Resultate. Für diese Betriebe wurde ein bottom-up Modell (BOTUMO) postuliert und entwickelt. Das Modell besteht aus einem produktionsabhängigen Term und einem batchzeitunabhängigen Grundverbrauchsterm. Der produktionsabhängige Term besteht aus einem von den Chemikalienspezifikationen abhängigen Term, einem von den Apparatespezifikationen abhängigen Term und einem zeitabhängigen Verlutsterm.

Durch diverse Messungen konnten Einzelapparate- und Einzeloperationsmodelle entwickelt werden. Diese Modelle benötigen ausschliesslich einfach zu bestimmende Substanz- und Apparatedaten und modellieren zudem die Verluste der verschiedenen Apparate. Die Modelle wurden so entwickelt, dass sie sich einfach auf andere Betriebe und Chemikalien übertragen lassen und nicht für einen spezifischen Betrieb bestimmt sind. Bereits aus den Einzelapparatemodellen ging hervor, dass die Verluste für Dampf- und Soleverbrauch signifikant waren. Für den Dampfverbrauch wurde ein Verlustkoeffizient von $4.2 \cdot 10^{-2}$ kW / m^2 / K und für den Soleverbrauch ein solcher von $1.7 \cdot 10^{-2}$ kW / m^2 / K gefunden. Hieraus kann geschlossen werden, dass über 50% des Verlustes beim Dampf auf das Heiz/Kühlsystem mit seinen Kondensatableitern zurückzuführen sind.

Zur Modellierung des Energieverbrauches ganzer Produktionsgebäude mit Hilfe des BOTUMO wurden die oben erwähnten Gleichungen in ein Excel® Modell integriert und summiert. Dieses Modell wurde zur Modellierung des Energieverbrauches des ganzen Produktionsgebäudes für einen und zwei Tage, eine Woche, sowie einen Monat verwendet. Die Produktionsdaten stammten entweder aus den Produktionsprotokollen (PR) oder den Betriebsvorschriften (PSP). Die Modellrechnungen zeigten sehr gute Genauigkeiten für die Modellierung von längeren Perioden (mit Hilfe der PSP Daten).

Analysen über die Periode von einem Monat zeigten, dass die Apparategruppe *Reaktoren und Nutschentrockner* die wichtigsten Energieverbraucher im untersuchten Gebäude darstellt (neben dem Infrastrukturverbrauch bei der Elektrizität). Detailliertere Analysen dieser Apparategruppe zeigten, dass ca. 30-40% des Dampfverbrauches für Verluste aufgewendet werden musste. Dies weist auf grosse Optimierungspotenziale hin.

Verschiedene Einsparpotenziale wurden eruiert und vorgeschlagen. Diese reichen von der Elimination von Rücklaufbedingungen bis zu einem völlig neuen Design für die klassischen Heiz/Kühlsysteme.

Diese Arbeit ist im Auftrag des Bundesamtes für Energie entstanden. Für den Inhalt und die Schlussfolgerungen ist ausschliesslich der Autor dieses Berichtes verantwortlich.

Abstract

Two different approaches for energy analysis and modelling of chemical batch plants (a top-down model and a bottom-up model) were conducted in this study. Brine, steam and electricity were the investigated utilities. The study is based on a thesis conducted at the ETH Zurich (Bieler 2004). A top-down model (TODOMO) consisting of a linear equation based on the specific energy consumption per ton of production output and the base consumption of the plant was postulated. This TODOMO showed to be applicable for batch plants of the following kind:

- Monoproduct batch plants
- Multiproduct batch plants with constant production mix
- Multipurpose batch plants in which only similar chemicals are produced

The results showed that the electricity consumption of infrastructure equipment was significant and responsible for about 50% of total electricity consumption. Base consumptions for the steam and the brine system were only minor. The specific energy consumption for the different buildings was related to the degree of automation and the production processes performed.

For the heating steam, a model only depending on air change rate and degree-days was applicable.

For multipurpose batch plants with highly varying production processes and changing production mix, the TODOMO was not applicable and produced inaccurate results. A bottom-up model (BOTUMO) was postulated for these plants. The model consists of a production dependent term and a production-independent term accounting for the infrastructure consumption. The production dependent term actually consists of a term related to the chemicals, another term related to the equipment, and a time-dependent loss term.

With the help of numerous measurements, different apparatus and unit operation models were built. These models use only easily accessible substance and apparatus information and account for the losses of the different apparatus. The models are therefore designed for being transferable to other batch plants and products and not limited to one specific plant. The single apparatus models showed that losses for steam and brine consumption are high. For steam consumption, a loss coefficient of about $4.2 \cdot 10^{-2}$ kW / m^2 / K was found while for brine consumption a loss coefficient of about $1.7 \cdot 10^{-2}$ kW / m^2 / K was found. More than 50% of the losses of the steam are therefore due to the heating/cooling-system design with its steam traps.

With the help of the above-mentioned equations, an Excel® model was built for the modelling of whole production plants according to the BOTUMO. Modelling of the whole production plant was performed for one and two days, one week and one month. The production data were taken from either the production record (PR) or the process step procedure (PSP). The modelling resulted in a high accuracy for the longer periods (PSP data is used as input).

Analyses of the modelling results for one month showed that the apparatus group *reactors and nutsche dryers* is the most important energy consumer in the building (apart from infrastructure consumption in the case of electricity). More detailed analyses of the energy consumption of this apparatus group showed, that about 30 to 40% of steam energy are lost and thus large optimisation potentials are revealed.

Different saving potentials, ranging from elimination of reflux conditions to invention of a new heating/cooling-system for a generic batch reactor, were identified.

This work was conducted under mandat of the Federal Office of Energy. The author is exclusively responsible for the content and the conclusions of this report.

Resumée

Dans le cadre de cette étude, deux approches différentes (un modèle top-down et un modèle bottom-up) pour analyser et modéliser l'utilisation de l'énergie dans une usine chimique de production en batch ont été conduites, qui prennent en considération l'électricité, la vapeur ainsi que la saumure. Cette étude est basée sur la thèse doctorale conduite à l'EPFZ (Bieler 2004).

Un modèle top-down (TODOMO) consistant en une équation linéaire basée sur la consommation de base de l'usine et sur la consommation spécifique d'énergie par tonne de production a été posé. Le modèle TODOMO s'est révélé applicable pour les usines de production en batch des types suivants :

- Usines de monoproduction (monoproduct plant),
- Usines de multiproduction (multiproduct plant) avec un spectre constant de produit,
- Usines flexibles à production multiples où seuls des produits semblables (chimiquement) sont synthétisés (multipurpose plants).

Les résultats ont montrés que la consommation électrique de l'infrastructure est significative et représente environ 50% de la consommation électrique totale, alors qu'elle est négligeable en ce qui concerne la saumure et la vapeur. La consommation énergétique spécifique des différents bâtiments a été corrélée avec le degré d'automation et le type de procédé de production. En ce qui concerne le system de chauffage, un modèle basé exclusivement sur le taux d'échange d'air et les degrés-jours est applicable.

Pour les usines à production multiples où des productions très diverses sont conduites, le modèle TODOMO n'est pas applicable et produit des résultats inexacts. Un modèle bottom-up (BOTUMO) a été posé pour ce type d'usine. Le modèle global consiste en une expression dépendante de la production et une seconde expression indépendante de la production qui représente la consommation de l'infrastructure. L'expression dépendante de la production est constituée d'un terme lié aux produits chimiques, un autre lié aux équipements et un terme représentant les pertes.

A l'aide de nombreuses mesures, des équations caractérisant différents appareillages et opérations ont été dérivées. Ces équations sont basées exclusivement sur des caractéristiques (de produits et d'appareillages) aisément accessibles et tiennent compte des pertes des différents appareils; elles sont donc aisément transposables à d'autres productions et d'autres usines et non limités à un cas particulier. Les équations dérivées pour les appareillages ont montrés que les pertes sont hautes pour ce qui concerne la vapeur et la saumure. Pour la vapeur, des pertes de $4.2 \cdot 10^{-2}$ kW / m^2 / K ont été constatées, alors qu'elles se montent à $1.7 \cdot 10^{-2}$ kW / m^2 / K pour la saumure. Plus de 50% des pertes de la vapeur dont donc dues au design du système de chauffage/refroidissement et à ses séparateurs de condensat.

Basé sur toutes les équations susmentionnées, le modèle global a été construit afin de représenter les usines complètes (BOTUMO). La modélisation a été conduite sur un jour, deux jours, une semaine et un mois de production. Les données de production ont été déterminées sur la base soit des protocoles de production (PR), soit des instructions de fabrication (PSP). La modélisation s'est montrée très précise pour les longues périodes (basées sur les PSP).

Les analyses conduites sur les résultats des modélisations ont montré que la groupe des appareils de type *réacteur et sécheurs* sont les plus gros consommateurs d'énergie dans le bâtiment (mis à part l'infrastructure en ce qui concerne l'électricité). Une analyse plus poussée de ces types d'appareillage a montré qu'environ 30% à 40% de l'énergie sous forme de vapeur est perdue, et a donc révélé un fort potentiel d'optimisation.

Cette étude a permis d'identifier de multiples possibilités d'économie, allant de l'élimination de conditions de retour de condensat en système fermé jusqu'à l'invention d'un nouveau système de chauffage/refroidissement pour un réacteur batch standard.

Ce travail est réalisé sous mandat de l'Office Fédéral de l'Energie. L'auteur est seul responsable du contenu de ce texte et des conclusions présentées dans ce rapport

Contents

List of Figures

List of Tables

1 Introduction

An introduction to the terminology of batch production is provided in (ISA 1995), in (Bieler 2004), and in (Blickenstorfer 1999).

A batch plant cannot be operated by itself. Many different processes, plants and operations have to be performed before a raw material enters the plant and after a substance (product) leaves the plant. A generic value chain of a chemical production is depicted in Figure 1-1. Basic chemicals like crude oil are extracted from nature, transformed and upgraded to intermediate chemicals that are the required raw materials for the pharmaceutical and fine chemical industry. These intermediate chemicals are most of the time produced with continuous processes in large amounts. Fine chemicals on the other hand, are high-value, low-tonnage products. These products are therefore often produced in batch processes to maintain the flexibility and efficiency of low production amounts. For a general overview of the chemicals produced in batch production, see (Parakrama 1985) or (Anonymus 2001). The same is true for the upgrading (i.e., formulating and mixing) of the fine chemicals. This is done often with the help of batch processes as well. The final industrial application and the end users often use batch processes too for their purposes. Therefore, batch processes are of high interest. Because of the difficulties related to the modelling of batch processes and the high prices often achieved on the market (compared to the total production costs), energy optimisation was only a minor issue so far. Today, prices of the fine chemicals are decreasing, production and raw material costs are increasing (i.e., decreasing margins). Moreover, environmental legislation gets stricter and energy consumption is therefore sanctioned (see e.g., (Burkhardt 2002; Eidgenossenschaft 1999; Ewers 2000; Gundersen 1991; Rásonyi 2002; Würsten 2003)). Therefore, the importance of minimising energy use is increasing. Moreover, modelling is required to declare and check the voluntary agreements of objectives for energy-savings in industry as mentioned in (BFE 2001a; BFE 2001b).

Figure 1-1: Value chain in the chemical industry (shaded: batch processes)

The shape of a batch reactor has little changed for the last 500 years (the stirred tank has remained the same from the alchemist's time until today), although new concepts are available and propagated today (e.g., micro-reactors etc. as described in (Höller and Renken 2000; Stitt 2002)). The uncanny resemblance between a 16th century gold plant depicted in Figure 1-2 and a modern fine chemicals plant, with both being dominated by the stirred tank reactor, has been noted by (Stankeiwicz and Moulijn 2000).

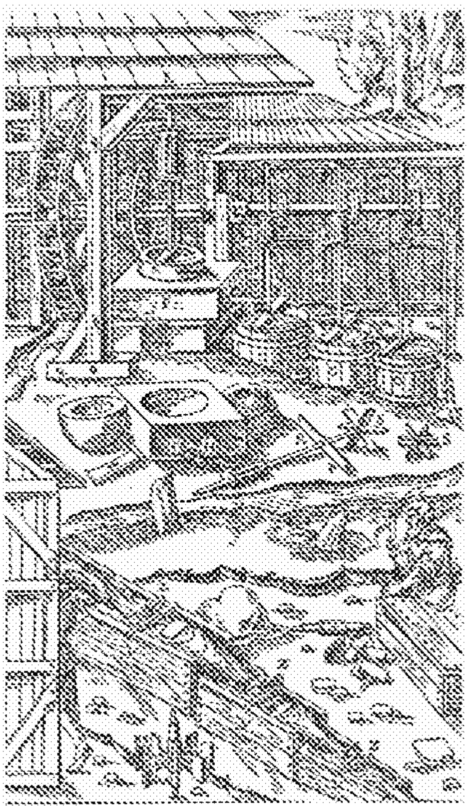


Figure 1-2: Engraving of a 16th century gold processing plant (Stitt 2002)

In (Villermaux 1995) another example of this fact is stated. He notes that the technology of the Concorde has almost nothing to do with that of the Wright brothers or Bleriot, and that they would probably not be able to fly it. By contrast, technical drawings of chemical processing apparatus, such as batch reactors, taken from patents filed in the 1880s are remarkably similar to those still in use and being installed today. Whether or not new concepts for batch reactors are required from an energetic point of view will be investigated in this study as well.

A batch plant usually consists of several parts, as depicted in Figure 1-3 and Table 1-1. The heart of the batch plant is represented by the batch production equipment (i.e., batch reactors, batch dryers, nutsche filters, etc.). In this equipment, the process input is transformed to the process output (i.e., the actual value is added to the product).

Another part of a batch plant consists of so called *special equipment*. This is equipment with special features, not common to the usual batch reactor like high-temperature devices, continuous equipment such as distillation columns for solvent recovery or continuous drying equipment, or equipment for filling and packaging. This equipment is, in contrast to the batch production equipment, very different from plant to plant depending on the kind of process output of the plant.

The *production infrastructure* is required for specific processes. Equipment like circulation pumps, vacuum pumps, etc. could fall in this category. These apparatus are not operated continuously for the whole building but specific for one or the other process.

The final part of a batch plant is represented by the *building infrastructure*. This infrastructure consists of heating and ventilation systems, general vacuum systems, waste-air treatment, etc. All equipment units that cannot be allocated to one specific process and that are therefore operated continuously or stepwise are considered as building infrastructure for the purpose of this study.

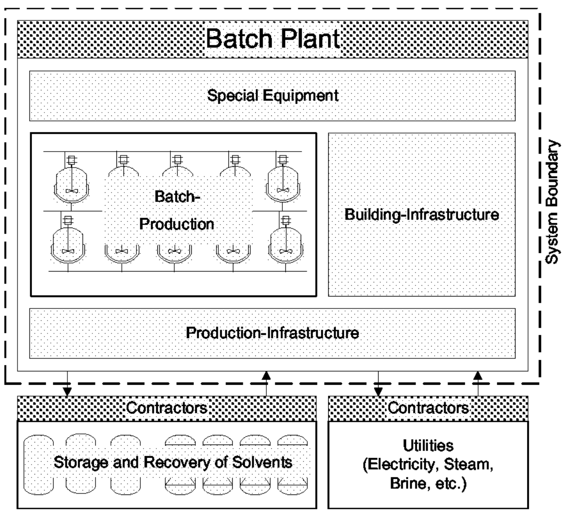


Figure 1-3: General structure of a batch plant

In general, allocation of the total energy consumption in such a building to its different parts is unknown, i.e., it is not known which part of a batch plant is the largest energy consumer and where savings would be most effective. Therefore, this study should provide industry with a tool for a fast and easy allocation of energy consumption in batch production plants for modelling, prediction and comparison of the energy consumption of different plants.

Table 1-1: Sections of a generic batch plant

Section	Description	Equipment Examples
Batch-Production	Standard unit-operations	Reactors; Distillation columns; Crystallisers
Special Equipment	Dedicated equipment used for special purposes or less common equipment	High-temperature equipment; Nutsche dryers; Continuous distillation columns
Production Infrastructure	Infrastructure needed for production but not related to one specific production process	Vacuum systems; Waste air treatment (absorbers, ventilation system)
Building Infrastructure	Infrastructure not necessarily needed for production but required to improve workplace conditions	Space heaters; Lights

The different utilities (e.g., steam, electricity) required in a production building are most of the time produced externally in a central facility for a complete site. Typically, cooling media production is an exception from this rule of centralized production. The term cooling medium, as used in this study, stands for ice or low-temperature fluids like brine (i.e., cooling water is not investigated because of the lack of measurements). Cooling media production is mostly done directly in the specific plant because decentralized production of cooling media is efficient and transportation losses would be significant in centralized production.

The recovery and storage of spent solvents is done either within the batch plant or by a contractor. However, large equipment is needed for this purpose. This equipment is considered independently (decoupled from batch-production). Optimisation of the regeneration operation can thus be done independently as well.

1.1 The Differences between Batch Plants

In batch production, different kinds of batch plants can be differentiated:

- The monoproduct batch plant
- The multiproduct batch plant
- The multipurpose batch plant

The characteristics of these different plants will be discussed shortly in the following sections.

1.1.1 The Monoproduct Batch Plant

A monoproduct batch plant is a plant that is designed especially for the production of one specific chemical. It is a dedicated plant with fix installation. The path of an amount of raw material through the plant is clearly defined. No or minimal manual operation is usually required since automation is elaborated and recipes are seldom changing (if cheap labour is available, degree of automation may be low as well). In an automated plant, data availability is most of the time good. Because of the constant production steps, focus is given to optimisation of the production process (e.g., energy savings by heat integration (Krummenacher 1997; Krummenacher and Favrat 2001)).

1.1.2 The Multiproduct Batch Plant

A multiproduct batch plant is a plant where different chemicals are produced throughout the year, but the same production steps are mostly performed in the same equipment (see (Rippin 1992) as well). Fixed lines of batch reactors are producing different products (probably different products on one line at different times of a year). The amounts of the different products may vary with sales requirement. Therefore, production mix may not stay constant and may have an influence on scheduling and utility requirements. Each line in a multiproduct batch plant may be considered as a (small) monoproduct batch plant (i.e., fixed material pathways, potential for specific optimisation) for each production period.

1.1.3 The Multipurpose Batch Plant

A multipurpose batch plant, on the other hand, produces different chemicals like the multiproduct batch plant, but in each equipment unit, different production steps might be performed (i.e., such plants are characterized by high flexibility; (Rippin 1992)). The units are most of the time independent from each other and connected via flexible pipes. This allows a construction of a production path for the purposes of one specific chemical, each time this chemical may be produced in the plant in a different way (i.e., in different reaction vessels). The pathway of a chemical in the monoproduct and the multiproduct batch plant is most of the time from top to bottom for reasons of ease of transportation (gravitation is helping to transport the chemicals). In multiproduct batch plants, this is probably considered as well, but not necessarily, because this would restrict the flexibility of the plant.

No or few dedicated equipment can be found in a multipurpose chemical batch plant. This implies that all the equipment items are capable to perform all possible unit operations and limits the optimisation potential.

The infrastructure part of the multipurpose batch plant may also differ from the infrastructure of the other two kinds of batch plants. Because of the multipurpose characteristic of these plants, the infrastructure is not optimised for one specific use. It is tried to operate as few infrastructure equipments as possible (cost savings) but to install the equipment as flexible as possible. This allows producing many different products. If a new product with new infrastructure requirements is introduced to the plant, the new infrastructure equipment has to be integrated in the former concept. This leaves room for over sizing and inefficiencies.

2 State of the Art

About 50% of industrial processes (Stoltze et al. 1995) and chemical production (Phillips et al. 1997) worldwide are batch processes.

Energy consumption of production processes contributes significantly to overall resource use. The fewer resources the production of a substance (or functional unit) uses, the more environmentally friendly the process is (assuming that all other parameters remain constant). Moreover, about 75% of man-made air pollution is caused by energy use (Wang and Feng 2000). Therefore, minimization of energy consumption is listed as the sixth principle of green chemistry (Anastas and Warner 1998).

The chemical industry is a large, and in certain sectors, intensive user of energy. For example, excluding man-made fibers, in 1985, it accounted for 10% of the UK's industrial output and 15% of its energy consumption; the latter value amounted for 34% if oil and gas feedstock were added. Despite substantial and continuing improvements in efficient energy use, the UK chemical industry's energy purchase bill was about £1.1 billion in 1985, with feedstock costing well over £1 billion in addition (Legge 1986). The US chemical industry sets in their "Vision 2020" the clear target to reduce energy consumption of chemical production and to improve energy efficiency (Eissen et al. 2002; ACS 1996).

A survey on the chemical industry in the U.K. showed that, on average for different chemical branches, the most energy is used for process heating (40%), with distillation (13%), drying (10%) and compression (10%) being the other major energy-consuming unit operations (Anonymus 1986).

Many papers, models and theories of the past and present research have dealt with energy modelling of continuous processes as stated in (Linnhoff 1993; Worrell et al. 2001; Zalba et al. 2003) or heat exchanger networks (Furman and Sahinidis 2002; Gundersen and Naess 1988; Jezowski 1994a; Jezowski 1994b; Zhao et al. 1998). Batch production is hereby most of the time neglected or the models are considered as too complex for industrial use (Stoltze et al. 1995). Similar methods for batch production are not yet well established. Furthermore, such studies are usually limited to heat-integration (Bouhenchir et al. 2001; Kemp and Macdonald 1988) and therefore rely on available storage capacity or constant production schedules. Other studies account for time-varying temperatures (Vaselenak et al. 1986) and rescheduling (Vaselenak et al. 1987). The use of these methods in batch production is limited because most of them are considered as too complicated, lengthy, demanding and complex to be of practical interest for most of the cases encountered (Stoltze et al. 1995). The fact that energy costs amount to about 5 to 10% of total production costs for common chemicals produced in batch operation (Vaklieva-Bancheva et al. 1996) limits the efforts undertaken in achieving high energy efficiency. A helpful overview of energy consumption and management in batch production is provided in (Grant 1996). Nevertheless, much literature is available on scheduling of batch plants, which allows a more efficient use of energy by reducing waiting and changeover times (see e.g., (Calderón et al. 2000; Papageorgiou et al. 1994; Reklaitis et al. 1997; Sahinidis et al. 1989; Suhami and Mah 1982; Verwater-Lukszo 1996; Vin and Ierapetritou 2000)).

A novel approach named as *Time Average Model* (TAM) or *Time Slice Model* (TSM) is introduced by (Linnhoff et al. 1988) and further used by several authors (e.g., (Krummenacher 1997; Stoltze et al. 1995; Zhao et al. 1998)). Both the TAM and the TSM adapt the concept of pinch analysis introduced by (Linnhoff et al. 1982) to batch processes. The TAM assumes that all batch operations can be performed at any time and in any order, so that no account is taken of scheduling or time availability of energy flows. The time dependent consumption of a batch reactor is averaged over the whole batch time for one process resulting in a mean consumption for the whole process. In other words, time is completely ignored as a constraint and the energy source and sink values become averaged over a chosen period. This results in a model similar to continuous processes that can be handled by pinch analysis. This model is easy-to-use but has, nevertheless, not much in common with the real behaviour of batch production and is therefore of no significant practical use. The TSM, on the other hand, does incorporate assumptions about time, e.g., cycle times and time availability. Time is then 'sliced' into periods during which process energy flows can be analysed and a separate model is calculated for each slice. For each of these slices, energy consumption is again analysed as an average consumption over the whole time of the slice. Both the TAM and the TSM, nevertheless, have no wide acceptability in industry. Furthermore, they have not been applied to different energy carriers (only examples for steam are available) and different products and processes in one unified model.

Reliable statements on energy efficiency and improvement potentials of production processes need standardized parameters characterizing energy consumption. It is only reasonable to set energy targets if the relation between the actual and the minimal practical energy consumption is known. In multiproduct and in multipurpose batch plants, this energy consumption has to be allocated to different products and unit operations. Focus may then be put on the greatest saving potential of the largest energy consumers. This prevents a wasting of the limited resources for re-engineering by using them for the most effective saving potentials.

Energy models for multiproduct and multipurpose batch plants are lacking in industry. It is known that energy consumption is, to some extent, related to production output, but exactly where energy is used is not known. Whether the dependence on production output is strong or whether the base load consumption of a building is dominating is not known. Energy consumption models on building level are needed for providing consumption forecasts to the energy supplier and for calculating total production costs.

Some authors mention that significant savings of energy cost (and consumption) in batch plants of up to 25% are possible (Allen and Shonnard 2002; Ashton 1993; Benz 2003; Krummenacher et al. 2002; Phillips et al. 1997; Rumazo et al. 2000). (Jiménez-González and Overcash 2000) state, that especially energy challenging in early process phases reduces the level of emissions during the whole lifecycle of the product. In this paper, energy lifecycle information is developed to support the decision-making process.

Besides these detailed papers mentioned above the basic concept of energy audit is essential for performing an energy analysis of a whole production plant. The concept of energy analysis is widely discussed in literature; some examples may be found in (Bhatt 2000a; Bhatt 2000b; Ganji 1999; Haman 2000; Hoshide 1995; Robert and Markus 1994). (Blickenstorfer 1999) provides a good overview of literature dealing with energy analysis.

No models are available in the literature to compute the energy consumption of batch processes, accounting for the consumption caused by the chemical process itself, the consumption due to the equipment and especially the losses of the different systems. This will be investigated and analysed in this study (see Chapter 4).

3 Goal of the Study

Energy consumption plays an important role in today's business since most of the processes are not possible without an appropriate energy source (Kürsten 1996). Allocation to different processes and products is, nevertheless, often not possible for batch production. As stated in the preceding chapter, energy consumption contributes quite significant to production costs and to environmental hazard in the producing industry. Nevertheless, accurate and ready-to-use tools for predicting or modelling the energy consumption of chemical batch plants are missing. Goals for energy savings or targets for focusing on improvement potentials are most of the time set according to common (engineering) sense or political targets. This is, contrary to continuous production processes, where detailed models for energy consumption and integration methods are available, an unsatisfying situation. Moreover, legislation needs tools to predict the energy saving potentials of plants to meet the goals set (see e.g., (Eidgenossenschaft 1999)) and the Kyoto protocol (see (http://unfccc.int/resource/docs/convkp/kpeng.html) for the text of the protocol and (Rásonyi 2002; Thöne and Fahl 1998; Würsten 2003) for some comments). The goals set in CO_2-legislation as mentioned in (Eidgenossenschaft 1999), lead to voluntary savings and agreements of objectives with industry as mentioned in (BFE 2001a; BFE 2001b) and in (BFE 2002). To succeed in these agreements of potential savings, detailed models for energy consumption are required. Without such models, it would not be possible to control whether or not the goals are achieved.

For all these reasons, easy to use tools should be available for energy modelling of chemical batch production plants. The thesis by (Blickenstorfer 1999) showed the possibility of energy modelling on building level for a specific kind of batch production (top-down approach for one kind of batch production plant as discussed below). Applicability of this approach to other buildings will be investigated in this study.

In this study, easy-to-use and adaptable single unit operation models (SUOM) on apparatus level are developed. The new approach of the study offers the possibility to model the energy consumption of a complete production plant with a detailed bottom-up model based on the SUOM with the help of easily accessible data. The required data consists of apparatus specifications, building infrastructure consumption, specifications of the chemicals and the production processes as well as operation times from the process step procedure. With the help of this model, it is possible to gather information on the energy consumption of a specific batch plant with a minimal of surplus measurements and data requirements. The data may be aggregated for different levels of analysis, as the user likes.

The applicability, usability, and accuracy of such models have to be investigated in this study. The models investigated should be simple enough to be useable in daily production and accurate enough to analyse the energy consumption of a production plant in detail. Such models would help legislation and particularly the production chemist and plant management to analyse and in a second step optimise the energy consumption of their production plants.

Intermediate results of the study may be found in (Bieler 2002).

4 Solution: Two Approaches for Energy Modelling

For the modelling of energy consumption, two basic models are postulated, elaborated and investigated in this study. One is a "Top-Down"-model (TODOMO) based on measurements of the whole building described in Chapters 4.1 and 5.1 and the other one is a "Bottom-Up"-model (BOTUMO) based on single unit operation models and measurements described in Chapters 4.2, 5.2, and 5.3.

The purpose of the two models is to model and allocate energy consumption of batch plants. The time horizon will be no shorter than one day. This limitation was set, because the short-term modelling would require clumsy integral equations that would need many input parameters usually unavailable in production business. Moreover, the important period for a production plant is one week or even one month. For those periods, accounting of the production output is available and contractors bill the energy consumption.

The following two subchapters will postulate the models of the TODOMO and the BOTUMO with their equations.

4.1 The Top-Down Approach

4.1.1 The Model for the Production Dependent Energy Consumption

For each utility, a model that computes the energy consumption of a building as a function of the specific consumption per ton of product output and the base consumption was postulated. The equation for the TODOMO is represented by Equation (3-1).

$$E_m = S_m \cdot PO + B_m \quad (3\text{-}1)$$

here, E_m is the overall consumption of a specific energy form in a specified period (i.e., longer than one day, mostly one month) in kWh per period, S_m is the specific consumption of one energy form per ton of products in kWh / t, PO is the production output on a weight basis during the period specified (including all products and intermediates leaving the plant, excluding solvents and aggregate) in t per period, and B_m is the so-called base consumption of the building of a specific energy form in kWh per period. The base consumption is the consumption of a warm production building that is ready to start production but in which no production process is actually running (i.e., base consumption measures infrastructure consumption and infrastructure losses).

Two different possibilities exist for the determination of the base consumption. Each building undergoes a period of revisions at least once a year. During this period, maintenance activities are undertaken and production is shut down. Therefore, it is possible to measure the consumption of the warm (ready to produce but not yet producing) and the cold (only safety equipment is running) building. Losses of the whole system have to be analysed in this way. A second possibility is the direct measurement of the consumption of the specific infrastructure equipment itself since it is known which apparatus is on stream during shutdown or production.

Such linear models were also postulated by (Blickenstorfer 1999). Models of this kind are only applicable to monoproduct or multiproduct batch plants or multipurpose batch plants with similar products as will be discussed in Chapter 5.1.

For multipurpose batch plants with large differences between their products and changing production mix, linear TODOMO are not applicable as will be shown in Chapter 5.1. For these buildings, that are the main research topic of this study, a new BOTUMO is postulated and discussed in the Chapters 5.2 and 5.3.

4.1.2 The Heating Steam Model

Production plants are heated by heating the fresh air entering the building. This is (unlike to residential buildings, where radiators are used most of the time) done by heat exchangers with condensing steam. This (comfort) heating steam is measured separately. A linear model only depending on degree-days (see (http://www.eia.doe.gov/neic/infosheets/degreedays.htm)) was first postulated according to Equation (3-2) but found to be not applicable.

$$SC = DSS \cdot DD + B \tag{3-2}$$

where, SC is the steam consumption in MWh / month, DSS is the degree-day specific steam consumption in MWh / °C / d, DD is the number of degree-days in °C · d / month and B is the base consumption of heating steam in MWh / month, which is unique for each building.

Since the air change rate of production buildings is significantly higher than for residential buildings because of safety reasons, the model was adapted to account for the air change rate. This model was found to be applicable for the heating steam consumption of batch plants and is depicted in the following equation:

$$SC = 0.32 \cdot ACR \cdot DD + B \tag{3-3}$$

where, ACR is the air change rate of a building in h^{-1}.

If no production infrastructure uses heating steam and if the main pipe of heating steam is closed during summer, the base consumption is almost equal to zero. Otherwise, the base consumption has to be measured or estimated before predictions of heating steam consumption can be made, as discussed in Chapter 5.1.3.1.

4.2 The Bottom-Up Approach

The basic equations for the BOTUMO, describing the concepts of calculating the energy consumptions for heating and cooling procedures (Chapter 4.2.1) and calculating the energy consumption of the electric equipment (Chapter 4.2.2) are presented here. These basic equations are combined in different way for the different unit operation models on single apparatus level presented in Chapter 4.2.3 and 5.2. The single unit operation models are summarised to result in a model of a whole plant (see Chapter 4.2.3 as well).

4.2.1 Equations for Heating and Cooling of Substances

In any book dealing with heat transfer and physical chemistry (e.g., (Atkins 1990) or (Wedler 1987) or (Perry et al. 1997)), the basic equations for the heating and cooling of substances can be found. The heating or cooling of a substance without phase change can be calculated by Equation (3-4).

$$\Delta H = \int_{T_1}^{T_2} m \cdot c_P dT \tag{3-4}$$

here, ΔH is the enthalpy change in kJ, T_1 and T_2 are the temperatures at the beginning and at the end of the heating process in K, c_P is the heat capacity of the product in kJ / kg / K and m is the mass of the heated substance in kg.

With the help of the assumption, that m as well as c_P stay constant in the investigated temperature range as stated by (Dahinden 2003), Equation (3-4) can be simplified, resulting in Equation (3-5).

$$\Delta H = E = m \cdot c_P \cdot (T_2 - T_1) \tag{3-5}$$

The generic equation for the energy consumption of a substance undergoing a phase change (i.e., crystallisation, freezing or evaporation) or performing a chemical reaction is presented in Equation (3-6).

$$\Delta H = E = m \cdot \Delta H_i \tag{3-6}$$

here, ΔH_i in kJ / kg signifies the heat of reaction ($_R$), evaporation (or condensation) ($_V$), freezing ($_M$), or crystallisation (or melting) ($_C$), respectively.

As stated in (Perry et al. 1997), heat losses through a solid wall are proportional to the temperature difference, the surface, and the time of operation and are insulation-specific coefficients as shown in Equation (3-7).

$$\Delta H = E = K \cdot A \cdot (T_{HJ} - T_{Am}) \cdot \Delta t \tag{3-7}$$

here, K is the heat transfer coefficient in kW / m^2 / K, A is the total surface area of the apparatus in m^2, T_{HJ} and T_{Am} are the temperature in the heating jacket of the apparatus and of the ambience in K, respectively, and Δt is the operation time in s.

4.2.2 Equations for Electric Equipment

The energy consumption of electric equipment is strongly related to its nominal power. The nominal power is a physical property describing electric equipment. Measurements of the actual power consumptions lead to Equation (3-8).

$$E = \gamma \cdot P_N \cdot \Delta t \tag{3-8}$$

here, γ is the part of nominal power consumed by the equipment, expressed in percent, P_N is the nominal power of the equipment in kW and Δt is the time of operation of the equipment in s.

As stated in (BBC 1976)[1] the efficiency of an electric motor decreases when not operated at nominal power. Moreover, shaft power is lost[2] in the transmission (about 5%) and by the use of frequency converters (about 10% because of imperfect sinus-curves of the current after the frequency converter). Shaft power of a stirrer is considered to directly contribute to heating of the vessels according to Equation (3-9).

$$E = \eta \cdot \gamma \cdot P_N \cdot \Delta t \tag{3-9}$$

here, η is the efficiency of the motor given in (BBC 1976) in %.

[1] Although this source is rather old, its findings are still valid today according to industry experts

[2] According to discussions with industry experts

According to (Perry et al. 1997), the power consumption of a vacuum pump can be calculated as follows:

$$P = p \cdot V \tag{3-10}$$

where, P is the power consumption in J (or kWh), p is the pressure at which the pump is operating in Pa, and V is the volume the pump is extracting from the vessel in m^3.

Power consumption of electric equipment may be calculated in general according to Equation (3-11) (see e.g., (Kneubühl 1994) for detailed explanation of the equation).

$$P = \frac{\sqrt{3} \cdot I \cdot U \cdot \cos\varphi}{1000} \tag{3-11}$$

here, P is the electricity consumption in kW, I is the current in A, U is the total voltage in V (i.e., 500 V), and $\cos\varphi$ is the power factor, specific to each motor.

The general equation for the mixing of a fluid inside a stirred vessel is of the form of Equation (3-12) (see e.g., (Mersmann et al. 1975)):

$$P = Ne \cdot \rho \cdot n^3 \cdot d^5 \tag{3-12}$$

where P is the power needed for mixing in kW, Ne is Newton's number, ρ is the density of the fluid in kg / m^3, n is the number of revolutions per minute in min^{-1}, and d is the diameter of the stirrer in m.

The general model for constant consumption is postulated according to the following equation:

$$E_m = C \cdot t \tag{3-13}$$

here, E_m is the consumption of the specific energy form $_m$ (steam, electricity, brine) in kWh, C is a constant consumption per time of the specific energy form, and t is the operation time in s.

4.2.3 Unified Equation for the Bottom-Up Modelling

The concept of the BOTUMO is given in Figure 4-1. The energy consumption of a production plant is split into infrastructure consumption and a production dependent consumption part. So far, this is a similar concept as the TODOMO discussed in Chapter 4.1. In addition to the TODOMO, the production dependent part is analysed by the BOTUMO as well. This will be discussed in the following part of this chapter.

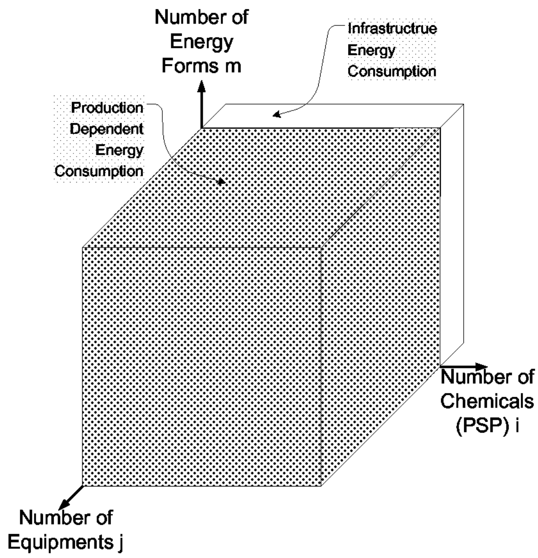


Figure 4-1: The basic concept of the BOTUMO

The model of a whole plant will be built similar to the TODOMO and according to the following basic equation:

$$E = E^P + E^I \cdot t \qquad (3\text{-}14)$$

here, E is the energy consumption of the whole building in kWh per period, E^P is the production dependent energy consumption in kWh per period, E^I is the energy consumption of the building infrastructure in kWh per s, and t is the length of the period in s per period. The infrastructure energy consumption is specific for each plant and measured or calculated on building level. The production dependent energy consumption on the contrary is related to the actual production and unifies the equations given in the Chapters 4.2.1 and 4.2.2 (see Chapter 5.2 as well).

The production dependent energy consumption is divided in a part that is related to the reaction mass, another part is associated with the apparatus and a last part that relates to the losses.

Equation (3-15) gives the basic concept of the production dependent energy consumption calculation.

$$E^P = E^{RM} + E^A + E^L \qquad (3\text{-}15)$$

where, E^P is the total energy consumption in kWh, E^{RM} is the energy consumption related to the reaction media in kWh, E^A is the energy consumption related to the apparatus in kWh, E^L is the loss of energy in kWh.

Each of these energy consumption terms consists of different parts: different forms of energy ($_m$), production in different apparatus ($_j$) and the production of different chemicals ($_i$). This leads to a split of the energy cube depicted in Figure 4-1 as shown in Figure 4-2.

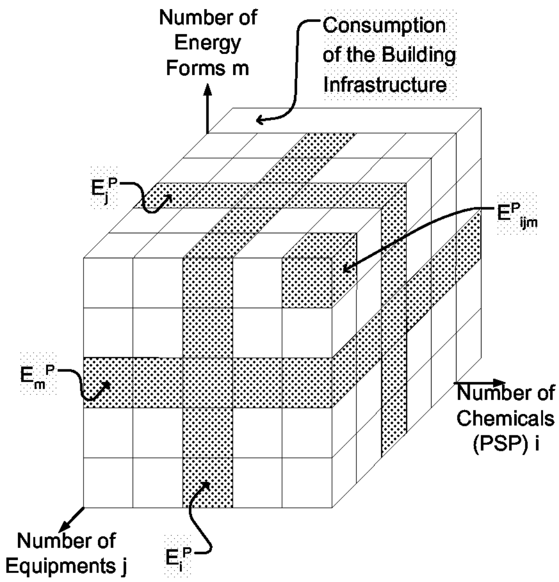


Figure 4-2: The principle of the BOTUMO

In Figure 4-2, E^P_{ijm} is the energy consumption of one specific chemical $_i$ (probably only one step of its production recipe), produced in one specific apparatus $_j$, requiring the energy form $_m$. The general equation for this calculation is shown in Equation (3-16).

$$E^P_{ijm} = \frac{E^{RM}_{ijm} + E^A_{ijm} + E^L_{ijm}}{SF_m} \qquad (3\text{-}16)$$

here, E^P_{ijm} is the above-mentioned energy consumption of one specific chemical produced in one specific apparatus with the help of one specific energy form in kWh per batch, E^{RM}_{ijm} is the energy consumption of one specific energy carrier in kWh per batch of the reaction mass of one specific chemical in a specific apparatus, E^A_{ijm} is the energy consumption of one specific energy carrier in kWh per batch in an apparatus of one specific production recipe, E^L_{ijm} is the loss or motor term of a specific apparatus, performing a specific recipe for one specific energy in kWh per batch, and SF_m is the scaling factor of the specific energy form (i.e., 1 for brine and electricity and 2350 kJ / kg for steam as discussed in Chapter 5.2.2 since steam is measured in t (or kg) in the plant).

The energy consumption of the reaction mass E^{RM}_{ijm} is defined by the following equation:

$$E^{RM}_{ijm} = F_m \cdot \sum_q \sum_k \left(c_{Pk} \cdot m_{ijk} \cdot \Delta T_{iq} + m_{ijkq} \cdot \Delta H_{ik} \right) \qquad (3\text{-}17)$$

where F_m is a dimensionless factor defining the kind of energy used (i.e., 1 for brine and steam and 0 for electricity), c_P is the heat capacity in kJ / kg / K, m_{ijk} is the mass in kg, ΔT is the temperature difference in K and ΔH is the enthalpy (of vaporisation, reaction, melting, etc.) in kJ / kg, the index $_k$ is an indicator for the different chemicals used in the step, and the index $_q$ is an indicator for the different process steps (e.g., temperature levels, unit operations) of the specific recipe.

The energy consumption dependent on the specifications of the reactor E_{ijm}^{A} may be explained by:

$$E_{ijm}^{A} = F_m \cdot \sum_q \sum_n c_{Pn} \cdot m_{jn} \cdot \Delta T_{iq} \tag{3-18}$$

where the index $_n$ is an indicator for the different aspects (i.e., materials) of an apparatus.

The losses and the consumption of electric motors E_{ijm}^{L} will be expressed by equations of the following type:

$$E_{ijm}^{L} = \frac{\sum_q \left(K_{jm} \cdot A_j \cdot \Delta T_{iq} - P_j^N \cdot \eta_j \cdot \gamma_j \right) \cdot t_{ijmq}}{3600 \, {}^{s}\!/_{h}} \tag{3-19}$$

where K is the heat transfer coefficient of the apparatus in kW / m2 / K, A is the total surface of the apparatus in m^2, ΔT is the temperature difference between the ambient temperature and the heating jacket in K, P_N is the nominal power of the motor in kW, γ is the relation of nominal power of the motor to the actual power consumption in %, η is the efficiency of the motor in %, and t is the operating time of one specific process step $_q$ in one specific equipment $_j$, producing one specific product $_i$, requiring one specific energy form $_m$ in s per batch. The factor 3600 s / h converts kWs in kWh.

Equations (3-17) to (3-19) are inserted into Equation (3-16). This is the base equation for the BOTUMO depicted in Figure 4-2. Now, each apparatus $_j$ represents for each chemical produced $_i$ and for every energy form $_m$ a single cubicle in the production dependent cube of Figure 4-2. With the help of the number of batches (n_i) of one chemical $_i$ produced in a certain period, a summation along all the three axes of the energy consumption cube presented in Figure 4-2 is possible leading to different results and finally to the total production dependent energy consumption E^P (Equation (3-26)). This could e.g., lead to the total energy consumption for the production of one specific chemical in all of the concerning apparatus E_i^P presented in Equation (3-23). The different summations are shown in the following equations.

$$E_{im}^{P} = n_i \cdot \sum_j E_{ijm}^{P} \tag{3-20}$$

$$E_{jm}^{P} = \sum_i n_i \cdot E_{ijm}^{P} \tag{3-21}$$

$$E_{ij}^{P} = n_i \cdot \sum_m E_{ijm}^{P} \tag{3-22}$$

$$E_{i}^{P} = n_i \cdot \sum_m \sum_j E_{ijm}^{P} \tag{3-23}$$

$$E_{j}^{P} = \sum_m \sum_i n_i \cdot E_{ijm}^{P} \tag{3-24}$$

$$E_{m}^{P} = \sum_j \sum_i n_i \cdot E_{ijm}^{P} \tag{3-25}$$

$$E^P = \sum_m \sum_j \sum_i n_i \cdot E^P_{ijm} \tag{3-26}$$

According to these summations, different statements like the energy consumption of one specific energy form for the production of all the chemicals in all the apparatus (i.e., Equation (3-25)) are possible.

The production dependent energy consumption of the whole plant given in Equation (3-26) is equivalent to the one given in Equation (3-15). This production dependent energy consumption may then be inserted in Equation (3-14) to result in the total energy consumption of a production plant.

These generic equations will be used to model the different kinds of unit operations. Therefore, the parameters (especially the loss coefficients of the different apparatus) have to be evaluated with the help of measurements as will be discussed in Chapter 5.2.

5 Main Results

5.1 Top-Down Modelling of Production Plants (TODOMO)

5.1.1 The Basic Equation for the Top-Down Modelling

Consumption of the different utilities was measured at the defined system boundary (see Figure 1-3). These data were collected on a monthly basis. In addition to these energy consumption data, the production output (tons of products) of the different buildings was determined on a monthly basis as well. The TODOMO is discussed in more detail in (Bieler et al. 2003) and (Bieler 2002). The measured values may be found in (Bieler 2004).

5.1.2 The Characteristics of the Different Buildings Investigated

Table 5-1 summarizes the characteristics of the investigated buildings. These buildings are typical for production in the specialty chemicals industry. Buildings 1 to 3 are multipurpose batch plants, conducting chemical reactions that use either organic compounds (Buildings 1 and 2) or water (Building 3) as the main solvent. A drying plant (Building 4; multiproduct batch plant), a multiproduct batch plant (Building 5) and a monoproduct batch plant (Building 6) complete the investigation. The buildings are of different sizes, and their production processes vary significantly, as shown in Table 5-1. The analysis of such a variety of different buildings permits the investigation of the applicability of general models for depicting the energy consumption of production buildings. The drying plant (Building 4) consists of several different dryers; mainly rotary vacuum dryers and filter presses. Furthermore, grinding and mixing equipment is available in the plant to shape the dried products and pack them for the customers.

Table 5-1: Characteristics of the investigated buildings

Building No.	Description	Number of major equipment pieces	Main Solvent	Variability of Products	Change of Production Mix	Range of Reaction Temperatures
1[3]	**Multipurpose batch plant**	**29**	**Organic**	**High**	**High**	**< -10 °C to > +200 °C**
2	Multipurpose batch plant	55	Organic	High	High	< -10 °C to > +100 °C
3	Multipurpose batch plant[4]	180	Water	Medium	Medium	0 °C to ~ +30 °C
4	Multiproduct Drying Plant	55	Organic and Water	High	High	+60 °C to > +100 °C
5	Multiproduct Batch Plant	74[5]	Organic	Medium	Medium	< -20 °C to > +250 °C
6	Monoproduct Batch Plant	8[5]	Organic	Low	None	< -10 °C to > +200 °C

[3] Building 1 is discussed and analysed in more detail in Chapters 5.2 and 5.3 with the help of a bottom-up approach

[4] See Blickenstorfer, C. (1999). "Analyse des Energieverbrauchs eines Mehrprodukte-Batch-Betriebes," Ph.D. dissertation, No. 13411, Zurich, ETH, http://e-collection.ethbib.ethz.ch/cgi-bin/show.pl?type=diss&nr=13411.

[5] Number excludes cooling machines

5.1.3 Analysis of the Different Energy Carriers

In the discussion and examination of the results obtained for the energy analysis of the different buildings, it must be kept in mind that the model is based on the total amount of chemicals produced (products and intermediates that leave the production plant). This is not equal to the degree of usage of the equipment, as different products have different production processes (especially in multipurpose batch plants). If, for example, the amount of chemicals produced in one month is only one-half of the amount of chemicals produced in another month, this could mean that the utilization of the equipment is only 50%. However, it could also mean that the chemicals produced in the former month have more complicated production paths that use more equipment, resulting in almost 100% usage of the equipment. Aside from this shortcoming, the monthly production provides a good picture of the average productivity of the different buildings and is easily accessible. In the following, the correlation of different energy consumptions with production output is studied.

Note that for clarity reasons and effective communication possibilities with industry, energy is accounted in MWh in this study. MWh can be converted to MJ by multiplying the value given in MWh by 3,600.

5.1.3.1 Steam

Steam is provided at two pressure levels and for two different purposes in most of the buildings. One purpose is the heating of the building for comfort reasons and the other is the usage for the production processes. Production steam is provided at two different pressure levels (i.e., 5 and 15 bar above ambient pressure) for providing heating utility at two different temperature levels. This steam is usually produced in a boiler house for a whole site at a pressure level of about 40 bar. This high-pressure steam is relaxed to the abovementioned pressure levels over steam turbines producing electricity as a by-product. Production steam and heating steam are investigated separately in the following subchapters.

Steam is a very important energy provider for industry, since according to US department of energy, about 45% of all fuel burned by manufacturers is expended on steam generation (see (Aggarwal 2002)).

Production Steam

For a comparison of steam, cooling media and electricity consumption, the energy content of one ton of steam was considered as 0.8075 MWh according to discussions with industrial representatives and values given in (Lide 1995).

The consumption of production steam as a function of the production output of the different buildings is shown in Figure 5-1 and summarized in Table 5-2.

The two multipurpose batch plants with largely varying production (Buildings 1 and 2) show the lowest correlation. The processes conducted in these plants vary significantly in terms of process temperature and time. Some of the chemicals have to be produced at more than 200 °C and some at room temperature or even below. Some of them show high heat of reactions and some low. Therefore, a correlation between steam consumption and total amount of chemicals produced does not at all exist for these buildings. The differences between the products are too large to obtain an accurate model with this simple approach.

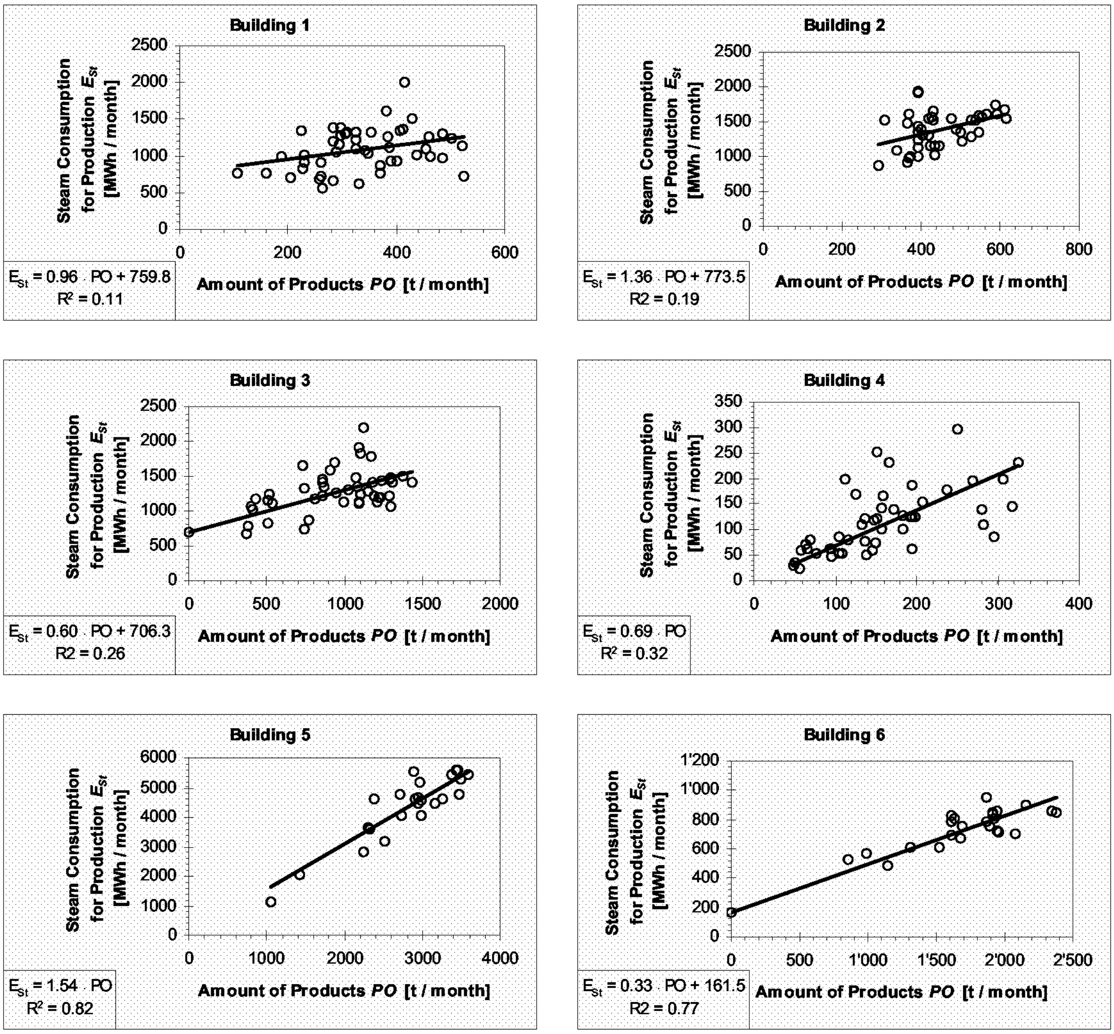


Figure 5-1: Consumption of production steam (5 and 15 bar) of the different buildings as a function of amount of products per month (according to Equation (3-1))

Building 3 shows a slightly better correlation. Here, the variations between the different products are smaller than in Buildings 1 and 2, since exclusively one family of chemicals is produced. These chemicals, although different, all have similar production processes and, most importantly, similar production temperatures.

The regression of the data for Building 4 shows almost no base consumption (no measurements at zero production were done for this building). The lack of a base consumption found by the regression is reasonable, given that steam consumption in a drying plant is shut down if nothing is dried and infrastructure losses are generally small, as shown by the measurements discussed below. The drying processes for different chemicals in horizontal vacuum rotary dryers are quite similar[6]. The heat capacity of most organic solvents is around 2 kJ / kg K and the heat of vaporization lies in the region of 1 MJ / kg (Lide 1995). Therefore, the main variation between the different drying processes lies in the drying time. This time depends on the amount and the relative moistness of the chemicals to be dried, as well as the adhesion of the solvent to the surface. Most products do not vary as greatly in these attributes than they do in the attributes of synthesis steps, and therefore, a better correlation is obtained for the steam consumption of this drying plant than for multipurpose batch plants.

[6] For a description of horizontal vacuum rotary dryers, see Mujumdar, A. S. (1995). *Handbook of Industrial Drying*, Marcel Dekker, Inc., New York.

Of the investigated plants, Buildings 5 and 6 show the best correlations between production steam consumption and production output. In these buildings, the production mix stays relatively constant (for Building 6, it is completely constant because only one specific chemical is produced). This explains the rather good correlations obtained for steam consumption of these buildings as compared to the other buildings.

The base consumption of production steam was measured only for Buildings 3 and 6. The base consumption accounts for a significant fraction of the production steam consumption. Nevertheless, the relative amount is smaller than for electricity. Here, base consumption means losses from steam pipes and equipment and steam for boilers, for example (if not included in the heating steam consumption). In contrast to electricity, only minor infrastructure equipment uses steam.

The measurement of the base consumption of Building 1 was conducted during a shutdown period (i.e., consumption of the cold building). These measurements showed that the consumption of production steam of this cold production building is significantly smaller than about 70 MWh / month (precision of the measuring device). The relative base consumption of the cold building is therefore much smaller than the average steam consumption for this building and less than 10% of the regressed base consumption of the warm building (about 760 MWh / month for Building 1 as shown in Figure 5-1).

Table 5-2: Summary of the different production energy consumption models obtained for the different energy forms ($_m$) in the different buildings according to Equation (3-1)[7]

Utility	Building	S_m [MWh/t]	B_m [MWh/month]	r^2	Base Load [%] 50% PO	100% PO
Electricity	1	0.28	130[8]	0.16	64	47
	2	0.23	137[8]	0.41	66	49
	3	**0.41**	**277.5[8]**	**0.89**	**49**	**32**
	4	0.16	48.6[9]	0.55	65	48
	5	**0.12**	**43.5[8]**	**0.86**	**17**	**9**
	6	**0.06**	**107[8]**	**0.9**	**60**	**43**
Production Steam[10]	1	0.96	759.8[9]	0.11	75	60
	2	0.73	773.5[9]	0.19	77	63
	3	0.6	706.3[8]	0.26	62	45
	4	0.69	0[9]	0.32	0	0
	5	**1.54**	**0[9]**	**0.82**	**0**	**0**
	6	**0.33**	**161.5[8]**	**0.77**	**29**	**17**
Cooling Media[11]	1	0.1	9[8]	0.03	26	15
	2	0.16	7.3[8]	0.30	13	7
	3	**0.23**	**0[8]**	**0.86**	**0**	**0**
	5	**0.04**	**0[8]**	**0.9**	**0**	**0**
	6	**0.01**	**0[8]**	**0.93**	**0**	**0**

[7] Applicable energy models are printed in bold face
[8] Measured data at zero production
[9] Result of the regression for zero production
[10] Energy content of steam is set to 0.8075 MWh/t according to discussions with industrial representatives and values given in Lide, D. R. (1995). "Handbook of Chemistry and Physics.", CRC Press, London.
[11] Energy (electricity) used for the production of the cooling media and not the energy content of the cooling media

Heating Steam

The heating steam consumption was set in correlation to the number of degree-days per month. The heating frontier was set to 12 °C. The daily mean temperatures were received from a meteorological institution nearby the production plants. Degree-days are explained in detail in the literature (see, e.g., (http://www.eia.doe.gov/neic/infosheets/degreedays.htm)).

The correlations between heating steam consumption and degree-days according to Equation (3-2) can be seen in Figure 5-2. Buildings 5 and 6 consume no heating steam, as these buildings are heated with condensate (i.e., hot water) originating from production heating, which is not measured separately. Therefore, only Buildings 1 to 4 are analysed.

The two multipurpose batch plants with significantly changing production (Buildings 1 and 2) show similar specific heating behaviours (slopes of the regression lines). The high base consumption (intercept at zero degree-days) of Building 2 appears extraordinary. Nevertheless, it can be explained by infrastructure equipment (such as heating of storage tanks) running on heating steam over weekend shutdown periods for safety reasons. This explains the inferior correlation (varying production infrastructure consumption) as well as the high base consumption.

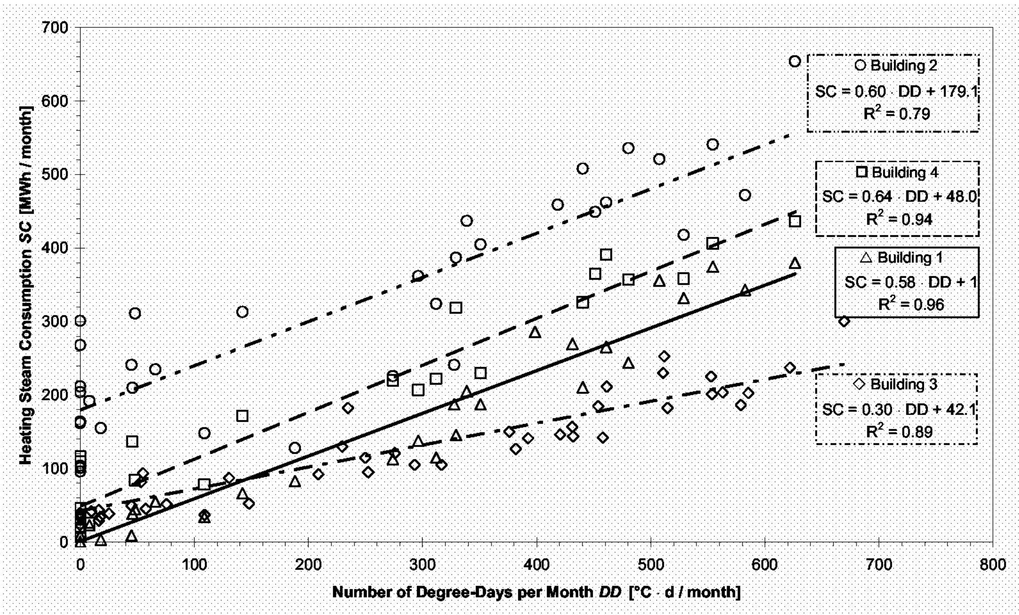


Figure 5-2: Consumption of heating steam (5 bar) as a function of degree-days per month (according to Equation (3-2))

Despite the different sizes of the two Buildings 1 and 2 (see Table 5-1), the specific energy consumption per degree-day (slopes of the regression lines in Figure 5-2) is similar for the two buildings. Building 3, which is the largest of the investigated plants, shows the smallest specific energy consumption. This is even more astonishing as the processes in this building produce only minor amounts of heat and are conducted at moderate temperatures (i.e., low irradiation of the equipment). This should result in a higher heating requirement for the plant. An explanation of this behaviour could be the heating regime of production buildings: Unlike apartment or office buildings, radiators are seldom found in production plants. Heating is performed mostly with the help of heating ventilators working with steam. Moreover, the air change rate in production plants is higher than in apartment buildings for safety reasons (about 2 h^{-1} versus about 0.5 h^{-1}). The fresh air has to be heated before entering the building. The number of times, the air volume of a building is exchanged is called air change rate *ACR* and is given in h^{-1}. It will now be considered, how this air change rate influences the heating steam consumption levels of the different buildings.

The result of this investigation is shown in Figure 5-3, where the normalized consumption of heating steam is plotted as a function of degree-days. The specific normalized heating steam consumption of the investigated buildings is about 0.32 (MWh · h) / (°C · d). The normalized base consumption of the investigated buildings still varies largely. As mentioned above, this can be explained by the varying use of the heating steam for production infrastructure (i.e., independent of ambient temperature). The good correlation shows that the normalised model according to Equation (3-3) is adequate for the heating steam consumption of production buildings

It may be seen from the investigations, that if no production infrastructure uses heating steam and if the main pipe of heating steam is closed during summer, the base consumption is almost equal to zero. Otherwise, the base consumption has to be measured or estimated before predictions of heating steam consumption can be made.

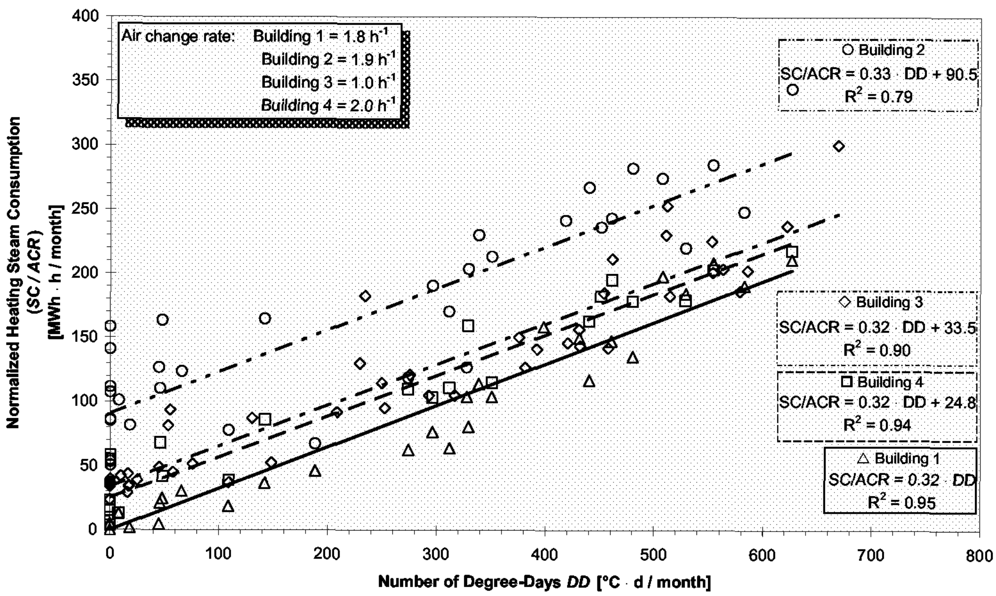


Figure 5-3: Normalized heating steam consumption (5 bar) as a function of the number of degree-days per month (according to Equation (3-3))

The main reason for the lack of a base consumption for most buildings is that the heating steam pipe is closed during summer times and therefore no losses occur when no heating is required. Some minor errors arise because the measuring location for the mean day temperatures (required for the calculation of the degree-days) was not located directly at the plants location, which might cause an error of ±1 °C.

The results are summarized in Table 5-3.

Table 5-3: Summary of the models for heating steam consumption obtained for the different buildings according to the normalised Equation (3-3)[7]

Building	$ACR \cdot 0.32$ [MWh/°C·d]	B [MWh/month]	r^2	$\overline{SC}$ [12] [(MWh·h)/(°C·d)]	ACR [h^{-1}]	Base Load [%] 350 *DD*	700 *DD*
1	**0.58**	**0.99**	**0.96**	**0.32**	**1.8**	**0**	**0**
2	**0.60**	**179.1**	**0.79**	**0.33**	**1.9**	**46**	**30**
3	**0.30**	**42.1**	**0.89**	**0.32**	**1.0**	**29**	**17**
4	**0.64**	**48.0**	**0.94**	**0.32**	**2.0**	**18**	**10**

5.1.3.2 Electricity

The electricity consumption data of the different buildings investigated are shown in Figure 5-4. The investigations exclude the electricity consumption for cooling purposes since this is discussed separately in Chapter 5.1.3.3.

For Buildings 1 and 2, the electricity consumption is barely correlated with the monthly production. The energy consumption of these buildings varies greatly between the different production processes, mainly due to differences in reaction time and in batch size, which are not always correlated with equipment size (standardized reactors with large motors).

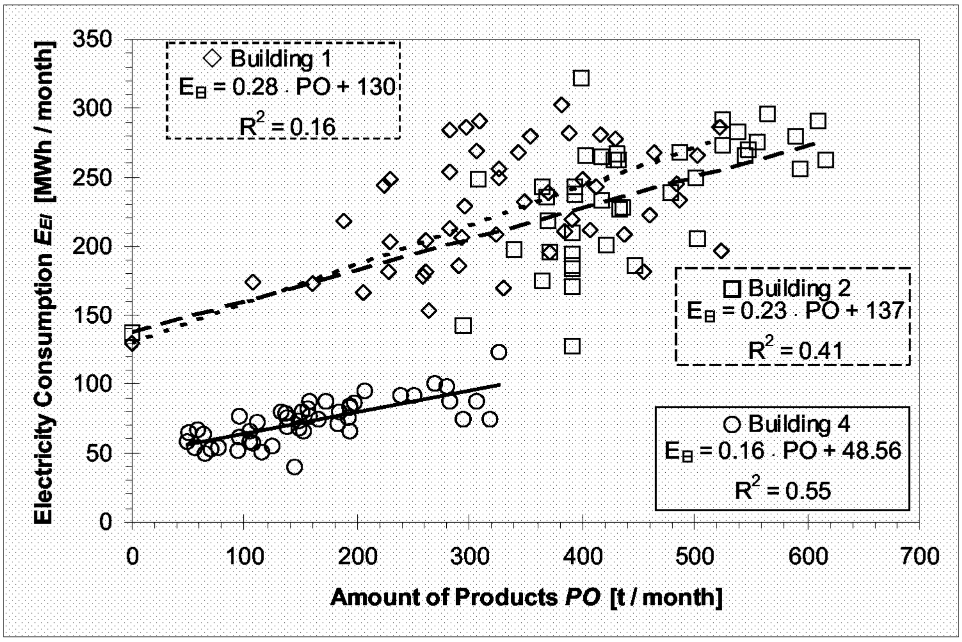
Buildings 3, 5 and 6 show a different behaviour as shown in Figure 5-4. For these buildings good correlations between electricity consumption and amount of chemicals produced are obtained. Building 3 shows high specific electricity consumption (slope of the regression line). This can be explained by the large stirring equipment used in this building. The large stirring equipment is installed because high stirring powers are sometimes required for the processes (e.g., for dissolving a solid). Although about 160 different chemicals are produced in this plant, the production processes are quite similar. This results in a good correlation between electricity consumption and production output.

Building 5 shows lower specific electricity consumption than Building 3. In Building 5, each production line is exclusively constructed for one product. The products originate from one family. The product mix stays constant over the year. The dedicated facilities and the uniformity of the production processes for the different products explain the good correlation obtained for this plant.

Building 6 shows a good correlation between electricity consumption and production output. Because only one product is produced in this building and the production process is highly automated, the differences between different batches are minimal. Therefore, this set of data shows the highest correlation coefficient.

Building 4 is completely different from the other buildings. The drying of different chemical products shows differences in drying time and initial moistness. The equipment sizes in this building do not vary largely. The electricity consumption is dominated by motors for vacuum pumps and stirring. This results in only minor differences between different products. Therefore, the correlation of electricity consumption and dried products lies between those of Buildings 1 and 2 and of Buildings 3, 5 and 6. The obtained results are summarized in Table 5-2.

[12] Specific normalized heating steam consumption



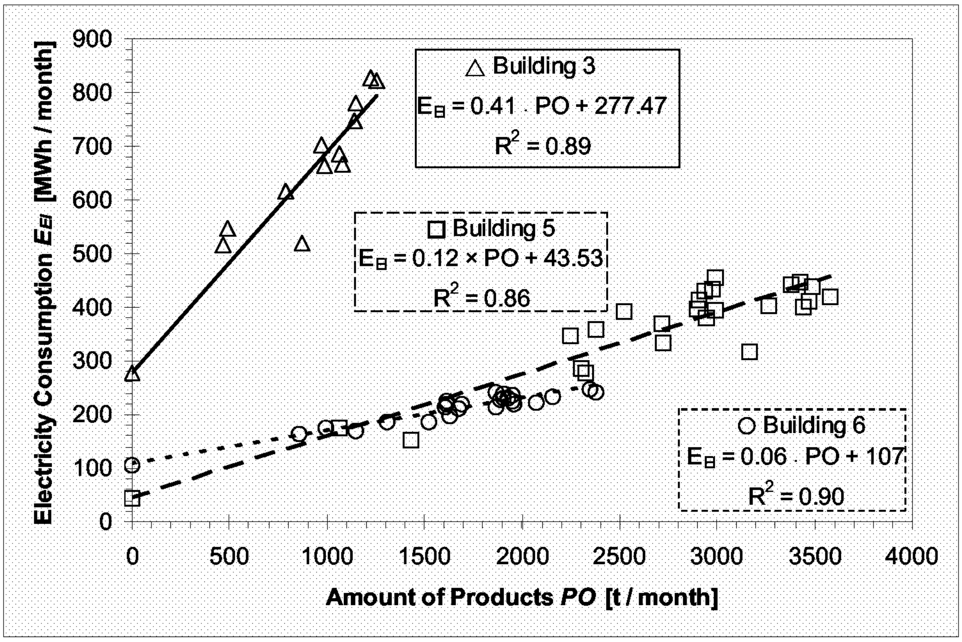


Figure 5-4: Electricity consumption (excluding electricity for cooling purposes) of the investigated buildings as a function of the amount of chemicals produced per month (according to Equation (3-1))

For Buildings 1, 2, 3, 5 and 6, measurements of the base consumption of electricity were conducted (measured values at zero production in Figure 5-4) as indicated in Table 5-2. For Building 4 no measurements of the base consumption were made.

In terms of electricity, base consumption means mainly infrastructure consumption, as losses are minimal. The proceeding of the measurements is described in (Bieler 2004). All buildings show high base levels of electricity consumption. Figure 5-4 shows that the infrastructure consumption of electricity contributes significantly to the total electricity consumption. The highly automated Building 6 shows a higher percentage of infrastructure consumption compared to the less automated Building 5. In automated buildings, much equipment is running independent whether it is in use. Automation shows only small consumption as stated in (Schalcher et al. 2003a; Schalcher et al. 2003b). Major consumers of electricity in this building are high temperature equipments requiring electricity. During shutdown periods, trace heating of these equipments is left active since shutdown would cause the product to crystallise in the pipes. Dedicated plants with manual operation like Building 5 show smaller levels of infrastructure consumption, if the processes do not need large and dedicated equipment, which would consume higher amounts of base load. In this specific building, fewer scrubbers are installed compared to the others. This results in a lower electricity consumption of the infrastructure. In addition, the electricity consumption in Building 5 is more dependent on production output than the consumption of Building 6 as shown by the higher slope of the Building 5 regression line in Figure 5-4.

The high flexibility of a multipurpose batch plant implies a high flexibility of the infrastructure equipment. The equipment is therefore built to handle the highest possible requirement of the plant. This explains the high base consumption of Buildings 1 and 2 as shown in Figure 5-4. The lower percentage of the base consumption of Building 3 as compared to Buildings 1, 2 and 4 (see Table 5-2) can be explained by the limited variability of the chemicals produced. This fact makes it easier to size the utility equipment.

5.1.3.3 Cooling Energy

The investigated buildings used two types of cooling media. For cooling above about ambient temperature, cooling water (taken from a river) was used. Because this water was not measured separately from the other water used for the production and no cooling towers were in use, the cooling water consumption was not investigated. For low-temperature cooling, three different cooling systems were in use. Buildings 1 and 2 use brine that was produced (i.e., cooled) externally. In Building 1, the internally used brine is cooled down with external brine using a heat exchanger for safety reasons, whereas in Building 2 the external brine was used directly. Building 3 used no brine at all; rather, the processes in this building used ice for direct cooling. This ice was produced internally with two ice machines. Building 4, as a drying plant used only water for cooling purposes. Therefore, this building was not considered in this investigation. Buildings 5 and 6 used brine that was produced internally. Here, the energy content of the cooling media was not measured. The investigated energy consumption is the energy consumption (electricity) required to produce the cooling media. Assuming a reasonable efficiency of the cooling machines (about 200% as stated in (http://www.aie.org.au/melb/material/resource/cop.htm ; Wang 2000)), the effective cooling duty could be estimated, but this was not done here for better comparison with the other utilities investigated.

The consumption of cooling media for the different buildings can be seen in Figure 5-5.

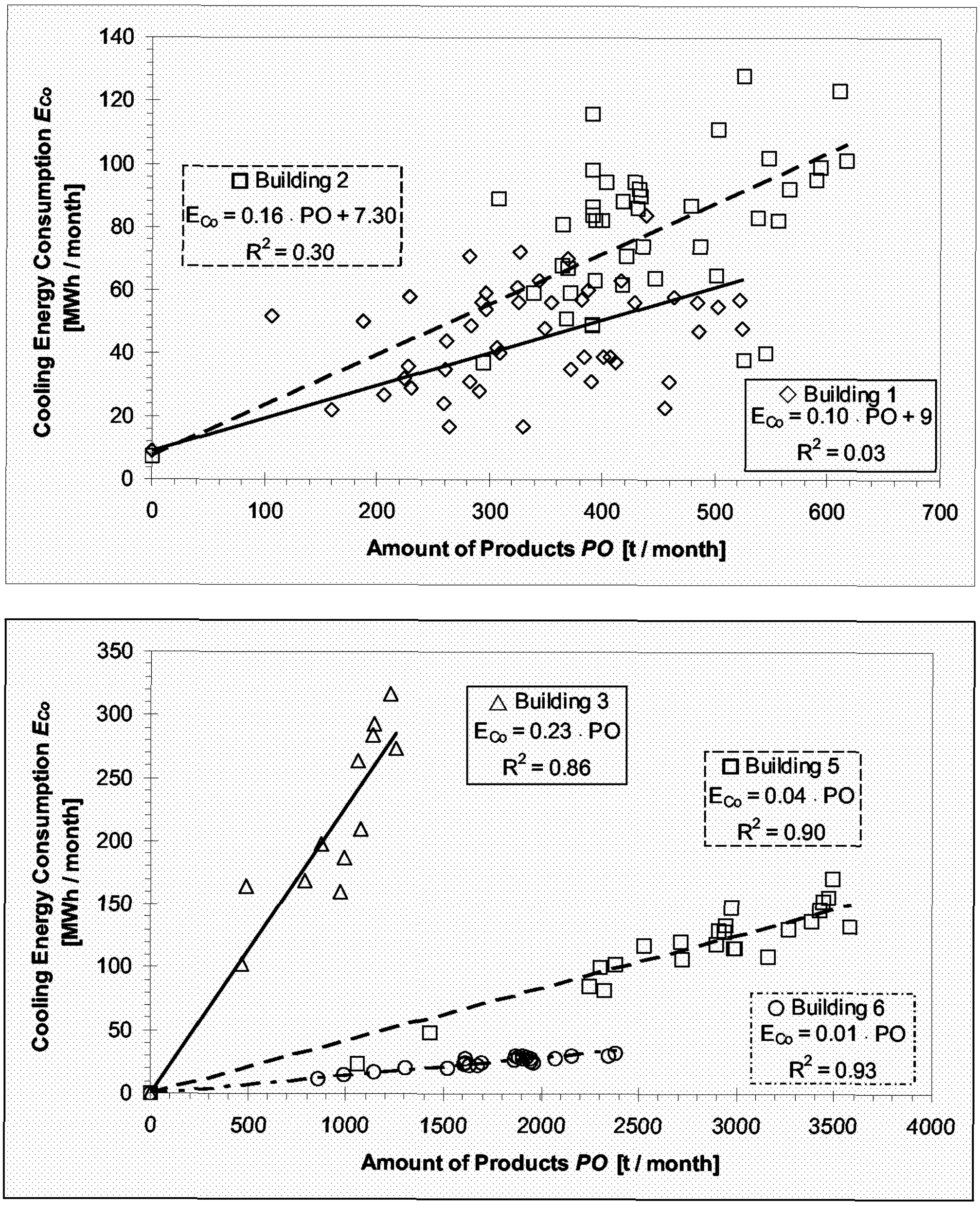


Figure 5-5: Consumption of cooling energy of the different buildings as a function of production output per month (according to Equation (3-1))

Buildings 3, 5 and 6 exhibit good correlations between cooling media consumption and production output. This is because of not only the internal production and the controlling mechanism, but also the uniformity of the production processes in each of these buildings.

The multipurpose batch plants with varying production (i.e., Buildings 1 and 2) show, once again, a different behaviour. The large variety of the products results in a poor correlation between cooling media consumption and amount of products. Models that are more detailed have to be built to model the energy consumption of such facilities.

The buildings that produce their cooling media internally (Buildings 3, 5 and 6) show no base consumption as shown in Figure 5-5. This can be explained by the fact that the cooling machines are shut down if not in use. The machines are controlled by measuring the cooling media consumption of the plant (i.e., the temperature of the backflow) and adapting the cooling power of the machines accordingly with frequency converters.

For Buildings 1 and 2, base consumption levels of about 10% of the average production consumption results. The infrastructure has to provide a base load even if no production occurs. Moreover, losses of the system are higher because of the longer piping systems (piping between the cooling machines and the different production plants). The higher base consumption of Building 2 might be due to the two brine systems (external and internal), which are joined with a heat exchanger. This heat exchanger has a specific heat loss (i.e., about 1 °C temperature difference between the supply temperature of the external brine and the heat exchanger outlet stream temperature of the internal brine) that results in a higher base consumption of the building. The results are summarised in Table 5-2.

5.1.4 Applicability of the Models

Generally, it can be stated that for multipurpose batch plants with highly varying production processes and changing production mixes (i.e., Buildings 1 and 2), energy consumption models according to Equation (3-1) are not suitable. The variations between the different products are too large to be modelled with highly aggregated energy models on a building level.

The results in the preceding section show that modelling the energy consumption on the building level according to Equation (3-1) is suitable for some production plants and not suitable for others. The postulated model for energy consumption on the building level is suitable for dedicated monoproduct batch plants (Building 6) or for multiproduct or multipurpose batch plants in which similar chemicals are produced or the product mix stays constant over time (Building 3 and 5). The buildings where an energy model according to Equation (3-1) can be applied are printed in bold face in Table 5-2.

For electricity consumption, the model expressed by Equation (3-1) was suitable for Buildings 3, 5 and 6. Figure 5-6 shows an example of the modelling of the electricity consumption of these buildings according to Equation (3-1) with the parameters given in Table 5-2. As mentioned above, the maximum production capacity (i.e., 100%) was taken as the highest observed production during the investigated period. The percentage contribution of base consumption to energy consumption is specific to each building. As can be seen in Figure 5-6, the total amount of energy consumed per unit of produced chemical decreases with increasing plant usage since the base consumption of the building stays constant. At higher plant usage, the base load can be distributed to a higher number of products. From an energetic point of view, it is therefore better to run a plant half a year at full capacity and shut it down for the rest of the year than producing at half capacity for the whole year. Considering only energy costs, higher plant usage results in lower production costs.

The modelling of the electricity consumption of Buildings 3 to 6 and the production steam consumption for Buildings 5 and 6 according to Equation (3-1) showed that a significant part of the energy consumption of a batch plant is independent of production (i.e., base load).

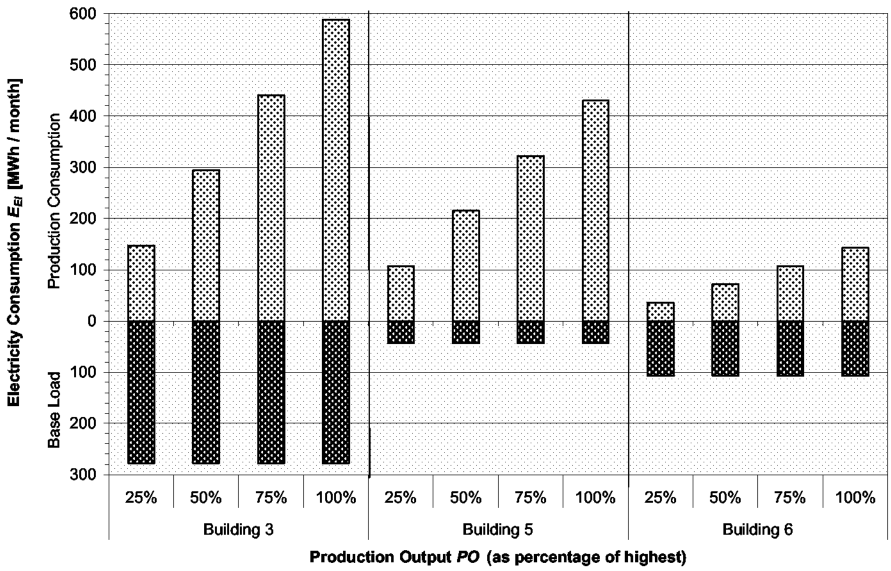


Figure 5-6: Modelled monthly electricity consumption as a function of capacity usage for those buildings where the model according to Equation (3-1) was suitable

For heating steam, a model according to Equation (3-3) was proposed. This model was suitable for all the buildings investigated (i.e., Buildings 1 to 4). The investigations showed that the heating steam consumption depends only on the number of degree-days and air change rate of the building. The corresponding base load depends on the infrastructure (both production and building) that is running with heating steam and therefore varies significantly between the different buildings. These results are summarized in Table 5-3.

5.1.5 Conclusions

For plants with only minor changes in production mix, it is possible to obtain a good description of energy consumption by use of Equation (3-1). For these buildings, one can allocate energy use per mass of chemicals produced after determining (measurement or estimation) the required parameters (i.e., base consumption, specific energy consumption per ton of chemicals produced). The energy consumption per ton of product depends significantly on the plant usage. The higher the plant usage, the smaller the ton-specific energy consumption because of the constant base-consumption of the building, thus providing possibilities to optimise the production plans of such buildings.

For the heating steam consumption of chemical batch plants, a model according to Equation (3-3) is suitable. The model depends only on the amount of degree-days, the air change rate, and the empirical base load and is therefore for general use for production buildings. Optimisation could be performed in terms of minimizing base consumption and optimising air change rate and room temperature (changing the heating frontier).

In cases where these equations are suitable, the allocation of energy consumption to produced amounts of chemicals is possible as is the forecasting of energy consumption or adequate costing. It is possible to distinguish the base load from production-dependent energy usage. This shows whether the consumption of the processes or of the infrastructure is most promising for optimisation. A detailed allocation of the energy consumption to single unit operations or products is nevertheless not possible with this top-down approach of energy investigations. This is a main drawback of the top-down approach: it precludes detailed optimisation. A better, although more intricate, possibility is therefore a bottom-up energy model. This model consists of a sum of detailed energy consumption models for single unit operations as shown in Chapter 5.2. These unit operation models, together with the production recipes, reflect the energy requirements of different products and, thus, allow an allocation of energy costs to single products. Furthermore, these detailed models reveal the amount of energy consumed for each production step of each product and how large the losses are. A model of a complete production building is possible by summarising the single apparatus and unit operation models and the infrastructure consumption as shown in Chapter 5.3. Therefore, the application of such a model leads to the identification of detailed improvement potentials in single unit operations and production steps (e.g., optimal choice of a solvent used in a certain operation, optimised insulation of an equipment unit).

The modelling of a multipurpose batch plant with varying production (i.e., Buildings 1 and 2) has to be done using this more detailed type of energy models. These bottom-up models will be investigated in Chapters 5.2 and 5.3.

5.2 Modelling of Single Unit Operations

Different measuring equipment was used for the measurement of the electricity, the cooling energy and the heating energy consumption. The measuring equipment and its accuracy is discussed in (Bieler 2004).

Only one of the six production plants discussed in Chapter 5.1 is investigated further on single unit operation level. Therefore, this building will now not be called Building 1 anymore (characteristics are presented in Table 5-1), but just (investigated) building for simplicity reasons.

The base equations for the BOTUMO are described in Equations (3-14) and (3-15). The different equations building the BOTUMO may be found in Chapter 4.2. In Chapter 5.2.1, an example of the model building for single unit operations and apparatus is presented for a reaction vessel. The different apparatus investigated are presented in Table 5-6. The details of the investigations for each apparatus may be found in (Bieler 2004).

For the conversion of kg of steam to kWh of energy consumption (and vice versa), values may be found in (Lide 1995). These investigations and discussions with industry experts led to the conclusion, that a value for the energy content of about 0.65 kWh / kg of steam (including cooling down of the condensed steam to the temperature of the water in the jacket) is reasonable. This value was taken for 15 bar as well as for 5 bar steam. The same value was taken for both pressure levels of the steam since heat of vaporisation is not changing greatly with changing temperature (according to the accuracy of this investigation).

5.2.1 Reactors

5.2.1.1 Description of the Equipment

A scheme of a standard batch reactor as it is operated in the investigated building is shown in Figure 5-7 together with its heating/cooling-system. The reactor consists of a vessel with its stirring equipment (for detailed description of the stirring equipment see (Bieler 2004)).

The heating/cooling-system consists of a heating jacket (either a double-jacket for most of the glass lined vessels or a construction with half-pipes for most of the stainless steel vessels) in which the heating and cooling fluids circulate.

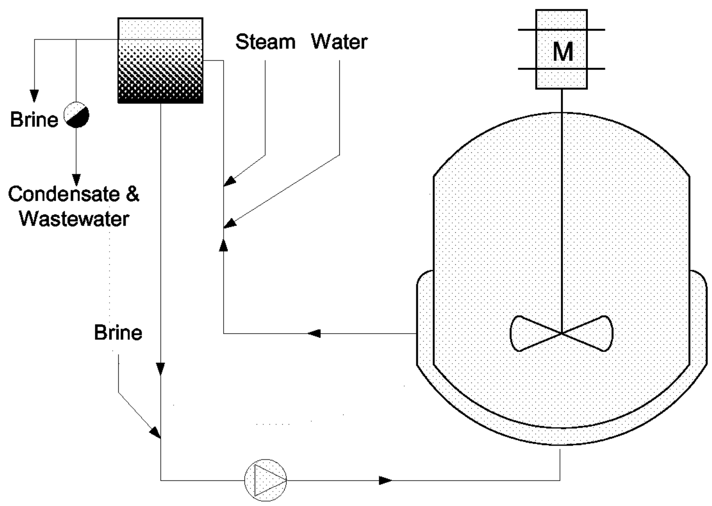


Figure 5-7: Scheme of a standard batch vessel with its heating/cooling-system

While heating, the system is filled with water (circulated by a pump). Steam (either 5 or 15 bar) is injected in the circulating water. This heats the water up to the desired temperature. The system is open to the wastewater system via an expansion vessel and a steam trap to prevent cavitation within the pump.

When cooling with water, the system operates similarly, except that the steam entrance is closed.

If the vessel is cooled with brine, water and steam entrances are closed and the outlet to the brine system is opened. The circulation pump has to be operated as well to allow free flow in the system. For brine, the system is a clear input-output-system, since the brine enters the system, flows through the jacket and leaves the system to the brine outlet immediately.

5.2.1.2 Measurements

Different measurements for the brine and the steam consumption of the reaction vessel are conducted. For all the different types of reaction vessels, different measurements were taken if possible. For brine, this was not possible, since only few reactors needed brine for their operation. Moreover, only some reactors were connected to the brine system.

Care had therefore to be taken not to interfere with daily production of the investigated building. For this reason, all measurements were taken during normal production with only minor disturbance of the production processes.

Steam

An example of the measurements performed is shown in Figure 5-8. It can be seen that at the beginning of a batch, the most steam is consumed (fast heating up of the reaction mass) and that a smaller amount of steam is used for holding the temperature at a constant value during the operation.

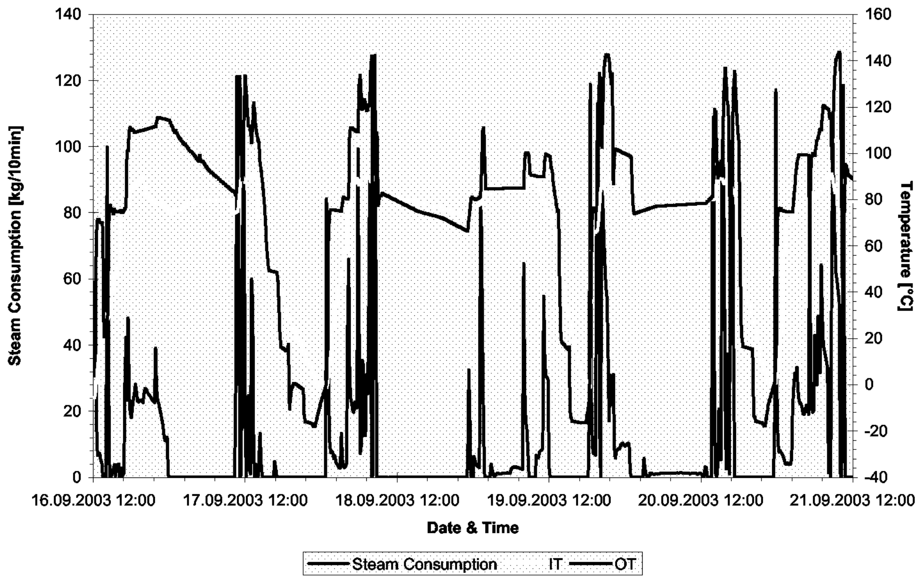


Figure 5-8: Example of the steam measurements for a 10 m³, glass lined reaction vessel heated with 5 bar steam

For the high temperature reactor discussed in the subchapter *Electricity*, measurements of the steam consumption were also taken. This vessel is only heated with steam up to a certain temperature during the starting period of each batch. Above this temperature, the electric heating is introduced for surplus heating power and above a significantly higher temperature, no steam is used at all and only electric heating is provided to the heating system. The special nature of this equipment is considered in the modelling (see below).

Brine

The measurements of the brine consumption showed to be complicated. Only some of the reactors were connected to the brine system. Moreover, many of the reactors using brine were connected to the brine system so badly that no measurements were possible (e.g., too short connection to the main pipe for the measuring equipment). This made it not possible to measure a good part of the reactors to have a significant spot check of the different systems.

Measurements of the hourly average of the brine consumption were performed. The temperature of the reaction mass (IT), the temperature of the jacket (OT), the brine flow in the jacket and the brine consumption according to Equation (3-5) were gathered as depicted in Figure 5-9.

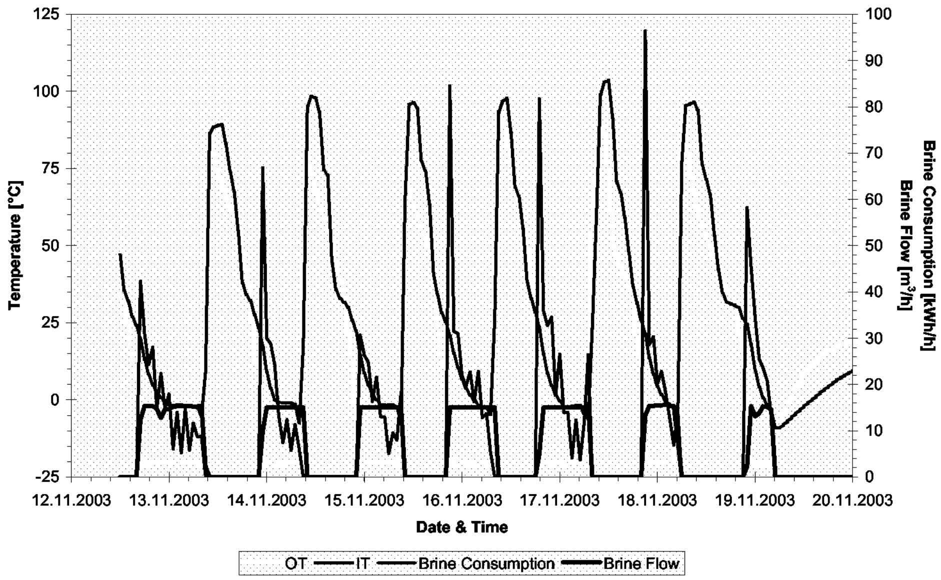


Figure 5-9: Example of a brine measurement for a 10 m³ stainless steel vessel

Electricity

The electricity consumption of the stirring and circulation equipment is discussed in (Bieler 2004). In this subchapter, the electric heating of one specific vessel will be investigated and discussed in detail.

The electricity consumption of the process control equipment is not measured or investigated. According to (Schalcher et al. 2003a; Schalcher et al. 2003b), the energy consumption of this equipment is negligible compared to the energy consumption of the controlled motors.

For one high-temperature reactor (4 m³ stainless steel reaction vessel), an electric heating aggregate is installed with a nominal power of 400 kW. This vessel is not heated directly, but is heated with a heating-oil[13] circuit. This circuit is heated either with steam (15 bar), or with electricity, or with both as described above, or is cooled with water through heat exchangers. The steam measurements of this vessel are discussed in the steam measurement paragraph above and will not be repeated here. Electricity measurements were performed with the help of a Memobox[14]. An example of these measurements is shown in Figure 5-10. The figure shows that a base consumption of electricity exists. This base consumption is

[13] Marlotherm®; for details see http://www.marlotherm.com

[14] See http://www.lem.com and Bieler, P. S. (2004). "Analysis and Modelling of the Energy Consumption of Chemical Batch Plants," Ph. D. dissertation, ETH, Zurich.

due to the circulation pump of the system that is running all the time. At the beginning of each batch, a high peak in electricity consumption is observed that shows the heating of the reaction mass. After this peak, only minor consumption is observed according to the measurements (the reaction is exothermic and helps therefore to balance the losses).

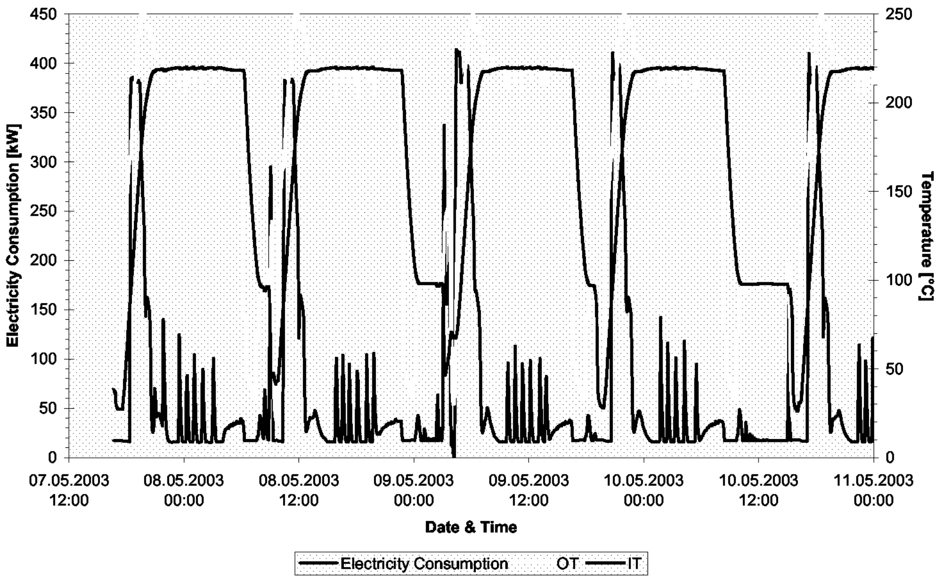


Figure 5-10: Measurements of the electric heating of the 4 m^3 high-temperature reaction vessel

5.2.1.3 Model and Conclusions

In contrary to the models described by (Bouhenchir et al. 2001), the models investigated in this study are applicable to existing plants and require only minimal supplementary measurements when transferred from one plant to the other[15].

The model for the stirrer and the circulation pump is described in detail in (Bieler 2004).

The models for heating and cooling of reactors are based on several assumptions, described in (Bieler 2004) in detail.

Steam

The model for the calculation of the steam consumption (either 5 or 15 bar) of the reaction vessels was postulated according to the generic model given in Equation (3-16). The general Equation (3-5) for heating up of the vessel and the substances, Equation (3-6) for evaporation of the solvent and the heat of reaction, Equation (3-7) for the losses, and Equation (3-9) for the heat input by the stirrer were combined to result in the following detailed equation of the steam consumption of a batch reactor:

$$\begin{aligned} E_{i,RV,St}^{P} = & \left(m_{RM} \cdot \left[c_{P}^{RM} \cdot \Delta T_{RM} + \Delta H_{R}^{RM}\right] + m_{ES} \cdot \Delta H_{V}^{ES}\right) \\ & + \left(\left[m_{A} \cdot c_{P}^{A} + m_{W} \cdot c_{P}^{W}\right] \cdot \Delta T_{A}\right) + \left(K \cdot A \cdot \Delta T_{Am} - \eta \cdot \gamma \cdot P_{N}\right) \cdot t \end{aligned} \qquad (5\text{-}1)$$

here, $E_{i,RV,St}^{P}$ is the production dependent steam consumption (either 5 or 15 bar) of a batch reactor in kJ, m are the masses of the reaction mass ($_{RM}$), the evaporated solvent ($_{ES}$),

[15] This has of course to be proven by further investigations (see Chapter 6 and Bieler, P. S. (2004). "Analysis and Modelling of the Energy Consumption of Chemical Batch Plants," Ph. D. dissertation, ETH, Zurich.)

the apparatus ($_A$), or the water in the heating/cooling-system ($_W$) in kg respectively, c_P represents the heat capacities of the reaction mass ($_{RM}$), the material of the apparatus ($_A$), or the water ($_W$) in kJ / kg / K, respectively, ΔT represents the temperature increases of the reaction mass ($_{RM}$), the apparatus ($_A$) or the temperature difference of the apparatus to the ambient temperature ($_{Am}$) in K, respectively, ΔH_R is the reaction enthalpy in kJ / kg, ΔH_V is the heat of vaporisation in kJ / kg, K is the loss coefficient in kW / m^2 / K, A is the surface area of the vessel in m^2, η is the efficiency of the stirrer in %, γ is the relation of nominal power to actual power consumption of the stirrer in %, P_N is the nominal power of the stirrer in kW, and t is the batch time in s. $E^P_{i,RV,St}$ may be translated to kWh by dividing kJ with 3,600 s / h.

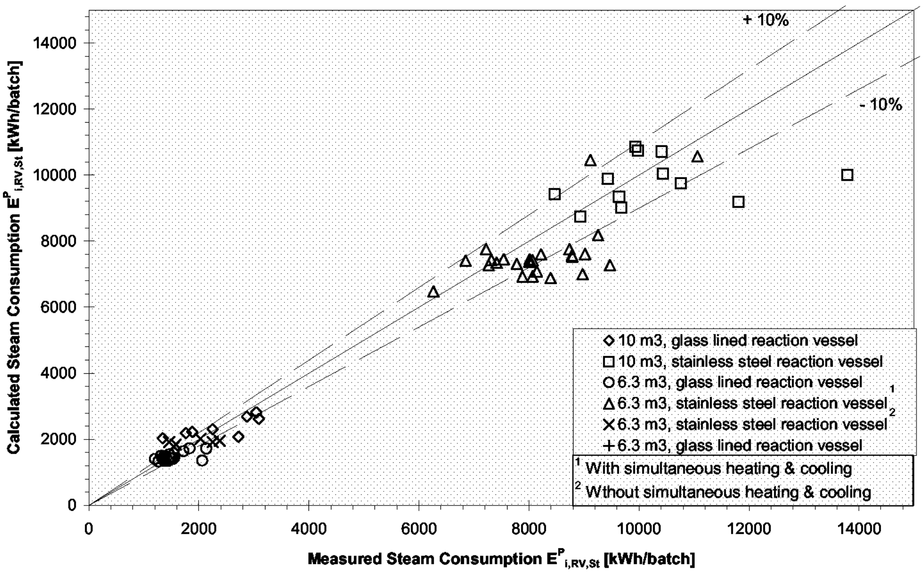


Figure 5-11: Modelling of the steam consumption of reaction vessels

With the help of this equation, modelling of the steam consumption of a reaction vessel was possible and the loss coefficient was fitted for the measured vessels according to the data. The modelling results are presented in Figure 5-11. It can be seen that the deviations between the measured and calculated steam consumptions are reasonable. This shows that the postulated model according to Equation (5-1) is valid.

With the help of this model, the steam consumption of a batch vessel may be analysed as shown in Figure 5-12. It can be seen that the losses are responsible for the biggest part of the steam consumption. As found by the modelling of the brine consumption (see next subchapter), about 50% of these losses are due to the radiation to the environment and the other 50% are losses through the steam traps and the pipes. This is because each kg of steam introduced to the system requires a kg of water to leave the system through the steam pipe as depicted in Figure 5-7. This means that the water leaves the system at the hottest point – without ever reaching the heat transfer area of the batch reactor. The normalization of the loss factor to an area basis is nevertheless valid since pipe and steam traps dimensions are proportional to the size of the vessel.

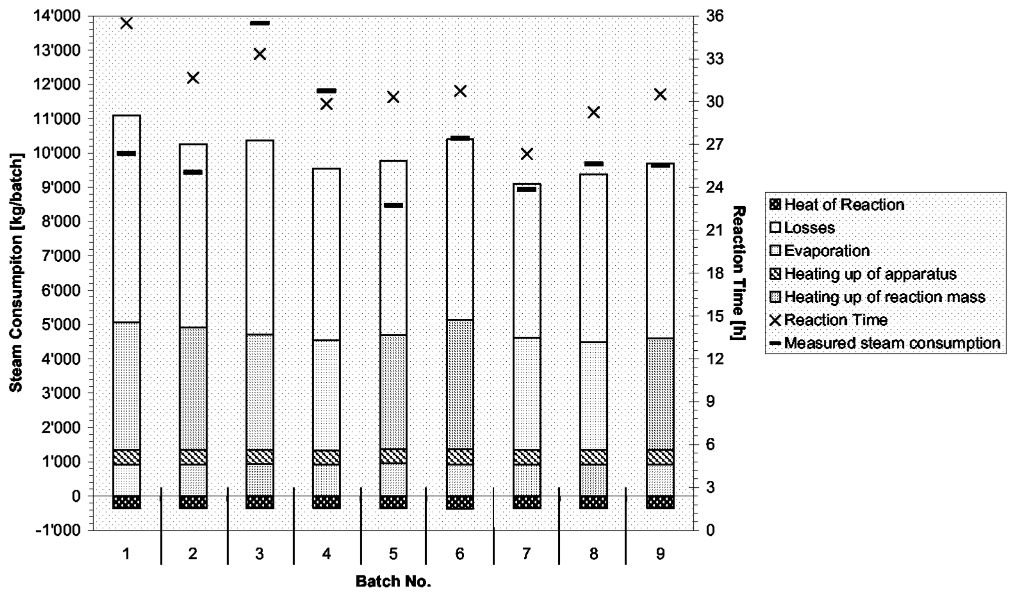


Figure 5-12: Modelling results of the steam consumption of a 10 m^3 stainless steel reaction vessel (in comparison with measured steam consumption and reaction time)

Out of the different measurements and models, different loss coefficients are found for the investigated batch reactors. These loss factors are summarized in Table 5-4. It is seen that the distribution of the loss coefficients from the best to the worst equipment is wide. An average of about $3.3 \cdot 10^{-2}$ kW / m^2 / K was calculated. The lower values represent batch vessels that operate at maximum performance and ideal conditions (i.e., the loss coefficient is in the same order of magnitude as the loss coefficient of the brine system as discussed in the next subchapter). These ideal conditions are nevertheless not attained all the time and for all the apparatus in a production plant. The influence of cleaning of a vessel is investigated in (Bieler 2004). In the random sample of the investigations, many vessels were found operating at nearly ideal conditions. Discussions with experts from the production plant and other industry experts showed that in usual operation, fewer ideal conditions would be found (compare (Dahinden 2003)). From these discussions, a loss coefficient about 25% higher was assumed more realistic (to account for the not ideal conditions in daily production). Therefore, a loss coefficient of about $4.2 \cdot 10^{-2}$ kW / m^2 / K was used in the modelling of the steam consumption of the reaction vessels and nutsche dryers.

Table 5-4: Calculated loss coefficients for the steam consumption of the reaction vessels and nutsche dryers[16] investigated

Reactor Type	K [kW/m²/K]
10 m³, glass lined	$1.8 \cdot 10^{-2}$
10 m³, stainless steel	$5.2 \cdot 10^{-2}$
6.3 m³, glass lined	$1.2 \cdot 10^{-2}$
6.3 m³, stainless steel[17]	$7.5 \cdot 10^{-2}$
6.3 m³, stainless steel[18]	$2.2 \cdot 10^{-2}$
6.3 m³, glass lined	$8.3 \cdot 10^{-3}$
6.3 m³, glass lined (dirty)	$4.2 \cdot 10^{-2}$
6.3 m³, glass lined (clean)	$3.7 \cdot 10^{-2}$
10 m², stainless steel nutsche[17]	$4.7 \cdot 10^{-2}$
10 m², stainless steel nutsche[17]	$4.7 \cdot 10^{-2}$
10 m², stainless steel nutsche[18]	$8.3 \cdot 10^{-3}$
Average	$3.3 \cdot 10^{-2}$

The measurements for the high temperature reaction vessel and the discussions mentioned in the electricity subchapter below resulted in an easier steam model for this apparatus than for the other equipment. This vessel requires steam just for the first part of the heating-up period. This is a period similar for all the different batches observed (reactor is filled the same way and the heating up is performed “as fast as possible”). Because of this, the steam consumption was modelled as a constant (base) consumption for each batch. The value observed in the measurements (about 530 kg / batch or 430 kWh / batch) was taken for the modelling.

Brine

Brine is used either for crystallization processes (i.e., cooling crystallization) or for reactions that have to be performed at low temperatures.

The general model for the cooling process is the same as presented in Equation (5-1) above for the steam consumption, just that this time, the reaction media is cooled down. Most of the time, no solvents evaporate and the reaction enthalpy is for crystallization processes replaced by the crystallization enthalpy, if known. For the processes conducted in the investigated building, no crystallization enthalpy was known. Because of the unique kind of the produced molecules, it was not possible to gather the crystallization enthalpies of analogues molecules. It was observed, that the crystallization processes often start at higher temperatures than the one from which on brine may be used (i.e., the cooling crystallization often starts at about 60 °C while brine is only used below 30 °C). No data was available on how much of the product is already crystallized when the switch to brine cooling is performed. Several discussions with industry experts on this problem were performed. These discussions lead to the assumption, that no significant part of the crystallization enthalpy is released while cooling with brine. Reaction enthalpy, nevertheless, is considered where applicable.

The investigations on whether the linear model according to the preceding chapter and Equation (3-16) is applicable are shown in Figure 5-13. The base consumption (i.e., heating up of the apparatus and the reaction mass) for this process is about 150 kWh per batch. The figure shows that a linear model with only a time dependent term models quite agreeably the brine consumption of this apparatus. The correlation coefficient is not too high, but because

[16] See Bieler, P. S. (2004). "Analysis and Modelling of the Energy Consumption of Chemical Batch Plants," Ph. D. dissertation, ETH, Zurich.

[17] With simultaneous heating & cooling

[18] Without simultaneous heating & cooling

of the large uncertainties and error possibilities for the brine measurement, as discussed in (Bieler 2004), better correlation cannot be expected.

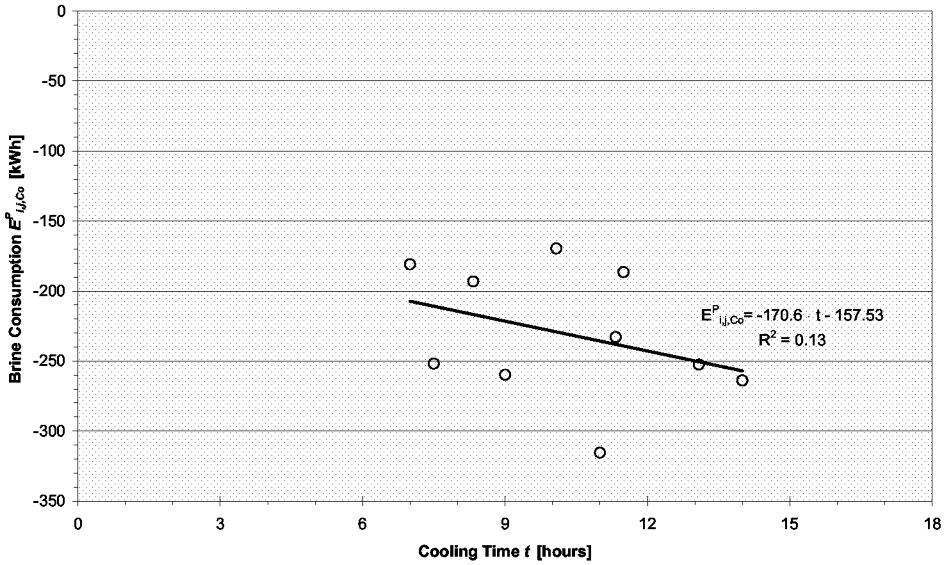


Figure 5-13: Measurements of the brine consumption of a 10 m³ stainless steel vessel (regression according to Equation (3-16))

The modelling results for the same 10 m³ stainless steel reactor shown in Figure 5-13 are presented in Figure 5-14. It can be seen, that the cooling down of the apparatus is only of minor importance for the brine consumption (because of the limited temperature difference). The cooling of the reaction mass is more important, since the media has a higher heat capacity than stainless steel and the apparatus contains a big amount of reaction mass that needs to be cooled down compared to the mass of stainless steel. Despite the high cooling times observed for the process, the losses are small compared to the losses during heating with steam. This can be explained by the small loss coefficient discussed below.

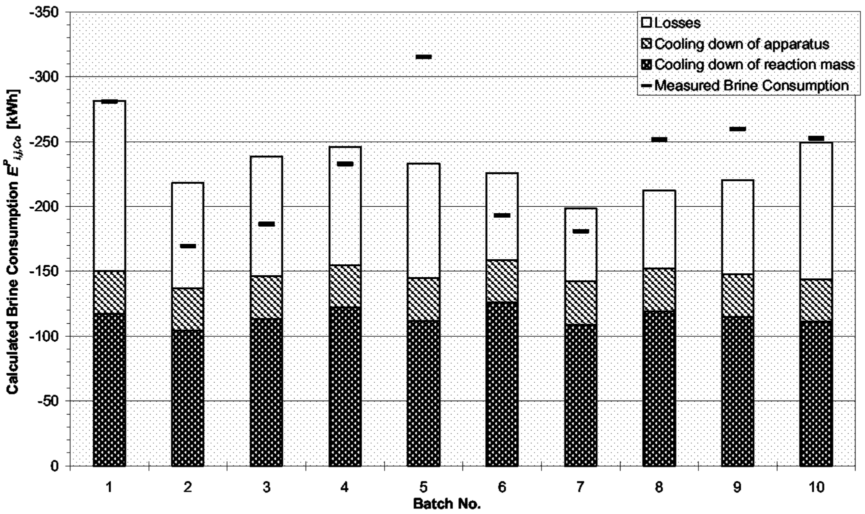


Figure 5-14: Modelling of the brine consumption of a 10 m³ stainless steel vessel (according to Equation (3-16); in comparison with measured steam consumption and reaction time)

All the loss coefficients investigated and found during the modelling of the different vessels are presented in Table 5-5. It can be seen that theses values are significantly smaller than the loss coefficients for the steam measurements presented in Table 5-4 in the subchapter above. This may be explained by the fact that for the brine measurements, the system is a complete input-output system and no losses occur through the steam traps. Simultaneous heating and cooling is also not possible while cooling with brine (this would be noticed instantaneously by contamination of the water). It can therefore be seen, that about 50% of the losses observed at the steam measurements were caused not by losses through irradiation but by losses through the steam traps and other suboptimal procedures during the heating period.

Table 5-5: Loss coefficients for the brine measurements of the investigated reaction vessels

Reactor Type	K [kW / m^2 / K]
10 m^3, stainless steel	$3.3 \cdot 10^{-3}$
10 m^3, glass lined	$5 \cdot 10^{-3}$
6.3 m^3, glass lined	$2.2 \cdot 10^{-2}$
4 m^3, glass lined	$3.3 \cdot 10^{-3}$

Modelling of the brine consumption with the found loss coefficients is depicted in Figure 5-15. As expected, the deviations between measured and modelled consumptions are larger than for the steam measurements. Deviations of 20% and more may occur. Because of the uncertainties in the measurement of the brine consumption and some other uncertainties of the parameters (e.g., neglecting of the crystallization enthalpy, see (Bieler 2004)), this is not surprising. Nevertheless, modelling of the brine consumption is possible by this simple equation and its accuracy is reasonable.

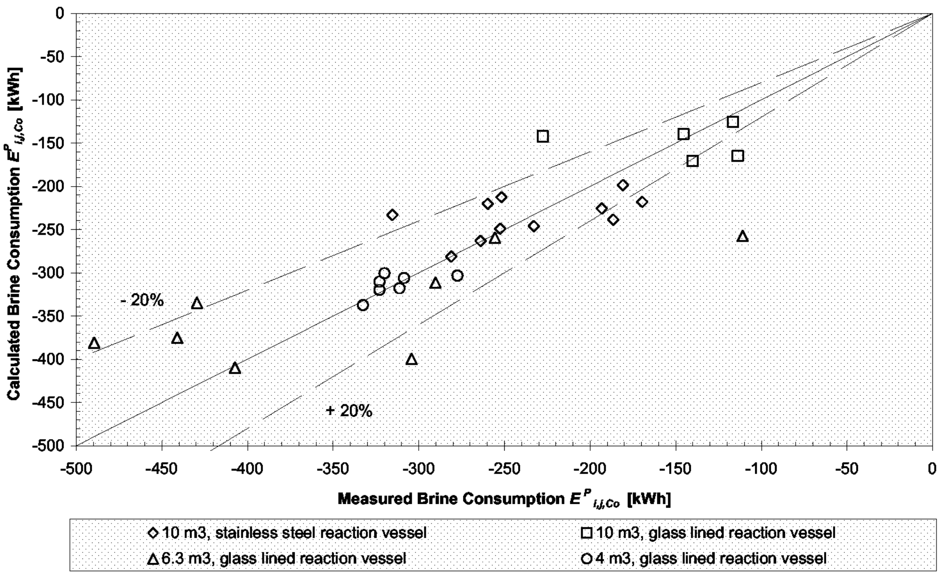


Figure 5-15: Modelling of the brine consumption vs. measurements (according to Equation (3-16))

The small values of the loss coefficient K depicted in Table 5-5 (compared to steam as shown in Table 5-4) are nevertheless not considered as reasonable for all of the apparatus for the same reasons discussed above for the steam measurements. As seen in Table 5-5, one of the investigated 6.3 m^3 glass lined reactors has a significantly higher loss value.

Since the brine consumption could only be measured for a few reaction vessels, it is not clear whether the high value of *K* for the 6.3 m^3 glass lined reactor is an exception or more standard for most of the vessels. In the 4 m^3 glass lined reactor, moreover, a difficult reaction is going on with evaporation of a reaction product that is not completely understood by the industry experts in energetic aspects. During discussions with industry experts, it was concluded, that a value of the loss coefficient *K* of about $1.7 \cdot 10^{-2}$ kW / m^2 / K is reasonable for reaction vessels for brine cooling. This value was taken as the standard value during modelling of the whole building (see Chapter 5.3).

Electricity for the High Temperature Reaction Vessel

The electricity consumption measurements of the high temperature reaction vessel shown above have a complicated behaviour not suitable for simple modelling. Since always the same product is produced in this reactor, a model according to Equation (3-8) was postulated for the base consumption (circulation pump) and according to Equation (3-13) for the consumption of heating energy respectively. Only one reactor uses electric heating.

Base consumption of the circulation pump may be extracted and is continuous. The base consumption is about 16.3 kW according to the measurements. It is consumed during the whole batch time. According to the nominal power of the circulation pump of 21.5 kW, this represents 76% of the nominal power (γ).

For the electricity consumption dependent on heating, an average value of about 100 kW was computed. Measurements of the batch time showed, that only minor deviations from the average value occur (see (Bieler 2004)). The deviations in batch time are about 4%. This is more accurate than the expected accuracy of the model. Therefore, the mean value could be taken as constant consumption during the whole batch time. This leads to a model similar to Equation (3-13). Now, *C* is the constant consumption of electricity of about 100 kW. Although this represents not exactly reality, it is sufficient to model the electricity consumption per batch with the required accuracy. Moreover, it makes the model significantly easier and allows a simple model without the requirements of many parameters.

5.2.2 Conclusions

Not all the different measurements and models are discussed in this report. All Measurements and models may be found in (Bieler 2004). For the different apparatus groups, equations were derived that are presented here.

For the heat-chambers, the following model was postulated:

$$E^{P}_{i,HC,St} = \frac{m_B \cdot c_P^W \cdot \Delta T_B + \left(m_A \cdot c_P^A + m_{Air} \cdot c_P^{Air}\right) \cdot \Delta T_A + K \cdot A \cdot \Delta T_{Am} \cdot t}{3600\, s/h} \tag{5-2}$$

here, $E^{P}_{i,HC,St}$ is the production dependent steam consumption of the heat-chamber in kWh, m_B is the mass of the filled barrel in kg, c_P^W is the heat capacity of water in kJ / kg / K, ΔT_B is the temperature rise of the barrel and its contents in K, m_A is the mass of the heating chamber (apparatus) in kg, c_P^A is the heat capacity of stainless steel in kJ / kg / K, m_{Air} is the mass of air inside the heating chamber in kg, c_P^{Air} is the heat capacity of air in kJ / kg / K, ΔT_A is the temperature rise of the heat-chamber in K, *K* is the heat transfer coefficient to the environment in kW / m^2 / K (loss coefficient), *A* is the surface area of the heat-chamber in m^2, ΔT_{Am} is the temperature difference between the outside wall and the environment in K, and *t* is the time in s. The scaling factor of 3,600 s / h is required for converting kJ in kWh.

For the batch distillation, a model according to the following equation was postulated:

$$E^{P}_{i,BC,St} = \left(m_S \cdot \left[c^{S}_{P} \cdot \Delta T_S + \Delta H^{S}_{R}\right] + \{1 + RR\} \cdot m_{ES} \cdot \Delta H^{ES}_{V}\right) + m_A \cdot c^{A}_{P} \cdot \Delta T_A + \left(K \cdot A \cdot \Delta T_{Am} - \eta \cdot \gamma \cdot P_N\right) \cdot t \qquad (5\text{-}3)$$

where, $E^{P}_{i,BC,St}$ is the production dependent steam consumption of a batch distillation column in kJ, m are the masses of the total solvent content of the reboiler ($_S$), the evaporated solvent ($_{ES}$), or the apparatus ($_A$) in kg respectively, c_P represents the heat capacities of the reaction mass ($_{RM}$) or the material of the apparatus ($_A$) in kJ / kg / K, respectively, ΔT represents the temperature increases of the reaction mass ($_{RM}$), the apparatus ($_A$) or the temperature difference of the apparatus to the ambient temperature ($_{Am}$) in K, respectively, ΔH_R is the reaction enthalpy in kJ / kg, ΔH_V is the heat of vaporisation in kJ / kg, RR is the dimension free reflux ratio, K is the loss coefficient in kW / m^2 / K, A is the surface area of the vessel in m^2, η is the efficiency of the stirrer in %, γ is the relation of nominal power to actual power consumption of the stirrer in %, P_N is the nominal power of the stirrer in kW, and t is the batch time in s. $E^{P}_{i,BC,St}$ may be translated to kWh by dividing kJ with 3,600 s / h.

For a centrifuge, discussions with industry experts lead to the following model:

$$E^{P}_{I,Z,El} = P^{F} \cdot m_{Su} \cdot t_F + (P^{O} + P^{Pu}) \cdot t_O - 0.2 \cdot P^{Br} \cdot m_{So} \cdot t_{Br} \qquad (5\text{-}4)$$

here, $E^{P}_{I,Z,El}$ is the total production dependent electricity consumption of a centrifuge, P^{F} is the power required for the feed in kW / t suspension, m_{Su} is the amount of suspension in t / batch, t_F is the feed time in s, P^{O} is the power consumption during operation in kW, P^{Pu} is the power consumption of the pumps in kW, t_O is the operation time in s, P^{Br} is the break power in kW / t solids, m_{So} is the mass of solids in t / batch, and t_{Br} is the breaking time in s.

The parameter values found in the above-mentioned investigations and the corresponding modelling equations are derived with the help of intense measurements during this study. All the measurements and model developments are described in detail in (Bieler 2004). With the help of the measurements, the parameters of the postulated models were developed. All the parameters are summarised in Table 5-6. The heat of vaporisation for both 5 and 15 bar steam (including cooling of the condensed water to average jacket temperature) is found to be about 0.65 kWh / kg according to values given in (Lide 1995) and discussions with industry experts.

Table 5-6: Summary of the Equations and Parameters[19] for the SUOM

Apparatus	Utility	Modelling Equation – see Page	Parameters & Values K [kW/m²/K]	η [%]	γ [%]	C [kW]
Reactor	Steam	(5-1) – 41	$4.2\cdot10^{-2}$	60	28	-
	Brine	(5-1) – 41	$1.7\cdot10^{-2}$	60	28	-
	Electricity[20]	(3-13) – 20	-	-	-	100
	Electricity[21]	(3-8) – 19	-	-	85	-
	Electricity[22]	(3-8) – 19	-	-	28	-
Nutsche Dryer	Steam	(5-1) – 41	$4.2\cdot10^{-2}$	60	28	-
	Electricity[21]	(3-8) – 19	-	-	85	-
	Electricity[22]	(3-8) – 19	-	-	28	-
Heat-Chamber	Steam[23]	(5-2) – 47	$4.2\cdot10^{-2}$	-	-	-
	Electricity	(3-8) – 19	-	-	64	-
Vacuum Pump	Electricity	(3-8) – 19	-	-	52	-
APOVAC	Electricity	(3-8) – 19	-	-	62	-
	Brine	(3-13) – 20	-	-	-	30
Steam Jet Pump	Steam	(3-13) – 20	-	-	-	93
Stirrer & Motor[24]	Electricity	(3-8) – 19	-	-	28	-
Infrastructure & Losses	Electricity	(3-13) – 20	-	-	-	180
	Steam	(3-13) – 20	-	-	-	200
	Brine	(3-13) – 20	-	-	-	20
Short Path Distillation	Brine	(3-13) – 20	-	-	-	3.6
	Electricity	(3-8) – 19	-	-	96	-
Falling-Film Evaporator	Steam	(5-1) – 41	$4.2\cdot10^{-2}$	60	85	-
	Electricity	(3-8) – 19	-	-	85	-
Horizontal Vacuum Rotary Dryer	Steam	(5-1) – 41	$4.2\cdot10^{-2}$	60	28	-
	Electricity[21]	(3-8) – 19	-	-	85	-
	Electricity[22]	(3-8) – 19	-	-	28	-
Batch Distillation Column	Steam	(5-3) – 48	$2.5\cdot10^{-2}$	60	28	-
	Electricity	(3-8) – 19	-	-	28	-
Centrifuge	Electricity	(5-4) – 48	P^F=750W/t, P^O=5-15kW; P^{Pu}=2kW; P^{Br}=1.8kW/t			

With the help of these parameters and the modelling equations for single unit operations, the modelling of a whole production plant according to Equations (3-14), (3-15) and (3-26) will be performed in Chapter 5.3.

[19] Shaded values are specific for the apparatus of the investigated building
[20] For heating of the high temperature reaction vessel
[21] Circulation pump
[22] Other equipment
[23] Other fixed values: c_P = 2.5 kJ/(kg K); m_S = 1.2 t (see Bieler, P. S. (2004). "Analysis and Modelling of the Energy Consumption of Chemical Batch Plants," Ph. D. dissertation, ETH, Zurich.)
[24] For all apparatus

The investigations on single apparatus level showed, that simple models according to the base Equation (3-16) are applicable to model the energy consumption of these apparatus.

For the generation of these models, extensive measurements had to be performed. These measurements took a big part of the work of this study. Measurements were not possible for all apparatus available in the building and extensive assumptions had to be made (see (Bieler 2004)). These assumptions were required to keep the models easy enough to be of use for daily business. The models should be easy enough for being applicable with the few data available in a standard way for most of the chemicals used in a batch production facility.

Differential equations were avoided in the models because not the timely energy consumption but the total consumption per batch is of main interest for production. This value is required not only for accounting the (standard) costs of a batch but also for comparing the actual utility consumption to the calculated utility consumption according to the production mass (see Chapter 5.1). If this is not possible with a TODOMO, the BOTUMO elaborated in this and the next chapter has to be applied. Deviations between reality and model could lead to the investigation of batches that performed badly or equipment failure.

The models of the equipment units and the whole plant show where the energy is consumed. With the help of this knowledge, optimisation potentials can be revealed. Changes in energy consumption caused by changes in the production mix will also be shown and accounted for more accurately than it is done until now.

Optimisation potential for the investigated processes lies mainly in two fields: the loss coefficient of the reaction vessels (steam and brine consumption) and in the nominal power of the stirring motors.

The loss coefficient of the reaction vessels influences directly the brine and steam consumption of these unit operations. As seen in the measurements mentioned in the preceding chapters, a big part (sometimes about 50% of total utility consumption) is lost. This loss is due to the stirrer and the circulation pump introducing heat to the system (for brine usage only), the radiation of heat from and to the environment, and the loss through the pipes and the steam traps (for steam usage only). The stirrer and the circulation pump have to introduce mechanical energy to the system. This energy is converted to waste heat through friction. Stirrers operated at low percentage of nominal power as the ones usually found in chemical industry have a poor efficiency, resulting in high amounts of waste heat. Better design of the motors could therefore lead not only to lower installation costs but also to lower operating costs. The losses through the walls of the apparatus could be minimised by improving the insulation of the apparatus. In the investigated plant, most of the reaction vessels were not insulated at the top because of flexibility reasons. This is definitely a significant factor for the losses. With the help of a flexible insulation that is easy to remove, the top could be insulated as well and the losses through the wall would decrease. The losses through the steam traps and piping system are significant and inherently related to the design of the reaction vessel depicted in Figure 5-7. Any other constellation could result in cavitation within the pump. It could be investigated, nevertheless, if installation of the steam inlet directly before the inlet to the vessel is possible. Heat transfer could be improved by this installation while not affecting the circulation pump. A drawback could be the occurrence of hot-spots in the heating jacket and a larger temperature difference from the inlet of the jacket to the outlet. Detailed investigations are therefore required for this possibility. Another possibility is staying with the design, as it is today and installing different kinds of steam traps. The main steam trap installed today is a steam trap with a floating ball. This type of steam trap is easily corrupted. Furthermore, it does not exactly divide steam and hot water. The other type is a thermodynamic steam trap. Here, a bimetal part opens and closes due to temperature and divides therefore clearly between steam and liquid. The thermodynamic steam traps known today in industry are not too practical for this purpose because they need to be adapted to the desired temperature manually. Probably in the future, an electronic solution to this problem is provided. With the help of these improvements, the losses of the system could be minimised.

The model equations for the different apparatus are summarised together with their parameters in Table 5-6. Some values are of general concern while others should be investigated again in a new building. The parameters specific to the equipment of the investigated building are shaded in the table. Although the development of these models required extensive measurements, the models are built to be adaptable to different unit operations, processes and buildings. For the modelling of a new building with new processes, only minor measurements for verification of the models and for investigating the base consumption of the building have to be performed. This is a big advantage when trying to provide the models company-wide while the basic unit operations and apparatus stay the same.

As mentioned above, the models developed in this section can be used for modelling the energy consumption of a whole plant according to the equations provided in Chapter 4.2. This is described and shown in the next chapter.

5.3 Bottom-Up Modelling of Multipurpose Batch Plants (BOTUMO)

The multipurpose batch plant investigated in this chapter is, as in the preceding chapter, Building 1 discussed in Chapter 5.1. The specifications of the building are presented in Table 5-1. In this chapter, it will be shown that the bottom-up approach is valid for this multipurpose batch plant for which the top-down modelling was not possible and delivered insufficient results.

The steam for heating of the building is not investigated further in this chapter, since the top-down modelling according to Equation (3-3) and discussed in Chapter 5.1.3.1 was applicable as presented in Figure 5-3.

5.3.1 Combining the Different Unit Operation Models to a Plant Model (BOTUMO)

5.3.1.1 Description of the Program for Modelling Multipurpose Batch Plants

The different unit operation models developed and postulated in Chapter 5.2 are based on the equations given in Chapter 4.2. As depicted in Figure 4-2, the single unit operation models have to be combined according to production data. These single models are then summed up with the base consumption of the building. This results in a model of the whole plant (BOTUMO).

This task is performed with the help of a dedicated Excel® model (called program in the proceeding of this study; see (Dahinden 2003) as well). The program will be shortly explained for better understanding.

The program is split in four layers as shown in Figure 5-16. The base data layer consists of the specifications of the standard substances, the apparatus used and the general modelling parameters given in Table 5-6.

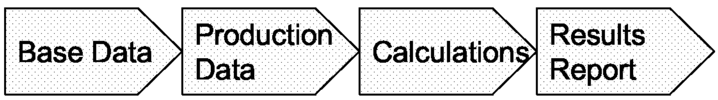


Figure 5-16: The four layers of the program

The production data layer contains the input sheet for the production data (either from production record (PR) or from process step procedure (PSP)), and the input and calculation sheets for the reactions, the heat chambers and for other special equipment (e.g., vacuum pumps).

The calculation layer contains the calculation sheets for the heating/cooling of the substances, the evaporation of substances and all the other calculations according to Equation (3-14) and (3-15).

The results are finally summarised and presented in the results report layer.

All these different layers and the interconnection of the different sheets available on each layer are shown in Figure 5-17.

The required input data for the different sheets for modelling are presented and explained in (Bieler 2004).

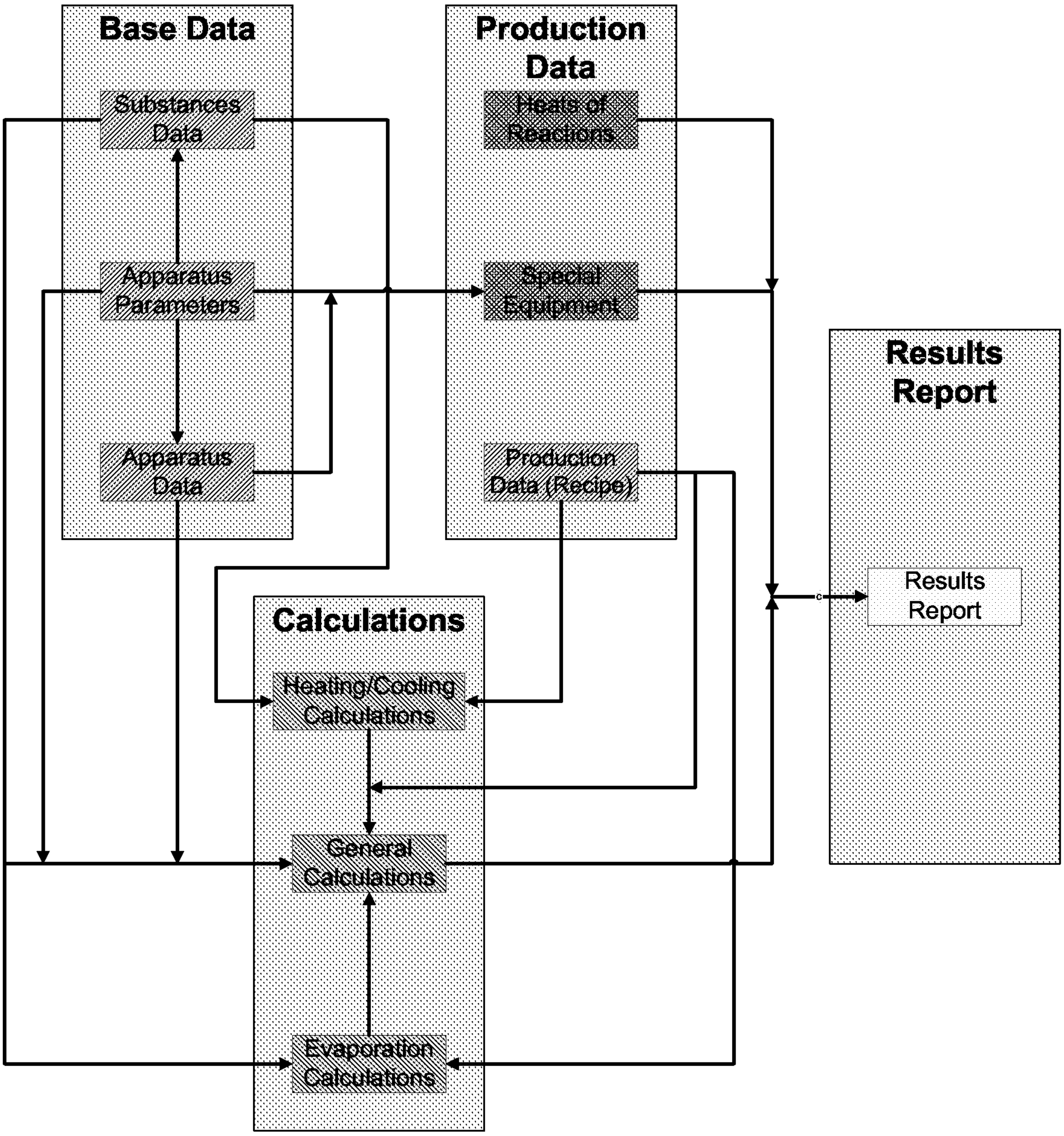


Figure 5-17: The different layers of the BOTUMO program and their contents[25]

5.3.1.2 Modelling and Report Generation

The modelling is performed by providing the input data to the production data layer mentioned above. The input data consists of the production steps for the different chemicals produced. Not all production steps need to be implemented, nevertheless. Only the inputs or removals of substances, the heating or cooling of the reaction media and the holding times in-between have to be provided. This reduces a long PR to a few lines in the worksheets of the production data layer. For daily production, this is done directly in the according sheets for the days of interest. This is, nevertheless, a big effort even for a small number of days in a medium building if no electronic form of the PR is available (as in the investigated building). The results for such a modelling, presented in the results report, are of the kind of $E^P{}_m$ pre-

[25] Hatched from bottom to top: input sheets; hatched from top to bottom: calculation sheets; crossed: input & calculation sheets; blank: results sheet; *Special Equipment* (e.g., heat-chambers) is listed separately and not together with the reactors in the sheet *General Calculations* for ease of calculation

sented in Equation (3-25). These can be summed up according to Equation (3-26) again to result in E^P or split to give all the different E^P's mentioned in Chapter 4.2.3.

When modelling a longer period than a couple of days (e.g., a week or a month), the modelling has to be performed with theoretical data extracted from the PSP. Therefore, a program (i.e., one Excel® workbook) is favourably built for each production process performed during the investigated period. This makes the data input easier and increases the flexibility and clearness of the program. In each program, only data of one batch of the specific chemical is entered according to the PSP and the guidelines mentioned above. This may therefore be considered as a condensed, electronic version of the PSP. As result, E^P_{im} as explained in Equation (3-20) is modelled in each worksheet. It is even possible to divide the model further to reach at the E^P_{ijm} (Equation (3-16)) level of modelling. All these different PSP models are then summarised in a summary sheet where the summation according to the different equations provided in Chapter 4.2.3 is performed. This modelling makes the program highly flexible and adaptable. A drawback is the speed of the calculation due to the many links between the different sheets that need to be updated. This could be overcome by a different modelling as described in Chapter 6.

5.3.2 Results of the BOTUMO

The results of the BOTUMO and the analysis thereof will be presented in the following chapters. Modelling was performed at different stages of detail.

The periods mentioned in the following paragraphs were taken during the year 2003 and are depicted in Table 5-7.

Table 5-7: Investigated periods

Period Name	Starting Time	End Time
One day	04.05.2003 06:00	05.05.2003 06:00
Two days	04.05.2003 06:00	06.05.2003 06:00
One week	05.05.2003 06:00	12.05.2003 06:00
One month	06.01.2003 06:00	10.02.2003 06:00

For the period of one day and of two days, the modelling according to PR and PSP data was performed similarly. For the longer periods, only the PSP data was used as input. When speaking about models for the period of one week or one month in the next sections, models using PSP data are meant.

The model incorporates not only models for each different chemical produced as will be shown in Chapter 5.3.2.4, but also for some special operation like re-concentration and distillation of the used brine, ethanol distillation in the falling-film evaporator, decalcification, cleaning, and preparation of the reaction vessels. These tasks are important for the total consumption and are modelled in the BOTUMO. For the discussions in Chapter 5.3.2.4, concerning the different products of the building, these tasks are, nevertheless not regarded since focus was put on the actual products of the plant.

5.3.2.1 Modelling of Different Periods

The modelling of different periods with the BOTUMO is possible with two different degrees of detail. In this section, the energy consumption of the different energy carriers for the whole building is presented. This is according to the E^P_m presented in Equation (3-25). The exact production data (extracted from the PR as mentioned above) can be used as input. This is tedious and time consuming even for short periods if no electronic version of the PR is available (see (Dahinden 2003)). For most of the multipurpose batch plants known to the author, no electronic data exist. Therefore, this approach is suitable for showing the accuracy of the model by comparing modelled results and measured data over short periods as discussed below. Nevertheless, it is not suitable for continuous control and prediction of the energy consumption of a production plant.

The production data extracted from the PSP on the other hand can be used for modelling of periods longer than several days (e.g., one week or one month). This data is entered only once for the modelling of longer periods according to the PSP data of one batch. As shown in Equation (3-26), the modelling of the whole plant may then be performed by multiplying the consumption of one batch by the numbers of batches produced during the investigated period and summation as intended. A sensitivity or uncertainty analysis (see e.g., (Stahel 1995; Vose 1996)) may then be performed to investigate the influence of the uncertain parameters to the result of the calculations (see Chapter 5.3.3 and (Bieler 2004)).

The possibility and accuracy of the BOTUMO of a building is based on the accuracy of the single unit operation models discussed in Chapter 5.2 (the generic equations are presented in Chapter 4.2). There, the models were tested and developed. The actual BOTUMO (i.e., the model of the whole plant) may only be tested on a total building level because of the lack of measurements of smaller parts of the plant.

For comparison, the consumption of the whole building was measured and calculated by three different methods for one and two days and by two different methods for one week and one month. For one day, the BOTUMO was provided with the data of the PR as well as with the data extracted from the PSP. The third method was the internal utility calculation used by the company at which this case study was conducted (called CPM: *C*ompany *P*roprietary *M*ethod). For periods longer than a few days, the data of the PR could not be extracted from the paper form because of lack of manpower. Therefore, the periods of one week and one month were modelled by the BOTUMO based on the PSP and the CPM.

For one common day of production, the results are depicted in Figure 5-18.

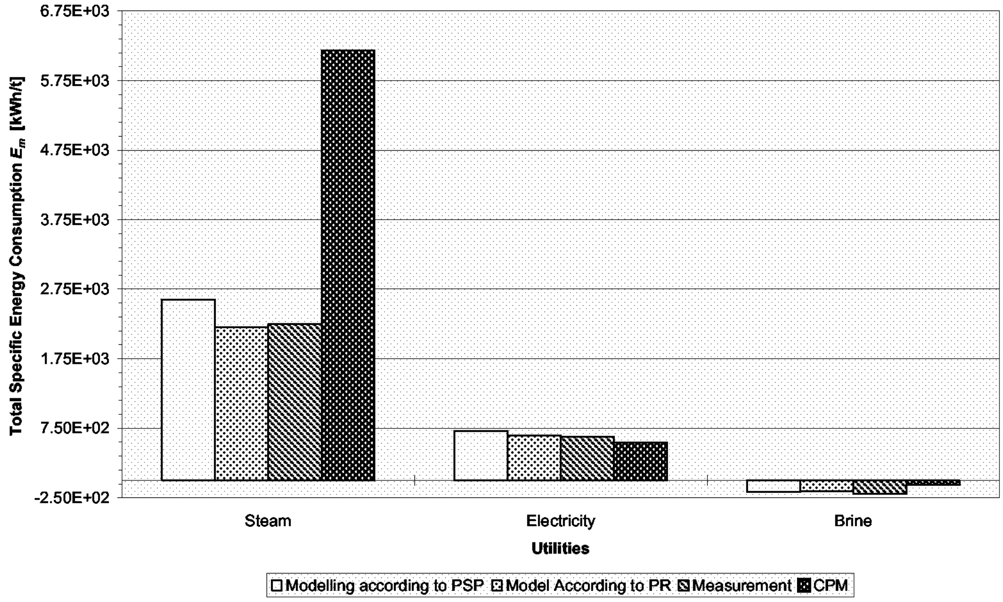


Figure 5-18: Modelling of the specific utility consumption (per t of product) of the whole building for one day of production according to Equation (3-14) and to a company proprietary method (CPM) in comparison with measured data

It is obvious that the modelling according to the CPM is the most inaccurate one. The CPM model is based on experience of daily production and incorporates the steam consumption for heating the building as well as the production steam while the measurements only account for the production steam consumption. The main interest is to give an approximate number of the (total) product cost. Since only total utility costs are considered, and since steam is cheaper than electricity and brine, the higher value is not that disastrous for the product cost but not satisfying anyway. The different deviations could level out each other in terms of costs. Moreover, deviations could level out between different months (consolidating over the year) since heating steam is not required for the whole year. Nevertheless, this is not satisfying since each product should be accounted for its specific costs. The detailed BOTUMO delivers results much more accurate than the CPM. The model based on data extracted from the PR deviates only slightly from the measured value. This is a good control for the accuracy of the model. The BOTUMO based on PSP data has a significant higher deviation from the measured value for the one-day period. This has several reasons. First, it is based on the standard values of the PSP. These standard times, temperatures, masses, etc. do not correlate fully with the actual ones. This implies a deviation inherent in the model especially for shorter periods, where different deviations from the standard parameter values are not levelling out. On the other hand, the model based on PSP data requires the number of batches produced (see Equation (3-26)). For one day, this number is a highly inaccurate and uncertain fraction of a whole batch, since products usually do not have batch times of one day. Some are started during the day and last probably longer, while others, started earlier are finished during the day investigated. An assumption on how many batches were produced (probably Batch 3 is actually starting, while Batch 2 is operating in the middle part of its PSP and Batch 1 is finishing) had to be made. The different parts of the batches under production were therefore summed up to result in a part of a standard batch (preferably one, but also ½ or other fractions were found) resulting in *virtual* batches. These *virtual* batches were used for the modelling (i.e., consumption of one standard batch times the number of *virtual* batches according to Equation (3-26)). This implies of course a deviation from reality that is reflected by the deviation from the measured value being bigger than for the model based on PR data. Nevertheless, this allows keeping the same model for all the periods investigated. Since longer periods than one day are in the focus of this study, a slightly larger deviation at short periods is acceptable.

The relative deviations of the different models are presented in Table 5-8. The modelling of the brine consumption shows the largest deviation between the BOTUMO and the measured values. This is explained by the difficulties and high inaccuracies inherent in the single apparatus measurements described in (Bieler 2004).

Table 5-8: Relative deviations of the different modelling methods for the investigated utilities according to Equation (3-14)

Period	Modelling Method	Steam [%]	Electricity [%]	Brine [%]
1 Day	PSP	16	14	-12
	PR	-2	3	-18
	CPM	175	-12	-67
2 Days	PSP	8	5	-19
	PR	-3	0	-5
	CPM	147	-19	-70
1 Week	PSP	1	-2	-27
	CPM	138	-28	-73
1 Month	PSP	-5	5	-16
	CPM	145	10	-51

The deviations between the model and the reality decrease when modelling larger periods. This is shown in Figure 5-19 for the modelling of one month. The relative deviations are given in Table 5-8. As discussed above, the model according to PR was performed for the period of one and two days only.

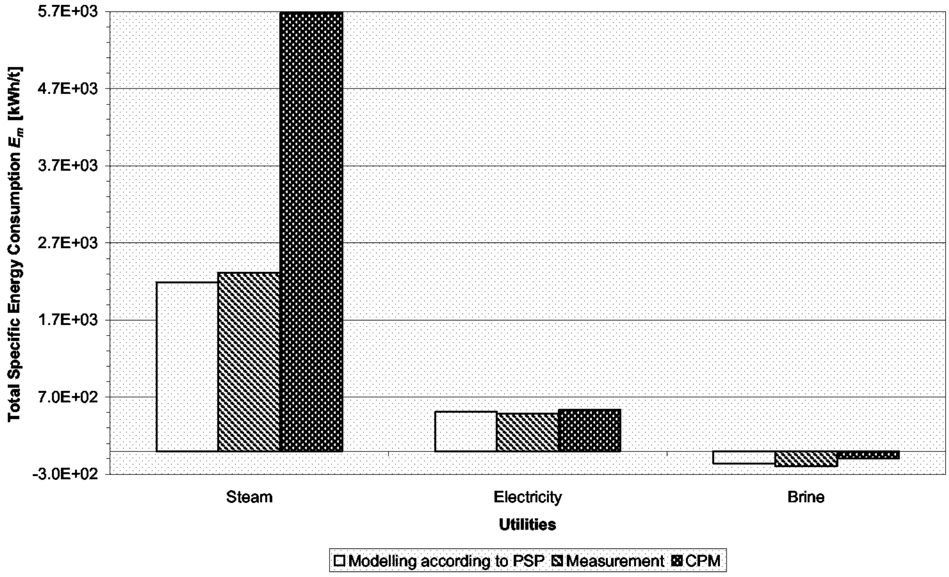


Figure 5-19: Modelling of the specific utility consumption (per t of product) of the investigated building for one month of production according to Equation (3-14) and to a company proprietary method (CPM) in comparison with measured data

The deviations for the CPM are again high. The reasons for this deviation are discussed above. The deviations of the PSP based model from the measurements are smaller for the longer period. This is due to several facts that will be discussed shortly. If the assumption that the batch time given in the PSP equals the mean time of the batch operation is correct as discussed in (Bieler 2004), the deviations due to time level out over long periods. For short periods, they could nevertheless account for significant deviations (i.e., levelling is not possible since only one batch is produced). The determination of the performed batches results in some batches not fully performed at the end and the start of each period. This is a drawback inherent in the BOTUMO as it is programmed (resulting in an easy and fast data input for long periods). The produced mass should be allocated according to the part of the total energy consumed during the part of the operation (i.e., if x% of the total energy of one batch are consumed in one day, x% of the total mass of the batch should be allocated to this period). Alternatively, the exact production reports provide the information of which parts of single batches are performed during the investigated period. Modelling of short periods is therefore preferably performed with PR data. The longer the period, the less influence these "edge-effects" have (the smaller is the contribution to the total consumption over the period). These are the two main influences for the decreasing of the deviation from the measurements for longer production periods.

For the modelling of brine, the deviations from the measured values are of the same order of magnitude for all of the investigated periods. This is due to the fact of the large uncertainty of the single unit operation models as mentioned in Chapters 5.2.1.2. It could be also a hint (since measurements are always higher than the modelled values) that the loss coefficient is larger for a standard batch vessel than the results of the single unit operation measurements indicate. Another possibility could be that the assumption of a minor contribution of safety cooling systems of some batch reactors was not correct and that these consumptions are higher than expected. Because of the impossibility of the measuring of these equipments, this could not be proved. The lack of a model for the enthalpy of crystallisation to the brine consumption could be another small contribution. For reaching at a solution, detailed measurements of crystallisations with known enthalpies of crystallisation should be performed. The measurement equipment could also be optimised to minimise the uncertainties in the temperature and flow measurements.

5.3.2.2 Analysis of the Energy Consumption of the Building

The analysis of the whole building for different periods as presented in the preceding chapter shows the applicability of the BOTUMO for energy modelling of whole production plants. The model is as accurate as could be expected considering the limitations of the measuring equipment and the straightforward modelling equations used (see Chapter 4.2).

The BOTUMO offers now the possibility of analysing the energy consumption of the modelled building in detail. This is analogous to Figure 4-2 and the equations presented in Chapter 4.2.3 only this time, the energy consumption is not summarised to result in the energy consumption of the whole building but divided to result in the energy consumption of single parts of interest. The analysis starts with the summation of the single energy carriers (i.e., steam, brine, and electricity) according to Equation (3-25) to find $E^P{}_m$. With the help of this analysis, it is possible to break down the total consumption per energy carrier to the different apparatus groups consuming energy in the building. This enables the analyser to put focus of energy analysis and optimisation on the apparatus group with the highest energy consumption.

The apparatus groups of the production plant requiring energy that were investigated separately are: the reactors and nutsche dryers, the heat provided to the building by the enthalpy of reaction, the consumption of the heat-chamber, the steam jet pumps (considered by people from production as large steam consumers), the external vacuum pumps (the APOVAC pumps are considered directly with the nutsche dryers and the general vacuum pumps are considered as infrastructure consumption) and the base consumption (building infrastructure).

Because of the accurate results received for the modelling according to the PSP data and the reduced "edge-effects" encountered for longer periods, the following investigations are performed of one month and sometimes for one week. The modelling for one week will be presented only for reasons of comparison with the results found for one month.

The modelling results are presented in detail in (Bieler 2004). For the relative values, the modelled consumption was divided by the total amount of products actually requiring the specific utility, while the base consumption was divided by the total amount of chemicals produced.

Figure 5-20 presents the results for the steam modelling. It is seen that the absolute value of the steam consumption of the reactors and nutsche dryers is the largest one. These apparatus should therefore be investigated in more detail (see Chapter 5.3.2.3). Furthermore, it can be seen that the base consumption is not as high as expected since no infrastructure equipment is using steam. The steam jet pumps on the other hand have no influence on total steam consumption either. This is due to the fact that these machines are only working when required and are shutdown if not in use.

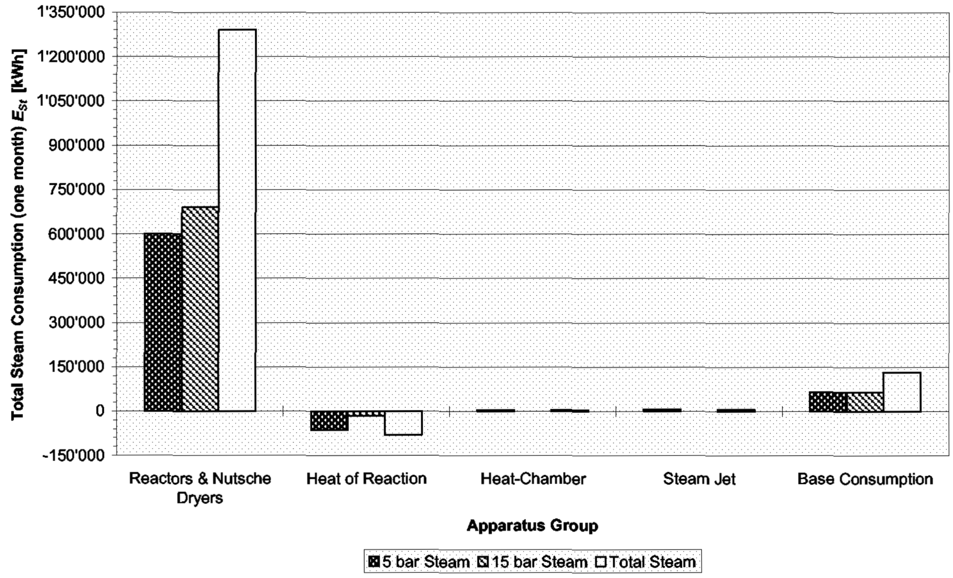


Figure 5-20: Absolute modelled steam consumption of the building during one month according to Equation (3-14) (PSP data)

In Figure 5-21, the modelled specific steam consumption for one month of production according to PSP data is presented. The base consumption is divided by the total mass of products of the plant while the other consumptions are divided by the actual amount of products requiring this utility. Therefore, the specific base consumption diminishes compared to the production dependent steam consumption. The heat of reaction provides a significant, though not large contribution to the heating steam (and reduces the heating steam consumption therefore). In terms of specific energy consumption, the reactors and nutsche dryers are the largest consumers. Focus has therefore to be put on these apparatus group. It will be analysed in more detail in the next chapter.

The analyses for brine and electricity may be found in in (Bieler 2004).

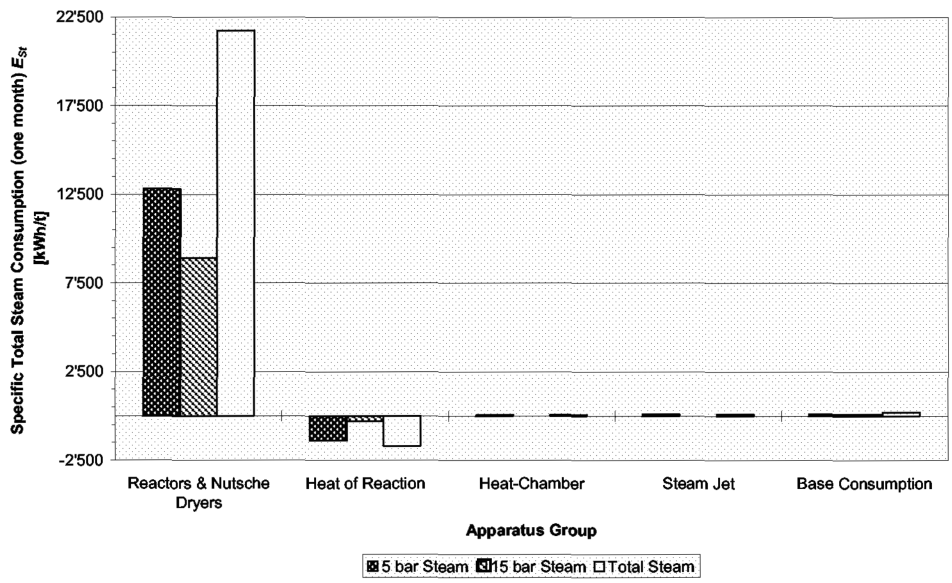


Figure 5-21: Specific modelled steam consumption of the building during one month according to Equation (3-14) (PSP data)

5.3.2.3 Modelling of Different Aspects of the Reactors and Nutsche Dryers

As in the preceding chapter, the model calculations presented in this chapter are all based on PSP data, since long periods are modelled. The results presented here are according to $E^P{}_m$ depicted in Equation (3-25). Not the whole $E^P{}_m$ is considered, but only the biggest consumer of energy, namely the apparatus group *Reactors and Nutsche Dryers* is investigated. Different aspects of the energy consumption of this apparatus group are investigated in the following paragraphs. Only the analyses of the steam consumption are presented here. Analyses of the electricity and brine consumption may be found in more detail in (Bieler 2004).

From the analyses in the preceding chapter it is seen, that the reactors and nutsche dryers are the most important energy consumers of the building, except for electricity consumption. Base consumption is extensively discussed in Chapter 5.1. No focus will be put on optimising or modelling the electricity consumption of the infrastructure of a production building in more detail in this section. For this continuous operation, models exist and industry has a significant experience in optimising the infrastructure consumption of buildings (see e.g., (SIA 1992; SIA 1995; SIA 1997) or (Gränicher 1997) or (Severson 1996; Sulzer 2003; Thumann 1983; Turner 1982)).

Furthermore, the continuous distillation will not be discussed in this paragraph. It is a significant consumer but is not a batch apparatus this study is dealing with. It is discussed separately in (Bieler 2004).

The BOTUMO (based on PSP data) was used for a detailed analysis of the energy consumption of the batch reactors and nutsche dryers.

Figure 5-22 presents the modelled specific steam consumption of the reactors and nutsche dryers. The different unit operations requiring steam, the stirrer input and the losses are investigated. The modelling is performed for one week and one month, both based on PSP data as described above. It can be seen that the different production mixes during the two periods result in different modelling results for the specific steam consumption. Different products require different amounts of steam during their production process. This results in differences in the (overall) specific steam consumption. The model accounts for the differences in the production processes (see Chapter 5.3.2.4). The different "edge effects" discussed above may have an influence on the product specific energy consumption as well. This will be discussed in detail in Chapter 5.3.2.4.

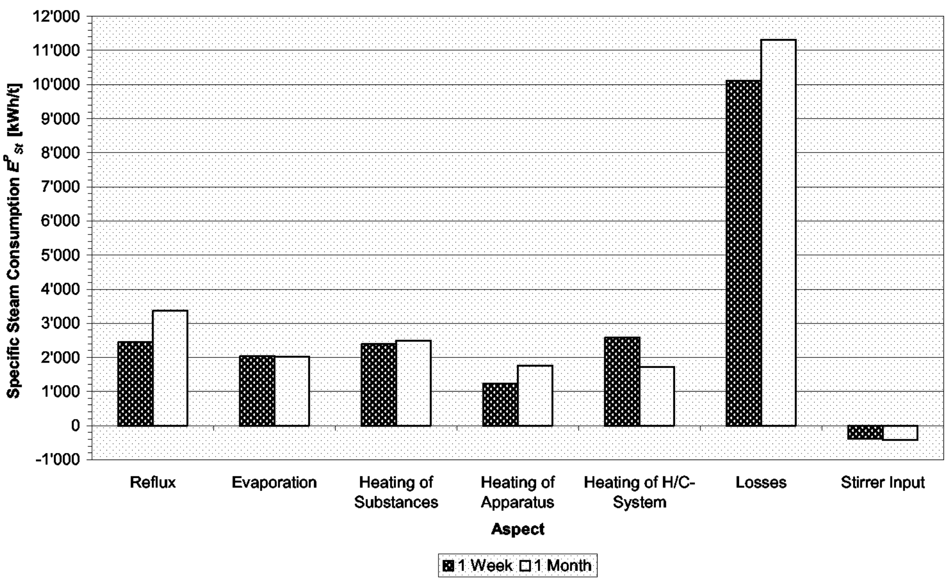


Figure 5-22: Modelled specific steam consumption of the reactors and nutsche dryers according to Equation (3-25) (PSP data)

Reflux conditions are used more often during the investigated month than during the investigated week.

The heating of the apparatus used a significantly higher amount of specific steam during the investigated month than during the investigated week. This is reflected also by the higher specific losses. Longer heating periods and higher process temperatures have an influence both on the loss coefficient and on the heating of the apparatus. The specific consumption of the heating of the apparatus and the heating/cooling-system could both be improved by moving products from smaller apparatus to bigger ones. This improves the relation between outside surface of an apparatus and its content. Since the weight of an apparatus (metal) is related to its surface area (surface area times thickness of the metal times the density of the metal equals the weight of a reactor), the specific energy consumption for heating the apparatus is decreased by increasing the size of an apparatus.

The heating of the heating/cooling-system uses less specific steam during the month than during the week. This is a hint that different apparatus were in use during the two periods (see Chapter 5.3.2.5 as well). An explanation could be that the apparatus used during the week were mostly reactors with thinner walls but with the same water content of the heating/cooling-systems as the reactors with the thicker walls (i.e., specifically bigger water content). This would increase the specific steam consumption for the heating/cooling-system and reduce the specific consumption for the heating of the apparatus.

Stirrer input may be neglected. It is only about 2% of total and of specific steam consumption. Losses, nevertheless, are significant and responsible for about 50% of total steam consumption for the reactors and nutsche dryers. About 50% of these losses are, as mentioned in Chapter 5.2.1, caused by the losses through the steam traps. The other 50% are caused by heat transfer through the outside wall of the apparatus. It is obvious that minimisation of the losses provides the best possibility to optimise the steam consumption of the reactors and nutsche dryers. An improvement of about 10% of the losses would result in a reduction of about 5% of total steam consumption for these apparatus while an optimisation of 10% for an improvement of the heating of the substances (i.e., lower process temperatures or solvents with lower heat capacity) would only result in about 1% of total steam consumption.

Focus may also be put on the steam consumption for reflux conditions. It is questionable whether these conditions are always required for the production process (e.g., drying of the solvent) or whether it is only a simple method for keeping process temperature constant. With today's possibilities of controlling the process temperature of an apparatus, reflux just for keeping a temperature would be useless. Detailed investigations of the different PSP could reveal the actual use of the reflux conditions and lead to an optimisation of the steam consumption of this specific unit operation.

5.3.2.4 The Differences between the Products

In the investigations of the TODOMO presented in Chapter 5.1, it was assumed that all the products of a multipurpose batch plant use about the same amount of specific energy. With the help of the BOTUMO, this assumption may be analysed. This will be discussed in this chapter. For some products, the modelling was performed during the "one week" (W) period and for the "one month" period (M).

The findings presented in this section are according to Equation (3-20) (i.e., E^{P}_{im}) presented in Chapter 4.2.3. The shading of the products presents an even more detailed analysis by presenting different aspects of the production processes (see (Bieler 2004) as well).

Figure 5-23 presents the specific modelled steam consumption for the different products as well as the chemical steps involved in the production of the different products. The steam consumptions of the different processes are presented as well.

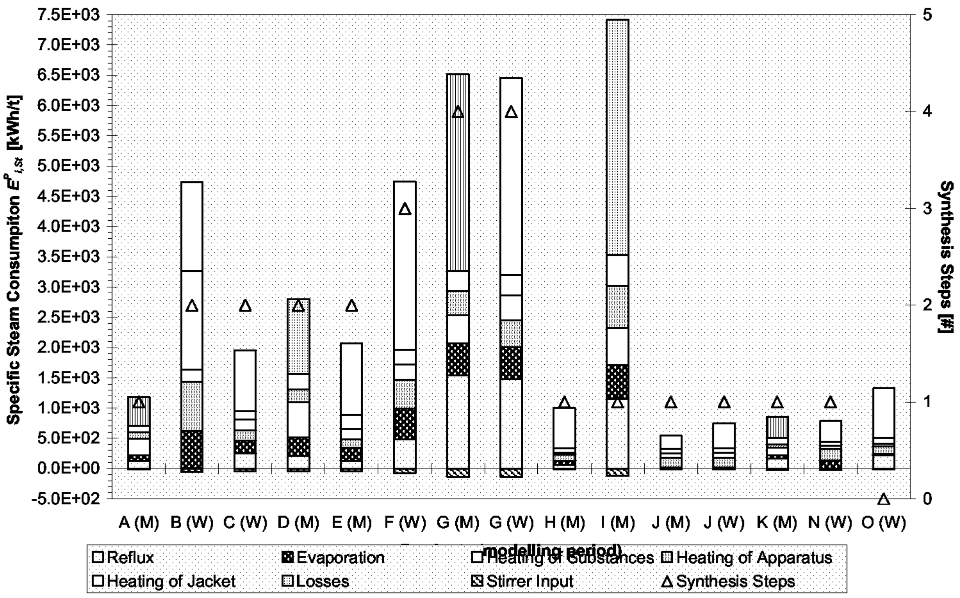


Figure 5-23: Specific modelled steam consumption of the different products (A, B,…,N, O) according to Equation (3-20) (PSP data) for the period of one month (M) and one week (W) and no. of synthesis steps involved in the productiton processes

The modelling of one month and one week for two products (G and J) shows the accuracy of the model for both periods. The aforementioned “edge effects” influencing the specific energy consumption for the two periods differently may be neglected. The model accounts for the differences in the production recipes but is only minor influenced by effects of inaccurate accounting of batches at the beginning and the end of longer periods. Therefore, the differences of total consumption for the two periods found in the former chapters are caused by differences in production mix and not by inaccurate accounting of the produced amount of chemicals.

From the picture it may be seen that the assumption of similar specific energy consumption for all of the different products postulated in Chapter 5.1 is not true for the specific steam consumption of the investigated building. The products vary widely in absolute steam consumption as well as in the specific consumption for the different unit operations required for the production process. The statement made in Chapter 5.1 that only production of one product or constant production mix of different products allows the top-down modelling of the whole production building is valid. The investigated building (Building 1 in Chapter 5.1) shows no constant production mix and the products are varying widely in specific steam consumption.

The different unit operations are discussed extensively in (Bieler 2004). It is seen, nevertheless, from Figure 5-23 that the losses are the most significant specific steam consumers for all the products. The losses are varying with the number of different vessels used (i.e., the total surface area), the batch times and the temperatures of the specific process.

Products with extensive reflux operation (i.e., long batch times), processes with high temperatures and production in several different vessels are found to be the major consumers of steam. Optimisation should therefore start with these products and for the apparatus with the highest specific consumptions (see Chapter 5.3.2.5).

Comparing the number of synthesis steps involved in the production of the different products with the energy consumption shows, that this number could give a first, rough estimate of the actual steam consumption as shown in Figure 5-23. Three different levels of energy consumption and number of synthesis steps can be seen: high, low, and medium. The only exceptions from this general rule are Products I and O. In the production process of Product O, no chemical synthesis step is involved, since it only comprises physical transformation (i.e., a solution is produced and dried). The physical steps require steam as well and therefore, the energy consumption of this product is not zero. For Product I it can be stated, that it requires long and energy intensive unit operations. The reaction is conducted at high temperature. Moreover, the product requires long reflux conditions that are conducted at high temperatures as well. Since losses are proportional to time (see Equation (3-7)), the losses increase although no chemical transformation is going on. This shows again, that a simple correlation of energy consumption with products is not applicable as discussed in Chapter 5.1. Nevertheless, the easy accessible data of the number of synthesis steps, enables the Chemist to have a fast cross-check of the modeled energy consumption data. Deviations have to be explained similar to the explanations above. If an explanation is missing, the model should be reviewed carefully to reveal mistakes or to find an explanation of the deviation.

5.3.2.5 The Differences between the Apparatus

The modelling described in this chapter was performed, according to E^P_{ijm} as depicted in Equation (3-16) (i.e., the consumption of each specific apparatus, consuming one kind of energy, and producing one specific chemical).

Figure 5-24 shows the specific steam consumption for each apparatus available in the investigated building during the one month modelling according to PSP data. It is seen that, although the apparatus have the same loss co-efficient, the specific steam consumptions per ton of produced chemical are quite different. This shows that the model accurately accounts for the different specifications of the apparatus and the different process conditions. The higher the process temperature, the longer the batch time, and the more solvent is evaporated (i.e., distilled or hold at reflux conditions), the more steam is consumed according to Equation (5-1).

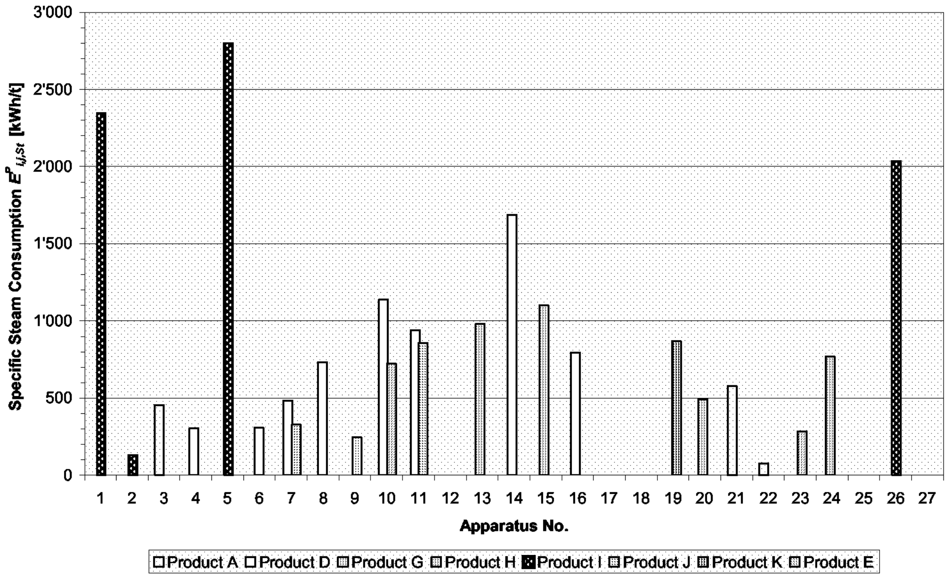


Figure 5-24: Modelled specific steam consumption of the apparatus (1, 2,…,26, 27) during one month according to Equation (3-16) (PSP data)

Furthermore it is seen, that some products (e.g., Product G) use several apparatus, while some products (e.g., Product K) use only one or two apparatus. This supports the findings of the last paragraph that the number of apparatus used by a production process has a significant influence on its energy consumption. Nevertheless, this is not the only or major influence since the high energy consumption of Product I is only distributed over four apparatus (see Figure 5-24).

Some production processes are performed in the same apparatus. Differing energy consumption may be due to differences in process times, temperatures, filling of the vessel, production processes, or physical properties of the chemicals. Investigations of performing the same production process in different apparatus were not performed but could be done with detailed production data according to the PSP.

The investigations of the electricity and brine consumption of the different apparatus may be found in (Bieler 2004).

5.3.3 Conclusions

The modelling of a whole production building according to PR and PSP with the help of the BOTUMO was performed. For such a BOTUMO the SUOM developed in Chapter 5.2 were put together and summarised according to the equations given in Chapter 4.2. The overall model was built according to Equations (3-14), (3-15), and (3-16). Summation resulted in a model according to Equation (3-26) (or, in other words, to Equation (3-15)). This production dependent energy consumption is then inserted together with the infrastructure consumption in Equation (3-14) to result in a model of the whole plant.

The modelling according to the PR results in more accurate outcomes of the model (in absolute terms). The results for short periods depict the problem that it is not exactly known how many batches are produced during a short period.

For modelling of longer periods than about two days, the PR showed to be a data source too tedious to acquire. It was too time consuming and complicated to extract the data. Therefore, a change to data extracted from the PSP was performed. For short periods (a few days), these models showed higher deviations from the measurements than the PR-based ones. Nevertheless, they showed to be significantly more accurate than the models used in daily production today. For longer periods (i.e., longer than about one week), the models built with the PSP data showed good accuracy when compared to the measurements of the whole building. The modelling according to PSP data is therefore possible and the BOTUMO applicable for longer periods.

With the help of the BOTUMO, it is possible to make detailed analyses of the energy consumption of a whole production plant. Unlike the black-box model presented in Chapter 5.1 (TODOMO), a breakdown of the total energy consumption is possible. The energy consumption (the specific as well as the absolute one) may be assigned to the different apparatus and products in the plant. Analogous to Figure 4-2, it is possible to distinguish the energy consumption of the whole building for all of the different utilities, apparatus and chemicals available in the plant.

The analysis showed that the specific energy consumption is varying widely for the different products. No mean specific consumption was found for the investigated building. This explains why the TODOMO presented in Chapter 5.1 was not applicable for the investigated building (Building 1). In the TODOMO, mean specific energy consumption is postulated for all the different chemicals available in a production plant. Modelling according to Equation (3-1) relies on this mean specific energy consumption.

As found in Chapter 5.2, losses are important for the steam and the brine consumption of a single apparatus. In this chapter, the losses showed to be important for the total consumption of brine and steam as well. Overall, the largest part of energy (apart from the electricity consumption of the infrastructure) is consumed by the apparatus group reactors and nutsche dryers. These apparatus show significant losses for brine and steam consumption. Focus should therefore be put on optimising the losses of brine and steam operations. For brine operations, the losses are smaller because only losses through heat transfer to the environment have to be considered. For steam, losses may occur through heat transfer through the wall, but also through suboptimally operating steam traps and through badly sealing valves etc.

The model was able to show differences between the different apparatus in terms of energy consumption as well. The model could therefore be used for comparing the production of the same chemical in different apparatus.

The results of the sensitivity analysis are discussed in (Bieler 2004) and are summarised in Table 5-9. The sensitivity analysis shows that the influence of most of the parameters is minor. Only the loss coefficients *K* and the times of the different process steps *t* have significant influence on the outcome of the models.

The loss coefficients *K* should therefore be investigated intensively in future studies. More measurements would lead to more exact parameter values. With the help of more exact parameter values, the model accuracy could be improved and the model would become more reliable. This would improve transferability of the model as well.

Table 5-9: Summary of the sensitivity analysis (see (Bieler 2004)) showing the deviation of the objective functions E_m according to Equation (3-14) for changes in the parameter values of ±20%; modelling period: one month

Parameter	Steam		Electricity	Brine
	15 bar	5 bar		
Stirrer efficiency	±0.3%	±0.3%	±4%	±1%
Stirrer input	±0.3%	±0.3%	-	±1%
Circulation pump efficiency	-	-	±2%	-
Vacuum pump efficiency	-	-	±2%	-
Heat-chamber ventilator efficiency	-	-	±0.1%	-
Short-path distillation efficiency	-	-	-2%	-
APOVAC efficiency	-	-	±1%	-
Enthalpy of vaporisation (steam)	±0.1%	±3%	-	-
Loss coefficient (steam)	±9%	±6%	-	-
Loss coefficient (brine)	-	-	-	±3%
Time	±9%	±6-8%	±6-7%	±9%

Time is the most influential parameter in the unit operation models as shown in Table 5-9. Care should therefore be taken to acquire the most exact values from the data given in the PSP. Sensitivity analyses should be performed again for a new building to investigate the margin of deviation of the model outputs according to this parameter.

5.4 Conclusions

The modelling of the energy consumption of batch production plants is possible. Two different approaches were performed for energy modelling of whole batch production plants: a top-down approach (TODOMO) and a bottom-up approach (BOTUMO).

The simpler of the two models, the TODOMO, has limited applicability and several drawbacks. This model is only suitable for modelling the energy consumption of production plants with products that have similar specific energy consumption. This is the case for monoproduct batch plants, for multiproduct batch plants with similar products and for multiproduct batch plants with constant production mix (on mass basis). For these buildings, it is possible to extract the infrastructure consumption from the actual production dependent consumption. This infrastructure consumption is responsible for a significant part of total energy consumption especially for electricity. The production dependent energy consumption results in a specific energy consumption for all the chemicals produced in the plant. The infrastructure consumption as well as the specific product consumption of energy may then be compared to the consumptions of other buildings. Furthermore, the production of the same chemical in several different plants may be compared in terms of energy. This shows whether or not the plants are comparable and which is the best of the investigated ones. Focus may then be put either on infrastructure or on production dependent consumption of energy. Optimisation potentials may be found by challenging the plants against the most efficient ones.

The BOTUMO on the other hand requires more modelling effort than the TODOMO but offers much more insight in the production processes and their energy consumptions. Therefore, it offers more insights in optimisation potentials than the TODOMO is able to provide. The BOTUMO may be used for multipurpose batch production buildings with highly varying production mix and a large variety of different production processes. The infrastructure consumption of the building may either be measured or found by the help of a TODOMO. For several unit operations and apparatus, specific models were postulated in this study and checked by measurements (see (Bieler 2004) as well). These measurements led to single unit operation models (SUOM) programmed in Excel® worksheets. These SUOM were checked on single apparatus basis (transferability and comparability) and found to be accurate considering the uncertainties given (i.e., uncertain parameter values and uncertain measurements). The summation of the different SUOM leads to a BOTUMO. Programming was done in Excel®. These SUOM (and therefore the BOTUMO as well) require only widely known parameters for the apparatus and the chemicals and are built simple enough for daily use in a production plant. With the help of these parameters, the generated SUOM and the BOTUMO are transferable to other batch production plants where no (or a limited number of) measurements have to be taken to adapt the model. The SUOM are fed with the production data originating from either PR or PSP. The PR data was nevertheless much too tedious to extract for a longer period than a few days. The BOTUMO based on the PSP data showed poorer accuracy than the one based on the PR for short periods (e.g., one day). When modelling longer periods (e.g., one month), the accuracy of the model based on PSP data was good.

The SUOM with the PSP data were then multiplied by the number of batches produced during the investigated period and summarised according to the general model provided in Equations (3-14) and (3-15) and Equations (3-16) to (3-26). The analysis of the energy consumption according to the modelled consumption showed several possibilities for energy savings (e.g., minimising the losses or optimising the nominal power of the stirrer motors). The model also showed, where the energy was consumed and which production processes should be investigated in more detail and which offer the best possibility for large energy savings as discussed in (Bieler 2004).

A model for the heating steam of production plants was elaborated as well. It was found that the heating steam consumption is only depending on air-change of a production building, degree-days and a base consumption that equals almost zero if no infrastructure equipment is connected with the heating steam system (see Equation (3-3)). This provides an easy-to-use tool for comparing the heating efficiency of a building with a standard one. Moreover, it shows how much heating steam could be saved by decreasing air-change or by removing infrastructure consumption.

The results summary of the modelling of the investigated plant during one month with the help of the BOTUMO are shown in Figure 5-25, Figure 5-26, and Figure 5-27 for steam, electricity, and brine consumption, respectively. The detailed analyses for the different energy carriers are described in (Bieler 2004).

In Figure 5-25, the total modelled steam consumption of the investigated building is analysed with the BOTUMO for the period of one month (with the help of PSP data). The total modelled consumption for this month is 1,354 MWh. This is the actual, modelled consumption, since reaction and stirrer input reduce the modelled consumption for about 80 MWh and about 23 MWh, respectively. The hatched fields in Figure 5-25 represent the consumptions not directly related to the chemistry of the process (i.e., base consumption, losses, etc.). This consumption is responsible for about 63% of total steam consumption. Steam savings should therefore start not with the actual production process but with the reduction of the base consumption, the losses, the heating of the vessels, etc. It can be seen from Figure 5-25 as well that the apparatus group *reactors & nutsche dryers* is responsible for the main part of the steam consumption (mainly because of the large losses). The more detailed modelling of this apparatus group was therefore appropriate to help understand its characteristics.

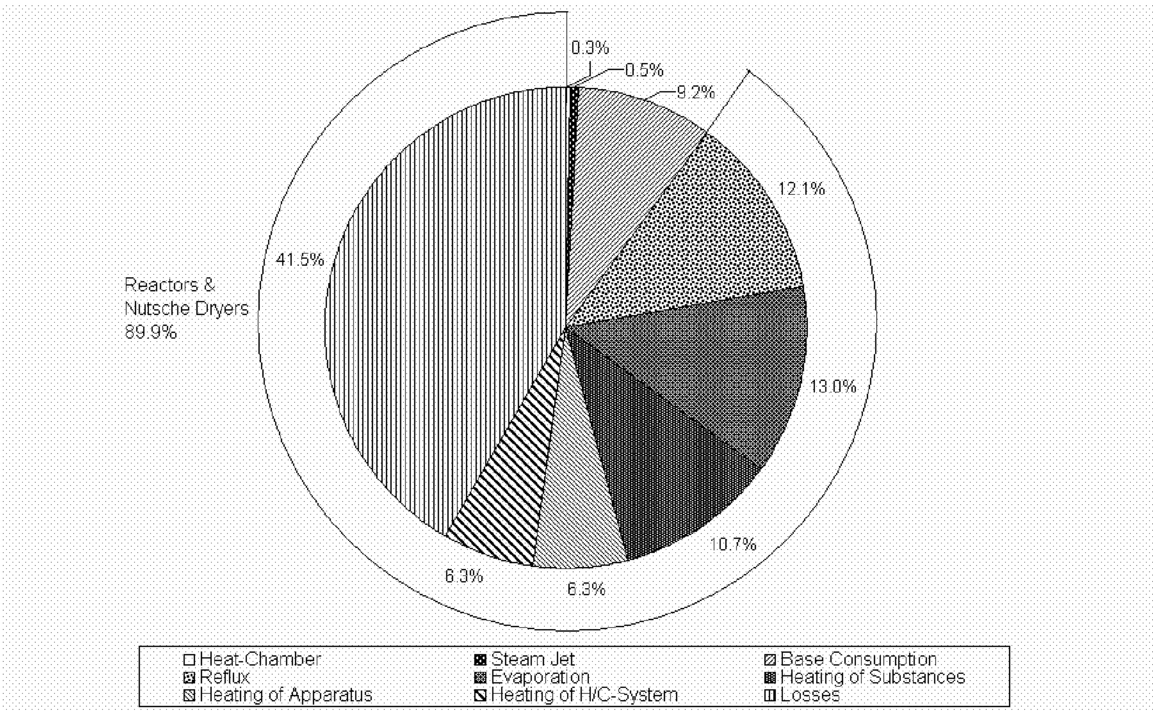


Figure 5-25: Analysis of the total modelled steam consumption of the investigated plant (period: one month; PSP data; total consumption: 1,354 MWh; heat of reaction: -80 MWh, stirrer input: -23 MWh)

Figure 5-26 presents the modelled electricity consumption for the period of one month. The modelling was performed with the help of PSP data. The total consumption of the modelled month is about 315 MWh. As the figure shows, about 50% of total modelled consumption is caused by the building infrastructure (base consumption). This finding corresponds with the findings of the different buildings in Chapter 5.1.3.2. As a rule of thumb, it seems therefore, that about 50% of the electricity consumption of a production building is consumed by the infrastructure equipment. Optimisation and minimisation should therefore start with the building infrastructure. About one third of the total electricity consumption is consumed by the apparatus group *reactors & nutsche dryers* and about one sixth by the vacuum pumps specific to processes. It is therefore essential to switch-off the vacuum pumps if not in use. The largest part of the consumption of the *reactors & nutsche dryers* is consumed by the stirrer motors (during the investigated month). Stirrer motors should therefore be tried to optimise. By reducing the nominal power of the stirrer motors, efficiency of the motors would be improved and electricity consumption would be reduced (see (Bieler 2004) as well).

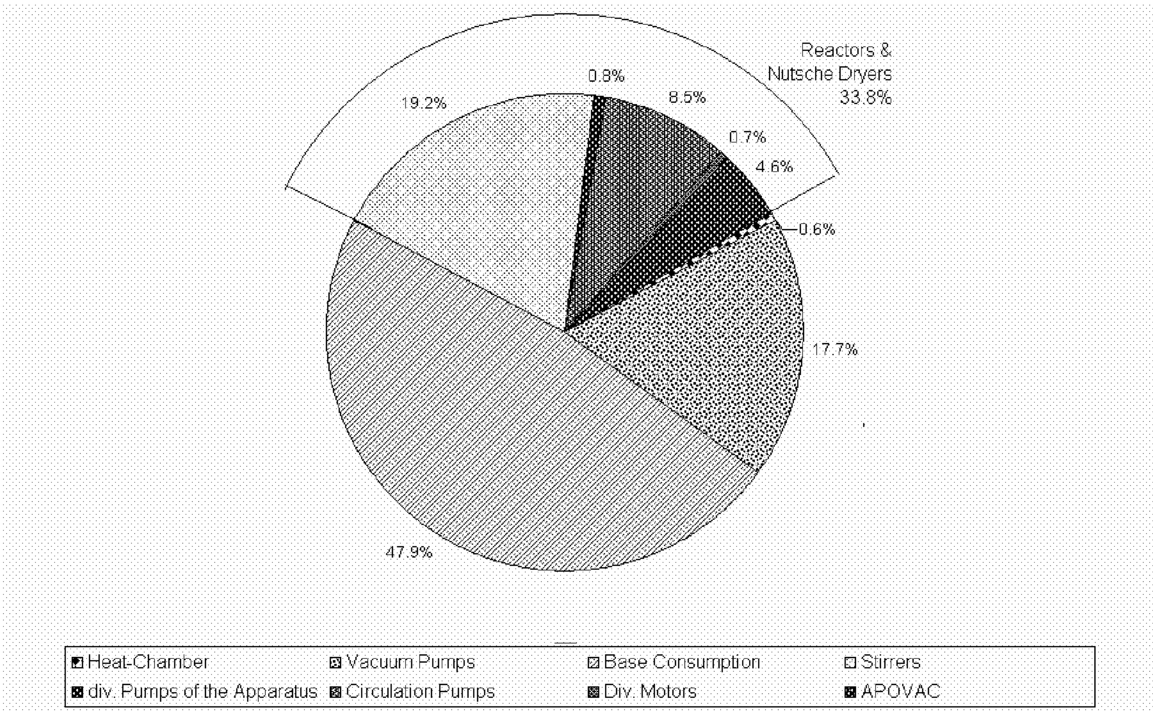


Figure 5-26: Analysis of the total modelled electricity consumption of the investigated plant (period: one month; PSP data; total consumption: 315 MWh)

The total modelled brine consumption for one month of operation of the investigated building is presented in Figure 5-27. The total modelled consumption is about 100 MWh for the investigated month. The model was based on PSP data. It can be seen that the apparatus group *reactors & nutsche dryers* is again responsible for the largest consumption (about 72% of total consumption; or about 80% of total consumption if enthalpy of reaction is included) of brine. As above (see e.g., Figure 5-25), heat of reaction is modelled and listed separately from the apparatus group for reasons of transparency. The hatched fields are once more the energy consumptions not related to and determined by the chemistry. These consumptions (i.e., base consumption, cooling of apparatus, losses and stirrer input) are open for optimisation or minimisation. Together, they are responsible for about 50% of total brine consumption. Therefore, significant reduction potentials in total brine consumption are revealed. The base consumption of the building (i.e., heat input from the main circulation pumps and losses through the walls of the pipes) is responsible for about one sixth of total consumption. This quite significant consumption may be optimised as well. Another main consumer group are the APOVAC pumps. Whether or not these systems really require the use of the low temperatures of the brine or if cooling with water would be sufficient should be challenged in further investigations. Significant savings would be achieved by the optimisation of this apparatus group.

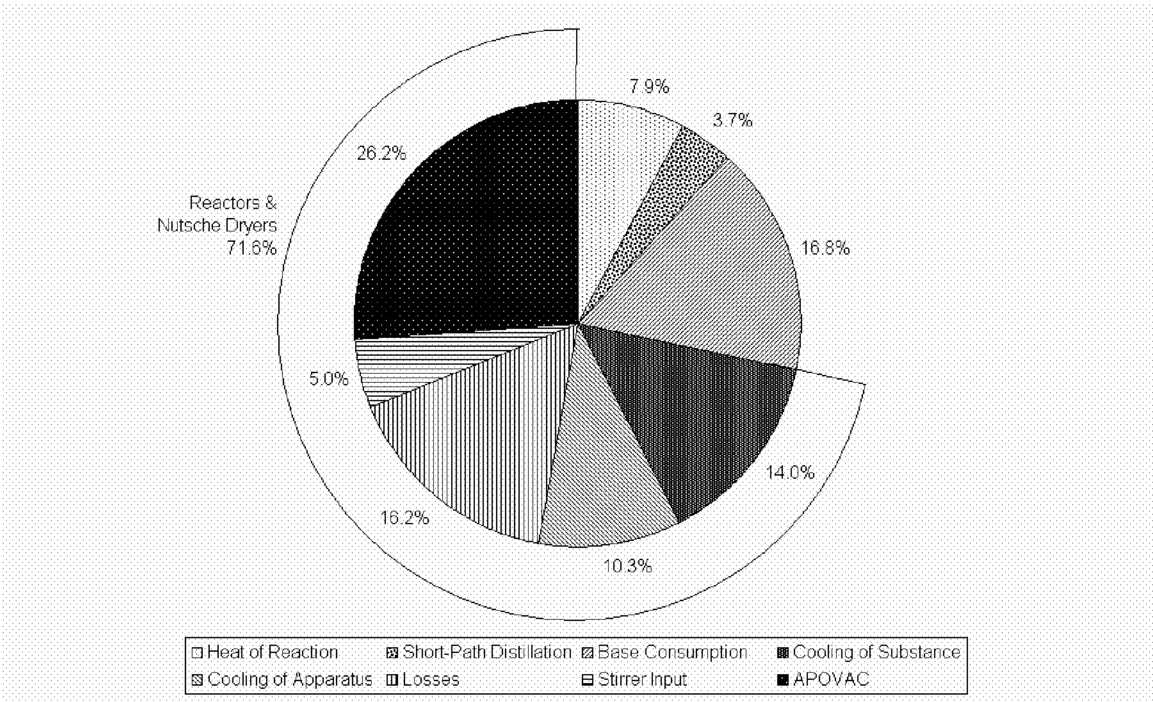


Figure 5-27: Analysis of the total modelled brine consumption of the investigated plant (period: one month; PSP data; total consumption: 100 MWh)

It can be seen from the abovementioned investigations on the total consumption of the different energy carriers, that a detailed analysis of an actual production mix is possible with the help of the BOTUMO. This allows the user to identify specific optimisation potentials. Focus may be put on the sensible unit operations and apparatus groups and energy targets may be set according to the possible savings found in a similar investigation as presented above.

6 Outlook

In future research, both the TODOMO and the BOTUMO should be tested on data of further production plants. Although the TODOMO was applicable to the plants investigated, its general applicability is not yet proven completely. The BOTUMO on the other hand has to be transferred to other production plants. In this study, the model was elaborated, built and tested on the same production plant. The possibility of transferring the SUOM to other plants exists. The models require only the most important product specific data, standard data of the apparatus specifications and the base consumption of the building. The base consumption may be found by measuring the different infrastructure consumers as it was done for this study or by performing a TODOMO on the available data. Since uncertainties would then be high for a multiproduct batch plant with high variability between products and in production mix, the direct measurement should be the method of choice. If apparatus are found in the further investigated production plants for which no SUOM exists, these apparatus have first to be measured and new models, according to the existing ones should be developed. Then modelling with the help of the PSP may be performed and the outcome analysed. Deviations from the measured value could be discussed and analysed according to the analyses in this study. If necessary, the models should be revised or adapted for the new plant or new, generally applicable models may be found.

Since measurement possibilities were limited in the plant investigated (especially the measurements of the brine consumption), additional measurements of unit operations requiring steam, electricity, and brine (with focus on brine) should be performed. These measurements would lead to a broader basis for the parameter values used in the BOTUMO (see Table 5-6). Uncertainties would decrease and modelling results would be more accurate and reliable. In addition, transferability would be improved with these measurements, since variability between more different apparatus of the same kind would be accessed in more detail.

If more accurate and detailed brine measurements would show a significant deviation from the measured values that could not be explained by uncertain parameters or random fluctuations in the outcomes of the model, several facts could be responsible for the deviations. First, the measured equipment should be extended by the safety heat exchangers of the reaction vessels. These heat exchangers help to prevent the solvents from venting in the waste air system. These equipment units could not be measured so far. Their consumption remains unknown until other measurements are introduced. Other minor consumers of brine (e.g., cooling down the washing solvents for filters) could also contribute to total brine consumption. Finally, and least importantly, the lack of simple models for incorporating the enthalpy of crystallisation could be responsible for some part of the deviation. Research should lead to simple, generally usable equations to incorporate the heat of crystallisation in the SUOM.

With the set of apparatus models developed in this study and with future additional apparatus models, investigations could be started how the energy consumption changes for a process, performed in different apparatus. This could mean, for example, to perform the drying of a product either in a nutsche dryer, or a horizontal vacuum rotary dryer, or a spray dryer. The different apparatus would result in different energy consumptions and would reveal the most energy-efficient apparatus for a specific product and unit operation. This would lead to a further application of the model for optimisation of the energy consumption of a batch process or a complete batch production building. The infrastructure, a specific apparatus or a specific energy use aspect (e.g., energy losses) could be checked for possibilities of optimisation. Optimisation in energetic means should be conducted together with optimisation or retrofit of the plant. Energy consumption may not be considered without considering aspects of product quality, plant usage, production schedule and the like. Therefore, incorporating the apparatus models in other programs performing retrofit of production plants could result in a further optimisation possibility and further objective functions for these programs.

It was seen that most of the times, the specific parameter values for the chemicals and products are not available in literature. This drawback was overcome by using the values of similar chemicals or standard values for organic compounds (e.g., a c_P of about 2 kJ / kg / K for generic organic compounds). For making the models usable for a broader range of products, it has to be considered to incorporate models for predicting the required physical values for these products (e.g., the group contribution theory discussed in (Daubert and Dannel 1985; Reid et al. 1987)). Another possibility would be to include data given in manuals (e.g., in (Daubert and Dannel 1984; Lide 1995; TRC 1998; VDI 1984)). This would make application in daily business easier since no physical data would be required from literature.

Similar to the models for brine, electricity and steam, other utilities could be implemented in the BOTUMO. This would increase the applicability of the model, improve the knowledge of the model by daily application and provide the plant manager with a single, simple management tool for challenging the utility consumption of his plant. Standard costs would be calculated more easily and utility requirement planning could be performed more accurate.

It is seen by the use of the Excel® model that the program is useful for a first challenging of the model equations and the BOTUMO itself. The advantage is, that the model may run on most computers available in industry and most people know the basic concepts of Excel® and may therefore be able to use the program. Nevertheless, several drawbacks are related to the use of a spreadsheet program. The equations are open to everybody and links between spreadsheets are easily corrupted by the transfer from one computer to another. Calculation time is a problem as well, since the many OLE-links between different spreadsheets required for the modelling of longer periods (PSP data) with the BOTUMO slow down calculation times significantly. The input of data to the spreadsheet is similar to the written input to the PR sheet. Therefore, data may be easily extracted from the PR data but many data points are required for modelling even short periods. Input of PSP data, on the other hand, requires more investigations and is not too intuitive. Nevertheless, less data is required, since each PSP is only entered once (and afterwards multiplied with the number of batches performed (n_i) according to Equation (3-26)). Since the basic equations of the models are all provided in Chapter 4 of this study, an easier user interface could be programmed that allows a simple input of the data. This would improve acceptability and transferability and would prevent that the base data (i.e., apparatus specifications and base consumptions) would be corrupted by user manipulations. Many of the analysis graphs, made by hand for this study, could be included automatically in the program, therefore making the standard analysis of a plant easier for the user.

The model could be used for modelling the energy consumption of processes only known from laboratory results as well. Incorporation of time calculations according to physical data (e.g., heating dynamics of the apparatus or reaction modelling as discussed in (Fogler 1999; Levenspiel 1999)) could be possible in early phases of reaction engineering. This would provide the Chemical Engineer in the research phase of a project with a first decision tool how to optimise energy consumption of his processes. He would see what effect his optimisation efforts would have on the final process. This would lead to more efficient optimisation and better design in terms of energy.

The measurements showed, that reaction vessels with 15 bar steam had lower loss factors than with 5 bar steam. This could be because the steam traps operate more efficient for higher pressures or because of better insulation or other reasons. Detailed investigations should be performed to find the reason of this fact or to show that it is a random finding related to the inaccuracy of the measurements.

Although this study is mainly focusing on chemical industry, in principle the model is not limited to the chemical industry. The basic concepts could be applied in any multipurpose batch production in industry. This opens doors for a generally accepted methodology for modelling, comparing, and analysing the energy consumption in industry. In today's challenging energy and environmental questions (see Chapters 2 and 3) this could lead to a better understanding of the processes and a focusing on the most promising saving potentials.

7 List of Abbreviations and Symbols

7.1 Abbreviations

APOVAC	Anti POllution VACuum
BOTUMO	BOTtom-Up MOdel
CPM	Company Proprietary Method
F1	Flow meter
F2	Flow meter
M	Month
P1	Pressure meter
PR	Production Record
PSP	Process Step Procedure
SUOM	Single Unit Operation Model
T1	Temperature meter
T2	Temperature meter
TAM	Time Average Model
TODOMO	TOp-DOwn MOdel
TSM	Time Slice Model
W	Week

7.2 Symbols

A	Surface Area	[m^2]
ACR	Air Change Rate	[h^{-1}]
B	Base consumption of energy	[MWh / period]
C	Constant	[div.]
c	Sound velocity	[m / s]
c_P	Heat capacity	[kJ / kg / K]
DD	Degree-Days	[°C · d]
DSS	Day-specific steam consumption	[MWh / °C · d]
E	Energy consumption	[kWh / s]
F	Energy defining factor (0 for electricity, 1 for steam and brine)	[-]
K	Loss coefficient	[kJ / m^2 / s / K]
IT	Temperature of reaction mass	[°C] or [K]
InT	Inlet Temperature	[°C] or [K]
m	Mass	[kg]
OT	Temperature of jacket	[°C] or [K]
OuT	Outlet Temperature	[°C] or [K]
P	Power	[kW]
PO	Production Output	[t / period]
RR	Reflux Ratio	[-]
S	Specific energy consumption	[MWh / t]
SC	Steam consumption	[MWh / period]
SF	Scaling Factor for steam	[kg / kWh]
t	Time	[s / period]
T	Temperature	[K]
ΔH	Enthalpy change	[kJ / kg]
γ	Power consumption of a motor to nominal power	[%]
η	Efficiency	[%]
ρ	Density	[kg / m^3]
ν	Kinematic viscosity	[m^2 / s]

7.3 Indices

1, 2	Start- & Endpoint
A	Apparatus
Air	Air
Am	Ambient
B	Barrel
BC	Batch Column
Br	Brake
C	Crystallisation
Co	Cooling
ES	Evaporated Solvent
El	Electricity
F	Feed
FFE	Falling Film Evaporator
HC	Heat-Chamber
HJ	Heating Jacket
I	Infrastructure
i	Chemicals type (PSP)
j	Apparatus type
k	Number of different specifications of a chemical (PSP)
L	Loss
M	Melting
m	Energy form
N	Nominal
n	Number of different specifications of a apparatus
ND	Nutsche Dryer
O	Operation
P	Production
Pu	Pump
q	Indicator for different process steps / unit operations of one recipe
R	Reaction
RD	Rotary Dryer
RM	Reaction Mass
RV	Reaction Vessel
S	Solvent
So	Solid
SPD	Short Path Distillation column
St	Steam
Su	Suspension
V	Vaporisation
W	Water
Z	Centrifuge

8 Literature

ACS. (1996). "Technology Vision 2020 - The U.S. Chemical Industry.", American Chemical Society, American Institute of Chemical Engineers, Chemical Manufacturers Association, Councin for Chemical Research, Synthetic Organic Chemical Manufacturers Association, Washington.

Aggarwal, S. (2002). "Boost Energy Efficiency in Plant Utilities." *Chem Eng*, 109(4), 70-73.

Allen, D. T., and Shonnard, D. R. (2002). *Green Engineering: Environmentally Conscious Design of Chemical Processes*, Prentice Hall PTR, Upper Saddle River.

Anastas, P. T., and Warner, J. C. (1998). *Green Chemistry: Theory and Practice*, Oxford University Press, Oxford.

Anonymus. (1986). "Where Energy is used." *Energy Management Focus*(9), 4-6.

Anonymus. (2001). "Facts & Figures for the Chemical Industry." *Chem. Eng. News*, 79(26).

Ashton, G. (1993). "Design of Energy Efficient Batch Processes." Energy Efficiency in Process Technology, P. A. Pilavachi, ed., Elsevier Applied Science, London, 1050-1062.

Atkins, P. W. (1990). *Physikalische Chemie*, VCH, Weinheim.

BBC. (1976). "Auswahl und Einsatz von Elektromotoren - Planungsunterlage." *D EM 60001 D*, Brown Boveri Company, Mannheim.

Benz, G. T. (2003). "Optimize Power Consumption in Aerobic Fermenters." *Chem Eng Prog*, 99(5), 32-35.

BFE. (2001a). "Anhang zur Richtlinie über freiwillige Massnahmen zur Reduktion von Energieverbrauch und CO_2-Emissionen." *003693825*, Bundesamt für Energie, Bern.

BFE. (2001b). "Richtlinie über freiwillige Massnahmen zur Reduktion von Energieverbrauch und CO_2-Emissionen.", Bundesamt für Energie, Bern.

BFE. (2002). "Energie- und CO_2-Management schafft Unternehmenswerte." *805.008 d*, Bundesamt für Energie, Bern.

Bhatt, M. S. (2000a). "Energy Audit Case Studies I - Steam Systems." *Appl. Therm. Eng.*, 20, 285-296.

Bhatt, M. S. (2000b). "Energy Audit Case Studies II - Air Conditioning (Cooling) Systems." *Appl. Therm. Eng.*, 20, 297-307.

Bieler, P. S. (2002). "Analyse und Modellierung des Energiebedarfes in Batch-Prozessen." *220185*, ETH Zurich / BFE, Zwischenbericht, Zurich.

Bieler, P. S. (2004). "Analysis and Modelling of the Energy Consumption of Chemical Batch Plants," Ph. D. dissertation, ETH, Zurich.

Bieler, P. S., Fischer, U., and Hungerbühler, K. (2003). "Modelling the Energy Consumption of Chemical Batch Plants - Top-Down Approach." *Ind. Eng. Chem. Res.*, 42, 6135-6144.

Blickenstorfer, C. (1999). "Analyse des Energieverbrauchs eines Mehrprodukte-Batch-Betriebes," Ph.D. dissertation, No. 13411, Zurich, ETH, http://e-collection.ethbib.ethz.ch/cgi-bin/show.pl?type=diss&nr=13411.

Bouhenchir, H., Cabassud, M., Le-Lann, M. V., and Casamatta, G. (2001). "A General Simulation Model and a Heating/Cooling Strategy to Improve Controllability of Batch Reactions." *Trans IChemE Part A*, 79, 641-654.

Burkhardt, P. G. (2002). "Windenergie, CO_2-Abgabe und Erfolgskontrolle." NZZ, Zurich, p. 17, 14.05.2002.

Calderón, Z., Grau, R., Espuña, A., and Puigjaner, L. (2000). "Scheduling of Multiproduct Plants Considering Energy and Waste Costs." *Hung. J. Ind. Chem.*, 28, 31-35.

Dahinden, D. (2003). "Modellierung des Energieverbrauches eines Chemischen Mehrzweckbetriebes," Diploma thesis, Zurich, ETH, 3-906734-34-X.

Daubert, T. E., and Dannel, R. P. (1984). "Data Compilation Tables of Properties of Pure Components.", AIChE Design Institute for Physical Property Data, New York.

Daubert, T. E., and Dannel, R. P. (1985). "Manual for Predicting Chemical Process Design Data.", AIChE Design Institute for Physical Property Data, New York.

Eidgenossenschaft. (1999). "Bundesgesetz über die Reduktion der CO_2-Emissionen." *641.71*, Bern.
Eissen, M., Metzger, J. O., Schmidt, E., and Schneidewind, U. (2002). "10 Years after Rio – Concepts on the Contribution of Chemistry to a Sustainable Development." *Angew. Chem. Int. Ed.*, 41, 414-436.
Ewers, H.-J. (2000). "Alternativen zum Konzept der Bundesregierung." *Gaia*, 9(1), 61-62.
Fogler, S. H. (1999). *Elements of Chemical Reaction Engineering*, Prentice Hall, Upper Saddle River (NJ).
Furman, K. C., and Sahinidis, N. V. (2002). "A Critical Review and Annotated Bibliography for Heat Exchanger Network Synthesis in the 20th Century." *Ind. Eng. Chem. Res.*, 41, 2335-2370.
Ganji, A. R. (1999). "Conducting an Energy Audit." *Chemical Processing*, 62(9), 64-70.
Gränicher, W. H. H. (1997). "Nationaler Energie Forschungs-Fonds NEFF 1997-97.", vdf Hochschulverlag AG, Zurich.
Grant, C. D. (1996). "Energy Management in Chemical Industry." Kirk-Othmer: Encyclopedia of Chemical Technology, J. I. Kroschwitz, ed., John Wiley & Sons, New York, 12-1-12-16.
Gundersen, T. "Achievements and Future Challenges in Industrial Design Applications of Process Systems Engineering." *4th International Symposium on Process Systems Engineering*, Montebello, Quebec, Canada, I.1.1-I.1.32.
Gundersen, T., and Naess, L. (1988). "The Synthesis of Cost Optimal Heat Exchanger Networks: An Industrial Review of the State of the Art." *Comput. Chem. Eng.*, 12(6), 503-530.
Haman, W. G. (2000). "Total Assessment Audits (TAA) in Iowa." *Resources, Conservation and Recycling*, 28(3-4), 185-198.
Höller, V., and Renken, A. (2000). "Neue Konzepte für chemische Prozesse." *CAV*(1), 62ff.
Hoshide, R. K. (1995). "Effective Energy Audits." *Energy Engineering*, 92(6), 6-17.
http://unfccc.int/resource/docs/convkp/kpeng.html. "Kyoto Protocol.", United Nations Framework Convention on Climate Change.
http://www.aie.org.au/melb/material/resource/cop.htm., Australian Institute of Energy.
http://www.eia.doe.gov/neic/infosheets/degreedays.htm. "Energy Information Sheets - Degree Days.", National Energy Information Center (NEIC).
ISA. (1995). "Batch Control Part 1: Models and Terminology." *ISA-S88.01-1995*, ISA, Raleigh, NC.
Jezowski, J. (1994a). "Heat Exchanger Network Grassroot and Retrofit Design. The Review of the State-of-the Art: Part I." *Hung. J. Ind. Chem.*, 22, 279-294.
Jezowski, J. (1994b). "Heat Exchanger Network Grassroot and Retrofit Design. The Review of the State-of-the Art: Part II." *Hung. J. Ind. Chem.*, 22, 295-308.
Jiménez-González, C., and Overcash, M. R. (2000). "Energy Optimization during Early Drug Development and the Relationship with Environmental Burdens." *J Chem Technol Biotechnol*, 75, 983-990.
Kemp, I. C., and Macdonald, E. K. (1988). "Application of Pinch Technology to Separation, Reaction and Batch Processes." Understanding Process Integration II, R. Smith, ed., The Institution of Chemical Engineers, Rugby, UK, 239 - 259.
Kneubühl, F. K. (1994). *Repetitorium der Physik*, B. G. Teubner, Stuttgart.
Krummenacher, P. (1997). "Energetische Integration von Batch-Prozessen." *SI+A*, 38(9), 757-763.
Krummenacher, P., and Favrat, D. (2001). "Indirect and Mixed Direct-Indirect Heat Integration of Batch Processes Based on Pinch Analysis." *Int. J. Applied Thermodynamics*, 4(3), 135-143.
Krummenacher, P., Zogg, M., and Geissmann, M. (2002). "Diskontinuierlich Energie sparen." *ENET-News*(53), 35-36.
Kürsten, M. (1996). "World Energy - A Changing Scene.", E. Schweizerbart'sche Verlagsbuchhandlung, Stuttgart.
Legge, R. (1986). "Chemicals and Energy - An Overview." *Energy Management Focus*(9), 3.

Levenspiel, O. (1999). *Chemical Reaction Engineering*, John Wiley & Sons, New York.
Lide, D. R. (1995). "Handbook of Chemistry and Physics.", CRC Press, London.
Linnhoff, B. (1993). "Pinch Analysis - a State-of the-Art Overview." *Trans IChemE Part A*, 71(6), 503-522.
Linnhoff, B., Ashton, G. J., and Obeng, E. D. A. (1988). "Process Integration of Batch Processes." Understanding Process Integration II, P. R. Crump, D. V. Greenwood, and R. Smith, eds., Institution of Chemical Engineers, Rugby, 221-237.
Linnhoff, B., Townsend, D. W., Boland, D., Hewitt, G. F., Thomas, B. E. A., Guy, A. R., and Marsland, R. H. (1982). *A User Guide on Process Integration for the Efficient Use of Energy*, The Institution of Chemical Engineers, Rugby, UK.
Mersmann, A., Einenkel, W.-D., and Käppel, M. (1975). "Auslegung und Massstabsvergrösserung von Rührapparaten." *Chem Ing Tech*, 47(23), 953-964.
Mujumdar, A. S. (1995). *Handbook of Industrial Drying*, Marcel Dekker, Inc., New York.
Papageorgiou, L. G., Shah, N., and Pantelides, C. C. (1994). "Optimal Scheduling of Heat-Integrated Multipurpose Plants." *Ind. Eng. Chem. Res.*, 33(12), 3168-3186.
Parakrama, R. (1985). "Improving Batch Chemical Processes." *The Chemical Engineer*, 417, 24-25.
Perry, R. H., Green, D. W., and Maloney, J. O. (1997). "Perry's Chemical Engineers' Handbook.", McGraw-Hill, New York.
Phillips, C. H., Lauschke, G., and Peerhoussaini, H. (1997). "Intensification of Batch Chemical Processes by Using Integrated Chemical Reactor Heat Exchangers." *Appl. Therm. Eng.*, 17(8), 809-824.
Rásonyi, P. (2002). "Aufgeschobene amerikanische Klimapolitik." NZZ, Zurich, p. 21, 23.02.2002.
Reid, R. C., Prausnitz, J. M., and Poling, B. E. (1987). *The Properties of Gases and Liquids*, McGraw Hill Inc., New York.
Reklaitis, G. V., Pekny, J., and Jogelekar, G. S. (1997). "Scheduling and Simulation of Batch Processes." Handbook of Batch Process Design, P. N. Sharratt, ed., Chapman & Hall, London, 24-60.
Rippin, D. W. T. (1992). "Batch Process Systems Engineering: A Retrospective and Prospective Review." *Comput. Chem. Eng.*, 17(Supplement), S1-S13.
Robert, H., and Markus, W. (1994). *Organisation und Energiemanagement*, Bundesamt für Konjunkturfragen, Bern.
Rumazo, C. A., Pryor, A., Mendoza, F. O., Villareal, J. C., Robledo, J. M., and Mercado, E. R. (2000). "Cleaner Production in the Chemical Industry." *Water Science and Technology*, 42(5-6), 1-7.
Sahinidis, N. V., Grossmann, I. E., Fornari, R. E., and Chathrathi, M. (1989). "Optimization Model for Long Range Planning in the Chemical Industry." *Comput. Chem. Eng.*, 13(9), 1049-1063.
Schalcher, M., Battaglia, U., and Bush, E. (2003a). "Energieverbrauch von Prozesssteuerungen (SPS)." *46 963*, Schlussbericht, Bundesamt für Energie (BFE), Bern.
Schalcher, M., Battaglia, U., and Bush, E. (2003b). "Projekt Energieverbrauch von Prozesssteuerungen." *46 963 / 87 079*, Jahresbericht, BFE, Chur.
Severson, D. S. "Benchmarking Process Energy Performance from Historical Data." *Eighteenth National Industrial Energy Technology Conference*, Huston, Texas, 87-91.
SIA. (1992). "Kühlleistungsbedarf von Gebäuden - SIA 382/2." *SIA 382/2*, SIA, Zurich.
SIA. (1995). "Elektrische Energie im Hochbau - SIA 380/4." *SIA 380/4*, SIA, Zurich.
SIA. (1997). "Energie im Hochbau - SIA 380/1." *SIA 380/1*, SIA, Zurich.
Stahel, W. A. (1995). *Statistische Datenanalyse; Eine Einführung für Naturwissenschaftler*, Friedrich Vieweg & Sohn, Wiesbaden a.o.
Stankeiwicz, A. I., and Moulijn, J. A. (2000). "Process Intensification: Transforming Chemical Engineering." *Chem Eng Prog*, 96(1), 22-34.
Stitt, E. H. (2002). "Alternative Multiphase Reactors for Fine Chemicals - A World Beyond Stirred Tanks?" *Chem. Eng. J.*, 90, 47-60.

Stoltze, S., Mikkelsen, J., Lorentzen, B., Petersen, P. M., and Qvale, B. (1995). "Waste-Heat Recovery in Batch Processes Using Heat Storage." *Journal of Energy Resources Technology; Transactions of the ASME*, 117(2), 142-149.

Suhami, I., and Mah, R. S. H. (1982). "Optimal Design of Multipurpose Batch Plants." *Ind. Eng. Chem. Process Des. Dev.*, 21(1), 94-100.

Sulzer, M. (2003). "Gute Gebäudetechnik - oder Die unendliche Uneinigkeit der Ingenieure!", Report, BFE.

Thöne, E., and Fahl, U. (1998). "Energiewirtschaftliche Gesamtsituation." *Brennstoff-Wärme-Kraft*, 50(4), 26-38.

Thumann, A. (1983). *Handbook of Energy Audits*, The Fairmont Press, Inc., Atlanta, Georgia.

TRC. (1998). "TRC Thermodynamic Tables.", Thermodynamics Research Center, College Station, Texas.

Turner, W. C. (1982). "Energy Management Handbook.", John Wiley & Sons, New York.

Vaklieva-Bancheva, N., Ivanov, B. B., Shah, N., and Pantelides, C. C. (1996). "Heat Exchanger Network Design for Multipurpose Batch Plants." *Comput. Chem. Eng.*, 20(8), 989-1001.

Vaselenak, J. A., Grossmann, I. E., and Westerberg, A. W. (1986). "Heat Integration in Batch Processing." *Ind. Eng. Chem. Process Des. Dev.*, 25(2), 357-366.

Vaselenak, J. A., Grossmann, I. E., and Westerberg, A. W. (1987). "An Embedding Formulation for the Optimal Scheduling and Design of Multipurpose Batch Plants." *Ind. Eng. Chem. Res.*, 26(1), 139-148.

VDI. (1984). *VDI-Wärmeatlas*, VDI-Verlag GmbH, Düsseldorf.

Verwater-Lukszo, Z. (1996). "A Practical Approach to Recipe Improvement and Optimization in the Batch Processing Industry," Ph.D. dissertation, Technical University of Eindhoven, Eindhoven.

Villermaux, J. (1995). "Future Challenges in Chemical Engineering Research." *Trans IChemE Part A*, 73, 105-109.

Vin, J. P., and Ierapetritou, M. G. (2000). "A New Approach for Efficient Rescheduling of Multiproduct Batch Plants." *Ind. Eng. Chem. Res.*, 39(11), 4228-4238.

Vose, D. (1996). *Quantitative Risk Analysis: A Guide to Monte Carlo Simulation Modelling*, John Wiley & Sons, New York.

Wang, S. K. (2000). "Handbook of Air Conditioning and Refrigeration.", McGraw-Hill, New York.

Wang, Y., and Feng, X. (2000). "Exergy Analysis Involving Resource Utilization and Environmental Influence." *Comput. Chem. Eng.*, 24, 1243-1246.

Wedler, G. (1987). *Lehrbuch der Physikalischen Chemie*, VCH, Weinheim.

Worrell, E., Price, L., and Ruth, M. (2001). "Policy Modeling for Energy Efficiency Improvement in US Industry." *Annu. Rev. Energy Environ.*, 26, 117-143.

Würsten, F. (2003). "Es braucht grosse Anstrengungen." *ETH Life*, http://www.ethlife.ethz.ch/articles/.

Zalba, B., Marín, J. M., Cabeza, L. F., and Mehling, H. (2003). "Review on Thermal Energy Storage with Phase Change: Materials, Heat Transfer Analysis and Applications." *Appl. Therm. Eng.*, 23, 251-283.

Zhao, X. G., O'Neill, B. K., Roach, J. R., and Wood, R. M. (1998). "Heat Integration for Batch Processes: Part 2: Heat Exchanger Network Design." *Trans IChemE Part A*, 76, 700-710.