SYNTHESIS OF ENERGY INTENSIVE INDUSTRIAL PROCESSES: METHODOLOGICAL ASPECTS AND A CASE STUDY OF A SUGAR CANE CONVERSION PLANT

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a Lise e
ai miei genitori
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Abstract

The topic of the present work is the synthesis of energy intensive industrial processes. The aims are to discuss methodologies already reported in the literature and to propose a new organized procedure for the generation and modification of system alternatives. The synthesis problem consists in the definition of the type and number of system components, their material connections and their operating parameters. The synthesis procedure proposed here starts with the definition of a Basic Plant Configuration which is the schematic representation of an original idea of the plant comprising all the components responsible for the chemical and mechanical transformations of the raw materials. Accordingly, the Heat Exchanger Network responsible for the heat transfer between system cold and hot streams is not comprised in the Basic Plant Configuration and the heat transfer feasibility is verified by using Pinch Analysis rules. This is also the approach of many studies published in the literature in the field of process integration, some of which are presented in Chapter 2. In the same chapter the synthesis of CHP systems is also addressed. This subproblem of the total site synthesis problem may be solved following different systematic procedures proposed in the literature. CHP systems are in fact a cost-effective way to locally satisfy the demand of productive processes for external heat and electricity provided that they are optimally sized. This can be done by applying computer-aided optimization procedures. A particular attention is given in this work to the formulation of the synthesis of steam networks, as a mixed-integer linear programming optimization of steam network superstructures. This and other methods proposed in the literature for the synthesis of energy systems are compared highlighting potentials, weaknesses and possible common criteria. The synthesis of a sugarcane conversion plant is studied in Chapters 3 and 4. In particular, in Chapter 3, the organized procedure for the generation and modification of process alternatives is applied and the process configurations for production of sugar and ethanol, also in combined mode, are discussed. Each plant configuration is optimized in order to minimize the process thermal demand. Main structural and operating parameters subject to optimization are those of the multi-effect evaporator and of the ethanol distillation subsystems. In Chapter 4 the synthesis of a bagasse fueled CHP system is studied and the potential for net electricity production to be sold to the market evaluated considering two options for the conversion of bagasse: combustion and gasification. The process for the combined production of sugar and ethanol and the CHP system are optimized simultaneously. In particular a two level optimization procedure is applied in this case. According to this procedure the structure and mass flow rates of the steam network are optimized in an inner step where the heat transfer feasibility is set as a constraint according to the Pinch Analysis rules. In an outer optimization step instead all the intensive parameters are optimized by means of a genetic algorithm based optimizer.
Sommario

L’argomento del presente lavoro è la sintesi degli impianti industriali ad alta intensità energetica. Gli obiettivi sono quello di discutere le metodologie già documentate in letteratura e di proporre una nuova procedura organizzata per la generazione e la modifica delle alternative di sistema. Il problema di sintesi consiste nella definizione del tipo e del numero di componenti di un sistema, le loro connessioni materiali e i loro parametri di funzionamento. La procedura di sintesi qui proposta inizia con la definizione di una Basic Plant Configuration la quale consiste nella rappresentazione schematica di un’idea originale del sistema, comprendente tutte i componenti responsabili delle trasformazioni chimiche e meccaniche delle materie prime. La rete degli scambiatori di calore responsabile per il trasferimento di calore tra i flussi freddi e caldi del sistema non risulta pertanto compresa nella Basic Plant Configuration e la fattibilità fisica dello scambio termico è verificata applicando le regole della Pinch Analysis. Questo è anche l’approccio di molti studi pubblicati in letteratura in materia di process integration, alcuni dei quali sono presentati nel Capitolo 2. Nello stesso capitolo si affronta il problema della sintesi dei sistemi di cogenerazione. Questo sottoproblema del problema di sintesi del sito industriale totale può essere risolto seguendo diverse procedure sistematiche proposte in letteratura. I sistemi di cogenerazione sono in realtà un modo economicamente efficace per soddisfare localmente la domanda dei processi produttivi di calore e di elettricità a condizione che siano ottimalmente dimensionati. Ciò può essere fatto applicando delle procedure di ottimizzazione che fanno uso di calcolatore. Una particolare attenzione viene data in questo lavoro alla formulazione della sintesi delle reti di vapore come un problema di programmazione mista intera lineare di un sovrastruttura di rete di vapore. Questo e altri metodi proposti in letteratura per la sintesi di sistemi energetici vengono confrontati evidenziando potenzialità, debolezze e possibili criteri comuni. La sintesi di un impianto di trasformazione della canna da zucchero è studiato nei Capitoli 3 e 4. In particolare, nel Capitolo 3, si applica la procedura organizzata per la generazione e la modifica di alternative processo e si discutono le configurazioni di processo per la produzione di zucchero ed etanolo anche in modalità combinata. Ogni configurazione dell’impianto è ottimizzata al fine di ridurre al minimo la richiesta termica del processo. I principali parametri strutturali e di design soggetti all’ottimizzazione sono quelli del evaporatore multi effetto e del sottoprocesso di distillazione dell’etanolo. Nel capitolo 4 si studia la sintesi di un sistema di cogenerazione alimentato con il sottoprodotto bagassa e si valuta il potenziale di produzione di energia elettrica netta da vendere ad un eventuale mercato elettrico considerando due opzioni per la conversione della bagassa: combustione e gassificazione. Il processo per la produzione combinata di zucchero e di etanolo e il sistema di cogenerazione sono ottimizzati simultaneamente. In particolare una procedura di ottimizzazione a due livelli viene applicata in questo caso. Secondo questa procedura la struttura e la portate di massa della rete di vapore sono ottimizzate in un’iterazione interna, dove la fattibilità fisica dello scambio termico è fissata come vincolo secondo le regole della Pinch Analysis. In un’iterazione esterna di ottimizzazione invece tutti i parametri intensivi sono ottimizzati per mezzo di un ottimizzatore basato su un algoritmo genetico.
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Chapter 1

Introduction

The conceptual design of an industrial process consists in the definition of a sequence of components transforming given raw materials into one or more useful products which can be profitably sold to a market. The production activity must in addition obey some social and environmental constraints.

In a preliminary step the designer is asked to find the optimum process in terms of structure, type, number of components and their operational parameters, along with the raw materials and utilities (external services) necessary to operate the process (e.g. electricity, heat, water, etc.). This is also addressed as a synthesis problem.

Typically, the designer can rely on the fact that some technological processes, which can be considered as predefined structures of an industrial plant, have already been discovered and have reached a high degree of reliability. Starting from a first design concept, the designer subsequently looks for process improvements by adjusting the process structure and operating parameters.

Even if the ultimate objective of process improvement is usually the maximization of process profitability, different are in general the aspects in which the attention of the designer can focus. Some general directions for improving the design of an industrial site are:

- Increase the production of useful products: identify new products that can be produced starting from the same raw materials or/and maximize production rates by choosing components with high performance.
- Investigate possible internal use of by-products.
- Reduce utilities consumptions: electricity and heat demands can be reduced with high process integration and by means of new technologies with lower energy consumption.

In this work the attention is drawn to the procedures for the synthesis of industrial plants in which significant improvement in profitability can be obtained by maximizing process energy efficiency, in particular by improving the heat and power integration between system components. This was the object of study of large body of literature especially in chemical process synthesis. A great contribution in this field is the work by Linnhoff on Pinch Analysis [84].

The productive processes characterized by continuous transformations involving multiple energy and material streams entering and exiting process components may in particular benefit from high process integration. This type of productive plants is also addressed as the “process” industry. The sizes of the plants belonging to this first category and the relatively constant and inflexible operation usually justify highly integrated configurations. Conversely, those plants commonly grouped under the “manufacturing” industry set typically feature intermittent transformations in which pieces of material are modified till they reach given product requirements, that is by means of batch processes. As a consequence thermal streams connected to the different batch operations, if any, are not equally distributed over the whole working time of the plant and integration opportunities are much more limited. Although the discussion focuses here on the synthesis of continuous and steady state processes, the same methodology could be extended to batch processes by using a multi-period formulation. A large body of literature is dedicated
to the application of process integration techniques to batch processes and multi-period problems. Some examples are [8, 92]. In addition, an important part of the so-called “manufacturing” industries present a layout in which different machines operate with mechanical transformations on the raw materials therefore showing a need for electricity or mechanical work (high-quality energy) rather than heat (low-quality energy). In these cases it is common to talk about process integration while referring to an extensive introduction of computer aided machinery or automation from which indeed the major benefits in process profitability can be drawn.

Conversely, process integration, in particular in chemical processes, is more related to the possibility of increasing productivity by matching heating and cooling needs between components and by recirculating material streams between components increasing chemical conversion performances. These procedures are also directly linked to the minimization of waste treatment or waste disposal. The interest for reusing by-products is becoming one of the key factors for a better plant economy also in the light of newly addressed environmental issues. In a more wide sense the use of waste-heat for power generation is another example. In addition to the contribution by Linnhoff, many papers in the literatures discuss the application of process integration techniques and their benefit in process economy and environmental impact also when dealing with multiple industrial sites [2, 45, 69, 72].

The improvement in the design of an industrial process is commonly obtained by applying heuristics or by taking advantage of the expertise of an engineering community. For instance, an interesting overview of guidelines for chemical process synthesis is reported in a recent book by Turton et al. [131]. However, a significant step forward in the systematic definition of structure and parameters of industrial processes can be achieved by using computer aided optimization procedures. A general discussion about this topic is found in [68] and [133]. The research in computer-aided optimization applied to industrial process design has been documented in a large body of literature, among which some famous examples are the works by Stoecker and Floudas [34, 127].

The change in process configuration, in terms of structure (number, type of components and their connections) and in terms of design parameters, affects in general both quality and quantity of the useful products and of the demand of external energy (utilities demand). When dealing with the design of an industrial plant, the utility system required to support plant operations is considered at the boundaries of the core of the industrial site consisting of the production facilities. Accordingly, the productive process is designed firstly and the utility system is designed in order to meet the process requirements. Another possible way to look at the synthesis problem of an industrial site is to consider the process and the utility system as parts to be optimized simultaneously.

In parallel it is possible to distinguish between two problems in the synthesis of an industrial process (for fixed input of raw material): 1. the definition of the structure and design parameters of the process components for obtaining maximum quality and quantity of products; 2. the design of the process and utility system leading to minimum consumption of primary energy for fixed quality and quantity of products. The second of these two different approaches, which are complementary to each other, is considered in this work.

In the literature the problem of the synthesis of the productive process is often separated from the problem of the synthesis of the set of components (e.g. the Heat Exchanger Network) which are entitled to integrate the energy demand and availability between main system components and to distribute energy (heat and electricity) from external utilities (e.g. fuel combustion) to the process by means of energy conversion technologies (e.g. through a Steam Network). An important step forward in the solution of this second synthesis subproblem was introduced by Linnhoff with the so called Pinch Technology [67, 84].

The problem of the systematic synthesis of basic components of energy intensive industrial processes (especially chemical processes) was the object of several works in the past decades. As an example we remember here the problem of the synthesis of distillation column networks in refineries which is quite challenging from the point of view of process structural alternatives [116]. A great effort in the mathematical formulation of the synthesis of a general process was made by Friedler. According to the approach introduced by Friedler, which is based on the graph theory, a general process is codified as a network of components (knots) linked by material and energy streams (edges) [39, 38, 54]. Another typical approach for process synthesis is to start with a superstructure including all possible components so that
the optimal process configuration is found as an outcome of mixed-integer programming optimization. Among others the contributions by Grossmann and Kravanja were significant in this field [60, 73, 141]. In the field of synthesis of energy system an interesting review on the methods for the design and synthesis optimization can be found in [37]. Among several works, interesting examples of advanced optimization procedure for the synthesis of energy system can be found in [24, 86, 48].

In parallel, a large body of literature has been dedicated to the synthesis of heat exchanger networks (HENs) and to the synthesis of optimal utility systems (where the productive process is instead considered as a fixed entity). In addition to the already mentioned contribution of the Pinch Technology (in particular the Pinch Analysis), different techniques were proposed in the past for the cost-effective synthesis of HENs. An elegant approach for the solution of this type of problems was suggested by Yee, Grossmann and Kravanja in a series of three papers [140]. This is based on a MINLP optimization of a pre-defined HEN superstructure. Recently, a one-step MILP algorithm was instead proposed by Barbaro et al. in [7]. Another procedure for the HEN synthesis based on properties of graphs was recently developed by Toffolo [128]. This method suggests to separate the optimization of the HEN topology (handled by a genetic algorithm) from the optimization of heat loads distribution (handled by a NLP deterministic algorithm).

### 1.1 Aims

The present work aims at discussing methodologies already documented in the literature and at proposing a new procedure for the synthesis of industrial processes with high heat and power requirements. This procedure is based on the organized generation and modification of plant configurations which have in common the same input of raw material(s). Each plant configuration must be subsequently optimized. The objective followed here is the process energy efficiency and for this purpose Pinch Analysis tools are used to evaluate minimum process demand of external energy and also to estimate opportunities for further modifications of plant configurations. Part of the work focuses therefore on the discussion of different strategies reported in the literature for design optimization underlying potentials, weaknesses and possible interactions. A case study of a sugarcane conversion plant is used to practically present the proposed synthesis procedure and to discuss how subproblems can also be solved by using more than one synthesis strategy. The plant configurations that are explored in this work are those for sugar production, for ethanol production and for combined production of sugar and ethanol. The additional use of bagasse for combined heat and power generation is also considered. The synthesis of the industrial site comprising the productive process and the CHP system is also called the total site problem.

Starting from an original idea of the process it is possible to define a general scheme of the plant corresponding to a given sequence of basic subprocesses. The issue is then to select the parameters and the actual structure of basic subprocesses. Once the idea of the process is fixed, it is possible to distinguish between two synthesis approaches corresponding to two different but complementary objectives. The focus can be either on the production of the maximum quantity and quality of desired product(s) from given raw materials (where the process energy demand is not taken into account), or on the optimal selection of components of the productive process and of the utility system and their optimal parameters that allow to reduce the process energy consumption while keeping constant the production rates of desired products. This second approach is considered in this work. All problems raised while designing an industrial process, like for instance which are the best components in the market and which is the best layout for the plant in order to achieve maximum profitability are not exhaustively discussed here. Conversely the aim is to present a methodology for identifying the best design options from an energy perspective.

Accordingly, the attention is drawn to the generation of process alternatives starting from the same type and amount of raw material and subsequently to the modification and optimization of the process structure following the objective of process energy efficiency. Plant configurations are modified following an organized procedure consisting in component staging, addition or change in material connections between components, addition or change of components. For a given plant configuration the so-called HEATSEP method is applied which consists in virtually cutting the thermal links between subsequent
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components and then including all the independent end-temperatures and mass flow rates within the set of
decision variables to optimize following the objective of minimum process thermal demand. Accordingly,
all the thermal streams are not matched in a pre-defined heat exchanger network and the heat transfer
feasibility is checked by means of Pinch Analysis rules. In order to better evaluate the heat integration
opportunities of a process, Pinch Analysis provides a set of graphical tools, the so-called composite
curves, which helps identify further process modification for the reduction of external utility demand.

This synthesis procedure is in particular applied in the present work to the case study of the sug-
arcane conversion plant. Starting from the same sugarcane input the plant configurations involving the
production of sugar and ethanol are explored. Many process design parameters are kept fixed in order
to keep constant the production rates of the product(s) for a given plant configuration. The structural
and operating parameters that are instead not specifically dictated by process requirements, and which
instead govern the heat loads and temperature levels of process thermal streams, are optimized. Part-
cicular attention is therefore drawn to the optimization of the pressure and concentration levels of the
multi-effect evaporator and of the ethanol distillation subprocess.

A large quantity of fiber called bagasse is discarded as by-product of the sugar and ethanol production
process. The chemical energy content of this by-product is large enough to balance the process energy
requirement. So the option of using bagasse for this purpose is also considered in this work.

Due to the size of some industrial process and their simultaneous needs for heat and electricity,
combined heat and power (CHP) systems may result a cost-effective solution for covering the process
energy requirement. This is usually easy to prove just by comparing the lower overall efficiency of the
separate production/consumption of electricity and heat with respect to the combined system.

Assuming that the value of a fuel is proportional to its exergy content (that is the potential for work
 generation), the use of fuel for heating purposes has a very low efficiency since usually the demand for
heat is at low temperature and a great part of exergy is lost within the boiler. The same heat requirement
can be satisfied in most cases with low grade heat for instance with a steam network delivering the heat
at various temperature levels with different pressure steam-lines. Nevertheless the exergetic efficiency
of the heating process does not change since the steam-line is nothing but an intermediate exchange
between the fuel combustion and the low-temperature heat sink and the centralized boiler producing low
pressure steam is still responsible for high exergy losses.

The high chemical exergy content of fuels can be used in a more efficient (i.e. cost effective) way by
converting it in useful work (in general electricity) and using only part of its exergy content for heating
purposes. This can be done by producing for instance high-pressure steam to be expanded in steam
turbines. Low pressure steam can be drawn from medium or low pressure turbine stages or directly from
the outlet of the turbine and then used for heating purposes. The utility system consists in this case in
a combined heat and power plant.

Thus, the option of using bagasse for combined heat and power is considered in the present work and
the total site problem is eventually addressed in which the objective followed is the maximum net power
production of while covering the process heat and power requirements. Even though the procedure for
the generation and modification of different system alternatives could be considered also for the synthesis
of the bagasse conversion subsystem, only two plant configurations are considered while the productive
process for combined sugar and ethanol production is considered fixed. These are the bagasse-fueled
steam cycle and the bagasse integrated gasification combined cycle. A synthesis subproblem involving
the definition of the steam network is considered. For this purpose a procedure for structural and
operating parameters optimization based on the definition of a steam network superstructure is used and
a two-level optimization procedure employed. In particular the same approach proposed by Marechal
et al., which implements Pinch Analysis rules introduced by Linnhoff [84] and integrates them with the
approach proposed by Grossmann for the synthesis of utility systems [50], is used.

As a consequence, a considerable part of the present work focuses on methodologies for the synthesis
of combined heat and power system. Since this type of systems can be considered within the set of power
generating plants based on thermal conversion processes, a part of the discussion in Chapter 2 focuses
on the comparison between different methodologies for the synthesis of energy systems highlighting po-
tentials and limitations.
The manuscript is basically divided into two parts. In Chapter 2, main methodological aspects are presented. These comprise an overview of Pinch Analysis tools, a discussion about the synthesis of steam networks, a general overview on methodologies on synthesis of power generating plants and finally the description of the organized procedure for the generation and modification of system structural alternatives. In this first chapter, two optimization procedures are basically presented and compared: the HEATSEP method (based on the definition of system basic plant configurations) and the two-level optimization procedure (based on the definition of system superstructures).

In Chapter 3 and 4, the synthesis of the sugarcane conversion plant is discussed. In particular, in Chapter 3 the organized procedure for the generation and modification of plant configuration is used for the synthesis of the sugarcane conversion plant for sugar, ethanol and combined and ethanol production. In this chapter, the HEATSEP method is used for the optimization of process parameters following the objective of minimum process energy demand. In Chapter 4, the synthesis of the total site configuration including the bagasse conversion subsystem is presented considering two alternatives: bagasse combustion and bagasse gasification. In this chapter, the two-level optimization procedure is considered.

Conclusions are drawn in Chapter 5 with particular reference to methodological aspects and to further directions of future research.
Chapter 2

Process integration and synthesis of energy systems

2.1 Pinch Analysis

In the field of process integration, heat and power integration techniques can play an important role in reducing the bill for external energy consumption of a boiler.

The basic idea at the basis of heat and power integration is to match the demand and availability of energy between subprocesses. The common case in fact is that of reducing the demand of external heat to be provided by combustion of fuel.

Different techniques were developed in the past for the design of the heat exchanger network (HEN) that maximizes internal heat recovery and possibly with minimum additional investment costs. Among others, the work by Linnhoff et al. on Pinch Analysis is important for the definition of a simple and effective methodology for heat and power integration [67, 84].

At the basis of the Pinch Analysis there is the need for the reduction of the heat requirement of a process in which material streams needs to be heated up (the set of the cold streams) and other material streams need to be cooled down (the set of hot streams).

2.1.1 The graphical interpretation of the heat integration problem

In absence of heat integration, the set of cold streams define a heating requirement and the set of hot streams a cooling requirement. These heating and cooling demands are equal to the summation of the respective thermal loads and need to be covered by external utilities (hot utility and cold utility). Thus the idea is to verify if part or the whole heating requirement can be covered by cooling some or all the hot streams of the process.

In Figure 2.1 the heat integration procedure as proposed by the Pinch Analysis is shown. The set of hot and cold streams are grouped into two poly-lines (blue for the cold streams and red for the hot streams) the so-called hot and cold composite curves. These are the basic graphical objects that give a straightforward representation of the heat integration opportunities between the cold and hot streams of a process. Composite curves are built by summing thermal capacities of all thermal streams appearing in each temperature interval and multiplying the composite thermal capacities by the temperature difference delimiting each interval (i.e. resulting in polylines in the temperature-heat load graph).

The horizontal extent of a composite corresponds to the sum of the heat loads (cold or hot) while the vertical extent gives the total range of temperatures in which process thermal streams are found.

If now the two curves are considered as the hot and cold part of a single theoretical heat exchanger, the hot composite curve can transfer heat only if in each point its temperature is higher than the that of the cold composite curve as shown on the right of Figure 2.1.

The amount of heat that can be potentially recovered by thermal integration is equal to that part of the hot composite curve that is superimposed onto the cold composite curve. Thus, starting from the
Figure 2.1: The graphical interpretation of the thermal integration as proposed by the Pinch Analysis

Without integration

With integration

SEPARATE HEAT AND COOLING CURVES

HEAT RECOVERY

Pinch Point

NEED FOR HEATING

NEED FOR COOLING

Temperature

Heat load

Temperature

Heat load

Figure 2.1: The graphical interpretation of the thermal integration as proposed by the Pinch Analysis

separate hot and cold composite curve, the heat integration potential can be graphically estimated by moving (horizontally) one composite curve as close to the other one as possible.

The heat transfer feasibility between cold and hot streams is in fact ensured until the two curves do not touch each other. This is the local condition in which the cold composite curve has the same temperature of the hot composite curve and theoretically corresponds to the condition in which heat is transferred through an infinite heat transfer surface.

As shown in Figure 2.1, the point (temperature level) in which the hot composite curve is at its minimum vertical distance from the cold composite curve is also called the process pinch point.

At the right side of this point the overall process acts as an heat sink, meaning that the heat demand imposed by the cold streams is greater than (or equal to) the cooling demand imposed by the hot streams. Conversely, on the left side of the pinch point the process acts as an heat source since the heat rejected by the hot streams is greater than (or equal to) the heat demand required by the cold streams.

This is the so-called MER condition (Maximum Energy Recovery) and reflects the fact that there is a maximum amount of heat that can be recovered by internal heat transfer within the system between cold and hot streams. In other words there is a minimum amount of heat that needs to be provided by an external source, called MER-hot utility, and a minimum amount of heat that needs to be rejected to an external sink, called MER-cold utility.

According to the Pinch Analysis the evaluation of the MER condition, (i.e. the maximum heat recovery), is done by solving the so-called problem table. This separates the heat integration problem into subproblems each related to a temperature interval. Temperature intervals are found by sorting (either in ascent or descent mode) the vectors of temperatures (inlet temperatures and outlet temperatures) of all the thermal streams that are included within the set of streams to be integrated. For each temperature interval the heat integration problem is ruled by Equation (2.1) which gives the thermal balance of the $u$ temperature interval.

$$R^u = \sum_{h=1}^{H^u} Q_h - \sum_{c=1}^{C^u} Q_c + R^{u-1}$$  \hspace{1cm} (2.1)

For given $U$ temperature intervals sorted descendingly so that the first interval ($u = 1$) is that at the highest temperatures, the cumulative heat load $R^u$ of the $u$ interval is obtained by adding the $Q_h$ heat
loads of all the $H^u$ hot streams and the $Q_c$ heat loads of all the $C^u$ cold streams operating at that interval plus the result of the thermal balance $R^{u-1}$ of the previous temperature interval $(u - 1)$ in the heat cascade. This last term of the equation derives from the intrinsic nature of the heat cascade problem that is the possibility for the heat to be transferred from higher temperature intervals towards the lower temperature intervals.

At the beginning of the procedure for the evaluation of the heat integration potential, the assumption is that there is no heat provided by an external heat source. This corresponds to writing Equation (2.1) for the first temperature interval $(u = 1)$ in the heat cascade and set $R^{u-1}$ equal to 0. In this way Equation (2.1) also gives for each temperature interval of the cascade, the relative horizontal distance between the cold and hot composite curves (at the knots separating the segments of each composite curve).

The heat transfer feasibility constrains the result of the thermal balance to be positive as expressed in Equation (2.2).

$$\forall \ u \in [1; U] \quad R^u \geq 0 \quad (2.2)$$

As a consequence of the assumption of no external heat source, this constraint can be either verified (leading to the so-called threshold condition) or not. The cases in which at the first attempt (that is for $R^0 = 0$) some of the $R^u$ cumulative heat loads are not positive are more frequent. In these cases, to ensure the feasibility of the heat transfer for a given $u$ temperature interval, it is sufficient to introduce an equivalent heat load at the first level of the cascade thus ensuring that $R^u = 0$. The heat cascade problem is completely solved when the heat transfer feasibility is guaranteed (by increasing the hot utility of that amount compensating the heat deficit of a temperature interval) for all the temperature intervals in the cascade. To avoid iterations, a straightforward procedure consists in evaluating Equation (2.1) for all the intervals, then find the maximum negative gap and add an equivalent heat load at the first level of the cascade $(R^0 \geq 0)$.

Eventually $R_0$ corresponds to the MER-hot utility $(R^0_{MER})$ that an utility thermal stream needs to provide to the process. In addition, the temperature level in which the condition $R^u = 0$ is verified gives the location of the pinch point in the heat cascade.

If instead of adding $R^0_{MER}$ to the first interval a greater amount of hot utility is considered, the extra heat $(R^0 - R^0_{MER})$ would create an excess of heat at the process pinch point. Accordingly, this excess of heat has to “pass through” the pinch point and be rejected to the cold utility. This translates into the general practical rule according to which, if the hot utility exceeds the MER amount, it causes an increase in cold utility thus leading to unjustified increase in process operating costs.

The ideal condition for the minimum MER (maximum theoretical internal heat recovery) is obtained when at the pinch point the hot composite curve has the same temperature of the cold composite curve (the two curves touch each other). This is theoretically possible for an infinite heat transfer surface that compensates for the infinitesimal temperature difference between the thermal streams participating in the heat exchange at the process pinch point.

Since it is not technically possible to guarantee an infinite heat transfer surface it is necessary to limit the minimum vertical (in the sense of the temperatures) distance between the hot and cold composite curve to a minimum allowable temperature difference $\Delta T_{min}$. This also changes the actual constraint in Equation (2.2) to another positive value $(R^u \geq R^{min})$ which nevertheless is let to be unknown since it depends on the heat capacities of the streams participating in the heat transfer at the specific temperature interval therefore cannot be in general estimated in advance. However, this does not change the nature of the heat cascade problem which again can be easily solved by introducing a graphical expedient. In fact the same procedure followed for the case of $\Delta T_{min} = 0$ can be reproduced by drawing the curves with corrected temperatures instead of real temperatures of the composite curves. This consists in vertically moving (in the sense of the temperatures) the two curve towards each other for a length equal to the previously defined $\Delta T_{min}$ (e.g. shifting up the temperatures of the cold composite curve and shifting down the temperatures of the hot composite curve of $\Delta T_{min}/2$). As a consequence, Equation (2.2) remains valid and the cascade problem can be solved following the same steps as before. Eventually, the actual thermal profiles can be recovered by shifting back the temperatures of the same quantity thus allowing to draw the actual relative position of the composite curves.
Once the heat cascade problem is solved, the hot and cold utility requirements are evaluated. A special case is the so-called threshold problem in which, for a given $\Delta T_{\text{min}}$, no hot utility demand is evaluated. This is also the case in which at the process pinch point the temperature difference between hot and cold composite curves is greater than the pre-defined $\Delta T_{\text{min}}$. This latter condition tells the designer that there is no need to reach reduced temperature differences between the hot and cold composite curve.

The higher temperature difference between the curves the lower is the corresponding heat transfer surface (i.e. the HEN capital costs) needed for the internal heat recovery. This is why for the threshold problem the most convenient solution is to maximize the distance between the hot and cold stream thus recovering the heat of the hot streams at higher temperature levels. This allows in fact to exploit the maximum forces for the heat transfer as done in Figure 2.3a. The temperature difference at the pinch point in this latter condition is therefore defined as the $\Delta T_{\text{Threshold}}$. Another way to express the same concept is by looking at the case in which the two curves are moved closer to each other as in Figure 2.3b. The thermodynamic result of the heat integration does not change since the cold utility remains the same (it just splits into two parts). Conversely, the reduced temperature differences lead to an increase in heat transfer surface (i.e. capital costs).

### 2.1.1.1 An example of application of Pinch Analysis

A simple example of application of Pinch Analysis for the evaluation of the minimum energy requirement (MER) of a process with four thermal streams is presented here (see table below). In order to solve the heat integration it is necessary to know at least the inlet and outlet temperatures ($T_i$ and $T_o$) and the heat load $Q$ of each stream. The heat capacity of a stream is calculated as the ratio between the heat load and the difference between the outlet and inlet temperatures (but can also be assessed as the product of the mass flow rate of the material stream by its specific heat).

<table>
<thead>
<tr>
<th>Stream</th>
<th>$C_p$ [kW/K]</th>
<th>$T_i$ [°C]</th>
<th>$T_o$ [°C]</th>
<th>type</th>
<th>$Q$ [kW]</th>
</tr>
</thead>
<tbody>
<tr>
<td>A</td>
<td>2.0</td>
<td>20</td>
<td>135</td>
<td>cold</td>
<td>230</td>
</tr>
<tr>
<td>B</td>
<td>3.0</td>
<td>170</td>
<td>60</td>
<td>hot</td>
<td>-330</td>
</tr>
<tr>
<td>C</td>
<td>4.0</td>
<td>80</td>
<td>140</td>
<td>cold</td>
<td>240</td>
</tr>
<tr>
<td>D</td>
<td>1.5</td>
<td>150</td>
<td>30</td>
<td>hot</td>
<td>-180</td>
</tr>
</tbody>
</table>

The streams can be classified in the two subsets of cold and hot thermal streams depending on their requirement of being heated or cooled. Accordingly, for each subset, a cascade of temperature intervals can be identified (each interval is denoted by the two end-temperatures $T_{lb}$ and $T_{ub}$). For each temperature interval the cumulative heat load $R$ can be assessed by considering the thermal contribution of each stream crossing the specific temperature interval (by multiplying the heat cascade of each stream by the temperature interval). The resulting cold and hot thermal cascades are shown in the following tables which are used to draw separately the cold and hot composite curves (cold composite curve and hot composite curve).

#### Cold streams thermal cascade

<table>
<thead>
<tr>
<th>$T_{lb}$ [°C]</th>
<th>$T_{ub}$ [°C]</th>
<th>Streams</th>
<th>$R$ [kW]</th>
</tr>
</thead>
<tbody>
<tr>
<td>20</td>
<td>80</td>
<td>A</td>
<td>120</td>
</tr>
<tr>
<td>80</td>
<td>135</td>
<td>A+C</td>
<td>450</td>
</tr>
<tr>
<td>135</td>
<td>140</td>
<td>C</td>
<td>470</td>
</tr>
</tbody>
</table>

#### Hot streams thermal cascade

<table>
<thead>
<tr>
<th>$T_{lb}$ [°C]</th>
<th>$T_{ub}$ [°C]</th>
<th>Streams</th>
<th>$R$ [kW]</th>
</tr>
</thead>
<tbody>
<tr>
<td>30</td>
<td>60</td>
<td>D</td>
<td>45</td>
</tr>
<tr>
<td>60</td>
<td>150</td>
<td>B+D</td>
<td>450</td>
</tr>
<tr>
<td>150</td>
<td>170</td>
<td>B</td>
<td>510</td>
</tr>
</tbody>
</table>

In order to compute the minimum thermal loads of hot utility and cold utility and the corresponding maximum process internal heat recovery, the two composite curves are firstly drawn in the way that the cold composite curve is horizontally aligned (i.e. in the sense of heat loads) to the hot composite curve (see red and grey bold lines in Figure 2.2). This corresponds to set the hot utility thermal load to 0. The actual need for hot and cold utility is assessed considering a minimum temperature difference (here we set $\Delta T_{\text{min}} = 10^\circ C$) that is sufficient to ensure the heat transfer feasibility between hot and
cold streams. Accordingly, the MER thermal loads of hot and cold utilities are evaluated by vertically moving the two curves near each other (i.e. in the sense of the temperatures) so that the heat transfer results feasible until the two curves touch each other in the so-called pinch point. Among other possible choices, the two curves are shifted here of a same quantity $\Delta T_{min}/2$ ($5^\circ C$). Accordingly new cold and hot stream thermal cascades can be built.

<table>
<thead>
<tr>
<th>Cold streams thermal cascade</th>
<th>Hot streams thermal cascade</th>
</tr>
</thead>
<tbody>
<tr>
<td>$T_{lb}$ [$^\circ C$]</td>
<td>$T_{ub}$ [$^\circ C$]</td>
</tr>
<tr>
<td>25</td>
<td>85</td>
</tr>
<tr>
<td>85</td>
<td>140</td>
</tr>
<tr>
<td>140</td>
<td>145</td>
</tr>
</tbody>
</table>

As shown in Figure 2.2, the cold composite curve with corrected temperatures (grey dashed line) not only touches the hot composite curve with corrected temperatures (red dashed line) but also crosses it thus leading to unfeasible heat transfer. Thus, the heat transfer feasibility must be recovered by adding a hot utility which thermal load is evaluated by solving the so-called problem table. This is built by considering the whole set of cold and thermal streams with corrected temperatures (merging together the previous hot and cold thermal cascades with corrected temperatures). This results in a new set of temperature intervals which, if sorted descendingly, returns the MER hot utility as the maximum deficit of heat load (minimum negative cumulative heat load). The cumulative heat loads are assessed by applying Equation (2.1). The unfeasible heat transfer appears at the temperature interval between 85 and 140$^\circ C$ (corrected temperatures). In particular the maximum heat deficit (20 kW) is found at 85$^\circ C$ giving the position of the pinch point in the diagram in Figure 2.2. Thus it is sufficient to add an equivalent positive heat load as hot utility to recover the heat transfer feasibility. This corresponds to shift the corrected cold composite curve of 20 kW so that the only contact point with the hot composite curve is the pinch point (blue dashed line).

Eventually the actual position of the cold composite curve (blue bold line in Figure 2.2) in the diagram can be recovered by subtracting the same quantity $\Delta T_{min}/2$ (in this case $5^\circ C$) from the corrected temperatures.

<table>
<thead>
<tr>
<th>Tub [$^\circ C$]</th>
<th>Tlb [$^\circ C$]</th>
<th>Streams</th>
<th>R [kW]</th>
<th>Hot utility [kW]</th>
<th>MER R [kW]</th>
</tr>
</thead>
<tbody>
<tr>
<td>165</td>
<td>145</td>
<td>B</td>
<td>60.0</td>
<td>80.0</td>
<td></td>
</tr>
<tr>
<td>145</td>
<td>140</td>
<td>B+C+D</td>
<td>62.5</td>
<td>82.5</td>
<td></td>
</tr>
<tr>
<td>140</td>
<td>85</td>
<td>A+B+C+D</td>
<td>20.0</td>
<td>0.0</td>
<td></td>
</tr>
<tr>
<td>85</td>
<td>55</td>
<td>A+B+C+D</td>
<td>55.0</td>
<td>75.0</td>
<td></td>
</tr>
<tr>
<td>55</td>
<td>25</td>
<td>A+D</td>
<td>40.0</td>
<td>60.0</td>
<td></td>
</tr>
</tbody>
</table>

**2.1.1.2 The grand composite curve**

Pinch Analysis uses the problem table (of which a definition was given on page 8) for accounting the thermal balance of all the temperature intervals of the process heat cascade. The MER (Minimum Energy Recovery) condition is found the minimum allowable distance between the hot and cold composite curve is reached. In Figure 2.1 this relative distance between the two curves corresponds in vertical sense to a temperature difference (which is the driving force of the heat transfer) and in horizontal sense to the net heat load between hot and cold streams. Each knot joining segments of the hot and cold composite curves corresponds to the temperature discontinuity in the heat cascade delimiting temperature intervals. Accordingly, the cumulative heat loads evaluated by solving the problem table give the horizontal distances between the two curves at those temperature points delimiting temperature intervals.

Another graphical tool for interpreting the heat integration problem between process streams is the graphical representation of the net heat load in the whole range of process operating temperatures corresponding to the horizontal distance of the hot and cold composite curves in MER condition along the whole range of process temperatures. This can be easily built by drawing the values of cumulative
heat loads at each temperature boundaries of the heat cascade intervals and joining them with straight lines. This alternative representation is called grand composite curve and is shown in Figure 2.4 where both the scales of real and corrected temperatures are used. As done for the solution of the problem table, when using the corrected temperatures the location of the pinch point is found at that temperature level in which the cumulative heat load is equal to 0. The grand composite curve with the corrected temperature returns clearly the location of the process pinch point as that point of the curve in contact with the axis of the temperatures.

2.1.1.3 Optimal placement of utility thermal streams

The grand composite curves is an useful graphical tool for deciding which is the right temperature level within the process heat cascade where to provide heat or cold to the process by means of utility thermal streams. The grand composite curve in fact shows immediately at what temperature the process requires heat (over the pinch point) or needs to release heat (under the pinch point).

The design of utility system has its first step in the definition of the hot and cold utility thermal profiles. The correct placement of the external utility can be done by the interpretation of the grand composite curve. The preliminary assessment of the optimal heat load and temperature level of the hot and cold utility is called also “balancing” of the process composite curves. According to the basic rule of Pinch Analysis, if an external heat source exceeds the process thermal requirement, the extra part of the utility heat “passes through” the pinch point and needs to be rejected to the environment.

In technical practice, at lower temperature levels, the easiest way to cool down the process is by means of water-cooling. This is in reality true only for processes operating over the environmental temperatures which do not need refrigeration (cooling load under the environmental temperature).

In addition, the easiest (and the more common) way to provide heat to a process is by means of fuel combustion. If however another external heat source at lower temperature level is available the designer might find convenient to use it in place of high temperature combustion.
Pinch Analysis

Figure 2.3: Example of threshold problem

\[ \Delta T_{\text{Pinch Point}} = \Delta T_{\text{Threshold}} \]

\[ \Delta T_{\text{Pinch Point}} = \Delta T_{\text{min}} \]

Figure 2.4: Example of construction of grand composite curve (dashed lines are used for real temperatures, solid lines are used for corrected temperatures)
Figure 2.5: The interpretation of the grand composite curve for the correct placement of utility thermal streams

In Figure 2.4 hot and cold utilities are pictured simply as heat loads without particular reference to temperature levels. The utility thermal streams have to be placed without altering the process heat cascade or, in other words, without increasing the same process thermal requirement. This can happen, for instance, when hot utility thermal streams do not have the necessary heat capacity and they are not able to provide the heat at proper temperature levels.

The grand composite curve provides the designer with a complete overview of the process requirements at all the temperature levels. The heat capacity of an utility thermal stream can be estimated by looking at the slope of each segment of the grand composite curve, since the case in which utility thermal profiles are parallel to the process thermal streams corresponds in general sense to an optimal match between process and utility thermal streams leading to minimum operating costs.

An example is given in Figure 2.5 where two different ways to provide the hot and cold utilities by means of isothermal streams are shown. The figure shows that there is no need for providing the hot and cold streams respectively at the highest and at the lowest temperature level of the process temperature range. In particular, there are some parts of the process heat cascade, highlighted with dashed areas, in which the process can sustain its own thermal needs. These areas in the temperature-heat loads diagrams are called heat pockets.

2.1.2 Using exergy for evaluating the “quality” of heat integration

The choice of the optimum set of thermal utilities can be done only after a proper assessment of the operating and capital costs of the utility system. The comparison of the left hand side with the right hand side of the grand composite curve in Figure 2.5 in reality shows again that there is no difference in total amount of heat (hot utility) or cooling load if the utility streams are placed at different temperature levels. If the specific costs of the heat loads are the same, there is no difference in terms of total operating costs. This is the case in which heat is supplied by combustion of a fuel and then used at different temperature levels.

Conversely, the two solutions proposed in Figure 2.5, which are both referred to the same process MER condition, differ from each other in terms of the “quality” (the temperature level) of the utility
thermal streams rather than on the “quantity” (the heat load).

The concept of exergy is a way to account for the “quality” of a material stream or energy stream. Exergy is in fact defined as the potential of a material or energy stream to produce work (or power if referring to exergy rate). In the literature the works of Tribus and Evans, Gaggioli and Frangopoulos were the first introducing on the use of exergy for the evaluation of thermodynamic and economic performances of energy systems [35, 36, 40, 129]. Among others, the books of Kotas, Bejan, Tsatsaronis, Borel and Favrat present a formulation of exergy in all its theoretical aspects [10, 12, 71]. For the sake of brevity the discussion about exergy is here limited to those aspects that are fundamental to understand its application to the Pinch Analysis.

In agreement with the Second Law of Thermodynamics, it is not possible to continuously convert a heat load at a given temperature level into power by means of a thermodynamic cycle without rejecting heat to a heat sink at lower temperature level. For fixed values of the absolute temperatures of the heat source \( T_H \) and the heat sink \( T_C \), the efficiency of converting the heat load \( Q_H \) into useful power \( W \) is given by the expression of the Carnot Efficiency as follows:

\[
W = Q_H \cdot \left( 1 - \frac{T_C}{T_H} \right)
\] (2.3)

According to the definition of dead state (the thermodynamic state of matter corresponding to null work potential), the minimum temperature level of a heat sink towards which it is possible to reject heat is the environmental temperature \( T_0 \). By imposing \( T_C = T_0 \) Equation (2.3) returns the maximum potential for power generation of a given heat load \( Q_H \) at temperature \( T_H \) as in Equation (2.4), thereby giving the exergy rate \( E_Q \) associated with the heat load \( Q_H \).

\[
E_Q = Q_H \cdot \left( 1 - \frac{T_0}{T_H} \right) = Q_H \cdot \tau
\] (2.4)

Accordingly, \( \tau \) (the Carnot factor) is the efficiency of a Carnot engine working between the temperature \( T_H \) and the environmental temperature \( T_0 \).

Equation (2.4) in fact refers to the exergy rate associated with a heat stream originating from a body at constant temperature \( T_H \). The same expression can be written for an infinitesimal heat stream \( \delta Q \) as in Equation (2.5).

\[
\delta E = \tau \cdot \delta Q
\] (2.5)

For general steady state thermodynamic process involving a material stream of mass flow rate \( \dot{m} \) passing from thermodynamic state 1 to thermodynamic state 2 as a consequence of a heating load \( Q \) and without any power exchange, Equation (2.5) can be related to the exergy rate associated with the change of state of the material stream. By neglecting the kinetic and gravitational terms, in presence of only a heating process the First Principle of Thermodynamics gives \( \delta Q = dH = \dot{m} \cdot dh \). In addition if the heating process is reversible (that is for infinitesimal temperature difference between the heat source and the material stream) the Second Principle of Thermodynamics gives \( dh = TdS \). Accordingly, the integral between state 1 and state 2 of \( \delta E \) gives:

\[
\int_1^2 \tau \delta Q = \int_1^2 (1 - \frac{T_0}{T}) \delta Q = \dot{m} \cdot \left[ \int_1^2 dh - T_0 \cdot \int_1^2 \frac{dh}{T} \right] = \dot{m} \cdot [(h_2 - h_1) - T_0 \cdot (s_2 - s_1)] = \Delta E |^2_1
\] (2.6)

\( \Delta E |^2_1 \) is the change in exergy rate of the material stream from state 1 to state 2 and, according to Equation (2.6), corresponds to the grey area in Figure 2.6.

When dealing with heat transfer above the environmental temperature, a positive input exergy rate is associated with heating cold streams while a positive output exergy rate is associated with cooling of hot streams. Conversely, opposite signs for \( \Delta E \) are found for heat transfer processes under the environmental temperature (for \( \tau < 0 \)).
Composites and grand composite curves can be re-drawn using $\tau$ (the Carnot factor) instead of using absolute temperatures in agreement with Equation (2.5). In so doing, the heat integration problem can be graphically represented in the so-called exergy (hot and cold) composite curves for which an example is given in Figure 2.7.

By applying Equation (2.6) to the whole set of process hot and cold thermal streams, the exergy rate associated with the heat transfer from the hot streams to cold streams can be evaluated as the region delimited by the hot composite curve and the H-axis for that part in which the hot composite curve is superimposed onto the cold composite curve. It is also possible to observe that the absolute value of decrease in exergy content for the hot streams is lower than the increase in exergy content of the cold streams. Thus, in all real (i.e. irreversible) heat transfer processes part of the exergy rate available from a thermal stream (hot stream when over the environmental temperature, cold stream when under the environmental temperature) is lost due to the actual temperature differences between hot and cold streams. In Figure 2.7 the exergy destruction due to the heat recovery between process hot and cold streams is highlighted in grey and it corresponds in fact to the difference in the areas delimited by the hot and cold composite curves for the part in which they vertically superimpose.

The representation of the exergy level of thermal streams can be extended to include the utility thermal streams, thus giving the overall amount of exergy loss that originates from all the heating and cooling processes during plant operation. As an example, the same process thermal streams shown in Figure 2.7 are now balanced with a hot utility and a cold thermal stream in Figure 2.8.

In the same figure the difference in terms of exergy loss between the hot utility at high temperature (isothermal stream at 700 K) and the same hot utility at lower temperature level is shown.

2.1.3 Evaluating opportunities for power generation through composite curves

For a given process MER condition, exergy composite curves give a straightforward indication about the convenience of reducing temperature difference between utility thermal streams and process thermal streams. This does not imply a reduction in energy consumption but results in the possibility of using utility stream with less specific exergy content (lower quality).

Yet, in practice, this does not result into a real benefit unless the price for hot utility thermal streams at lower temperature levels is lower than that at higher temperature level. If fuel combustion is chosen for covering the hot utility requirement of the process, and if the process operates at relatively low temperatures compared to the combustion temperatures, it might be convenient to exploit part of the exergy content of the fuel for power generation.

So, a combined heat and power system can be introduced.

In the first book of Linnhoff on Pinch Analysis [84], exergy is not used explicitly as a mean for
Figure 2.7: Example of hot and cold composite curves (left), grand composite curve (center) and exergy composite curves (right)

Figure 2.8: Balanced exergy hot and cold composite curves: (a) with hot utility stream at 700 K, (b) with hot utility stream at 500 K
evaluating heat integration opportunities for combined heat and power systems. The same basic concepts expressed so far in an exergy analysis perspective were in fact extrapolated by the interpretation of composite and grand composite curves of processes.

According to Linnhoff’s formulation on the optimal placement of CHP systems with respect to the process heat cascade, a thermal engine is correctly placed either when it releases heat to the process over the pinch point or converts heat released by the process below the pinch point into power. Conversely, heat pump is correctly placed, with respect to the process heat cascade, if it operates across the pinch point (where the process behaves like a heat source) above the pinch point (where the process operates as a heat sink). The previous exergy formulation of the heat integration problem can be used to confirm these rules. As an example, the case in Figure 2.8a is now revised, in the light of power production, in Figure 2.9.

![Figure 2.9: Balanced exergy hot and cold composite curves: (a) with hot utility at 700 K, (b) with a thermal engine operating between 700 and 500 K](image)

Starting from the assumptions that a hot utility is available at 700 K and the highest temperature level of the process is at 500 K, it is possible to convert the heat at 700 K into power. Using a thermal engine part of the heat is rejected to the process at 500 K (in reality a temperature difference must be considered to ensure feasible heat transfer). In the exergy composite curves diagram the power production is represented as the difference between the area included between the two thermal streams, that is the difference between the exergy entering the thermal engine at 700 K and the exergy flow leaving the thermal engine at 500 K and supplied to the process. This difference is equal to $Q_1(1 - T_b/700) - Q_2(1 - T_o/500)$ and corresponds to the shaded area in Figure 2.9b.

When dealing with the design of thermal utilities, the designer usually has to choose thermal machines like thermal engines or heat pumps that are available in the market. Thus, the design of proper combined heat and power system is constrained by the size of existing energy systems like gas turbines or steam cycles. Thus, it is less common to design from scratch a thermal engine that works between two temperature levels, whereas it is more common to find the thermal engine that thermally matches the process in optimal way directly in manufacturers’ catalogs. Still, the interpretation of the process grand composite curve is the key point for the selection of the CHP system.

When looking only to the thermodynamic performance (i.e. to total site operating costs), the general rule is that a thermal utility (or combination of more thermal utilities) is properly placed when its thermal profile follows the profile of the process grand composite curve. Accordingly, a first selection of the utility system can be done just by observing for instance that process streams with horizontal profiles can be optimally coupled with evaporating and condensing streams like those generated by steam.
networks. Conversely, oblique profiles of process streams can be coupled to those associated with cooling of combustion gas or exhaust gases coming from an internal combustion engine.

For a better understanding another example in which process thermal streams show primarily horizontal thermal profiles is introduced in Figure 2.10.

The case analyzed in Figure 2.10 reflects the typical case of food industry or similar processes in which the evaporation of water is an important energy-consuming sub-process, as it is discussed in the next chapters about the application of process integration methodologies to a sugar-cane conversion process. Evaporation is in fact performed in more than one stage in order to exploit the heat integration potential between subsequent stages (effects). As it is appears in the same figure, the process thermal requirement is mainly related to the operation of the first effect. According to the guidelines for the design of CHP systems proposed by Linnhoff, a horizontal profile of part of the grand composite curve would suggest the use of steam condensation as hot utility. A steam boiler results in one of the most common choice and the heat is here delivered (distributed) to the process by means of a steam line.

A useful way to show the resulting integration of the utility with the process is the so called integrated grand composite curve of the utility streams as proposed by Maréchal and Kalitvenzeff [89] and shown in Figure 2.11a for the case of the steam line at 3 bar that is used to cover (balance) the hot utility requirement of the process previously introduced (see Figure 2.10).

The integrated grand composite curve of a particular subset of streams “A”, is built using the same procedure as for the standard grand composite curve. Theoretically, this is equal to considering the heat integration of subset “A” as independent of the set “B” of the remaining streams. Here subset “A” includes the thermal streams of the utility system and subset “B” the process streams. In order to highlight the integration of utility thermal streams and process thermal streams, subset “A” (blue grand composite curve in Figure 2.11) is represented as integrated with set “B” (red lines in the same figure). This corresponds to graphically flip the grand composite curve of subset “A” towards the grand composite curve of set “B” and move them closer until they touch each other. This latter point is in fact a pinch point meaning that, with respect to subset “B”, subset “A” behaves as a heat sink over that temperature and as heat source under that temperature. If in particular subset “A” includes the streams of an utility system, like in Figure 2.11, then this point is called utility pinch point.

Figure 2.10: Example of process with several evaporations and condensations: a) hot and cold composite curves; b) grand composite curve

A schematic representation of the steam boiler configuration is shown in Figure 2.11b. For a maximum steam pressure around 10 to 15 bar fire-tubes boilers may be installed (and this may be the case of a steam line at 3 bar). However, for reasons of consistency with further representations of the steam network, water-tubes boiler is considered in this analysis. The scheme in Figure 2.11b refers to the general situation...
in which the water preheating, evaporation and possible steam super-heating are counter-current with respect to the combustion gases.

In Figure 2.11a the corresponding integrated grand composite curve of the system is presented. For sake of simplicity, the thermal profiles associated with the heat transfer between heat of combustion and the steam production in the boiler is not shown.

In fact, it is worth observing that, when heat is generated through combustion in a boiler the total amount of heat to be generated dictates the operating costs independently of the temperature and pressure levels at which heat is used. So, the operating parameters of a steam network built for heating purposes only are chosen mainly to minimize capital costs. In particular, the major issue is related to the minimization of the operating pressure, which, on the other hand, is constrained by process temperatures and overall pressure drops. Heat integration opportunities are therefore to be exploited in the process design to lower the heat loads and the temperature levels at which steam has to be delivered.

For the case in Figure 2.11a, where the heat demand is associated with the first evaporation level only, the choice of the steam pressure is particularly simple. In reality it is also possible to note that the temperature difference between the steam line (saturated steam at 3 bar) and the process stream (the first effect of the multi-effect evaporator) is still considerably high, consequently leading to some exergy losses. So, it is possible to reduce the pressure at which steam is delivered to the process. More complicated steam networks could be considered if the heat was required and provided at different temperature levels. However, in technical practice, when steam pressures are below a certain level (medium low temperature heat demand), the benefit in capital costs derived from producing steam at different pressures is not that big and it could be convenient to deliver heat at the maximum pressure and to use a system of throttling valves to match the desired local temperature level. This is also a way to reduce the plant complexity that would be introduced by multiple pressure steam production.

The case of combined heat and power production deserves instead a completely different analysis.
2.2 Synthesis of steam networks for combined heat and power production

According to the guidelines on process integration introduced by Linnhoff\cite{84}, a thermal engine (machine producing mechanical power by means of a thermal cycle) is well integrated to a generic thermal process when it does not alter the process heat cascade. This is either the case in which the thermal cycle releases heat to the process heat sinks (over the process pinch point), or the case in which the process heat sources (below the pinch point) is used as thermal source for the thermal cycle. In order to clarify the methodological aspects deriving from the design of the proper CHP system for a given process, we investigate in the following the first of the two options since it is the most common one.

A thermal engine seldom appears as a device receiving heat from a single external source at constant temperature and producing power while releasing heat to a single external heat sink at constant temperature as commonly represented in theoretical dissertations. Most likely the so-called thermal engine is a general name to indicate a gas turbine, a reciprocating combustion engine or a steam engine.

Internal combustion engines are less suitable than steam plants for the generation of heat at different temperature levels. In fact fuel is used in open-cycle combustion to upgrade the enthalpy content of the thermodynamic medium itself (air). After this enthalpy content is converted into useful power (mechanical or electrical work over time), at the engine discharge the thermodynamic medium has a still quite high heating potential. Thus, this is the place where a possible heat integration with other entities (an industrial process or even a bottoming cycle) takes place. Technically this corresponds to use a gas to gas or gas to liquid heat exchangers that allows to recover the heat of the exhaust gases for other heating purposes.

Gas turbines and reciprocating combustion engines are in fact always used as topping cycle (at the top of the heat cascade) and this let the design of these machines to be tackled as a rather independent procedure. As a result the design of CHP system adopting this type of machines consists often in purchasing the right number, size and type of machines that are available in catalogs provided by different producers.

A steam cycle (a Rankine cycle consisting of a loop of compression, evaporation, expansion and condensation) is instead a more flexible thermal engine. Firstly, different fuels can be used to run the cycle, being this a close cycle that requires an external combustion. Secondly the operating parameters can be adjusted to meet different requirements in terms of power production and heat production thus leading to different efficiencies. Furthermore the structure of the cycle can be adapted not only to match process heat sinks but also process heat sources when already available from medium temperature levels. In the light of a full heat integration between the steam cycle with an industrial process, a steam cycle is in fact regarded as a modular part of a general steam network. Accordingly, steam cycles can be superimposed to each other to form a complex structure of which hot and cold streams are thermal interfaces that interact not only with each other but also with the industrial process thermal streams. Theoretically this corresponds to include the whole set of thermal streams related to the steam cycle operation into the overall heat integration problem and let the topology (type and number of steam expansion and heat exchangers) to be defined as a result. When necessary, that is when the industrial process is not able to generate the heat acquired for power generation, additional hot utility can be provided by fuel combustion which typically takes place in water-tubes boilers.

In the following paragraphs the design of a steam network is analyzed with particular emphasis on efficiency (i.e. operating costs) while the minimization of capital costs is considered as a subsequent issue to be investigated only by an extensive thermo-economic analysis that is beyond the scope of the present discussion.

The design of a CHP system based on a steam network can be reduced to the definition of the structure and the optimal operating parameters of the steam network that covers the process heat requirement and a part or the total of the process power requirement. Indeed a CHP system results particularly convenient when its simultaneous production of heat and power, which are usually of the same order of magnitude, are mostly absorbed by the process. So, the common criterion for the design of a CHP system is to verify that that the ratio between the process heat and power requirements is equal to the ratio between the combined heat and power production. However, when this condition is not verified a
CHP system can still be a profitable plant solution provided it is properly sized. In particular, due to the difficulty of storing or selling the extra amount of heat, a possible design strategy is to find the best trade-off between electricity sales and purchases and plant capital costs, with the constraint that all of the heat production is used within the industrial site.

Technical feasibility of power generating steam cycle starts from some MW of installed power. For a better understanding of the concepts presented hereafter, a numerical example is given. We suppose here that the heat required by a process is around 145 MW and its electrical/mechanical power demand is around 16 MW which are values that justify the design of a steam network also for power generation (CHP system).

In addition we assign costs to fuel and electricity as boundary conditions of the problem. In the case of natural gas with a lower heating value \( LHV = 46M J/kg \) (around 39 \( MJ/Nm^3 \) considering a density \( \rho = 0.84kg/Nm^3 \) ) the specific cost \( c_{fuel} = 0.3€/Nm^3 \) is assumed. The cost of electricity \( P_{en} \) imported from the network is \( c_{el} = 0.15€/kWh \) and the price of the electricity \( P_{out} \) sold to the network is \( p_{el} = 0.1€/kWh \) in case of positive net power production \( P_{net} \) (total power produced \( P_{CHP} \) minus process electricity demand \( P_{pro} \)).

The total operating cost function can be written as follows:

\[
c_{tot} = \dot{V}_{fuel} \cdot c_{fuel} - P_{out} \cdot p_{el} + P_{in} \cdot c_{el} \tag{2.7}
\]

The problem of the minimization of the operating costs can be therefore seen as a linear optimization problem where the variables are the power and the fuel consumption. In reality these costs depend on the performance of the particular steam cycle (network) and on the mass flow rates involved. If structural and operating parameters of the steam network are fixed and the CHP system is considered to be operated at its design point (nominal power), a fairly good approximation of the problem is to consider power and fuel consumption as linearly dependent on mass flow rates. A better discussion about the feasibility of this type of assumption is discussed in one of the subsequent sections.

An alternative way to interpret the problem is to visualize Equation (2.7) in a 3-D diagram in which a given couple of values of fuel consumption \( \dot{V}_{fuel} \) and net power production \( P_{net} \) corresponds to a value of total operating costs \( c_{tot} \). Depending on the possibility of selling electricity and on the fuel consumption, the resulting value of total operating costs can be positive (positive cash flow exiting the plant) or negative (positive incoming cash flow). Theoretically all possible values of net power production and fuel consumption can be obtained in a given range. Thus in the same diagram all cost scenarios are represented as a cost surface. This in fact results from merging together two plans: one corresponding to the case of selling the net electricity to the market (positive values of \( P_{net} \) ) and the other one to the case of buying electricity from the network (for negative values of \( P_{net} \) ), being the price (cost) of electricity different in the two cases. Obviously, different slopes of the cost surface can be found for different specific costs of electricity and fuel \( \left(p_{el}, c_{el}, c_{fuel}\right) \).

Now, as previously mentioned, power production and total fuel consumption are not independent variables but are physically linked to each other by means of the performance of the particular CHP system considered and the overall heat and power requirement of the industrial process for which the CHP system is designed. In parallel, the characteristics related to different structures and operating parameters of the CHP system can be represented as vertical plans (the loci of design operation points in terms of couples \( \left(\dot{V}_{fuel}, P_{net}\right) \) ), each one corresponding to one CHP configuration). Their equations can be written considering the operation of the CHP system in different conditions depending on the sizes and on the process demands for heat and electricity.

As a result the actual operating cost function for a particular system is the intersection of the cost surface associated with Equation 2.7 with the characteristic of the CHP system (that fixes the relation between fuel and power generation). This intersection (between planes) is shown in the lines \( ABCD \) or \( ABCE \) that are obtained for two different CHP systems (different performances) as explained in the following.

For a given set of operating parameters and structure of the steam network it is possible to relate the net power production \( P_{net} \) to the electric efficiency \( \eta_{el} \) as follows:

\[
P_{net} = \dot{m}_{fuel} \cdot LHV \cdot \eta_{el} - P_{pro} \tag{2.8}
\]
Figure 2.12: Graphical interpretation of the cost problem for optimal design of a CHP system
Accordingly, assuming that it is possible to cover the electricity demand directly with the power produced by the CHP and neglecting contractual limits of local power exchange and that the process heat demand has to be totally covered by the CHP system (in the example that we make this corresponds to 145 MW):

\[ P_{\text{net}} > 0 \Rightarrow P_{\text{out}} = P_{\text{net}}; P_{\text{in}} = 0 \]  \hspace{1cm} (2.9)

\[ P_{\text{net}} < 0 \Rightarrow P_{\text{out}} = 0; P_{\text{in}} = |P_{\text{net}}| \]  \hspace{1cm} (2.10)

As a consequence, the result of the overall energy balance can fall into one of the following situations:

1. \( Q_{\text{CHP}} = Q_{\text{pro}}; P_{\text{CHP}} < P_{\text{pro}} \rightarrow \) Buy electricity
2. \( Q_{\text{CHP}} = Q_{\text{pro}}; P_{\text{CHP}} = P_{\text{pro}} \)
3. \( Q_{\text{CHP}} = Q_{\text{pro}}; P_{\text{CHP}} > P_{\text{pro}} \rightarrow \) Sell electricity
4. \( Q_{\text{CHP}} > Q_{\text{pro}}; P_{\text{CHP}} > P_{\text{pro}} \rightarrow \) Sell electricity, sell heat or use condensing turbine.

In the example, the power requirement is lower than the heat requirement by about one order of magnitude (16 MW compared to 145 MW). Assuming that all the heat has to be provided by the CHP system and cannot be bought from a district heating system, a CHP system can reproduce one of the aforementioned cases. However, for other processes with higher power requirement, it may happen that once the heat requirement of the process is covered by the CHP system, the power produced by the CHP system is still less than the amount required by the process.

Heat generation discussed in the previous Section (the case of a boiler in Figure 2.11a) can be seen as trivial CHP condition for which the part of power generation is reduced to zero (see point A in Figure 2.12). For this case the heat demand \( Q_{\text{pro}} \) is equal to 145 MW resulting in a fuel consumption of around 3.7 \( \text{Nm}^3/\text{s} \) \( (\dot{V}_{\text{fuel}} = Q_{\text{pro}}/(LHV \cdot \rho) \) neglecting the efficiency of the steam boiler for simplicity).

All the other possible CHP configurations yield to bigger values of fuel consumptions and power generation.

For a given industrial process, the structural and operating parameters for the optimal CHP system can be chosen by observing the operation requirements of the process (e.g. by looking at its composite and grand composite curves). For instance if, again, the process in Figure 2.10 is considered, the CHP system must deliver heat with a steam line at a temperature slightly higher (minimum temperature difference) than the first evaporation effect. However when the aim is power generation a high pressure steam line is required.

Still, there might be different options for the design of the steam network both in terms of structure and in terms of operating parameters. In the light of a generalized and possibly systematic approach (i.e. to be translated into calculation codes) for the synthesis of a CHP systems, the optimal design is presented here as the design which minimizes operating costs (objective function). In presence of a fair estimation of the investment costs and other economic indexes, CHP net present value or even process profitability can be used as more accurate objective functions.

Following the choice of the operating costs as objective function, different CHP systems are compared. The discussion is supported hereafter by a graphical representation of the linear programming optimization procedure.

### 2.2.1 CHP system with total heat recovery for process heating

In this section we analyze the case in which all the heat produced by the CHP system is used for heating purposes within the process.

For the process in Figure 2.10, we propose firstly a simple steam network including a back-pressure turbine. One steam production header at high pressure drives the steam to the expansion. At the turbine outlet, steam is used for process heating purpose only. Once the minimum steam pressure has been defined by estimating the minimum temperature of the process heat demand, the overall pressure ratio of the expansion (i.e. the specific power production) is found. After having transferred its latent
heat to process streams, the condensate stream is then re-directed to the boiler to feed again the steam boiler.

An overview of the corresponding structure can be seen in Figure 2.13b.

In Figure 2.13a the resulting utility integrated grand composite curve is presented. This representation highlights that an utility pinch point is activated. Accordingly, the process heat requirement is completely balanced by the utility thermal load and for greater fuel consumption an excess heat would be generated and eventually rejected to the cold utility as pointed out in the general rules for heat integration proposed by Linnhoff and previously discussed.

Since the heat requirement of the process is quite high with respect to the process power requirement for the case in the example, extra net power is generated and is sold to the market. In Figure 2.12 this situation corresponds to point \( C \). Higher steam mass flow rates for greater power production would provide additional power generation but not additional heat to be used in the process. Conversely, all the configurations between point \( A \) and point \( C \) are those in which, neglecting the boiler efficiency and other heat losses in the plant, the energy content of the fuel is totally converted into power (part used by the process and part sold to the market) and heat used by the process and no heat is rejected to the environment. We conclude therefore that the total efficiency (ratio between the useful energy output and the energy input) is equal to the 1 (that is in reality to the only boiler efficiency). Conversely, those configurations in which part of the fuel is only used for power production appear beyond point \( C \). In these cases, depending on the steam cycle efficiency, some heat is inevitably released to the environment at the turbine condenser.

We firstly analyze the structure, thermal integration and a the impact in total site operating costs of those configurations belonging to the first subset (between \( A \) and \( C \) in Figure 2.12). This includes all the steam networks that cover the total process heat demand either with a dedicated steam line (like for instance the steam line at 3 bar just for heating the first evaporation effect) or with the steam exiting the turbine (back pressure steam line). In fact the share of process thermal requirement covered by this back-pressure steam-line can range between 0 (configuration in which the power generation is reduced to 0) to the total amount of hot utility (145 MW in the example). With reference to Figure 2.14b this is equivalent to the all the ratio \( x \) (in the range \([0; 1]\)) between the steam flow rate used for power production and the total steam produced at 80bar. \((1 - x)\) gives instead the portion of the steam diverted directly to process heating (steam header at 3bar).

The intermediate solution in which the available heat at the exit of the back pressure turbine is not sufficient for covering the process thermal requirement and some extra heat has to be delivered by an independent steam-line at the same pressure, can be practically realized at least in two ways. One possibility is to produce the additional steam by means of a separate steam production line. This would result in a boiler design that comprises two separate water heaters and two evaporators (the steam for heating purpose could be also superheated but usually saturated steam is sufficient). A second possibility is that in which all the steam is produced at the same pressure and, if not used for power production, is expanded through a throttle valve like in Figure 2.14b. In this case only one steam production line is required. It is apparent that the extra work used to pump all the water mass flow rate to the maximum operating pressure is lost when steam is laminated from 80 to 3bar. However the extra cost for the greater number of heat exchanger units in the first case may be not justified, being the resulting thermodynamic benefit quite small.

In the example considered we fixed the process power requirement \( P_{\text{pro}} \) to 16MW. Assuming that the part of steam diverted to the back pressure turbine (80 → 3 bar) produces electricity with an efficiency \( \eta_{el} = 0.20 \), it is possible to re-write in a more explicit way Equation 2.8 for the set of steam networks corresponding to Figure 2.14b as follows:

\[
\dot{V}_{\text{fuel}} = \frac{1}{LHV \cdot \rho} \cdot (Q_{\text{pro}} + P_{\text{CHP}}) = \frac{1}{LHV \cdot \rho} \cdot (Q_{\text{pro}} + P_{\text{net}} + 16\text{MW})
\]

(2.11)

The resulting cost function, graphically equivalent to the intersection between the costs surface and the CHP characteristic plane set by Equation 2.11, corresponds to the segment \( ABC \), being point \( A \) related to the boiler operation \((x = 0, P_{\text{net}} = -P_{\text{pro}})\), point \( B \) to the situation in which \( P_{\text{net}} = 0 \) \((P_{\text{CHP}} = P_{\text{pro}})\). Point \( C \) the situation in which all the process thermal requirement is covered totally by the back-pressure
Figure 2.13: Back pressure turbine: (a) integrated grand composite curve (blue: steam network thermal streams, red: heat of combustion and low-temperature process thermal streams), (b) plant flow-sheet

Figure 2.14: Back pressure turbine and additional steam production for heating purpose only: (a) integrated grand composite curve (blue: steam network thermal streams, red: heat of combustion and low-temperature process thermal streams), (b) plant flow-sheet
steam line \((x = 1)\) and an exceeding power is produced \((P_{CHP} > P_{Pro})\) and sold to the market.

From Equation 2.11 it it possible to evaluate the corresponding fuel consumption of point \(C\) by using first principle relation between \(Q_{pro}\) and \(P_{CHP}\):

\[
\dot{V}_{fuel}^C = \frac{1}{LHV \cdot \rho} \cdot \frac{Q_{pro}}{1 - \eta_{el}}
\]  

In Figure 2.14a the integrated grand composite curve of the steam network in Figure 2.14b is represented. In agreement with the rules of heat and power integration, the cold utility is not altered by the presence of the power generating system since the heat released by the turbine is totally used for heating purposes (cold utility equal to the case in Figure 2.11).

### 2.2.2 CHP system with partial heat recovery and integrated additional power generation

In the previous pages, the steam network configurations in which all the heat available at the outlet of the steam turbines is used for heating purposes within the process were analyzed. Here we consider instead those steam networks embedding a steam power cycle which produces excess heat compared to the process heat requirement as a consequence of steam expansion for the only purpose of additional power generation.

Following the graphical interpretation of the operating costs minimization problem proposed in Figure 2.12, this second subset of steam network configurations are those yielding to greater fuel consumption and electricity production than configuration at point \(C\) (which was previously defined as the point of the operating cost surface corresponding to the case in which the heat produced by the CHP system is exactly equal to the process thermal requirement). In other words, this subset groups those configurations that need to reject part of the heat to a cold utility. In the light of the heat and power integration rules this corresponds to the condition in which some of the heat of combustion passes through the whole heat cascade and crosses the utility pinch point. In fact, even if the thermal balance is altered and the total site heat integration is not more that of the MER condition, there could be an economic interest in using the same facility for a bigger power production even if part of the heat is rejected to the environment and part of the electricity is sold to the market. This is often justified by economy of scale factors, that is the reduction of the specific investment costs for bigger installed power, along with the possibility of using the CHP facilities that are in any case required by the industrial process.

CHP plant were object of attention of governments in the last decades. At the basis of this interest there is the possibility for a better use of fuel and eventually for a reduction of the total energy bill. In order to promote the installation of such systems, a series of legislative tools were developed like, for instance, different fiscal policies and subsidies.

In this context, one of the crucial points that politicians and technician still need to face is the definition of indexes that allow to distinguish between purely power generating plants and CHP plants. The newly issued European Directive in this field (see [30]) prescribes the criteria that high-efficiency cogeneration must fulfill. Once a CHP system is considered to be high-efficient it is given access to subsidies, the amount of which may depend on specific legislation of the member states. According to the European Directive cogeneration production from cogeneration units shall provide primary energy savings of at least 10% compared with the references for separate production of heat and electricity and production from small scale and micro cogeneration units (that is for electrical power less than 10MW) providing primary energy savings may qualify as high-efficiency cogeneration. The index of primary energy savings \(PES\) of a CHP plant is defined as follows:

\[
PES = 1 - \frac{E_t}{E_r} \frac{\eta_{es}}{\eta_{ts}}
\]  

(2.13)
where \( E_c \) is the annual amount of energy corresponding of the fuel input used to produce the sum of useful heat output \( E_t \) and electricity \( E_e \) from cogeneration, \( \eta_{es} \) and \( \eta_{ts} \) the efficiency reference values for separate production of electricity and heat respectively.

For the case here examined in which additional power production is considered, we should therefore bear in mind that, behind the indication provided by the representation in Figure 2.12, the real profitability of the CHP plant for greater power production than point \( C \) could be affected by the reduced impact of subsidies. These are in fact only limited to the case in which the major part of heat produced by the CHP plant is used for heating purposes in the process.

Let’s consider the case in which a greater steam flow rate is used in the same steam network configuration as in 2.13. For the same operating parameters of the back pressure steam turbine, the extra heat available at the back pressure (3 bar steam line) is rejected to the cold utility, as shown in Figure 2.15, thus leading to quite high exergy losses.

For the whole spectrum of higher steam mass flow rates, the corresponding cost function is shown in Figure 2.12 by the segment \( \overline{CD} \). The steam network characteristic that identifies a plane that originates an intersection with the costs surface can be expressed as follows:

\[
\dot{V}_{fuel} = \frac{1}{LHV \cdot \rho} \cdot \frac{P_{net} + P_{pro}}{\eta_{el}} \tag{2.14}
\]

It is possible however to exploit in a better way the energy content of the extra part of generated steam by means of a further expansion of steam directly to the cold utility temperature level. This is practically done by adopting a condensing turbine.

From the point of view of a generic process flow diagram, there is no distinction between a steam condensation for heating purpose (like the steam line at 3 bar) and that at the cold utility level, being different only the type of the heat exchanger involved. On the other hand, in addition to the possibility of exploiting a bigger enthalpy gap for lower outlet pressure (typically in the range of 0.1 to 0.05 bars), better conversion performances are usually achieved with a condensing turbine than with a back pressure turbine because of the more favorable conditions of steam expansion at lower pressures.

Thus the efficiency of the cycle performed by this additional part of steam mass flow rate \((m_{steam} \cdot (1 - y)) \) in Figure 2.16b) is bigger than that of the back pressure turbine cycle performed by the remaining part \((m_{steam} \cdot y)\). If in reality there is no physical distinction between the two cycles, it is convenient to interpret the steam network configuration in Figure 2.16a as the superimposition of the cycle performed by the steam flowing through the condensing turbine and of the cycle performed by the steam flowing through back-pressure turbine. In this way in fact it is easy to separate the contribution of the two steam flow rates to the overall electric efficiency.

If \( \eta_{el}^{BPT} \) is the electric efficiency of the back-pressure turbine cycle (for the numerical example we consider here \( \eta_{el}^{BPT} = 0.2 \)) and if \( \eta_{el}^{CT} \) is of the condensing turbine cycle (for the numerical example we consider here \( \eta_{el}^{CT} = 0.3 \)), the overall fuel consumption can be expressed as follows:

\[
\dot{V}_{fuel} = \frac{1}{LHV \cdot \rho} \cdot \left[ \frac{Q_{pro}}{1 - \eta_{el}^{BPT}} + \frac{P_{net} + P_{pro} - P_{BPT}}{\eta_{el}^{CT}} \right] \tag{2.15}
\]

\[
P_{BPT} = \frac{Q_{pro} \cdot \eta_{el}^{BPT}}{1 - \eta_{el}^{BPT}} \tag{2.16}
\]

Equation 2.15 defines the steam network characteristic with combined back-pressure and condensation turbine which outline the interception \( \overline{CE} \) with the costs surface in Figure 2.12. This segment shows a more convenient slope in terms of operating costs, which reflects better performance for power generation obtained with this second subset of steam network configurations with respect to the case of only back-pressure turbine (\( \overline{CD} \)).

Figure 2.16a shows the corresponding integrated grand composite curve representation of the coupling of the steam network of Figure 2.16b with the process considered in the example. In the same figure it is also possible to note that total site heat integration would lead not only to heat recovery within the process itself as already shown in Figure 2.10 but also between the process and the steam network. This thermal integration can be practically realized by using part of the process hot streams under the process.
Figure 2.15: Discovering opportunities for additional power generation through the interpretation of the integrated grand composite curve.

Figure 2.16: Back pressure turbine and additional condensing turbine for additional power generation: (a) integrated grand composite curve (blue: steam network thermal streams, red: heat of combustion and low-temperature process thermal streams), (b) plant flow-sheet.
pinch point for preheating water before the steam boiler. In large steam plants water is pre-heated by steam draw-offs derived from some medium and lower temperature stages of the turbine. The solution is still valid also for the case of CHP plant. However, total site heat integration shows the opportunity of water preheating by using process thermal streams, which would otherwise reject heat to the cold utility, instead of high quality steam produced in the boiler. This means also that part of the energy content of the fuel passes through the all total site heat cascade, from combustion to steam production and from the process to the steam generation.

It should be pointed out that usually hot process thermal streams are available at rather low temperatures compared to the steam cycle temperatures. In addition, if temperature levels of these streams are high enough to guarantee water preheating like in the example, the solution of doing water preheating with process stream is competitive with that using draw-off steam lines, only if the number of hot process thermal streams involved is small. Conversely, when a great number of heat exchanger units is needed, the increased plant complexity that may rise from this strong thermal integration, is not economically counterbalanced by the slight increase in thermodynamic performance of power production.

The two options for water pre-heating are shown in gray in Figure 2.16b. Obviously, it is also possible to have both the two solutions together (water preheating with process streams and steam draw-offs) when only part of the water heating at low pressure can be achieved with process hot streams.

2.2.3 The MILP formulation of the problem of the synthesis of CHP systems

![Graphical interpretation of the minimum operating costs problem](image)

Figure 2.17: Graphical interpretation of the minimum operating costs problem, fuel cost $c_f = 0.3\$/Nm³, electricity cost: (a) $p_{el} = 0.1\$/kWh, (b) $p_{el} = 0.08\$/kWh

Starting from the analysis of the process energy requirements and in particular of its grand composite curve it is possible to select the optimal configuration leading to highest performances among the whole set of possible configurations of CHP systems. In fact, as previously pointed out, different CHP concepts can be adopted depending on the desired level of integration between process and utility system and capital costs that can be afforded.

Within a same technology, different structural and operating parameters can play a crucial role in determining process and CHP profitability. In particular, the case of the steam network was chosen as a paradigmatic case in which the high number of structural alternatives suggests the use of a systematic procedure for the synthesis. In the previous sections, starting from the boiler configuration, the structure of the steam network was heuristically complicated in order to comprise several options (back pressure turbine, condensation turbine, possible draw off or regeneration with process stream). Further improvements in efficiency can be achieved by using multiple pressure levels for steam production or re-heating.
(part of the steam can be diverted again to the furnace for additional super-heating before entering the last expansion stages).

In the following paragraphs, a possible approach for the systematic synthesis of steam network is presented. The problem of the synthesis of the CHP system could be tackled in a more general way by including also other power generating technologies like reciprocated internal combustion engines or gas turbines possibly in combined mode with the steam network. However, we consider here steam networks only, being a quite paradigmatic case due to the discrete number of structural options that can be considered. This topic is discussed in more detail in Section 2.3.

The systematic synthesis of the CHP system, like any other thermal system, is proposed here as the solution of an optimization problem in which structural and operating parameters are treated as decision variables and operating costs (the difference between cost of the fuel and the revenue from the electricity sold to the network when exceeding the process power requirement) are the objective function.

An expression of the objective function was previously given in Equation 2.7. Total cost function has been expressed in a more explicit way as the intersection between the costs surface (resulting from all the possible combinations of fuel consumption and power generation) and the characteristic (design points) of possible steam network configurations (Figure 2.12).

In Figure 2.17 the same graphical representation proposed in Figure 2.12 is shown in 2-D sight for two cases in which different prices were assumed for the electricity to be sold to the grid. Steam networks characteristics are represented as solid lines. A relative magnitude of the total operating cost is shown in colors (the more blue the surface the lower are the operating costs). Values for \( P_{\text{net}} \) are limited within 60 MW, which was chosen considering that the CHP operation should not compete with the separate electricity production market in which values for nominal power are normally of hundreds of MW. This range of \( P_{\text{net}} \) comprises all the solutions between the “trivial” point \( A \), in which \( Q_{\text{pro}} \) is covered by a boiler and \( P_{\text{pro}} \) is totally imported from the grid, up to 60 MW in which all the process heat and power requirements are satisfied by the CHP system and extra electricity is sold to the market while extra heat is rejected to the environment by means of the condenser.

The two plots in Figure 2.17a and 2.17b present same steam network characteristics but different cost surfaces obtained for different values of specific price of electricity \( p_{\text{el}} \) as reported in the respective captions. The dashed line for \( p_{\text{net}} = 0 \) sets the boundary between import and export of electricity. Segment \( AC \) refers to the back pressure turbine progressively covering all the process heat requirement. For bigger steam mass flow rates the heat available at the turbine outlet exceeds the process thermal requirement and the cost function follows the segment \( CD \). Segment \( CE \) instead refers to the case in which additional power production is achieved by an independent condensation turbine. Segment \( AK \) refers instead to the characteristic in which heat for the system is provided by a boiler and power is generated by independent steam cycle. In both the two plots the best solutions front line is the polyline \( ACE \). When additional electricity generation is well paid, the best solution coincides with maximum achievable power generation (which is limited here to 60 MW). On the contrary when electricity is less well paid, back-pressure turbine configuration (point \( C \)) results the best solution.

2.2.3.1 Modeling a steam network superstructure

According to the linear characteristics of the various CHP systems considered so far (where intensive parameters are in fact considered fixed and only mass flow rates of steam and fuel are adjusted), the problem of finding the optimum configuration leading to minimum operating costs can be formulated as a comparison between the optimum points of the various configurations considered, which can be found by solving separate linear programming problems.

Alternatively, a mixed integer linear programming (MILP) problem can be formulated in order to found the optimal configuration at once by letting the solution algorithm to select the optimal structural branches of a CHP system superstructure by means of the activation of binary (or integer) variables. In the present section the formulation of such superstructure for the synthesis of CHP systems based on steam networks only is discussed. In particular, the attention is drawn towards those assumptions on the modeling of steam network that ensure linear characteristics so that the synthesis of steam network can be solved as a MILP problem.
Steam networks have been previously generated by observing the process grand composite curve and identifying the opportunities for integrating utility systems with the process. The characteristics (relation between fuel consumption and power generation) have been also evaluated once the structure and the energy flows from and to the process have been defined.

Since the aim is to systematically assess the best structure and design parameters of the steam network, a superstructure can be defined in order to include all the possible solutions of the synthesis problem. In this field Dhole and Linnhoff proposed the so called “Totalsite” methodology that was supported by graphical considerations on the heat sources and sinks within the total site heat cascade [22].

Previous studies in the field of computer-aided chemical engineering achieved same or even better results relying in a more rigorous mathematical programming. The method discussed in detail in the following pages was developed and presented in the past by Papoulias and Grossmann et al. [105] and is based in a MILP optimization approach proposed by Grossmann and Santibanez [50] which dates back to the 80’s. The mixed integer linear formulation of the synthesis problem relies on the model of a system superstructure including different technologies and not only the steam network. The same methodology was implemented by Marechal and Kalitvenzeff in different works about process synthesis [90, 91] and is mainly applied to the optimal synthesis of a steam network.

An exhaustive one step strategy including the whole spectrum of plant options and values of operating parameters necessary leads to a MINLP formulation of the problem. This is mainly due to non-linear relations between design parameters and thermodynamic and cost performances, and to the combinatorial complexity introduced by structural alternatives. In the last decades, the increase robustness of deterministic optimization procedures encouraged the researchers to develop MINLP models for the synthesis of utility systems. Among others we remind here the work of Bruno et al. [16]. This latter work focuses in fact on the formulation of the utility system and its annualized costs (operating costs plus capital costs over life-time) including a set of non-linear equations used for estimating thermodynamic states of different utility streams (mainly exhaust gases and steam). Still, the pressures of steam lines are considered as boundary conditions that are supposed to be fixed a priori.

The idea of fixing the pressures of steam lines or even temperatures as boundary conditions might result as a limitation of the problem formulation. In technical practice these are often already known by the process engineer who is most likely to tackle the problem of selecting the best combination of a discrete number of pressure lines rather than dealing with continuous range of values for steam pressures. These can be for instance fixed by process requirements or can be already indicated by catalogs of steam turbine producers. The same can happen for the choice of the temperatures of steam headers.

On the other hand, it is convenient to rely on a systematic way of selection of all the operating parameters. This is done by decomposing the overall synthesis problem into a two-level (nested) optimization problem. In a inner optimization step, structural parameters and mass flow rates are assessed on the basis of heat and power integration rules, whereas other intensive parameters which have a non-linear relation with heat loads and power loads are handled in an outer optimization loop. The complete optimization procedure is discussed later in this section.

The core procedure for the synthesis of a steam network for optimum heat and power integration with a given process is in fact the inner MILP optimization problem. The basic idea is to define a superstructure that includes several pressure levels for steam generation and consumption. The key point of the methodology is the codification of steam network structures and the way it is used to build the aforementioned superstructure. A way to address steam network structure is to use the graph representation.

Basic structural elements for steam networks are:

- steam headers distributing steam to the process and to steam turbines.
- condensate headers that collect condensate streams and send them to the boilers.

The linearity of the problem, which allows to formulate the synthesis of steam networks as a MILP problem, is ensured by the definition of the thermodynamic states of these elementary steam and condensate headers. Temperatures and pressures are the same in every point of a single steam or condensate header.
which therefore correspond to given points in the Mollier’s diagram. In the light of the graph representation of the steam network, headers can be conceptually represented as graph knots in which mass and enthalpy balances can be expressed as function of the incoming and outgoing streams. In parallel, condensate and steam headers are linked to each others by means of thermodynamic transformations, which appear as edges of the graph of the steam network. The steam mass flow rates involved in these transformations are the continuous decision variables of the problems.

The steam network consisting in just one pair of steam-condensate headers is shown in Figure 2.18a as a directed graph where condensate header and steam header are represented respectively as a black and a white knot. Water heating, steam production and steam condensation are represented as heating/cooling loops connecting the condensate and steam headers. According to the graph representation, two directed edges connect the condensate knot with the steam knot.

Water has to be heated to produce steam thus generating a cold stream and steam distributes heat by means of condensation thus generating hot streams. Combustion is required to provide the necessary heat for water evaporation and can be represented as a combination of two hot sources (radiative heating and convective heating). A cooling water stream has also to be considered to complete the formulation of the superstructure. This in fact lets open the possibility for the steam network to exchange heat either with the process (in the case of back-pressure turbines) or with the environment (in the case of condensing turbines).

A minimum possible steam network is defined by one steam header and one condensate header. This corresponds to the trivial case of the boiler in which the steam network is substantially at the same pressure everywhere and it is mainly used for distributing heat within the process by means of condensations. A more accurate model should take into account distributed and concentrated pressure losses. In most cases in fact these pressure losses implies the need for water pumping at the inlet of the boiler and some power is spent to drive pumps. Pressure losses are not taken into account in MILP model except for the case in which expansion is consider. In this latter case pressure gaps between inlet and outlet of turbines and pumps are set \textit{a priori} as the difference between pressures of different steam and condensate headers (which are fixed as boundary condition of the problem).

In the Figure 2.18, a graph representation of an elementary steam cycle is also reported. Starting from the elementary boiler structure it is in fact possible to introduce another elementary structure (1 steam header plus 1 condensate header) at higher pressure level (see Figure 2.18b). When two pressure levels are introduced, expansion and compression devices can realize a power cycle in which net power production is the algebraic summation of the electric power required by the pump and the power generated by the turbine. Thermodynamic transformations between steam knots and condensate knots at different pressure levels introduce new edges in the graph representation.

![Figure 2.18: Graph representation of the steam networks superstructure: a) elementary steam boiler, b) steam cycle](image)

The following graphical rules are given for building the steam network superstructure:

- \textit{Elementary structure consists of one condensate knot plus one steam knot at the same pressure}
Knots are vertically displayed according to their pressure level, thus lower knots correspond to lower pressure levels.

- A condensate knot is connected by a pumping transformation plus water heating (cold stream) to another condensate knot at higher pressure level - 1 direct edge

- A steam knot is connected by throttling and expansion transformations (2 direct edges) to another steam knot at lower pressure level

Better explanations of the latter two rules can be given considering that, since thermodynamic states of the knots are defined a priori (which means by an external routine or by heuristic choices of the designer) some structural degrees of freedom must be ensured anyway. For instance the temperature of the condensate header at higher pressure is not necessarily equal to the temperature at the pump outlet or to the saturation temperature at that pressure. In this way if more that one edge is entering a condensate knot (for instance starting from two other condensate knots at different pressures), its temperature can be differently adjusted by independent water pre-heatings. In addition, as it will be explained later, it is necessary to guarantee some steam throttling between steam header knots at different pressures. If this can be in contrast with the idea of recovering the maximum share of exergy of high pressure steam, it is necessary to introduce a degree of freedom in order to adjust mass and enthalpy balances since thermodynamic states of steam headers are defined a priori. Furthermore it could me more convenient to produce steam at higher pressure and use it for heating purpose only (i.e. by-passing the steam turbine) than to use two independent steam production lines at two different pressures (one for power production and heating and one for additional heating only). An alternative way to handle pre-defined thermodynamic state at the knots, is to close enthalpy balances at the knots either with some water or some steam mass flux rate which need to be minimized while maximizing the steam mass flux rates flowing through the expansions for power generation.

In order to overcome the combinatorial complexity related to the definition of multiple different utility networks, a superstructure is used to include all the possible steam expansions and their respective mass flow rates between pre-defined state \((p, T)\) of steam and condensate headers. According to the MILP formulation, instead of optimizing and comparing different design solutions for the steam network, binary variables are used to activate parts of the same superstructure.

Binary variables are assigned to each steam header knot, which automatically activates also the respective condensate header knot at the same pressure level. Remaining decision variables are all the steam mass flow rates that flow from an header to another (following graph edges). In reality, by observing mass balance equations at the knots and the topology of the steam network (the mass flowing between two condensate headers has to be equal to the mass counter-flowing between the corresponding steam headers), the number of steam mass flow rates \(n\) to be optimized is limited to \(n = 3 \cdot (q - 1) + 1\) where \(q\) are pressure levels (couple of steam and condensate headers at the same pressure level), being 3 the unknown mass flow rates for each additional pressure level as it shown in Figure 2.19.

For instance, for a steam network configuration with three rows of condensate and steam headers like in Figure 2.19, seven are the steam mass flow rates to be assessed. In fact for a given row of condensate and steam header, an elementary boiling cycle can be considered thus allowing to use a bigger quantity of steam for process heating at that pressure level in addition to the steam that is further used for steam expansion till lower pressures levels.

The linear relation between mass flow rates and heat and power loads, is ensured by a previous assignment of values to the state variables like pressure and temperature (boundary conditions) at the graph knots (steam and condensate headers) which in fact have a non linear relation with steam network performance. Following the structural rules previously mentioned, one could observe that for a couple of condensate and steam knot only three state variables \(((p, T))\) need to be defined since the two headers operate at the same pressure (these variables can be therefore included in the outer-level decision variable set for a more general synthesis approach). In addition, isentropic efficiencies for pumps and turbines are other boundary conditions expressing the performance of the energy conversion devices (when costs are not expressed as function of isentropic efficiencies these are however left as boundary conditions even
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at the outer-level optimization step being otherwise maximized up to their upper-bound limit). These boundaries conditions for the MILP problem, can be fixed in the way that the resulting steam network structure found by the solution of the MILP problem can be optimally integrated with the process. In fact it is usually possible to identify \textit{a priori} the temperature levels at which the heat (that is steam condensation) is required by the process. Later in this section a two-level optimization approach is introduced where instead these boundary conditions of the MILP heat and power integration problem are further optimized in a outer-optimization loop.

Figure 2.19: Example of steam network superstructure

The overall set of decision variables deriving from the formulation of the MILP problem for the synthesis of the optimal steam network comprise the binary variables $i_q$ associated with the activation of the $q$ couple of steam and condensate headers at given pressure levels, plus the steam mass flow rates $m_j$. In addition, since the steam network requires a hot source for steam production, it is necessary to consider for instance a combustion that can be represented as a combination of radiative a convective heating like in Figure 2.18 resulting from the reaction between fuel and air. For given combustion performance parameters as fixed boundary conditions (to avoid non-linearity), the fuel mass flow rate $m_f$ is also to be added to the set of decision variable. It is also necessary to consider an environmental cold utility (for instance water) that can act as additional heat sink at lower temperature levels, i.e. the water mass flow rate $m_w$ is to be added to the set of decision variable as well.

In Figure 2.19 the edges between condensate and steam knots are identified as cold and hot streams respectively with letter $C$ and $H$. These streams, together with process thermal streams, participate in the total site heat integration. This is done here by applying the Pinch Analysis rules which can be expressed in a mathematical way by the inequality constraint on the cumulative heat loads as in Equations (2.1) and (2.2).

Steam network investment costs can also be expressed as linear function of mass flow rates. According to the MILP formulation, cost functions are governed by binary variables related to the activation or each single branch of the superstructure. Normally equipment cost are strongly non-linear which may induce to use MINLP formulation in place or more simplified MILP one as proposed here. Nevertheless, the estimation of investment costs can be separated into a sequence of linear functions (segments corresponding to size interval), each of which is assigned a binary variable, however leading to a dramatic increase of the computational effort. The expression of the total annualized costs can therefore be used as the objective function of the synthesis problem. Here, for sake of simplicity, we consider to search for the configuration leading to the minimum operative cost.

In agreement with Equation (2.7), the general MILP optimization problem can be expressed as follows:
\[
\begin{align*}
\min \quad c_{tot} &= \dot{V}_{fuel} \cdot c_{fuel} - P_{out} \cdot p_{el} + P_{in} \cdot c_{el} \\
&\quad \forall m \in M = \{m_1, \ldots, m_j, \ldots, m_n, m_f, m_w \in R^{n+2}; m^{low} \leq m \leq m^{up}\} \\
&\quad \forall i \in I = \{i_1, \ldots, i_l, \ldots, i_q \ldots\} = \{0, 1\}^s \\
\text{s.t.} \quad R_0 &= 0 \\
&\quad R_u = 0 \\
&\quad R^u = \sum_{h=1}^{u} Q_h - \sum_{c=1}^{C_u} Q_c + R^{u-1} \geq 0 \\
&\quad u \in U \subset N \\
&\quad \text{where } Q_h = g(i, m) \text{ and } Q_c = h(i, m)
\end{align*}
\]

\(\dot{V}_{fuel}\) and \(P_{in}\) and \(P_{out}\) are eventually expressed as linear combinations of the integer (binary) and real decision variables \((i, m)\) according to the linearized model of the steam network previously described.

In fact in the general optimization problem different prices are assigned to the electricity that is purchased from the grid and to the electricity that is sold to the grid. Depending on the type of contract stipulated with the electricity distribution company and on the legislation that rules the electricity market, there are basically two options for selling or purchasing the surplus or deficit of electricity.

One option is to sell all the electricity produced by the CHP system and to buy all the electricity needed by the process (which is here considered fixed to the value \(P_{pro}\). Under this assumption, \(P_{in} = P_{pro}\) and \(P_{out} = P_{CHP}\) so that the objective function \(c_{tot}\) can be written as follows:

\[
c_{tot} = \dot{V}_{fuel} \cdot c_{fuel} - P_{CHP} \cdot p_{el} + P_{pro} \cdot c_{el} 
\]

The second option is to sell and to buy only the net flow of electricity \(P_{net} = P_{CHP} - P_{pro}\) appearing at the boundaries of the industrial site. This assumption was in fact stated already in Equations (2.8) and (2.9) and considered throughout all the discussion of graphical interpretation of the operating costs minimization problem in the previous sections. According to this second contractual option, a conditional statement must be included in the optimization problem so that

- if \(P_{net} < 0\) then \(P_{in} = P_{net}\) and \(P_{out} = 0\) so that the objective function can be written as follows

\[
c_{tot} = \dot{V}_{fuel} \cdot c_{fuel} + P_{net} \cdot c_{el} 
\]

- elseif \(P_{net} > 0\) then \(P_{in} = 0\) and \(P_{out} = P_{net}\) so that the objective function can be written as follows

\[
c_{tot} = \dot{V}_{fuel} \cdot c_{fuel} - P_{net} \cdot p_{el} 
\]

Conditional statements introduced non-linearities in the formulation of the optimization problem. As a consequence the only way to solve the global optimization problem in the presence of this second contractual option is to solve two separate problems by adding additional constraints: one for \(P_{net} < 0\) with Equation (2.19) as objective function, one for \(P_{net} \geq 0\) with Equation (2.20) as objective function. Eventually the optimal solutions of the two optimization problems are compared and the global minimum found. Alternatively, a single optimization problem can be found provided that \(P_{in}\) and \(P_{out}\) are expressed as function of different set of variables but with the same linear coefficients (being in fact both \(P_{in}\) and \(P_{out}\) expressions of the same \(P_{net}\) respectively when \(P_{net}\) is defined negative or positive). Two new binary variables must be used to control the activation of two different sets of boundary conditions that allow either to obtained Equation (2.19) or Equation (2.20).

It can be concluded that the complexity of the optimization problem dramatically increases in this second case since the number of decision variables is at least double than in the case all the electricity produced by the CHP system is considered to be sold to the market and all the process electricity demand is accounted as fixed purchased electricity.

The idea of using couples of steam and condensate headers at same pressure level as elementary structural components for the steam network superstructure introduces generality to the topological
Figure 2.20: Examples of solutions of optimization of a steam network superstructure
definition of steam networks. In fact, as described in Figures 2.18 and 2.19, for each couple of steam and condensate headers, both steam production (cold thermal streams) and steam condensation (hot thermal streams) are defined as possible thermal processes at that pressure level. In this way the choice of producing rather of condensing steam at that pressure is left as a result of the synthesis problem.

Alternatively, it is possible to consider since the beginning a larger variety of elementary structural components. It must be observed that in most cases it is possible to discern a priori the pressure levels of a steam network superstructure at which steam is to be produced or condensed, being few the cases in which both condensation and production must occur at the same level, thus limiting the number of possible combination to be investigated through the optimization procedure. Accordingly, a less general but more efficient topological description of steam network is to consider as additional elementary structural components, steam production headers and steam condensation headers. A steam production header connects a condensate header to a steam header and generates cold thermal streams. A steam condensate header connects a steam header to a condensate header and generates hot thermal streams. This is however still consistent with the more general formulation of the superstructure previously discussed, the only difference being the fact that given structural constraints (only production or condensation between the couple of steam and condensate headers at the same pressure) are considered as characteristics of separate structural element. This modeling approach is also at the basis of the computational tool for solving heat and power integration problems which embeds the MILP formulation of steam network superstructures. For this topic the reader is referred to the Appendix.

In addition to possible boundary conditions for some steam mass flow rates, the deterministic optimization problem can handle other linear equality or inequality constraints. Some of these are used for modeling the heat integration problem which in Equation (2.17) is given in explicit form. In particular, as already mentioned in Section 2.1.1, once the heat cascade is subdivided into $U$ temperature intervals, the heat transfer feasibility imposes that the algebraic summation of the $Q_h$ and $Q_c$ heat loads, respectively of the $H_u$ hot streams and $C_u$ cold streams, with the net heat $R_{u-1}$ coming from the previous temperature interval in the cascade is positive. Furthermore, since no other hot or cold utility are available, the cumulative heat loads and the extreme temperature intervals of the cascade have to be equal to 0. This in fact implies that the resulting utility system is able to balance completely the process thermal requirements. Other inequality constraints can be for instance used to limit the expansion works to be greater than a minimum value or the total power to be less than a maximum value.

For a given process, for instance that in Figure 2.10, a steam network superstructure can be built as that in Figure 2.19 by setting the pressures and the temperatures of the three couples of steam and condensate headers. As shown in Figure 2.17 the MILP optimization can lead to different solutions depending on the values of price of fuel and electricity. For the same starting superstructure, the change of other boundary conditions or constraints can obviously lead to multiple solutions. As an example in Figure 2.20 different steam network configurations are presented as solutions of the MILP problem for the same process (which requires heat at a maximum temperature of 120°C) and starting from the same steam network superstructure consisting in three couple of steam and condensate headers at 80, 2.5 and 0.05 bar.

In particular, all the three solution were obtained for the same specific cost of fuel but with different price of electricity and by setting some additional constraints. The first steam network consisting in a simple back-pressure turbine was obtained for a low price of electricity (as in Figure 2.17b) so that the optimal solution consists in maximizing power generation until all the process thermal requirement is covered. Yet, the revenue from the electricity sale is not enough to justify an additional production of electricity by means of a condensing turbine. The second solution (in the middle of Figure 2.20) was found for the same values of fuel cost and electricity price with the only addition of particular constraints. On the one hand the maximum power generation was constrained to be lower than the power generation obtained in the previous solution, so that the optimal point is found when this constraint is active. On the other hand an equality constraint is set so that the remaining process thermal requirement is covered by an additional production of steam at 2.5 bar. Conversely, the third solution was obtained for a good price of electricity sold to the grid (as in Figure 2.17a) so that the extra production of electricity by means of a condensing turbine results convenient. As a consequence part of the steam is eventually condensed at 0.05 bar. The optimal solution is found when the constraint in maximum power generation
2.2.4 An optimization procedure for the synthesis of CHP systems

In the previous section different steam networks were generated on the basis of the analysis of the process grand composite curve. Figure 2.21 shows synthetically the main steps of the methodology here presented. Starting from the process thermal streams, which are considered fixed by the requirements of the production sequence, the total minimum energy requirement is evaluated. Pinch Analysis is used to evaluate the total thermal requirement.

Once the opportunity of installing a CHP plant is of interest, the information about MER thermal requirement and process power demand is useful to understand the size range of the utility systems therefore the technology that can be included in the overall evaluations. Furthermore another selection of possible energy conversion devices is done by observing the process grand composite curve which give the idea about thermal loads and temperature ranges that have to be covered by the process. Still the possibilities in terms of number, size and design parameters result in most cases quite numerous therefore an utility superstructure is considered and the afore-mentioned MILP optimization procedure is performed for the definition of the ultimate CHP system design.

Since the formulation of the synthesis problem in terms of MILP problem cannot handle the evaluation of the optimum values of design parameters at the same time, a second optimization step is considered in order to systematically optimize those design parameters upon which the objective function (or more than one) have a non-linear dependency. These are usually pressures and temperatures that are used to fix the thermodynamic states of the branches of the superstructure in order to ensure the linearity of the MILP problem.

Accordingly, a two levels optimization strategy is used for a systematic solution of the synthesis problem: in the inner level, utility structure and mass flow rates are optimized with a deterministic MILP algorithm, in the outer level the optimization of thermodynamic state variable is performed. A similar approach can be found in a work by Papalexandri et al. [104].

The proposed optimization algorithm is presented in more detail in Figure 2.22 for the case in which the synthesis of the CHP system yielding to minimum operating costs is considered. Process thermal streams are imposed as boundary conditions. In addition some utility superstructure parameters can also be imposed as boundary conditions which set constraints to the MILP optimization problem. This latter subset of boundary conditions may comprise for instance the number of pressure levels of the...
steam network, the maximum power production, the maximum number of energy conversion units (like maximum steam expansion stages or maximum number of gas turbines or reciprocating combustion engines in case of a more general synthesis problem).

The optimization procedure starts with the definition of the first array of values for the “non-linear” superstructure parameters (typically the pressures and the temperatures of the steam network headers as previously explained. In the inner optimization loop which is handled by a deterministic algorithm (for instance a Branch and Bound algorithm), the optimal structure and mass flow rates of the utility system that minimize operating costs while covering process demand are assessed.

The value of the resulting operating cost is stored and a new array of values for the thermodynamic variables is issued and the algorithm repeated. This outer optimization loop can be easily processed by a genetic algorithm which is a valuable optimization strategy when dealing with high number of decision variables and multiple sub-optimal points. In addition genetic algorithms are particularly convenient when the search space is discontinuous or with discontinuous derivatives. An example can be the case in which different utility pinch points are activated for different values of the pressure of a steam line which can lead to a discontinuity in the value of fuel consumption and power production (i.e. operating costs). These particular features of the heat and power integration between a CHP system and a fixed industrial process are on the other hand already visible from the analysis of the utility integrated grand composite curves as shown in Figure 2.20. The procedure followed by the algorithm for the definition of the optimal CHP structure and design parameters consists in finding the right match between a sequence of convex (steam production) and concave (process heat pockets) thermal profiles. The search space near the optimal solutions result therefore highly discontinuous. This in in particular true for high number of process thermal streams which complicates the zig-zag profile of the process grand composite curve.

Once one of the end-criteria of the genetic algorithm is reached, the minimum operating cost and the optimal structure and design parameters of the CHP system found. Typically, if the starting superstructure is large enough to include different type of energy conversion devices or for instance a large number of steam and condensate headers for the case of the steam network, there are several different configurations that can achieve values of the objective function around the optimum.

It is possible at this stage to operate in different way in order to refine the procedure of the selection of the optimal utility system. Firstly it is usually convenient when possible to add new objective functions to the optimization that can count for competing aspects. This is in fact the case when different CHP systems lead to similar operating costs but might result in different total investment costs. An option could be therefore that of running a new optimization with two objective functions (operating costs and capital costs). When looking for minimum operating and investment costs a convenient approach could be that of using the annualized cost function thus avoiding multi-objective optimizations.

The critical point of the algorithm is how the CHP superstructure is conceived. On the one hand the idea is to widen the analysis as much as possible in order to include all the possible systems. On the other hand it is preferable to reduce the search space in order to limit the computational effort. The interpretation of the process grand composite curve is an important operation which can support the engineer in stating a proper set of optimization constraints.

Eventually, once the final CHP configuration is obtained the total site Heat Exchanger Network (HEN) must be defined in order to estimate size and number of the total site heat and power equipment. This HEN in fact comprises the heat-exchangers entitled for the process internal heat recovery and for the heat transfer between the process and the CHP system. The synthesis of the HEN structure is another important step of the overall synthesis problem and is considered here as a separate problem the discussion of which is beyond the scope of the present work. Indeed, the reader might note that, if the HEN synthesis is tackled only in a subsequent step, the result of the HEN synthesis problem depends strictly on the result of the CHP synthesis problem. Rigorously, when capital (or annualized) costs are used as optimization criterion for the selection of the optimal CHP system, they should include the share of HEN capital costs so that for each set of structural and design parameter of the CHP system it would be necessary to estimate simultaneously the structure and design parameters of the HEN. On the other hand, in order to limit the computational effort for the solution of the synthesis problem, it is usually preferable to separate the detailed HEN synthesis problem from the CHP synthesis problem, thus allowing to chose different optimization algorithms for the solution of the two subproblems.
Synthesis of steam networks for combined heat and power production

Figure 2.22: Two-level optimization strategy for the synthesis of the CHP system according to a minimum operating cost objective
2.3 On the synthesis of power generating plants

In this section methodological aspects related to the application of heat integration techniques to the synthesis of power generating plants are discussed. The examples that are used to illustrate the major concepts are limited to the maximization of the thermodynamic performances of the various systems and the impact of investment costs on the profitability of plants is not analyzed in detail.

In previous sections the structure and the performance of CHP systems were shown to depend on the thermal and power requirements of the industrial process which they are designed to support. In the light of heat and power integration of the total site (process + CHP system), as presented in Section 2.1.3, the CHP thermal streams are considered in an unique set of thermal streams to be integrated together with the process thermal streams.

Conversely, when talking about power generating plants, systems structure and design parameters are optimized only following the objective of maximum profitability of power generation. In addition ecological indicators, like those provided by the Life Cycle Analysis, are useful tools for supporting the engineer in choosing the cleanest technologies. These latter indicators are often converted into economic quantities for instance by considering the additional operating costs due to emission control or cleaning of plant exhaust streams as the additional income obtained by carbon emission trading when dealing with renewable energy systems.

In analogy with the synthesis of industrial processes, the synthesis of power generating plants consists in the selection of the number and types of components, and their connections, that are able to convert in the most profitable way raw materials into useful products. Thermal power plants in particular convert fuel into electricity which is the most convenient form of energy to be transmitted through a distribution network.

In the field of power plant design, quite advanced plant configurations were developed in the past which are able to reach efficiencies up to 50-60 % (in case of advanced combined cycles). As already introduced by Linnhoff [84], some of the concepts of process integration apply also to the case of the synthesis of the optimal heat transfer section responsible for the internal heat recovery within power generating plants. In fact the main design choices in plant structure and design parameters can be justified in the light of the general criterion of maximum internal heat recovery.

2.3.1 The synthesis of steam power plants

The case of a steam cycle designed for power generation only is a paradigmatic case in which the structure of the system (e.g. different steam draw-offs for water pre-heating) can be justified in the light of thermodynamic benefits derived from the internal heat integration of the steam cycle. This case, already mentioned by Linnhoff in [84], is here briefly discussed since it reproduces most of the concepts already introduced in Section 2.1.3. The MILP formulation of the steam network synthesis problem can be used to find the optimum structure of a steam power plant for power generation only. Temperature and pressures of the steam lines need to be fixed as boundary conditions of the MILP problem as previously discussed in Section 2.2. In fact, when they cannot be fixed a priori as a consequence of other design constraints, they can be optimized in an outer-optimization step as previously presented in Figure 2.22.

An example of the interpretation of the steam cycle synthesis problem in the light of the heat and power integration rules previously introduced is given in Figure 2.23. The synthesis of such a rather complex structure can be shown as the outcome of the heat integration problem between a hot thermal profile of the combustion gases, the steam network modeled as in Section 2.2.3.1, and the cold utility thermal profile (the cold water used at the steam condenser). In the example in Figure 2.23, a cycle with one reheat and three steam draw-offs is shown.

The choice of the optimal structure and design parameters of a steam cycle can be obtained by means of a MILP optimization problem in which steam mass flow rates are the decision variables to be maximized (in order to maximize power) subject to the constraints of the heat cascade problem resulting from the heat integration problem of all the cold streams associated with water heating and steam production, and hot streams associated with steam draw-offs.
On the synthesis of power generating plants

2.3.2 The synthesis of combined cycle power plants

The same synthesis approach based on a MILP formulation, in which the heat integration is embedded as a set of inequality constraints according to the heat cascade problem, can be extended to the synthesis of a combined cycle by including within the set of thermal streams to be optimally integrated (e.g. for maximum power generation) also the hot streams of a gas engine. It is in fact possible to express the contribution of a general gas engine to total power production as a linear function of the gas mass flow rate by fixing as boundary conditions those design parameters that have non linear relations with power production and heat loads (typically the compression pressure ratio and the temperature at the inlet or outlet of the turbine). Following the afore-mentioned methodologies, these parameters can be possibly included in the set of decision variables to be optimized in an outer optimization step.

In the case of the combined cycle power plant, for which a simple scheme is given if in Figure 2.24, the gas turbine exhaust gases are used as a heat source for the steam cycle. It is apparent that the optimum plant configuration depends on the heat integration between the cold streams of the steam cycle and the cooling of the gas turbine exhaust gases. Accordingly, once the intensive variables are fixed, the heat and power integration problem is solved by finding the optimum value of the steam mass flow rate (or more than one in case of several steam lines) for given value of the gas mass flow rate performing the gas turbine cycle. This is equivalent to fix the mass flow rate of the fuel entering the gas turbine and is consistent with the idea of maximizing the energy conversion of a given amount of available “raw material” (fuel in this case).

The synthesis problem of the combined cycle can be complicated by setting a steam network superstructure that includes for instance a second pressure level and some steam draw-offs. The synthesis approach would not differ from what already described for the case of the only steam power plant represented in Figure 2.23. The reader might observe in fact that the activation of a second line of steam production (second pressure level) depends only on the slope of the hot streams. In the case of steam boiler a
great amount of heat is transferred to the steam by means of radiation which can be considered to be preponderant with respect to convection for temperature higher than 1000°C. On the other hand, in the case of the combined cycle, the temperature of the hot gases at the outlet of the gas turbine is much lower than those of the coal fired boiler for instance. This results in a less steep thermal profile of the hot streams which in most cases implies the need for a two pressure levels steam generation to reach high efficiencies. Since the gas turbine outlet temperature depends on the pressure ratio and therefore on the share of total power provided by the gas turbine, this eventually leads to consider a second optimization step for estimating optimal values of temperatures and pressures.

The choice of fixing one of the several system mass flow rates is in fact a way to fix at least one heat load as a boundary condition of the heat integration problem. Other possible ways to fix the size of the power generating system are either to fix the value of power generation (and letting the value of the fuel consumption and all the steam and gas mass flow rate to be evaluated as a result of the optimization) or to fix another mass flow rate within the system for instance a steam mass flow rate. In the general case in which more than one steam or condensate headers are considered as part of the steam superstructure, this latter choice is less convenient since it may set a constraint to the problem thus limiting the optimization algorithm to search for the optimal solution in a restricted area that could exclude the actual global optimum.

It is worth noting again that the linearity of the heat integration problem is ensured also in the case of the combined cycle since mass flow rates affect only the heat and power loads. As a consequence the synthesis of a combined cycle can be expressed as a heat and power integration problem of independent cycles. These are the gas turbine cycle and all the independent steam cycles embedded in the steam cycle superstructure. Rigorously, while the gas turbine cycle and the steam network contribute separately to power generation and to the heat cascade due to their material separation (they exchange only heat at the HRSG), the contributions of independent steam cycles (which are considered to occur within all possible loops between steam and condensate headers) can be separated only by linearizing the response of the steam network to the change of steam mass flow rates. As previously discussed in Section 2.2.3.1, in presence of steam networks with multiple steam and condensate headers (thus leading to consider more than one steam independent cycle), since temperature and pressure of each steam and condensate header are fixed along with turbine isentropic efficiencies, it happens that, as a result of steam expansion with different expansion ratios, steam mass flow rates at different temperatures mix into a same steam header. This leads in general to different values of enthalpy to that imposed by fixing temperature and pressures as boundary condition of the MILP problem. Thus, enthalpy balances must be ensured by using some additional steam or water mass flow rates which represent virtual cycles (i.e. not appearing in the final steam network structure) that reduce power output (since they do not participate in power generation through expansions). This expedient is particularly valid only within a given range of values of intensive parameters, out of which virtual mass flow rates become too large and have to be treated as unfeasible solutions. Still, this linear model of steam network allows to estimate with acceptable accuracy the values of heat and power loads of a high number of configurations.

2.3.3 On the limits of the MILP formulation of the synthesis of energy system

A big limit to the application of the aforementioned synthesis method to more complex systems can arise in the case in which the change of the mass flow rate of one or more branches of the system structure reflects in a non-linear change on the system performance. When dealing with power production plants, this happens for instance when different compounds work in separate parts of the total system and are mixed together in others. In these circumstances, the heat and power integration problem cannot be easily handled as done for the previous problems (as a linear programming problem) because enthalpy balances are ensured only with given set of values of overall system mass flow rates which cannot be adjusted independently to maximize heat integration (that is power generation).

In addition, when power cycles operate with subsequent splittings and mixing of multiple compounds, it can happen that the system configuration with the maximum internal heat recovery does not coincide with that with the maximum total power production. In these other cases the application of the criterion
based on the increase of the mass flow rates of the different subsystems until the maximum heat recovery is obtained, as done for the case in Figure 2.23 and 2.24, can only lead to suboptimal solutions.

It is possible to conclude that the methodology presented in Section 2.2.3 can be a valid tool for the synthesis of power generating plants only when systems can be partitioned in independent subsystems which interact only in terms of heat transfer.

In order to discuss the limits of the aforementioned synthesis methodology when dealing with more complex energy systems, we consider here as an example the case of conceptual design of a fuel cell system fueled with syngas for which a schematic representation is given in Figure 2.25. The system consists in a gasifier in which the solid fuel react with an oxidizing agent to produce syngas. Before entering the fuel cell, syngas is purified and upgraded with an additional reforming stage. Electricity is generated by means of red-ox processes within the fuel cell. Part of the unreacted fuel exiting the fuel cell can be burnt in a additional post combustor to provide some heat to be used within the system. In most cases such a system is not able to sustain itself without part of the product gas being by-passed and burnt in a separate combustion stage. In the light of the heat integration problem, the system can be subdivided into three subsystems which in fact interact only in terms of heat transfer as shown in Figure 2.25. The mass flow rates of these subsystems are not independent of each other being the total gas mass flow rate passing through the gas cleaning and the SOFC and through the auxiliary combustor equal to the syngas mass flow rate within the gasification subsystem. This bond can be easily expressed by imposing that the total syngas mass flow rate is equal to the sum of the two downstream mass flow-rates, thus imposing a linear constraint on mass flow rates.

Even though the modeling of the system requires a quite complex set of strongly non-linear equations, once the mass and energy balance of the three subsystems is performed for given values of the intensive parameters, the heat integration problem can be solved in a separate step. As a result of the optimization of mass flow rates, allowing to achieve maximum power generation, the minimum by-pass mass flow rate of syngas diverted to the extra combustion (i.e. not contributing to power generation) is evaluated. Within each independent subsystem it is in fact possible to express heat loads as linear functions of the syngas mass flow rates. Accordingly, these mass flow rates can be optimized by means of linear programming. An outer optimization loop can be used to find the best values of other design parameters. The internal heat recovery can be shown by means of the process cold and hot composite curves, an example of which is given in Figure 2.26 for the system in Figure 2.25.

The example is a rather simple case of structural optimization and the use of binary variables could be avoided since only three branches are considered, two of which (the gasifier and the gas cleaning and SOFC subsystems) are necessarily present in the final structure.

Following the same approach additional energy conversion subsystems can be added. For instance,
on the basis of the outcome of the heat and power integration, which is represented in terms of process hot and cold composite curves as in Figure 2.26, it is possible to evaluate the opportunity of placing additional energy conversion devices that allow to convert part of the exergy that is otherwise rejected to the cold utility. The system composite curves show that the post combustion of the unreacted fuel after the SOFC, it is enough to cover the gasification and the reforming thermal demands. This also means that in this particular case, further combustion of by-passed gas is not needed. In other words for the given values of design parameters the heat integration problem is of the threshold type. Being the process pinch point at the maximum temperature interval of the heat cascade, the addition of a “bottoming” cycle can be of interest. For instance a steam network superstructure can be added to the superstructure in Figure 2.25 and the synthesis of a more complex SOFC-steam cycle combined power plant explored.

The heat and power integration of this latter system, shown in Figure 2.27, does not appear anymore of the threshold type. In particular the maximization of power generation coincides with maximum heat recovery or, in other words, with the activation of multiple pinch points along the system heat cascade.

Now we are interested in further complicating the system topology by adding recycles of material streams. The approach followed so far, based on the optimization of mass flow rates by means of heat and power integration rules, is no more helpful for instance with a slightly different plant structure like in Figure 2.28. Exhaust gases from the fuel cell are quite rich in steam and SOFC outlet temperature is particularly high. These characteristics are similar to those of the gasification reactions. The recirculation of flue gases into the gasifier can yield to a quite big improvement in plant performance. This in turn implies that the option of separating the plant into sub-systems is no more possible and the MILP formulation used to optimize the heat and power integration of subsystems cannot be implemented. It is simple to observe in fact that, however the system is decomposed in different subsystems, it is not possible to express the heat and power loads of different subsystems to the overall heat cascade and power generation by means of a set of linear equations on mass flow rates.
Figure 2.27: Example of composite curves of an integrated gasification combined SOFC and steam cycle power plant: a) hot and cold composite curves b) integrated grand composite curve (blue: steam network thermal streams, red: all the other plant thermal streams)

Figure 2.28: Example of integrated gasification SOFC power plant with recirculation of steam-rich flue gases into the gasifier
2.3.4 On the decomposition of the synthesis problems in optimization sub-problems

When dealing with the synthesis/design of systems, the separation of the contributions of different subsystems to the overall objective function can be of interest for reducing the complexity of optimization algorithms and possibly the computational effort. This in fact can allow to separately optimize different subsystems and to express the global objective function as a summation of effects of the subsystems at their optimal design points.

Decomposition strategies by Von Spakovsky

Following the idea of reducing the burden of carrying out the analysis of the whole system at once, some efforts were spent in the last decades by Von Spakovsky et al. for the definition of a methodology of decomposing system optimization in a sequence of optimization problems of subsystems [99, 134].

The idea is that the more are the subsystems the simpler is the model of each single system and its respective optimization problem. Benefits in adopting this type of decomposition strategy in big optimization problems are due to the fact that solving several optimizations of small subsystems requires less computational effort than solving the global optimization at once. However, the global value of the objective function must be recovered by re-assembling somehow the system integrity by recovering the physical relations at subsystems boundaries. According to the decomposition strategy suggested by von Spakovsky, this is done by setting proper coupling functions which are used to link the change in the subsystem objective function to the change of the boundary conditions. In particular, the objective function of the global problem must be expressed as some linear combination of the objective functions of the local problems.

In a recent publication of Lazzaretto et al. [81], this methodology is applied to the optimization of simple power plants like combined cycle with one or two pressure levels. Basically subsystems are separated either by cutting material boundaries or thermal boundaries. For the case of a combined cycle two subsystems can be identified more or less following the two elementary cycles (Brayton topping cycle and Rankine bottoming cycle). According to the first approach, the two subsystems are separated at the level of the pipe of the exhaust gases feeding the hot side of the HRSG. According to the second approach the separation is done by virtually cutting the hot and cold sides of the HRSG.

While material cuts are univocally defined by the mass and chemical balance at each mixer of splitter, Pinch Analysis shows how in general internal heat recovery can practically occur by connecting in different way hot and cold thermal streams. For instance, for the case in Figure 2.25 the three subsystems can be disjointed by cutting the material connection at the splitter (highlighted with a red circle in the figure). However, since the HEN structure is not defined in advance, there are no indications on how to set the thermal boundary conditions (thermal coupling functions) between the three subsystems. We already show that in the case the HEN structure is not given a priori, the heat transfer feasibility can be found by applying Pinch Analysis rules to the whole set of the system thermal streams (thus including the thermal streams of all the subsystem simultaneously). Eventually the problem must be solved by accounting the contributions of all thermal streams to the (global) heat integration problem which is in contrast with the idea of complete separation between subsystems. If the aforementioned decomposition strategy can be of success when the separation of subproblems coincides with physical separations between subsystems, the same strategy cannot be easily applied to the case in which system optimization involves subsequent change in system topology like for instance the topology of the HEN for the internal heat recovery.

Superimposition of elementary thermodynamic cycles

An alternative strategy for separating the analysis (design optimization or synthesis) of an energy system into subproblems involving separate subsystems is to identify elementary cycles. This methodology was proposed by Lazzaretto et al. in some recent articles [76, 97]. In the case of the combined cycle for instance the separation of the two elementary cycles is apparent as shown in Figure 2.24 where the arrows indicate the direction of the heat transfer between the hot side of the Brayton cycle and cold side of the Rankine cycle. Indeed, the same observation is at the basis of the two-level optimization strategy
proposed in the previous section. The separation of the two elementary cycles allows to optimize their respective mass flow rates by means of the heat and power integration problem which is formulated as a MILP problem.

In a general sense an elementary cycle consists in a sequence of thermodynamic transformations (e.g.: compression, heating, expansion and cooling). An elementary cycle can be complicated considering staging of components and possible additional cooling processes (between compressions) or reheating subprocesses (between expansions) and can be used therefore to reproduce several cycle configurations. This way to interpret the topology of thermal cycles convinced the same authors to develop a methodology based on increasing system complexity by staging components and cutting thermal links between subsequent stages (some aspects of this methodology are also applied in the present work for the synthesis of the sugar cane conversion process in Chapter 3).

The same approach leads to interpret the topology of some advanced power systems as a superimposition of elementary cycles. For instance this is the case of the steam injected gas turbine cycle (STIG cycle), for which a schematic representation is given in Figure 2.29.

![Figure 2.29: Representation of the STIG cycle according to the method of the superimposition of elementary cycles: a) Basic Plant Configuration b) $T - s$ diagrams of the two elementary cycles (Brayton cycle and high temperature Rankine cycle)](image)

The idea at the basis of the development of the STIG cycle was to reduce emissions produced by high temperature combustion of fuel in gas turbines by injecting water or steam in the combustion chamber. In so doing, the kinetics of some of the reactions that promote $NO_x$ formation is altered and the production of this pollutants reduced. No particular increase in efficiency was technically observed, due to the fact that steam was injected directly in aero-derivative gas turbines which were not designed to accommodate mass flow rates much bigger than the design point mass flow rate. Theoretical studies of the STIG cycles were performed by Rice in the beginning of the '90s [113, 114]. These analyses show instead that thermal efficiencies can be similar to those of the combined cycles. Nevertheless, STIG cycles were found to be too-expensive and water consumption too high.

The reason for high thermal efficiencies can be found by studying the thermal coupling between the two elementary Brayton and Rankine (high temperature) open cycles. In fact the two cycles can be considered as sequences of thermodynamic transformations that start independently (respectively from the air compressor and water pump sections) and superimpose on their last parts (combustion, expansion and at the hot side of the HRSG). Steam is generated in fact by cooling the hot gases at the outlet of the expansion which partially consists of the steam mass flow rate itself. In other words, in addition to the heating capacity of the exhaust gases of the so-called elementary Brayton cycle, the auto-regeneration of the steam elementary cycle is also exploited. This can be done because the high temperature Rankine cycle does not perform the same thermodynamic transformations as in standard steam cycles and reaches instead the same temperature obtained in gas turbine cycles. Thus at the outlet of the expansion the
steam is hot enough to cover the thermal demand of the first part of the cycle before the combustion chamber inlet indicated with a black point along the isobaric heating in the T-S diagram of the $R_HT$ cycle in Figure 2.29b.

![Figure 2.30: Analysis of the STIG cycle according to the superimposition of the elementary cycles: Thermal efficiency as a function of the percentage of air in the total mass flow rate of exhaust gases](image)

An analysis of the STIG cycle and its evolutions in the light of the methodology of the superimposition of the elementary cycle is reported in [97]. Some results are shown in Figure 2.30. In particular thermal efficiency is plotted with respect to the quota of air mass flow rate of the hot air (Brayton cycle thermodynamic medium) in the total mass flow rate (air plus steam) for turbine inlet temperature of $1200^\circ C$ and different maximum operating pressures of the cycle. It is possible to notice that maximum efficiencies are obtained for a particular values of the afore-mentioned ratios. These values coincides also with the maximum heat integration at the HRSG between steam generation (cold thermal streams) and the exhaust gases (hot thermal stream).

Thus the question is whether the contributions of the two elementary cycles to the cycle thermal efficiency can be considered or not proportional to the respective mass flow rates. If so, for given values of design parameters of the two independent cycles (turbine inlet temperatures and pressures), the system model could be described with a set of linear combinations of the mass flow rates. Accordingly, the synthesis methodology based on the two-level optimization strategy described in Section 2.2.3 could be used as presented for the case in Figure 2.25.

In particular, the linearization of the STIG cycle model would imply that the total expansion work can be expressed as a linear combination of separate expansions of the two compounds (environmental air and steam) that are considered to perform distinct elementary cycles. This would mean that the actual expansion occurring in a single turbine as in the real STIG cycle can be described as virtually occurring in two turbines, one for the steam expansion and the other one for the hot air expansion.

For the case of the steam networks, it is quite straightforward to describe the overall steam expansion as a superimposition of multiple expansions between a discrete number of steam and condensate headers since steam is the unique compound undergoing thermodynamic transformations. For given isentropic efficiencies, temperatures and pressures of steam headers, steam turbine specific work can be considered constant and steam network power output can be evaluated as a linear function of mass flow rates flowing in separate (superimposed) steam cycles (corresponding to independent loops between steam and condensate headers). When dealing with multiple compounds instead, for given values of the design parameters the specific work obtained from the expansion of one compound is different from that of the
other one (the $\lambda$ ratio between specific heats is different for different compounds). For instance in the case of the STIG cycle, for fixed values of the turbine inlet temperature, pressure ratio and isentropic efficiency, the outlet temperatures of two separate expansions of steam and hot air differ from each other and are also different from the actual final temperature of the expansion of the mixture of the two compounds and the aforementioned MILP formulation of the synthesis problem cannot be therefore considered.

As a consequence, in presence of mixtures of different compounds, the superimposition of elementary cycle does not lead to the description of systems in terms of linear combinations of mass flow rates of single compounds.

2.3.5 On the separation of the heat transfer section in the synthesis of thermal power plants

Although it is not always possible to handle the synthesis problem by solving the heat integration problem between sub-systems, it is apparent that Pinch Analysis offers a quite straightforward way to treat the heat transfer between different system streams. Mainly, heat integration rules can be used to verify the heat transfer feasibility between system thermal streams without considering a priori a HEN in which the system internal heat transfer occurs thereby letting the optimization of the design parameters of the main system components to be tackled as a separate problem from the HEN synthesis problem.

This latter concept is at the basis of a general methodology proposed by Lazzaretto et al. the application of which is presented in several papers about the synthesis and design optimization of different types of energy systems [77, 78, 79, 75, 128]. The reader is in particular referred to [80] for an exhaustive description of the theoretical aspects of the methodology named HEATSEP.

According to this methodology the synthesis of a thermal power plant starts from the definition of a “Basic Plant configuration” (BPC) which represents the “basis” design concept of the plant or, in other words, a technical representation of a preliminary idea of the plant. The plant BPC is in particular defined by a heuristic choice of a type of technology. In most cases various factors, which cannot take into account in a computational algorithm, play a major role in the preliminary step of conceiving the BPC.

Compared to the actual plant configuration that is expected to be the result of the synthesis problem, the BPC can be considered as the embryonic state consisting in all the components responsible for chemical or mechanical conversions and their physical connections. With reference to the case of the integrated gasification SOFC system a representation of a possible BPC was already given in Figure 2.28.

The reader might observe that heat exchangers performing the internal heat transfer are not present in this type of representation. The definition of the HEN responsible for the internal heat transfer is in fact left as a separate problem which can be solved once the ultimate structure and the optimal design parameters of the BPC are found. Nevertheless, the feasibility of the internal heat transfer must be verified every time the BPC is modified or one of its parameters changed. Among different methods, Pinch Analysis is chosen to check the heat transfer feasibility between system thermal streams.

For this purpose the HEATSEP methodology suggests to highlight the internal heat transfer section by virtually cutting thermal links between subsequent components and including all the heat sources and heat sinks related to the operation of basic components (for instance reactors). This preliminary construction step is represented in Figure 2.31 for the case of the integrated gasification SOFC system.

In the light of the formulation of the synthesis or the design improvement procedure in terms of a mathematical problem, a set of decision variables must be defined. These are selected among the main structural or design parameters. The number of decision variables is in principle related not only to the size of the system and its complexity but also to the desired dimension of the problem and eventually on the affordable computational complexity. However, according the idea of introducing virtual thermal cuts between components, a minimum number of decision variables exists. These are the temperatures that are introduced by the thermal discontinuity within cuts.

In addition other decision variables can be chosen. For instance, referring to the example in Figure 2.31, in addition to the set of the temperatures already shown in the figure, other convenient decision
variables can be the mass flow rates of the exhaust gas recirculation and that of the oxidizing agent entering the gasifier.

Conversely, the number of decision variables can be possibly reduced by technological limitations or process requirements. For instance, in the case of the integrated gasification SOFC system, it is possible that the temperature of the particles filter is constrained to be below 500°C. This is typically imposed by the convenience of cooling the product gas under the condensation temperature of the alkali metals, so that metallic particles can solidify and be mechanically removed by the particles filter. In addition, since the SOFC operates at high temperatures, the product gas must undergo a subsequent reheating process. Thus the performance of the system most likely does not benefit from additional cooling of the gas under the temperature limit imposed by the particle filter (500°C). As a consequence it is possible to fix the temperature $T_{5}$ as a constant parameter.

We now look for the values of the decision variables that optimize the power generation of a given system BPC. The so-called HEATSEP methodology does not give any particular indications about the optimization algorithm to be used. This might depend on each particular case and on the way the problem of synthesis or design improvement is stated. The unique feature of the methodology is rather the way the selection of the decision variable is formalized and the way the internal heat transfer is handled throughout the optimization procedure. In particular the heat integration is not treated as an inner optimization step like it is done according to the two-steps procedure described in the previous sections. In fact, as already discussed for the case in Figure 2.28, the maximization of the power generation (of plant efficiency) does not coincide in general with the maximization of the internal heat recovery. Accordingly, the focus is no more on the maximization of the mass flow rates of independent subsystems, which was previously handled as a linear optimization problem, but on the maximization of the plant performance with respect to the whole set of decision variables. The heat integration via Pinch Analysis is therefore included only as a constraint in the optimization and can be generally expressed as in Equations (2.1) and (2.2).

According to this methodology, the synthesis or the design improvement procedures are formulated as a complete non-linear (mixed integer when using a superstructure) optimization problem which is solved in one step optimization algorithm.

For the design of a generic power generating system, a schematic representation of the optimization procedure is proposed in Figure 2.32. At the top the procedure values are assigned to the decision variables and the system flow-sheet is used to perform mass and energy balances. As a result, a set of
Figure 2.32: Procedure for the system design optimization according to the HEATSEP method
hot and cold streams is identified and the problem table is set according to the Pinch Analysis rules. Since the input fuel mass flow rate is kept fixed as a boundary condition of the problem, the heat transfer feasibility is ensured only if the heat integration problem results of the threshold type. This means that there is no need to solve the problem table by finding the system pinch point and the MER hot utility. On the contrary a system design point (a solution of the mass and energy balance for given values of the decision variables) can be discarded once the cumulative heat load in one of the intervals of the system heat cascade is found negative (Pinch Analysis rule). If the internal heat transfer is found feasible the solution is acknowledged as a valid system design point, and system performance indicators (thermal efficiency, exergetic efficiency, operating costs, annualized costs, etc.) can be evaluated. The new array of values for the system decision variables is then chosen by the optimization algorithm. When possible, a deterministic algorithm can be used to performed the optimization loop. However, it is worth reminding that the way the heat transfer feasibility is ensured throughout the algorithm, leads to a highly non-linear constraint with discontinuous derivatives. Whenever it is possible to handle such a constraint, the non-unimodal characteristic of the search space is another limitation to the implementation of deterministic algorithm. A possible strategy is to use robust sequential quadratic programming in combination with an heuristic algorithm that can help explore different subsets of the search space. An alternative strategy could consist in using genetic algorithms which can handle in an easier way objective functions with complex behavior, at the expense of a higher computational effort. An important difference between the pseudo-deterministic approach and genetic algorithms is the way in which the heat transfer constraint is processed by the optimization algorithm. While in the first approach this is implemented as a non-linear constraint which cuts out the unfeasible domain of the search space, in the second approach it is evaluated as a penalty factor to the objective function (which smoothens the search space boundaries).

Another important advantage of the so-called HEATSEP method is the fact that the formulation of the synthesis or design optimization problem does not rely on values of cold and hot thermal streams. In fact the set of thermal streams to be integrated is built after the mass and energy balances are performed and depend on the value of the decision variables only. This feature introduce generality to the problem and can lead to optimal internal heat transfer configurations that are not expected before the complete solution of the optimization problem.

On the use of virtual hot utility for balancing unfeasible heat transfer
We suppose now to tackle the same design optimization problem (for instance for the system presented in Figure 2.28) following the two-level optimization strategy described in Section 2.2.4 and in particular in Figure 2.22. The system cannot be subdivided into separate subsystems which add linear contributions to the objective function (for instance power generation). Accordingly, all the mass flow rates of the system must be considered as decision variables or as dependent variables. So the first step of the algorithm is totally equivalent to that in Figure 2.32. However, the heat integration problem is solved as a separate inner problem and an additional hot utility is evaluated when additional heat demand is needed to balance the system thermal requirement. This is handled by adding a virtual combustion to the problem formulation and its heat load expressed as a linear function of an additional fuel mass flow rate. The result of the MILP internal optimization loop is the presence or not of this additional combustion and the amount of additional fuel. This is subsequently introduced as a penalty factor to the final objective function. This latter procedure is schematically represented in Figure 2.33.

The synthesis of an energy system can be defined as the problem of defining type, number of components and their connections. The synthesis problem, as it was lately described in this Section, was almost reduce to the HEN synthesis responsible for the internal heat transfer. It is apparent that the major problem that the methodologies so far described aims to solve is in fact how to optimize design parameters of an already defined basic plant configuration without dealing with the definition of the actual HEN.

On the other hand, the synthesis problem is much more general and aims at finding in a systematic way the best BPC among a set of possible competing BPCs. There can be many different ways to realize a same idea of energy conversion system. For instance these different BPCs can be conceived by trying different connections between material streams and components (compare Figure 2.25 and 2.28). To
some extent, a systematic procedure for generation of different plant configurations was shown for steam network in Section 2.2. However it was recently shown that the general problem is not easily reduced to such linear or MILP formulation and deserves a much larger type of formulation.

In the next section, the synthesis of an industrial plant and of the utility system required to support the plant operation is discussed with particular emphasis on the way new BPCs can be generated.

![Diagram](image)

**Figure 2.33:** Procedure for the system design optimization according to the two-level optimization strategy
2.4 A generalized approach for the synthesis of energy intensive industrial processes

Major aspects of the methodologies for heat and power integration were discussed in the previous sections. Pinch Analysis rules result the ultimate tool for the definition of optimal thermal interactions between thermal streams within a system. These rules were applied to the case of CHP plants designed for supporting industrial sites. As a result of the heat integration of process thermal streams, the process grand composite curve were used for identifying process requirements in terms of heat loads and temperature levels. Accordingly, we discussed in Section 2.2 the design of CHP system in order to cover these thermal demands along with process power requirements. Possibly extra power can be used to generate additional electricity to be sold to the market. Some of the aspects related to the systematic synthesis of CHP systems for a given process, with particular emphasis on the topology of steam networks, were also discussed and eventually algorithms were also presented in detail.

In addition, the problem of the synthesis of systems for power generation only was the object of discussion in Section 2.3. While CHP systems commonly feature the coupling of relatively standardized technologies like internal combustion engines and steam cycles (networks), advanced configurations of power plants can present more complex characteristics which complicate the definition of a general methodology for the system synthesis. In fact, when system performance has non-linear dependency on mass flow rates, these cannot be evaluated by only analyzing the heat integration by means of the system grand composite curve (as done instead when linear models apply). In those cases in which the performance of a system cannot be described as a linear combination of the performances of subsystems, the application of the Pinch Analysis rules remains nonetheless the basic tool for the separation of the problem of the synthesis of the internal heat transfer section to the problem of the synthesis of the system basic components, that is here called the Basic Plant Configuration (BPC).

This latter methodology, also referred a the HEATSEP method (see Section 2.3.5), is based on the idea of identifying the BPC and modifying it in order to find improvements in process performance while checking heat transfer feasibility by means of Pinch Analysis rules.

In the present work we want to give indications on how to improve the structure and the design parameters of energy intensive industrial plants. The boundaries of the set of streams and components that are subject to modifications are not only those of the CHP system or those of a general energy conversion system but those of the total site. They include therefore also the components and their connections that are involved in the production process of particular goods (in general more than one).

According to Pinch Technology [67, 84], it is common to call process that part of the overall system that is responsible for the production of desired products and is considered fixed in the heat and power integration problem both in terms of performance and mass flow rate (as discussed in Section 2.1). Conversely the parts of the overall industrial plant that can be adapted to the process depending on its energy requirement are addressed as utilities. The distinction is not only physical but also methodological since in Linnhoff’s methodology the process is a rather fixed entity that is not subject to modifications.

The reason for highlighting a methodological separation between process and utility besides a physical one, relies on the fact that process design parameters are seldom imposed by energy saving related issues. In most cases transformations and their respective heat and power demands within a process are dictated by the productive process itself. Thus most of the process components and their design parameters necessarily remain fixed in order not to alter the way the raw material (or more than one) is converted in useful product (or more than one).

Here the approach is instead to extend the analysis to the effects of process modification in total site energy performance. Thus the formalism introduced by Linnhoff is hereafter mostly used to distinguish the location of components or streams within the total site than to identify separate subproblems.

In Figure 2.34 a general overview of the synthesis problems is given. The first simple problem considered at the beginning of the chapter is the thermal integration of process thermal streams. Hot and cold utility thermal streams are considered in order to cover process heating and cooling demands that cannot be satisfied by internal heat recovery (problem a). If then these thermal and power demands must be covered by a CHP system, another independent synthesis problem has to be tackle which involves the definition of the types and number of CHP energy conversion systems (problem b). In this
latter problem however, the heat integration is not extended to the CHP system and the relation between process and utility system consists only in a heat load sufficiently hot to cover the process heat and power demands. This may refer to those cases in which the CHP system is designed in order to generate a given amount of steam at some pressure as required by productive subprocesses thus not leading to fully heat integrated configurations. In these cases the selection of the devices for combined heat and power production can be done without analyzing in detail the heat integration opportunities between the process and the CHP systems, just by evaluating the total steam and electricity requirements of the productive process.

A different problem which was largely discussed in previous sections is that of considering process and CHP thermal streams as part of a unique set of thermal streams to be integrated (problem c). Thus the structure and the design parameters of the CHP system are exclusively designed for a given process.

The ultimate general problem (problem d) is that of considering the process no more a “fixed entity”. In this case in fact some of its structural features along with design parameters can be changed in order to better accommodate the CHP system and vice-versa.

![Conceptual boundaries of different total site synthesis problems](image)

Figure 2.34: Conceptual boundaries of different total site synthesis problems: a) Process thermal integration, b) Separate synthesis of CHP system for given process thermal and power demands, c) Synthesis of heat and power integrated process and CHP system, d) Total site synthesis

The general problem behind the search for the optimal total site configuration remains that of converting in the best way with available technologies the raw material in something that can be profitably sold to the market. This way of thinking at processes can be somehow acknowledged as a top-down approach of synthesis: from the raw material (top) to the products and by-products (down). Conversely when following a bottom-up approach, both the process and the required raw materials are to be designed in order to generate a fixed amount of product.

The bottom-up way of thinking at industrial process evolution seems to reflect the step of complete substitution of the production chain and raw material for the production of a specific product. In the particular case of sugar and ethanol production this would mean for instance to consider the opportunity of producing ethanol from fermentation of ligneo-cellulosic biomass rather than yeast fermentation of sucrose-rich juice.

Between the two, it seems on the other hand that the first approach reflects the actual evolution of industrial processes in which new products or by-products are produced by adding few additional components and rerouting part of the raw or intermediate materials. This approach is considered here and a procedure for the synthesis of energy intensive industrial processes is proposed accordingly. The same approach is followed also in the subsequent chapters where the synthesis of sugar-cane process is examined (sugar cane is converted into sugar, into ethanol, and then also into electricity),

In the light of the total site synthesis problem, the general problem concerns the definition of the structure, that is the number, type of components and their connection of both the so-called process and utilities, and their design parameters. While the complexity of the synthesis problem can possibly
be reduced by neglecting some trivial structural modifications or some trivial decision variables, the objective of the synthesis is to broaden the analysis towards more interesting configurations.

Starting from an original idea of the plant, different questions are posed: what are the possible new products to be generated? Is it possible to improve the conversion of the same given raw material? Which criteria are followed while modifying process design parameters?

According to the top-down approach an initial (original) idea of the process is conceived by the engineer and the so called Basic Plant Configuration is defined. This idea results into a process flow-sheet which does not include heat exchangers as discussed in Section 2.3.5.

When dealing with the design of energy intensive processes there is the interest in knowing how process modifications (that is the change in process design parameters) impact on the total site thermal and power demands while keeping constant the quality and the quantity of the main products.

This first Basic Plant Configuration is therefore analyzed in the light of the HEATSEP method in order to explore improvement in process performance by changing process design parameters. The method was so far applied to the search for optimal heat integration within thermal power plants (Section 2.3.5). When dealing with the internal heat recovery associated with thermal power plants, most of the temperature values, deriving from cutting of thermal links between components, can be included in the decision variable set. Conversely, in an industrial process most of the temperatures are in general already dictated by process requirements and therefore cannot be included in the set of decision variables.

The initial optimized BPC configuration is subsequently modified in order to explore possible better total site configurations. It is clear that in general, as soon the process is modified, it might happen that conversion performances change accordingly. This is not always true if for instance the modifications do not change reaction kinetics or mechanical transformations. Accordingly, among the whole set of process components and their operating parameters, only those that are responsible for thermal and power demands are considered to be modified. After the BPC is optimized, heat loads and temperatures of thermal streams remain defined. These data are then used for building the HEN responsible for the internal heat recovery section.

The final aim of the research, which main methodological aspects are discussed in the present work, is to propose a systematic way for the synthesis, possibly to be translated into a calculation algorithm. By now only an organized procedure for the generation/modification of process BPCs is given. This consists in the following structural modifications:

1. Staging of components.
2. Change in material connections between components by adding material splits or mixers.

In more detail, while staging of components and change in material connections between components are modifications which do not alter the basic concept behind the BPC, the addition of new components result in the definition of a new BPC. After the BPC is modified design parameters of the BPC must be optimized. Here the objective of the BPC design parameters optimization is to increase process energy performance or in other words the process primary energy savings (under the assumption of constant input of raw materials and constant production rate). The optimization procedure considered here follows the objective of minimum process hot utility demand which is evaluated by solving the heat cascade problem. This objective function is chosen for the optimization of the design parameters of the sugarcane industrial site in Chapter 3.

While electricity and heat do not appear in general among the products of an energy intensive industrial process (with the only obvious exception of power generating plants), there are few cases in which part of the raw material can be converted into heat and electricity thus letting to partially or completely cover the heat and power demands of the productive process. Accordingly, when an excess of electricity and heat can be produced by a CHP system fueled by on-site by-products (like the case of the bagasse within the sugarcane process) it is convenient to perform design parameters optimization in order to estimate the maximum net power production. Electricity (along with heat in presence of a district heating network) is in fact the valuable product that can be maximized while minimizing the heat and power consumption of the productive process (the part of the total industrial site responsible
for the conversion of raw materials into material products). This objective function is chosen for the optimization of the design parameters of the sugarcane conversion industrial site in Chapter 4.

In the field of energy systems and chemical processes important indications about heat and power integration can result from the analysis of the process grand composite curve. Changes in the original PBC can be interpreted and possibly conceived by using the integrated grand composite curve representation which allows to analyze the impact of one subsystem, for instance that is modified in subsequent synthesis steps, in the total site heat cascade.
Chapter 3

Synthesis of the sugarcane conversion process

The methodology presented in the previous chapter about the synthesis of energy intensive industrial processes, is used here to identify the optimal plant configurations and design parameters of an industrial facility converting sugar-cane into sugar and ethanol. A variety of structural alternatives can be considered for the synthesis of large sugarcane conversion processes. In addition the process is highly energy intensive thus representing an interesting case study for the application of the methodology so far introduced.

Those readers who have an expertise in the process of conversion of sugar-cane may find some technical solutions proposed throughout the following discussion already consolidated. In fact, the idea is to show the evolution of the topology of the sugarcane conversion plant as a result of a structured synthesis procedure, the guidelines of which were presented in detail in Section 2.4 for a general case of a energy intensive industrial process.

The chapter is organized in three main sections in which the synthesis of three basic concepts of sugarcane conversion process are presented. These are the sugar production, ethanol production and combined sugar and ethanol production processes. At the beginning of each section a base case Basic Plant Configuration (BPC) is defined and the maximum potential of thermal integration is evaluated by means of Pinch Analysis rules. The HEATSEP method, previously discussed in Section 2.3.5 as a methodology for the optimization of power generating plants, is here applied in order to perform parameter optimization of the BPCs following the objective of minimizing the process thermal demand under the hypothesis of constant mass flow rate of the sugarcane input (138 kg/s). Accordingly, thermal links between subsequent components are virtually cut and all the independent end-temperatures and mass flow rates are included in the set of decision variables along with all the other independent design parameters that can affect the process thermal demand.

Following the aforementioned organized procedure for the modification of BPCs, new BPCs are subsequently generated starting from the base case by adding step by step additional stages of components and by introducing new material connections by means of splitters and mixers. Eventually some components are substituted and some others are added according to a different process concept therefore leading to a new base case BPC.

The process grand composite curve is interpreted in order to locate the sub-processes, which modification (both in terms of structure and design parameters) can lead to further minimization of process thermal demand. This Pinch Analysis tool gives in fact a straightforward indication not only about the process thermal demand (corresponding to the horizontal extension of the curve at the higher temperature level) but also about the possible thermal pockets in the process heat cascade (relative large temperature intervals in which the process behaves as a heat source separated by temperature intervals in which the process behaves as a heat sink) that can be better balanced by optimizing structure and parameters of some subprocesses therefore affecting some or all the thermal streams participating in the process heat cascade.
For sake of consistency between the process configurations explored step by step in the following pages, the conversion performance of each process component (the way chemical and material transformations occur within a component) is considered constant, remaining fixed in this way the quality and the quantity of the product obtained from sugarcane conversion. In fact, in the presence of combined production of sugar and ethanol it is possible to change production rates of each single product, for instance in the sugarcane conversion process by diverting in different ways intermediate flows of sucrose-rich juice. If component performances are kept constant, the total conversion of raw material does not change. This is possible only if component characteristics do not change in a quite large range of components sizes which, for the sugar-cane conversion plant can be considered related to the volumetric flow rate of sucrose-rich juice (or syrup). The possibility of intervening in process productivity by exploiting by-products that were in a previous instance rejected as waste-products is also left open. In particular, among the possible process modifications that increase productivity of the sugar-cane conversion plant, the recycling of the molasses into juice fermentation and the use of bagasse for the production of heat and electricity are considered here, being extensively employed in modern sugarcane conversion processes. In the case of the sugar-cane conversion process we refer to productivity as the aggregated production of sugar, ethanol and electricity with respect to the fixed input of sugarcane. This concept can be also referred to as process profitability that is the ability of the process to produce money as a net income between process expenses and the sell of goods. A common criterion for accounting process profitability is the Net Present Value of the industrial site after its life time.

The following assumptions are considered in the analysis:

- Steady state conditions: effects of process dynamics are not considered.
- Continuous process: within a given process configurations all components operate continuously.
- Design point operation: for a given set of components, production efficiency is considered at its nominal value. Components are considered to operate only at optimal conditions for mechanical and chemical transformations.
- The total input of sugarcane mass flow rate is fixed at 138.9 kg/s.
- The potential for heat integration is solved according to the Pinch Analysis rules under the hypothesis of 4°C of minimum temperature difference between hot and cold streams.

There could be several possible starting configurations for the conversion of the available sugarcane, since this raw material is potentially convertible into different products with already high-reliable technologies. In the case of the sugarcane, the processes for the production of white sugar, rum or ethanol are already quite well known. Yet, the choice here is to start from the concept of a factory producing only white sugar and progressively including additional process alternatives until the process layout will comprise the combined production of ethanol and sugar. Starting from this latter basic plant configuration, the problem of the optimal configuration (structure and parameters) of the total industrial site including the process and a bagasse fueled CHP system is separately discussed in Chapter 4 following the objective of maximum net electricity production.

The selection of the components and their design parameters affecting the sugarcane material conversion is based on the work of Ensinas et al. [27, 28] in which the analysis of the heat and power consumption of a combined sugar and ethanol production plant is reported.

The reader is referred to the Appendix for a better description of all the computational tools used for modeling, simulating and optimizing the plant configurations analyzed in this chapter.
### 3.1 Production of sugar

Sugar cane basically consists of water (mass fraction 73-76%), soluble solids (10-16%) and dry fiber (11-16%). Soluble solids are the chemical compounds that must be extracted from raw biomass and then converted into the desired products. In particular, the main compound involved in sugar production is sucrose, which makes up the major part of the soluble solids (up to 88% of the soluble solid mass fraction). Other types of sugar like glucose and fructose, salts, and other organic compounds are the components of the remaining part of the soluble solids [119]. In Figures 3.1 and 3.2 the main transformations carried out in a sugarcane conversion process are described in terms of change in composition of material streams.

![Diagram of sugarcane conversion process]

**Figure 3.1:** Overview of composition from raw cane to bagasse and sucrose-rich juice

A typical sugar cane factory converts sugarcane into white sugar. This is done in principle by smashing the cane, extracting the sucrose-rich juice and crystallizing the sugar by means of boiling and drying. A simple overview of the process is shown in Figure 3.3.

A description of the main sub-processes involved in the conversion of the sugar cane into sugar is presented in the following paragraphs.

The sugar cane is firstly chopped by a set of knives and then smashed in a set of mills in which water is added in order to dissolve the soluble solids and extract them from the original fibrous cane structure.

These operations occur within the juice-extraction sub-process. Water (10-35% of the cane weight) is added counter-currently in the last mill with a part of juice recycled backward in order to increase the extraction (imbibition). From each mill the extracted juice is collected in a tank then strained. The first row of mills produce a juice (crusher juice) with 12-17% sugar content. In the last mills, the juice obtained have 1-3% sugar content. At the outlet of the extraction sub-process the juice is dark colored, at 4-5 pH with high water content and 10 - 15%wt of solids.

At the outlet of the extraction, juice is sent to the juice treatment section. The juice extracted from the biomass in fact still presents a quite high content of undesired organic compounds which have to be removed. In particular the undesired "inverting process" may be occur under some uncontrolled process conditions:

\[
C_{12}H_{22}O_{11}(\text{sucrose}) + H_2O ⇌ C_6H_{12}O_6(\text{glucose}) + C_6H_{12}O_6(\text{fructose})
\]  

(3.1)

The inverting reaction is the hydrolysis of sucrose (polysaccharide) in fructose and glucose (invert sugar) which have a lower sweetness (saturated sucrose-water solution is referred to as sweetness equal to...
Synthesis of the sugarcane conversion process

1, whereas fructose and glucose have around 0.85 sweetness and therefore are undesired in the sugar production). The reaction is driven by the presence of an acid environment (low pH) or by an enzyme (invertase). In the case of an acid environment the reaction speeds up with the temperature increase instead in the case of enzymatic hydrolysis high temperature can inhibit the activation and cooling may instead favor the reaction. Thus, in the treatment section, addition of chemicals (lime and sulfuric acid) and juice heating take place. The juice is heated up almost to the boiling point 115°C (105°C is usually a better process condition) in order to destroy invertase and avoid downstream enzymatic inverting processes [119]. The juice is treated in a clarifier with lime (CaO) in order to increase the pH and stop the acid sucrose inversion. Then some sulphuric acid is used to precipitate some inorganic material. The precipitated form goes to a filter and washed. The filter cake is rejected and part of the water is recycled in clarifier.

Since the sugar production consists mainly of the extraction of the sucrose and its crystallization, juice is firstly concentrated up to its saturated concentration 62-69%wt (thick juice) in the evaporator and then crystallized.

The juice coming from the clarification process has usually a sugar content around 10-16% (thin juice). The temperature of the juice along the evaporation has to be under the discoloration temperature that is 132°C [119].

In the case of the use of multiple shells evaporators, an independent hot stream would be required for each shell and, on the other side, the vapor phase (basically the water and low-boiling substances from the juice) of each evaporation unit would be simply extracted, condensed and sent to sewage treatment.

Since evaporation is one of the points in the overall plant with the highest heat demand, the heat of the vapor exiting each evaporation unit is technically exploited within the evaporation process itself by means of multi-effect evaporators. A schematic representation of such equipment is given in Figure 3.4 in which an evaporator with 5-effects is presented.

Multi-effect evaporators are used in the pulp and paper and food-processing factories. Single evaporation units are usually of the type of the Robert Calandria evaporator. In the first effect of the multi-stage evaporation system, steam from a separate boiler is used for heating up the juice. The steam condenses and exits the evaporator at the bottom side (this results in a condensate stream of pure water to be recycled to the steam boiler). At the juice side the vapor phase exits the unit on the top. This vapor phase is used as an heat source for the next effect (multi-effect evaporator strategy). The main princi-
Figure 3.3: Scheme of a sugarcane mill for production of sugar (©encarta.msn.com)

Figure 3.4: Co-current five-effects evaporator
ple of the multi-effect evaporator is to evaporate the juice in subsequent stages at progressively lower pressures. At lower pressures the saturation temperature also decreases and evaporation can be carried out using part of the vapor of an evaporation unit operating at higher pressure (considering a technical temperature difference between the vapor phase at the hot side and the liquor at the cold side).

There could be different configurations depending on the relative paths between cold and hot streams (juice and vapor) as in the design of heat exchangers networks. In Figure 3.4 a typical co-current configuration is shown where the steam follows the same sequence of effects of the juice. According to desired concentration increase in each single effect, which fixes the water mass flow rate to be evaporated from the juice, the steam coming from a unit is only partially diverted towards the subsequent unit, the exceeding part of the heat usually being employed for other heating purposes in the process.

The minimum operating pressure for commercial Calandria unit is around 0.10-0.2 bar. In addition to the pressure change along the multi-effect, the temperature of the liquor also decreases from the first effect to the last effect [119] (usually from 130°C to 90°C), the temperature depending on the pressure when the juice evaporation takes place.

The last operations that are needed for the production of the massecuite (dense water-sugar mixture) and of the sugar (solid granular white or brown sugar) are: evaporating crystallization, cooling crystallization and centrifugation. These are grouped within the crystallization sub-process.

The thick juice has a content of 60-70%wt sugar available at the outlet of the evaporation and the product stream is subsequently concentrated up to the 85-92%wt crystalline sucrose content. The by-product of the process is the molasse (solid content = 85-89%wt, sugar content = 50-60%wt, non sugar content = 32-40%wt). In evaporating crystallization the thick juice is heated up in pans at 0.2-0.3 bar at the evaporating temperature of 65°C-80°C till metastable crystallization conditions. The crystallization is promoted by the seeding of some microcrystals such that crystals grow till the desired size. To complete the process, mixers and centrifuges centrifuge off the sugar. Up to 85%wt of the sucrose is produced through only evaporating crystallization and centrifugation. The remaining syrup can be still use for the production of other white sugar by means of cooling crystallization. The principle is to separate the sugar by reducing the temperature and therefore the solubility of the sugar in water. The sugar is cooled from 65°C to 35°C. The surface water content must be further reduced down to 0.03-0.05% with a subsequent air-drier downstream the crystallization units.

3.1.1 Modeling assumptions

In order to evaluate the electricity and thermal demand of each of the generated process configurations, a mathematical model of the sugarcane factory is considered. The juice properties are expressed as a function of the following juice characteristics:

- **B** Solid content [%] expressed as the mass percentage of solid material in the juice
- **Z** Purity of juice [%] expressed as the sucrose mass percentage of the solid part
- **cp** Specific heat [kJ/kg-K] of the corresponding sucrose-water mixture

The following expression reported in the literature [102] is used to evaluate the thermodynamic properties of the sucrose-water mixture as a function of solid concentration **B**, sucrose concentration expressed as the product between **B** and **Z** and the temperature **T** [K]:

$$ cp = 4.1868 - a \cdot B + b \cdot B \cdot Z + c \cdot B \cdot (T - 273.15) $$

with $a = 0.0297; b = 4.6\text{E-5}; c = 7.5\text{E-5}$.

Multi-stage evaporation is a way to locally (that is within this sub-system) reduce the process thermal demand by means of a better heat integration between evaporating units.

Since the multi-effect evaporator is also the component showing the major potential for process integration, a detailed model of this component is considered. The main operating principle of the multi-effect evaporator is the pressure cascade which is an effective way to minimize the heat requirement for evaporation. In fact steam saturation temperature is lower at lower pressure. It is therefore convenient
Figure 3.5: Possible configurations of multi-effect evaporator: (a) counter-current, (b) co-current, (c) mixed

to exploit the latent heat of the steam that is evaporated in one effect to heat up the juice in a subsequent effect. This can be done only if this second effect operates at a lower pressure which corresponds to a lower saturation temperature.

Crucial design parameters for multi-stage evaporation are:

- Number of effects: the higher the number the lower is the reduction in total energy requirement.

- Solid content profiles along the evaporator: heat loads of different effects depends on the amount of water to be evaporated that is on the desired increase in solid concentration.

- Operating pressure profile: the juice stream can follow co-current, counter-current or mixed configurations.

In Figure 3.5 three configurations are presented. Counter-current configuration requires forced circulation, since the juice enters the effects progressively at higher pressures which can complicate plant operation. Forced circulation helps in ensuring the right velocities for good heat transfer. Co-current configuration is usually adopted when the quality of the juice may decrease in presence of high heat rates which are generally achieved with the counter-current layout. Co-current works with natural circulation so that temperatures differences have to be designed properly to ensure both circulation and heat transfer. Mixed configuration is never justified unless vapor streams are used for other heating purposes that are external to the operation of the evaporator itself (this may be the case when total site heat integration is considered). Juice streams can also be split into more streams thus leading to more integration opportunities.

For the test case of the sugar cane factory, the co-current solution may result the optimal one as proposed for the base case scenario so far considered, because of a better control of maximum temperatures which can be critical for juice quality over 115°C. However different solutions for the multi-effect evaporator are investigated following the objective of a minimum process thermal requirement. For doing this a detailed model of the evaporating unit was implemented.

The design of a multi-stage evaporator is often a trade-off between investment costs which are related to the number of units and exchange surface, and operating costs which are related to the thermal requirement of the first effect, being this heat demand usually satisfied by hot steam coming from a boiler. Furthermore, depending also on the type of configuration desired, temperature differences affect also natural circulation in the case of co-current configuration and pressure differences between effects affect the value of the pumping work in the case of counter-current configuration [11].

As previously mentioned, the multi-effect evaporator is in reality a local heat exchanger network which is often employed in food-process and pulp and paper industry as the main tool for reducing the process hot utility. According to the idea of separating the problem of the HEN synthesis from the problem of the synthesis of the rest of the plant, all the thermal matches between effects as appearing in the stand-alone multi-effect evaporator (see Figure 3.4) are discarded. The resulting structure of this
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sub-process consists only of the sequence of units separating water from the juice as shown in Figure 3.6 for the case of five-effects evaporator.

Since the heat recovery within the multi-effect evaporator is obtained by properly choosing the operating pressure of each unit (which will be included among the set of decision variables to be optimized along with the concentration increase across each unit), the multi-effect evaporator model must be included in the total plant BPC.

Following this modeling approach, which was already proposed in the literature [109], different evaporation units remain connected to each other only at the cold juice side (from lower solid content to higher solid content), the sequence of evaporation stages remaining fixed a priori as a necessary condition to ensure congruity of juice properties between units.

Under the hypothesis of exploiting the maximum share of heat of the steam exiting each effect, condensation of the steam streams and further cooling of the condensate till environmental temperature are considered. In addition to these two hot streams, for each unit a cold stream corresponding to the isothermal evaporation is generated.

In Figure 3.7b typical shape of the composite and grand composite curves of one evaporation unit are given along with some general indications about how decision variables can affect the thermal profile of the unit and heat integration of the process.

With reference to Figure 3.7 the following equations are used to model the behavior of the evaporation of the sucrose-water mixture (where the subscript $J,i$ refers to the stream of juice exiting the effect $i$ and entering the effect $i+1$, the subscript $V_o,i$ refers to the stream of vapor exiting the effect $i$ and entering the effect $i+1$, $b$ is the solid content equal to $B/100$).

\[ \dot{m}_{V_o,i} = \dot{m}_{J,i} \cdot (b_{J,i} - b_{J,i-1}) \]  
\[ \dot{m}_{V_o,i} \cdot h_{V_o,i} + \dot{m}_{J,i} \cdot h_{J,i} = \dot{m}_{J,i-1} \cdot h_{J,i-1} + Q_i^+ \]  
\[ T_{V_o,i} = T_{J,i} + T_{sat}(p_i) + dT_{evap} \]  
\[ dT_{evap} = 3.7 \cdot b_{J,i} - 5.8 \cdot b_{J,i}^2 + 18 \cdot b_{J,i}^3 \]

In particular Equation 3.2 is the mass balance where $\dot{m}$ is the mass flow rate of a given material stream. Equation 3.3 is the enthalpy balance where $h$ is the specific enthalpy of a given material stream and $Q_i^+$ is the positive heating load that must be provided to the effect by a hot utility or by another hot thermal stream to be found in the system (in stand-alone co-current multi-effect evaporators this is the heat provided by the steam coming from the upstream effect). Equation (3.4) is the equality constraint between the temperatures of the vapor and the juice at the outlet of the effect, where $T_{J,i}$ is expressed as the saturation temperature of the vapor $T_{sat}$ at the operating pressure of the effect $p_i$ plus the delay of evaporation $dT_{evap}$. In fact, as solutions of salts or sugars in water typically feature an alteration in thermal properties compared to pure water, a relation is also imposed between the real evaporation temperature and the solid content in the juice. For a given pressure, the sucrose-water
mixture evaporates at a temperature slightly higher than the saturation temperature of the water at that pressure. This is taken into account in Equation 3.4 where $dT_{\text{evap}}$ is the delay of evaporation of the sucrose-water mixture with respect to the water. This latter parameter depends in general on both solid concentration and temperature (pressure) of the mixture and can be determined by using different correlation formulas reported in the literature [107, 110]. A good estimation of $dT_{\text{evap}}$ for sucrose-water mixture is reported in Equation 3.5. A comparison between this latter correlation and some others found in the literature is given in Figure 3.8.

By varying the pressure $p_i$ and the concentration of the single effect it is possible to vary the thermal load and the operating temperature of each effect.

### 3.1.2 The base case scenario for sugar production

The synthesis of the process for the conversion of sugarcane into white sugar is discussed in the following paragraphs. According to the proposed methodology a BPC is defined and the relative heat and power consumption along with the sugar production rate are evaluated.

A schematic representation of the BPC includes all the components which perform chemical or mechanical conversion of the main material streams (e.g. sugarcane $\rightarrow$ juice $\rightarrow$ sugar). Firstly a base case BPC for the sugar production is presented. Afterwards this base case BPC is modified and optimized according to the organized procedure previously introduced.

Conversion of juice within sub-processes is modeled by recollecting parameters and juice characteristics from a previous study about design improvement on a sugarcane factory for combined sugar and ethanol production [27, 28]. The power consumption of each subprocess was evaluated by multiplying the value of average specific power consumption found in the reference work by the mass flow rate of sugarcane or juice.

A schematic overview of the base-case BPC for sugar production is presented in Figure 3.9 where the BPCs of the different sub-process are shown as black boxes. In the same figure sugar yield and flow rates of the main material streams along with heat and power requirements of the sub-processes are reported.

The total heat and power demands of the so-called base case scenario is evaluated by summing up the heat and power demands of the single processes without considering process integration. In particular for the case of the multi-effect evaporator of this base case scenario, only local heat integration is considered. In this preliminary design a co-current configuration with three effects evaporation system is considered. At this stage number of effects and operating parameters are estimated by simply separating the whole evaporation load in three equal loads (according to a rule of thumb equal loads correspond to equal heat transfer surface for same $\Delta T_{ml}$ that is equal sizes of evaporation units) and setting the operating temperatures of the three effects at intervals of $10^\circ C$. The corresponding values of Solid contents and
operating pressures of the three units are: $B_1 = 19.8$, $p_1 = 1.65\text{bar}$; $B_2 = 30.3$, $p_2 = 1.16\text{bar}$; $B_3 = 65$, $p_3 = 0.70\text{bar}$. Accordingly the heat cascade of the three equal evaporation effects is exploited and the local heat demand of the multi-effect evaporator is evaluated as the thermal requirement of the first of the three effects. The first unit is in fact in technical practice the one receiving the steam from the centralized boiler. For all the other sub-processes, the local heat demand is evaluated by summing up the cold stream loads (those thermal streams that are locally responsible for a hot utility demand).

As reported at the bottom of Figure 3.9, the base case sugarcane conversion plant presents a considerably high heat demand (179 MW). While the power demand (16.6 MW) is proportional to the mass flow rate of the processed materials (sugarcane, juice, syrup and sugar), the heat demand can be potentially reduced by adopting a more heat integrated plant configuration.

### 3.1.3 Minimization of the process thermal requirement

For the same operating conditions of the base case scenario we now want to focus on the reduction of the process heat demand. Firstly, all the cold and hot streams in the process are identified. The aim is to maximize step by step the internal heat recovery. According to the rules of Pinch Analysis, all the material streams that need to be rejected to the environment are cooled down till the environmental temperature. All the hot streams undergoing a condensing process before being cooled down to the environmental temperatures, generate a poly-line in the common temperature-heat load diagram consisting in an isothermal segment (condensation) and in an oblique line (water sub-cooling) as already presented in Figure 3.7 for a single evaporation unit. As a result of the solution of the cascade problem, those streams that are not used for heating purposes are eventually cooled down by an environmental cold utility.

For a better investigation of process integration opportunities a detailed analysis of the BPC of each sub-process is required. In the following figures of these BPCs, thermal streams are represented with a
circle reporting letter H and the heat load in red when they are hot streams, letter C and heat load in blue when cold.

In particular the local heat integration of the multi-effect evaporator that was previously considered for evaluating the heat demand of the base case BPC, as reported in Figure 3.9, is discarded. Conversely the cold stream (juice to be concentrated) and the hot stream (vapor to be condensed and removed) of each unit are left to participate separately in the process heat-cascade problem as shown in Figure 3.6.

The BPC of the juice-extraction sub-system is firstly described in Figure 3.10. The outlet temperature of the knives cooling water at 50°C is cooled down to 25°C. Lubrication oil exits knives and crushers and is cooled down by a water stream. In principle oil could be considered as a hot stream to be exploited in the process heat cascade however since oil/water circuit is typically already integrated with the design of crushers and knives, the hot water stream after oil-cooling is considered instead (hot stream to be cooled down from 50°C to 25°C).

Juice heating represents the thermal stream with the biggest load within the juice treatment sub-process shown in Figure 3.11. Within this sub-process, some vaporization also occurs and two sources of steam are identified, one departing from the juice heater and the other from the recycling stream. These by-products streams, which are usually quenched and eventually sent to the sewage treatment, are now included as hot streams in the overall heat integration problem. Accordingly, steam is condensed and
the condensate is then cooled down till the environmental temperature. These two streams can in this way be exploited for other heating purposes within the process.

Figure 3.11: Basic configuration of the juice treatment subprocess

After the treatment, juice is sent to the multi-effect evaporator. In the light of the previous discussion about the modeling of the multi-effect evaporator (Section 3.1.1), hot and cold streams generated by each unit are identified as separate thermal streams that are included in the overall heat integration problem (thus allowing the heat recovery of all the steam departing from each effect to be exploited for heating purposes in other parts of the plant). The only physical connection that remains untouched with respect to the original configuration is the cold juice stream to be concentrated.

In fact it is not given a priori that the use of hot steam of a unit within the a subsequent unit leads to the minimum total site thermal demand.

The resulting BPC for the multi-effect evaporation sub-process is shown in Figure 3.12.

Figure 3.12: Basic configuration of the multi-effect evaporator subprocess

Sugar crystallization is conceptually quite similar to the evaporation, the only difference consisting in the fact that, in presence of a syrup at saturation concentration, water evaporation causes sugar crystals
to precipitate. Since sugar crystals need to be removed and centrifuged for white dry sugar production, it is convenient to separate this latter evaporation step from the former one occurring without precipitation of crystals (carried out within the multi-effect evaporator). As shown in Figure 3.13 and in analogy with the multi-effect BPC configuration, each pan generates a cold stream (evaporation heat load) and two hot streams (steam condensation and water sub-cooling).

In the same picture, the BPC of the drying sub-process is also represented. Sugar drying is the last part of the process in which humidity of the sugar is reduced to a minimum value.

![Figure 3.13: Basic configuration of the crystallization and drying sub-process](image)

Following the idea of exploring gradually the minimization of the process energy consumption, the first set of thermal streams to be integrated including only the thermal streams originating within the multi-effect evaporator and crystallization sub-processes is considered. The choice to first analyze the heat integration of these two sub-processes, which feature subsequent evaporations and condensations, is in agreement with the idea of matching similar thermal profiles (in this case latent heat), which was already mentioned by Linnhoff [84].

The result of the heat integratation of the multi-effect evaporator plus the crystallization thermal streams is reported in Figure 3.14.

The corresponding total process heat demand, evaluated by adding the hot utility demand of the heat integrated evaporation and crystallization sub-processes (the horizontal extent of the grand composite curve in Figure 3.14) to the thermal requirements of the extraction and the juice treatment sub-processes, passes from 179 MW of the base case scenario to 141 MW. This value corresponds in fact to the summation of the heat load of the first evaporation effect to the separate heat demand of the juice treatment section, the juice extraction being the source of only hot streams at low temperature levels.

From the interpretation of the process grand composite curve in Figure 3.14 it is also possible to notice that heat integration opportunities can technically only be achieved by diverting the steam produced by the last evaporation effect to the two crystallization pans, since these two components together require less than half of the total heat available from the multi-effect evaporator. Compared to the base case scenario in which the thermal requirement of the crystallization sub-process is considered to be covered by steam produced by the centralized boiler, the alternative solution of using the steam produced by the last evaporation effect does not introduce any additional capital costs and can be considered a pure saving in operating costs.

The overall process heat integration is finally studied by including all the thermal streams of the other two sub-processes (juice extraction and treatment) within the set of thermal streams to be integrated. The resulting grand composite curve of the process is shown in Figure 3.15.

The total process heat demand is further reduced to only the heat duty of the first evaporation unit (around 100 MW), the reduction corresponding to the 41 MW of the juice treatment. With respect to
Synthesis of the sugarcane conversion process

Figure 3.14: Heat integration between evaporation and crystallization thermal streams

the base case scenario of Figure 3.9 where sub-processes were considered totally independent from the thermal point of view (no heat integration), the reduction amounts to almost 79 MW. Compared to the previous solution in which no further capital investment was observed for achieving a considerable reduction in process thermal demand, total site heat integration can be obtained only at the expense of some investment in heat transfer equipment, being necessary to add some heat exchangers in order to fulfill the objective of total heat recovery through the process heat cascade under the first evaporation load. The benefits in process profitability can however be estimated only after the HEN is also defined and total investment costs assessed, two evaluation that here omitted since are beyond the scope of the work.

In the previous section the BPC of the process converting sugarcane into sugar was generated by recollecting data from the literature and by considering a multi-effect evaporator (with three effects with equal loads), which appeared to be the locus of major heat consumption. An important reduction in the process thermal requirement was obtained by exploiting heat integration opportunities.

The suggested organized procedure for the reduction of the total process energy demands proceeds with the identification of new opportunities of process integration by adjusting process parameters. This has to be regarded therefore as a parameter optimization step rather than a structural modification that would lead to new BPC.

In the previous chapter, different approaches for the optimization of system design parameters were presented with particular reference to the case of the power generating system. In particular, in presence of sub-systems in which thermal loads can be regarded as proportional to local mass flow rate, it is convenient to separate the problem of the optimization of the optimal intensive parameters (pressures, temperatures, etc.) to the problem of the optimal mass flow rates maximizing the internal heat recovery. With reference to the particular case of the industrial BPC converting sugar-cane into white sugar, mass flow rates are considered fixed at their maximum values since they are related to the conversion efficiency of the raw material into sucrose rich juice and sugar. Thus the only set of parameters that can be possibly optimized are operating temperatures and pressures of the various sub-processes.

A particularly effective way to identify, in an organized way, the set of process temperatures that
Production of sugar

Heat pockets
(possible cold utility stream)

Figure 3.15: Grand composite curve of the base case BPC (sugar production) with total heat integration can be optimized was presented in the previous chapter under the name of the HEATSEP method [80]. This approach consists in exploring the benefits that intermediate coolings or heatings can bring to the reduction of the process heat demand.

When dealing with optimization of industrial processes, the introduction of thermal cuts between subsequent components in most cases has to cope with process requirements which constraints the temperatures of the material streams within small ranges. As an example, in the case of the juice heating within the treatment sub-process, the value of the final temperature for the juice is constrained to be around 115°C since discoloration problems can occur for higher values and juice treatment is less effective for lower temperatures.

For the case of the multi-effect evaporator, possible thermal cuts can be considered in the juice stream just before the first evaporation unit and between the other units. This would allow the temperature of juice entering each unit to vary independently of the actual operating temperature of the unit. Juice pre-heating up to the temperature of the first unit is in fact possible, while juice cooling before evaporation is not thermodynamically reasonable. In the base case condition the juice leaves the treatment sub-process at 98 °C while the first effect works at the maximum allowable temperature of 115°C before discoloration. Thus, part of the heat load of the first unit is spent on juice heating instead of actual evaporation. If juice was pre-heated before entering the unit, an oblique thermal stream in the process composite curve from 97°C to 115°C would be generated. This thermal load is equal to almost 10 MW but only 5 MW could possibly be covered by other thermal stream in the process at that temperature level, this being the point in the process operating at the highest temperature.

In addition, for the case of thermal cuts of the juice stream between units, in the case of co-current configuration, juice leaving a unit enters the subsequent one already at higher temperature. As a consequence juice cooling would be unnecessary while additional juice heating would lead to evaporation which in fact occurs within subsequent units.

As a conclusion the actual benefits that the placement of an intermediate heat exchanger and the optimization of their temperatures would bring to the minimization of the process heat demand can be neglected. Furthermore, other process operating parameters to be optimized are at this step of the
Synthesis of the sugarcane conversion process

analysis found only within the multi-effect evaporator (unit operating pressures and solid content at the outlet of each unit) and, as it appears in Figure 3.15, there is not so much space for further improvement of the thermal profiles of this latter component, being the grand composite curve of the process already near to the activation of multiple pinch points. It is worth pointing out that the design of the multi-effect evaporator for the base case scenario was proven to be, in the subsequent steps of process thermal integration presented in Figures 3.14 and 3.15, already a fairly “good” design. This has been envisioned, while generating the base case BPC, by setting the simple system of Equations ((3.2), (3.3)) plus the equality of the loads of the evaporation units.

3.1.4 Introducing modifications of the BPC

![Grand Composite Curve](image)

Figure 3.16: Grand composite curve of Case S1 - total heat integration of sugar production plant with five-effects evaporator

As already discussed in the previous paragraphs, further improvements in process thermal requirement are expected to be introduced by some structural changes of the BPC. According to the aforementioned methodology we now look for possible staging of components within the sub-processes, which would keep the BPC intact (that is the concept of producing sugar by means of the four sub-processes as in Figure 3.9). Subsequently alternative material connections between components and new components are also explored which however would lead to significant modification of the process configuration and eventually to new BPCs.

Following the idea of staging components, we observed that more stages can be introduced within the multi-effect evaporator. This structural choice is conceived by looking at the grand composite curve of the overall process in Figure 3.15 which shows that there is still space (in terms of heat pockets within some temperature intervals) for further staging of evaporation. The heat pocket between the third stage and the crystallization thermal profile for instance extends in a temperature interval large enough to accommodate at least another evaporation stage. Furthermore it is also possible to fit another stage below the crystallization profile in the heat cascade (between the crystallization and possible cold utility streams). As a consequence a co-current five-effects evaporation is here explored.

As a preliminary design criterion we suppose again to split the total evaporation load in five equal
parts following the same rule of thumb that was used for the case of three effects for the base case scenario.

Since the crystallization temperature is fixed at 344 K (71°C), the last evaporation effect is considered to operate at a temperature of 334 K (51°C) corresponding to an interval at 10°C lower than the crystallization temperature. The design parameters for this new multi-effect evaporator configurations are: $B_1 = 17.1, p_1 = 1.66\text{bar}; B_2 = 20.9, p_2 = 1.18\text{bar}; B_3 = 27.1, p_3 = 0.81\text{bar}; B_4 = 38.2, p_4 = 0.54\text{bar}; B_5 = 65, p_5 = 0.16\text{bar}$. For this new configuration, referred to as case S1, heat integration of the total site is studied. The resulting grand composite curve is shown in Figure 3.16. The overall heat demand is around $62\ MW$ which corresponds to a reduction of other $38\ MW$ with respect to the case in which three effects were used (Figure 3.15).
3.2 Production of ethanol

There are two general ways to produce ethanol: synthesis and fermentation. Synthesis of ethanol from ethylene was demonstrated since the beginning of the last century while other ways are those starting from methanol. Since methanol can be produced by using carbon monoxide and hydrogen there are many pathways for the industrial synthesis of ethanol [70].

A more common way to produce ethanol is instead yeast fermentation of sugar which is at the base of all the production of alcoholic beverages (spirits). Continuous yeast fermentation of sucrose-rich juice is here considered being this the common pathway for ethanol production starting from sugarcane.

Ethanol is produced by yeast fermentation of sucrose according to the following relation:

$$C_6H_{12}O_6 \rightarrow 2C_2H_5OH + 2CO_2$$  \hspace{1cm} (3.6)

Part of the carbon in the substrate (sucrose) is used for the yeast metabolism and some other organic substances are also produced. The actual part of sugar that is converted into ethanol is therefore less than what is available at the inlet of the biochemical reactor. Fermentation is mainly anaerobic and is exothermic so the reactions need to be under specific conditions of oxygen concentration and temperature conditions. Since the reaction is exothermic, for an effective conversion of all the sucrose into ethanol and $CO_2$, cooling of the substrate is needed. If oxygen is present instead, glycolysis is promoted and the sugar is reduced to water and $CO_2$. Furthermore since ethanol inhibits yeast activity, the final concentration of the ethanol in the reactor has to be lower then 10%vol. Yeasts are also present somehow in the biomass but are usually added to the biomass along with some nutrients (minerals) that are useful for yeast growing. In order to recycle the yeast in a continuous process, a centrifuge is used to separate the yeast and the ethanol rich wine is sent to ethanol distillation.

The process can be seen as a complex set of reactions that produce basically $CO_2$ and a liquor with 10%vol maximum of ethanol (similar to wine or beer). At the outlet of the reactor yeast is usually recycled and reinjected at the inlet. The overall process can be batch-wise or continuous. Depending on the type of process the optimal fermenting substrate (sucrose) can range between 10-20%wt in water.

In Figure 3.17 a schematic representation of the yeast fermentation reactor (fermentor) is presented. The fermentation process is considered to occur at 28°C leading to a high thermal load of the cooling process of the juice/syrup coming from upstream components. Carbon dioxide is produced and vented out.

The assumption made in modeling yeast fermentation is that the ethanol production depends linearly on the quantity of sucrose in the must (the thick juice prepared for the yeast-fermentation) entering the fermentor as expressed with the empirical relation reported in Equation (3.7) where $m_{eth}$ is the ethanol yield in volume, $m_{must}$ is the mass flow rate of must, $P_{must}$ is the mass fraction of sucrose in the must and $\eta_{YF}$ is the efficiency of the yeast fermentation process which was fixed at 0.9. In reality, for a given selection of yeasts, there might be an optimal concentration of sucrose in the substrate that leads to the optimal ethanol yield. With different sucrose concentration of the must, it is possible to find a selection of yeasts that reflect the ethanol production characteristics of Equation (3.7).

$$m_{eth} = m_{must} \cdot P_{must} \cdot 0.489 \cdot \eta_{YF}$$  \hspace{1cm} (3.7)

The value of the sucrose concentration at the inlet of the fermentor found in the reference work from which the main process data were derived (see [27]) is 17.5% (this value in fact corresponds to the product of solid content value $B$ times purity $Z$ of the juice). In reality the optimal value may depend on the availability of such concentrated juice. In the sugar production base case scenario, the concentration of sucrose after juice treatment is around 14.5%. If no other components are considered before the juice fermentor, this also corresponds to the sucrose concentration of the juice at the inlet of the fermentor. For the standard case of juice at 17.5% of sucrose concentration an ethanol concentration of 6.8%vol in the wine was obtained according to data found in the literature about performance characteristic of fermentors. For the same performance parameters, when the inlet juice is available at the sucrose concentration of 14.5%, the evaluated ethanol concentration in the produced wine is 5.83%vol.
Ethanol is produced by means of subsequent distillation of the liquor from the fermentation. Distillation of ethanol from a water-ethanol mixture is performed at the azeotropic point (78.15°C at atmospheric pressure) yielding a distillation vapor with 95.5% weight basis of ethanol (89.2% mol.) at maximum.

Since fermented mashes coming from the fermentation sub-process generally consists of a complex mixture of water and organic compounds, of which ethanol is the most interesting one, distillation products can differ in quality. If part of the heavy organic compounds are removed as bottom products of the distillation, an important part of aldehydes and ethers are still present in the head products of a first distillation column. When high grade ethanol is to be produced these substances need to be removed by an extractive distillation column. Subsequently hydrous azeotropic ethanol can be distilled in a rectifying column. Yet, if motor fuel ethanol is to be produced, aldehydes and ethers are left as part of the product, since these substances are easily processed in combustion engines.

Anhydrous high grade ethanol or motor fuel can be produced by adding a tertiary compound to the hydrous mixture by means of the so-called tertiary azeotropic distillation.

Ethanol distillation is particularly interesting from the thermal integration point of view. The distillation process, the multi-effect evaporator and the crystallization share the common feature of generating multiple hot and cold streams at different temperature levels which mostly consist in isothermal heat loads. The influence of structural and operating parameters of ethanol distillation in the process thermal integration is analyzed by means of a detailed process flow-sheeting of common ethanol distillation configurations. Distillation is a separation process in which the desired products are evaporated from a solution and subsequently condensed through a sequence of stages.

In the case of wine produced by yeast fermentation the mixture can be approximated to a water and ethanol mixture. In all cases water is mixed with alcohol the mixture has a unconventional behavior in terms of vapor and liquid equilibrium. Accordingly a thermodynamic model based on the Nonrandom-Two-Liquid activity coefficients model was chosen for simulating the energy and mass balances of ethanol distillation. The NRTL is extensively used for simulating vapor-liquid equilibrium of solutions with highly polar components like Ethanol [111] and is a common properties model package in many flow-sheeting software [4].

The water-ethanol equilibrium at environmental pressure is reported in Figure 3.18 in which the azeotrope point can be recognized where the vapor and liquid concentration profiles touch each other (78.14°C, 89.2% mol.).

A preliminary analysis of the ethanol and water distillation reporting the mass balance between distillate and condensate is reported in Figure 3.19 for different operating pressures. As a result it is possible to assume that the behavior of the mixture is basically the same from the mass balance point of view. The McCabe-Thiele approach applied to the case of distillation of ethanol/water mixture gives an indication of the number of stages necessary to obtain a desired concentration of ethanol in the distillate. As a result a quite high number of stages with a considerably high reflux ratio is necessary to obtain
Figure 3.18: Boiling point diagram of ethanol-water mixture at 1.013 bar

Figure 3.19: Molar fractions of ethanol in water-ethanol mixture in boiling conditions
Production of ethanol

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azeotropic concentration. The assumptions behind the McCabe-Thiele approach are rigorously poor for the case of non-ideal mixture like water-ethanol. In fact this approach is mainly based in assuming Costant Molar Overflow that is constant vapor and liquid flow-rates through the whole distillation column. This is true only if latent heats of chemical components are more or less the same, if specific heats remain constant along the column, if no additional heat is provided to or removed from the column and if there is not heat of mixing between components [125].

In Figure 3.19 is also possible to notice that at different pressures the mass balance profiles are almost overlapping. The application of the McCabe-Thiele approach leads to estimate the same number of stages and re-flux ratio for different operating pressure (ratio between the condensate and distillate flow rates).

This means that, for given values of ethanol concentration in the inlet stream and in the desired outlet streams, the evaluation of optimal reflux ratio and number of stages can be made in first approximation regardless of the change in operating pressure.

Conversely, the effect of pressure is important for the temperature levels at which the distillation columns operate and the entity of the thermal demand also changes since inlet temperature of the wine remains fixed throughout the whole analysis. It is in fact apparent that the higher the pressure the higher is also the temperature range at which the vapor-liquid equilibrium appears (for higher operating pressures the diagram in Figure 3.18 shifts towards higher values of T). As a consequence, for the same characteristics and operating parameters of the column (for fixed concentration and rates of the bottoms and distillate), re-boiler and condenser work at higher temperature levels which also means that large exergy losses occur when the heat available at the distillation condenser is totally released to the environment.

Since in addition pressurized distillation columns are also more expensive because of the higher resistance of the construction materials to stand greater operating pressures, it is not convenient in general sense to choose a high operating pressure of a column and, on the contrary, it is convenient to adopt a vacuum system to lower the interval of operating temperatures, thus allowing to exploit low temperature waste heat when available. However, once distillation is carried out in stages (series of columns), the heat of condensation released by the condenser of the first column can be potentially exploited for covering the re-boiler heat duty of a second column when this operates at lower pressure than the first one. This concept of exploiting the heat cascade of two or more columns (sequence or parallel) is conceptually equal to the stages in the multi-effect evaporator system.

If the boundaries of thermal integration are extended to the overall process, it is also possible that depending on the thermal profiles of other subsystems, the minimum process thermal demand is achieved for pressures of the columns that would not be convenient if distillation was thermally independent of other sub-systems. Thus, in the following optimization of the process design parameters, operating pressures of the columns are considered among the decision variables.

3.2.1 The base-case scenario for ethanol production

In the light of the proposed methodology we are now interested in exploring the benefits in process thermal demand that is achieved by introducing new components and connections between pre-existing components of the sugarcane conversion process.

In particular the substitution of the evaporation and of the crystallization subprocess (which are the main parts of the sugar production BPC) with yeast fermentation and subsequent ethanol distillation is discussed in this section.

This results in the definition of a new BPC of the sugarcane conversion process which leads to production of ethanol only, while combined sugar and ethanol production BPC is analyzed in Section (3.3). The demand for external energy in the ethanol production process is assessed here for constant mass flow rate of sugarcane input (138.9 kg/s).

Process parameters and characteristics of the conversion sub-processes are based on data recollected from the literature [27, 28]. Hydrous ethanol is obtained from distillation, the sub-process in which ethanol is separated from the fermented wine and water is removed as a bottom (liquid) product. The evaporation of part of the water in the juice by means of an upstream evaporation sub-system as done for
In the present section we firstly consider the option of producing motor fuel ethanol from sugar-cane. In the base case scenario, motor fuel ethanol is distilled in a single stripping-rectifying column and design parameters of the local distillation sub-process are fixed according to indication found in the literature [27, 125].

Aspen Plus was used to simulate the distillation model in detail presented in Figure 3.21. The following parameters are considered fixed in the analysis:

- 35 stages (trays)
- Reflux ratio (Condensate to Distillate ratio) = 7
- Distillate to Feed ratio = 0.07

The base case scenario of ethanol production is shown in Figure 3.20 along with the ethanol yield and heat and power demands. For a fixed input of sugarcane of 138.9 kg/s a total production of almost 9.8 kg/s of hydrous motor fuel ethanol is evaluated.

In more detail, the concentration of the wine obtained at the outlet of fermentor is around 5.8%vol as a result of the yeast fermentation of a juice with a sucrose concentration of 14.4%.

The concentration of ethanol in the distillate is around 94% which is slightly lower than the azeotrope concentration at the same pressure. Accordingly the specific thermal energy consumption of the distillation column is around 528 kJ for each kg of wine feeding the column. An overview of the thermal streams generated within the distillation subprocess is shown in the Table 3.1.

For the non-integrated plant configuration a total thermal demand of 149 MW was evaluated. The slight reduction in total heat demand with respect to the sugar production is due to the lower specific energy consumption of ethanol distillation from the water-ethanol mixture compared to the pure water evaporation in the case of sugar production.
3.2.2 Minimization of the process thermal requirement

As reported in the schematic representation of the BPC (Figure 3.20), the plant thermal requirement is related only to the juice treatment and the ethanol distillation operations.

Total site heat integration is studied here. In addition to the thermal streams already identified for the juice extraction and juice treatment subprocesses, the thermal streams resulting from the operation of yeast fermentation and ethanol distillation (see Figures 3.17 and 3.21) are included within the whole set of process thermal streams to be integrated. The resulting total site grand composite curve is reported in Figure 3.22.

A potential reduction of the heat demand from almost 149 MW of the BPC without heat integration, down to 86 MW in the case of total heat integration is evaluated.

The ethanol production plant is in fact a paradigmatic case showing the benefits of heat integration in the plant economy. In the juice treatment section, juice has to be heated up to discoloration temperature (105°C) while in the subsequent fermentation stage it has to be cooled down to around 28°C. These heating and subsequent cooling steps can be effectively integrated bringing a significant reduction in thermal demand as shown in the grand composite curve in Figure 3.22. In addition, a detailed analysis of the grand composite curve shows that the juice stream after treatment is still hot enough to preheat part of the wine before the distillation column.

As discussed for the case of sugar production in Section 3.1, most of the process operating temperatures are fixed by process requirements with only one exception, in the case of the ethanol production, for the outlet temperature of the wine pre-heater before distillation. The wine produced by the yeast fermentation can in fact be heated up to whatever temperature before entering the distillation column. Inside the distillation column the wine is heated up to the boiling point for evaporation and this corresponds to an almost isothermal heat requirement at quite high temperature. Thus, it is reasonable to reduce this heat duty (at reboiler side) as much as possible (till the actual evaporation heat load) and
pre-heat the wine for distillation by means of convective thermal streams when available, for instance with the hot juice coming from the treatment Section (an equivalent condition was previously shown for the case of pre-heating before the multi-effect evaporator). This was in fact already considered in the base case BPC where wine is pre-heated up to (around) the re-boiler operating temperature of the distillation column. Since there is no thermodynamic benefit from pre-heating the wine up to a different temperature we neglect this temperature as a decision variable. In addition, for the base case BPC, no significant other decision variables are identified in the process. We move therefore directly to the next step of the proposed organized procedure.

3.2.3 Introducing modifications of the BPC

In this section components staging and changes in material connection between components are investigated in order to investigate new heat integration opportunities which possibly will lower the process energy demand. In fact, these changes in BPC will not affect the original concept of the process, the structure which remains of the base case scenario (see Figure 3.20).

In particular the attention is here drawn to the possible modifications of the distillation sub-process as it appears to be the locus with the highest heat consumption. Accordingly, different values of the overall process thermal requirement are assessed for each possible change in ethanol distillation.

Two main alternative configurations for ethanol distillation are considered in the following paragraphs:

- two parallel columns both producing hydrous ethanol: this corresponds to split the wine stream at the outlet of the fermentor into two different portions that are processed in two separate columns (Case E1 in Figure 3.23a).

- a sequence of a stripping and a rectifying column: this corresponds to perform distillation of hydrous ethanol in two stages (Case E2 in Figure 3.23b).

In addition we introduce the possibility of operating the columns at various pressures. In fact, if looking at a single column, the higher is the pressure the higher is the thermal requirement of the re-boiler. Conversely, when two distillation columns operate at different pressures, a reduction in total heat requirement

![Figure 3.22: Grand composite curve of the base case ethanol production with total heat integration](image-url)
Production of ethanol

Figure 3.23: Multi-column ethanol distillation a) parallel of two stripping-rectifying columns b) sequence of stripper and rectifier

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<td>$T_{in}$ [K]</td>
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<td>93.30</td>
<td>92.80</td>
<td>92.40</td>
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</table>

Table 3.2: Thermal streams for the single stripping-rectifying column at different operating pressures
can be obtained by exploiting the separation of the total heat duties of boiling and condensation into different temperature intervals thus leading to more heat recovery opportunities.

For this purpose a simulation of the distillation column at different operating pressures was first carried out.

As a choice in the present analysis, the design parameters of the distillation columns (number of stages, feeding stage, reflux ratio and distillate to feed ratio, are kept equal to the values assumed for the base case. This is in agreement with the fact that for the case of the ethanol-water binary distillation, the vapor-liquid equilibrium is not as pressure-sensitive as it is shown in Figure 3.19. Since design parameters for the base case scenario were estimated heuristically in order to obtain a fair compromise between minimization of the column thermal demand and maximization of purity of distillate, the same values are expected to lead to the same compromise for higher operating pressures.

If for the case of the environmental distillation the ethanol concentration is around 94% in mass, this concentration is reduced by two or three percentage points when the pressure increases up to 5 bar which was considered as upper bound for the range of the investigated pressures. This is in agreement with the fact that the actual ethanol purity is slightly less than the azeotrope concentration and for higher operating pressures the azeotrope concentration decreases. As a consequence the market value of the product changes, since the higher water content is an undesired component which will lower the higher heating value of the distillate. Besides, pressurized distillation equipment is also more expensive, so it is reasonable to adopt pressurized distillation only when the reduction in process utility demand counterbalance the lower selling price of the product and the additional investments. This can be evaluated however only by means of a thermo-economic analysis of the plant which is beyond the scope of the present work. An example of thermo-economic analysis applied to the syntheses of a sugarcane conversion plant can be found in [27].

In particular for case E1 (parallel of distillation columns), the same parameters were used for each stripping-rectifying column as in the base case scenario. The overall ethanol yield is not changed compared to the base case scenario. Results of Aspen simulation for a single stripping-rectifying column are reported in table 3.2 for different pressures. It is apparent that in case E1 (parallel of columns)
only sizing issues would justify the use of two columns operating at the same parameters and no better thermal management would be obtained with respect to the base case scenario. Once one of the two columns operates at higher pressure, the temperature levels of both the reboiler and the condenser of that column are shifted up in the total process heat cascade. In so doing, the total heat duty introduced by ethanol distillation can be split in different stages, revealing a high potential for heat integration. According to the approach so far used for the minimization of the process thermal demand, we let open the possibility of integrating not only thermal streams of the two columns within the distillation itself, but also with the other thermal streams in the overall plant.

We here propose the example in which one of the two columns is operated at 4 bar, being in principle possible to adopt whichever value of the operating pressure as long as the temperature of the re-boiler of the column at lower pressure (in this case environmental pressure) is lower than the temperature of the condenser of the pressurized column thus leading to maximum heat integration opportunities. In presence of a mass splitter diverting the two portions of wine to separate columns, the distillation sub-process can be further separated into two different sub-systems corresponding to the two columns with heat and power requirements proportional to their respective input mass flow rates of wine. As already discussed in the previous chapter, the minimization of the process thermal demand can therefore be formulated as a linear programming problem in which decision variables are mass flow rates. The case of the parallel of two stripping-rectifying columns is however a simple example of a problem of this nature and a sensitivity analysis is sufficient to evaluate the optimal splitting fraction.

For case E1 minimum thermal demand can be obtained by simply splitting the wine mass flow rate in two equal mass flow rates towards the two columns. A grand composite curve of the overall process (from sugarcane to ethanol) for case E1 is reported in Figure 3.24. The total hot utility requirement of case E1 is equal to 47.8 MW (38 MW less than in the heat integrated base case).

It is worth pointing out that when thermal streams of the distillation sub-process are locally integrated, the optimum splitting fraction of wine to be diverted to the pressurized column might be slightly different from half of the mass flow rate, due to the difference in heat loads between the columns operating at different pressures as reported in table 3.2. In presence of total site heat integration instead, the optimal splitting fraction at the wine splitter is in general different and the fact that in case E1 the optimal condition is when wine is split into equal portions is just a coincidence. For the same type of ethanol distillation plant but in presence of different thermal streams originating in other sub-processes, the optimal value of the splitting fraction can completely differ from case E1.

Figure 3.25: Aspen Plus flowsheet of high grade ethanol distillation in a sequence of stripper and rectifier
<table>
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<th>pressure [bar]</th>
<th>1.0132</th>
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<th>3</th>
<th>4</th>
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<tr>
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</tr>
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<td>406.75</td>
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<td>93.50</td>
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<td>92.90</td>
<td>92.50</td>
</tr>
</tbody>
</table>

Table 3.3: Thermal streams for the sequence stripper-rectifier column at different operating pressures

*Synthesis of the sugarcane conversion process*
Process thermal demand in case E2 (sequence of columns) can become twice as much the thermal requirement of a case with one column since, for the same column characteristics (same number of trays and reflux ratio), the share of high-boiling substances (in this case modeled as water) to be evaporated and passed to the second column is bigger therefore increasing the re-boiler heat duty of the first column.

In technical practice, sequence of distillation is considered when from the first stripping column head products still consists in a mixture of ethanol and undesired compounds that need to be removed in subsequent stages for obtaining rather pure hydrous ethanol as final product. Case E2 does not refer in fact anymore to the distillation plant used for motor fuel ethanol production but to the case of high grade hydrous ethanol production where aldehydes and ethers are removed in an intermediate extraction column and the water-ethanol mixture needs to be rectified in a second column. In the intermediate extractive column, the undesired substances are removed as head products of high pressure distillation while the ethanol rich stream is removed as a bottom product. This intermediate step is not requiring high thermal energy. In addition the choice of approximating the wine to ethanol-water mixture prevent us in modeling the separation of aldehydes or ethers. As a consequence the high grade ethanol distillation is modeled as a simple sequence of stripper and rectifier.

The heat integration of a sequence of distillation columns was the objective of several studies in the literature [1, 23, 64]. The discussion here is done in the light of a generalized approach of modifying the structure of the process and looking at the overall process heat integration and is based on the assumption that wine is a mixture of only ethanol and water.

For the case of high grade ethanol distillation, operating parameters are fixed according to data recollected from an actual plant and found in the reference study [27]. The following parameters are considered fixed in the analysis:

- wine inlet : 90°C, 5.8%vol ethanol
- Stripping column: 25 stages, Reflux ratio = 1, Bottom to Feed ratio = 0.87
- Rectifier: 50 stages, Reflux ratio = 4.5, Distillate to Feed ratio = 0.46

In Figure 3.25 a picture of the Aspen flow-sheet of the distillation plant based on the sequence of stripper and rectifier is given. In particular, according to the indication found in the literature, a relatively small loss of ethanol from the total amount of ethanol available in the input wine exits the stripper column as a vapor head product. This is an alternative way to account for the loss of ethanol that remains partially mixed with other heads by-products of the actual distillation process in presence of all the other undesired hydrocarbons.

Results of detailed simulation of the sequence of stripper and rectifier are reported in table 3.3 for different values of the operating pressure. A total production of 8.68 kg/s of high grade ethanol is produced starting from 140 kg/s of wine at 5.8%vol available at the outlet of the fermentor. As already shown for the single stripping-rectifying column, reboiler and condenser thermal loads are sensitive to the change in operating pressure. This is mainly caused by the increase of the boiling temperature with the increase of the pressure which leave a higher portion of preheating to be carried out in the first column while the wine inlet temperature was considered fixed at 90°C. This fact would suggest to further optimize this temperature for achieving additional reduction in process thermal demand.

As done for case E1, in order to exploit the heat integration potential of the two columns, the operating pressure of the stripping column in case E2 was set to 4 bar.

As a result of the heat integration of this latter BPC (case E2) a total process hot utility of 92.6 MW is evaluated which corresponds to an increase of 7 MW with respect to the base case scenario (Figure 3.22). As expected, the potential reduction of total energy requirement is much higher in the case of motor fuel ethanol than in the case of production of high grade ethanol. This is related to the more complex, and energy expensive, distillation configuration for the production of high grade ethanol which is however supposed to be paid off by a higher price of the product than in the case of motor fuel ethanol.
3.3 Combined sugar and ethanol production

In Sections 3.1 and 3.2 the analyses of two different concepts of sugarcane conversion plant were analyzed. Two sets of Basic Plant Configurations were generated and their heat and power demands evaluated.

Another plant option, already quite well known in technical practice, is that of combining the production of ethanol and sugar in a single plant (i.e. in a single BPC). This alternative solution of converting part of the sugarcane into sugar and the remaining part in ethanol at the same time is explored in the following in the light of the organized procedure for process synthesis that was introduced in the previous chapters.

The combined production of ethanol and sugar is particularly convenient since both processes are substantially based on the separation of sucrose from dry fiber and water of the sugarcane. In fact ethanol and sugar production BPCs partially feature the same sub-processes (juice extraction and treatment). In technical practice juice for ethanol production is treated without the addition of sulfural species so that sulfur is not present in the final product. Accordingly the juice treatment should be divided into two subprocesses (one for the juice for ethanol production and one for the juice for sugar production). However estimation of the thermal streams generated from the operation of the treatment section is not substantially affected by considering these subprocesses as one subprocess.

After the juice-treatment sub-process the juice is split into two parts, one diverted to the sugar production and the other one to the ethanol production. The splitting fraction is a critical design decision variable that affects process configuration and heat integration.

The BPC of the combined sugar and ethanol production is presented in Figure 3.27.

For a base case scenario we assume that the juice is split into two equal parts after the juice treatment section. As already shown for the sugar production process, the number of effects used for the evaporation is a particularly important structural parameter that helps reducing the process thermal demand. In addition, the more are the effects, the more flexible is the distribution of the overall evaporation thermal load between different temperature intervals. Here we consider five effects evaporator, this configuration showing the minimum thermal requirement in case of only sugar production (see Figure 3.16 compared
Combined sugar and ethanol production

Figure 3.27: Base case BPC for combined sugar and ethanol production, and possible modifications (dashed lines) for increasing ethanol yield

...to 3.15). This is in fact not expected to be the optimal configuration in the case of combined sugar and ethanol so a detailed discussion of structural and design parameters optimization is given in the following paragraphs.

In Section 3.2, different plant configurations for ethanol distillation were discussed. Between the two main alternatives of distilling motor fuel ethanol in two parallel columns and high grade ethanol in a sequence of stripper and rectifier, we consider this last option for the case of a combined ethanol and sugar production process.

As shown in Figure 3.27, in the base case scenario of combined sugar and ethanol production, almost 4.3 kg/s of high grade hydrous ethanol and 7.2 kg/s of sugar are obtained, being the two products yields proportional to the mass flow rates of treated juice diverted respectively to the two separate production sequences. Under the additional assumption that the total evaporation load is equally distributed into the 5 effects and that both the stripping and rectifying columns work at environmental pressure, the total heat demand of the process, that is the addition of the separate heat demands of the different sub-processes, is around 164 MW (of which 31 MW is the local heat demand of the thermal cascade of the 5-effects evaporator).

For the same operating parameters of the various subsystems, total site heat integration is considered. The resulting grand composite curve is reported in Figure 3.28 where it is possible to recognize the zig-zag profile typical of the various steps of evaporation of water within juice concentration (multi-effect evaporator) and of ethanol distillation. The overall thermal requirement of this base case scenario is around 92 MW corresponding to almost a 72 MW reduction with respect to the base case scenario without total heat integration.

3.3.1 Minimization of the process thermal requirement

The optimization of those parameters that in the previous analysis were discovered to influence particularly the thermal requirement of the sugar and ethanol processes is carried out.

In particular, by observing Figure 3.28 we notice that the temperature levels of the environmental distillation and those of the first evaporation effects overlap each other resulting in the particular shape of the grand composite curve. In this condition it behaves strongly as a heat sink over the pinch point and as a heat source under the pinch point. Since the two sub-processes have quite high local heat demands,
a high total process thermal demand is obtained even with total heat integration of the process.

A better solution is therefore expected to be obtained by exploring different set of parameters of the multi-effect evaporator and distillation subprocesses. Accordingly, operation pressures along with the evaporation loads (increase in solid content) of the five effects plus the operating pressure of the stripping column are optimized in order to reduce the total process heat demand.

The adjustment of each of these parameters has a non-linear response of the process thermal demand (objective function). In addition the total site thermal integration is evaluated by taking into account simultaneously all the changes in operating parameters (i.e. thermal loads and temperatures). This prevents the optimization to be tackled in separate steps. The presence of several horizontal thermal loads results into strong discontinuity of the objective function within the range of variation of the decision variables. The constraint imposed by the heat cascade problem to ensure feasible heat transfer is also strongly non linear and discontinuous. While robust deterministic solvers would probably require less computational effort, genetic algorithms are more often used for solving this type of problem [42]. This optimization strategy is based on a random generation of design points (arrays of values of decision variables) and several selection of optimal configurations. The optimization procedure can rely therefore in quite standardized code.

The results reported in the following were generated by means of an optimization code developed by Leyland at EPFL [82].

Similar works about the optimization of thermal profiles of multi-effect evaporator are reported in the literature [109, 136]. In principle it could be possible to also include within the set of decision variables the operating pressure of the rectifying column. However, compared to the stripper column, the rectifier is responsible for a small part of the local heat demand of the distillation sub-process and its reboiler heat duty can be covered by the heat released by the condenser of the stripper column operating at higher pressure.

Eventually the optimization problem can be described as follows:

\[
\min \text{ Process Hot utility}
\]
considering the following decision variables with their respective lower and upper bounds in square brackets:

- \( p_i \): operating pressure of the \( i \)-effect \([p_{i-1} \ 0.1 \text{bar}]\) (the first effect operating temperature is fixed at 115\(^\circ\)C)
- \( B_i \): solid concentration at the outlet of the \( i \)-effect \([B_{i-1} \ 65\%] \) (the outlet concentration of the last effect is fixed at 65\%)

while stripper pressure is considered as a parameter and two cases are discussed (environmental distillation and stripper at 4 \( \text{bar} \)). Optimization results show that the pressure of the stripping column is the parameter with the greater influence in the value of the total process heat demand. In fact if the stripping column works at atmospheric pressure, the optimization of the multi effect evaporators can reduce the total heat demand of the process down to 69 \( \text{MW} \) (case CSE1). Among several possible configurations yielding more or less the same result in terms of minimum thermal requirement, one configuration is presented in detail in Figures 3.29, 3.30 and 3.31. In these two latter pictures the integrated grand composite curves of the three main subprocesses are presented. In particular the multi-effects evaporator configurations was obtained with the following values of decision variables:

1. 1\(^{st}\) effect: \( B_1 = 23.5\% \); \( T_1 \) fixed at 115\(^\circ\)C
2. 2\(^{nd}\) effect: \( B_2 = 27.5\% \); \( T_2 = 82\,^{\circ}\)C \( (p = 0.5 \text{ bar}) \);
3. 3\(^{rd}\) effect: \( B_3 = 50.7\% \); \( T_3 = 64\,^{\circ}\)C \( (p = 0.21 \text{ bar}) \);
4. 4\(^{th}\) effect: \( B_4 = 53.5\% \); \( T_4 = 55\,^{\circ}\)C \( (p = 0.13 \text{ bar}) \);
5. 5\(^{th}\) effect: \( B_5 \) fixed at 65\%; \( T_5 = 55\,^{\circ}\)C \( (p = 0.13 \text{ bar}) \);

The integrated grand composite curve of the multi-effect evaporator shows that an optimal condition is reached by carrying out a big part of the evaporation at the first effect so that the steam coming out from this effect can be used to feed the stripper and rectifier reboilers. In addition, the 4\(^{th}\) and the 5\(^{th}\) effect operate at the same temperature (pressure) which means that practically these last evaporation steps can be carried out in a single unit. It is worth comparing these results (case CSE1) with a second case (case CSE2) in which the pressurized stripper is considered (4 \( \text{bar} \)). If the stripping column is instead operated at 4 \( \text{bar} \), the optimized thermal profile of the multi-effect evaporator can further reduce the process heat demand down to 62 \( \text{MW} \) (see Case CSE2 in Figure 3.32) which is around 7 \( \text{MW} \) less than case CSE1.

As soon as the stripper operating pressure is increased, it is more convenient to leave a bigger part of the evaporation to be carried out in the subsequent effects (compare Figure 3.33 with Figure 3.30). Still optimization results show that it is not necessary to split the evaporation in more than four effects since the last two effects are found to overlap each other in the optimal condition. The multi-effects evaporator configurations was obtained with the following values of decision variables:

1. 1\(^{st}\) effect: \( B_1 = 19.5\% \); \( T_1 \) fixed at 115\(^\circ\)C
2. 2\(^{nd}\) effect: \( B_2 = 25.7\% \); \( T_2 = 84\,^{\circ}\)C \( (p = 0.54 \text{ bar}) \);
3. 3\(^{rd}\) effect: \( B_3 = 31.4\% \); \( T_3 = 68\,^{\circ}\)C \( (p = 0.28 \text{ bar}) \);
4. 4\(^{th}\) effect: \( B_4 = 49.4\% \); \( T_4 = 58\,^{\circ}\)C \( (p = 0.16 \text{ bar}) \);
5. 5\(^{th}\) effect: \( B_5 \) fixed at 65\%; \( T_5 = 57\,^{\circ}\)C \( (p = 0.14 \text{ bar}) \);
Figure 3.29: Grand composite curve of case CSE1 - total heat integration of the combined sugar and ethanol production plant with atmospheric distillation.

Figure 3.30: Case CSE1 - integrated grand composite curve (blue: multi-effect evaporator thermal streams, red: all the remaining process thermal streams)
Figure 3.31: Case CSE1 - a) integrated grand composite curve (blue: distillation thermal streams, red: all the remaining process thermal streams) b) integrated grand composite curve (blue: crystallization and drying thermal streams, red: all the remaining process thermal streams)

Figure 3.32: Grand composite curve of case CSE2 - total heat integration of the combined sugar and ethanol production plant with stripping column operating at 4 bar
Figure 3.33: Case CSE2 - integrated grand composite curve (blue: multi-effect evaporator thermal streams, red: all the remaining process thermal streams)

Figure 3.34: Case CSE2 - a) integrated grand composite curve (blue: distillation thermal streams, red: all the remaining process thermal streams) b) integrated grand composite curve (blue: crystallization and drying thermal streams, red: all the remaining process thermal streams)
3.3.2 Introducing modifications of the BPC

In Figure 3.27 it is possible to notice that, among other process by-products, molasses, which have a quite high sucrose content (73% of solid content, 58% of which is sucrose), are rejected as a by-product of the sugar crystallization sub-process. This amount of sucrose can be diverted to the must preparation right before the fermentor in order to increase the ethanol yield of the yeast fermentation. In reality, yeast metabolism can be inhibited by excess of sucrose content in the must and ethanol content in the product [70]. According to data found in the reference work [27, 28] we fix this limit at 17.5%. By mixing molasses with juice coming from the treatment section, the sucrose content is found to be lower than this value therefore some syrup, obtained by juice concentration in the multi-effect evaporator, is also added to the must.

These new materials are represented with dashed lines in Figure 3.27. As a consequence of the increased sucrose content in the must, yeast fermentation produces wine at 6.8% vol. of ethanol. Ethanol yields are also expected to increase so that the distillate to feed ratio of the rectifier is increased up to 0.55 while other parameters of the distillation are kept constant as in Section 3.2.3. Due to a higher content of ethanol in the wine a slight reduction of the heat consumption of distillation per unit of produced ethanol is obtained.

The choice of diverting different portions of sucrose to the ethanol production or to the sugar production is in fact the key design point of the combined production plant. The assumption made in modeling yeast fermentation is that the ethanol production depends linearly on the quantity of sucrose entering the fermentor as expressed with the empirical relation seen in Equation (3.7). According to this assumption, from the point of view of process productivity, there is no reason to increase the sucrose concentration of the must from 12.7% (the base case scenario) to higher values, except for the obvious case in which this increase in sucrose content is obtained by recycling some by-products like molasses.

In other words, the part of sucrose that is added to the must to obtain the new sucrose concentration of 17.5% by diverting some syrup at the outlet of the multi-effect evaporator could be added by simply diverting more juice just after the treatment process. Yet, if the final amount of ethanol production and sugar production are kept constant, the only difference between adding syrup or not to the must before fermentation is the relative difference in thermal and energy demand and capital costs between the two alternative solutions of further concentrating the must before fermentation and of distilling a wine with less ethanol content.

While this topic is quite relevant from the point of view of the final decision on process structure, the actual optimal configuration cannot be found only by analyzing the thermal and power consumption as primarily done in the present work. The optimal configuration may in fact also depend on the choice of promoting one production rather the other (e.g. because the difference between price of ethanol and cost of ethanol is higher than the same difference for the sugar) and when balancing the capital costs of process sub-systems (e.g. evaporating water in multi-effect evaporator is less expensive than distilling ethanol from water).

The split ratio $x_1$ (ratio between juice to ethanol production over the total juice mass flow rate at the juice splitter) is chosen as a parameter in order to investigate different possible process configurations. A sensitivity analysis is used to evaluate the split ratio $x_2$ (ratio between syrup to ethanol production over the total syrup mass flow rate at the syrup splitter) that ensures the required sucrose concentration (17.5%) of the must at the inlet of the fermentor. Since all the molasses from the sugar crystallization are mixed with the must, the production range of ethanol is then constrained to the minimum juice and syrup quantities that can dilute the molasses to a mixture with 17.5% of sucrose content. Viceversa, the complementary parts of syrup sets the upper limit for the sugar production. Figure 3.35 shows these quantities and the relation between the split fractions of the juice splitter and that of the syrup splitter. The overall sugar production can range between 0 and about 10.5 kg/s whereas the high grade ethanol production can range between 3.9 and about 9.3 kg/s.

If the juice is split into two equal parts after the treatment section (as done in the base case in Figure 3.27), a great part of the syrup has to be added to the juice to obtain the desired sucrose concentration which makes the ethanol production dramatically increase at the expense of reducing the sugar yield. Thus, to compare the new BPC in terms of energy consumption and sugar and ethanol production
with the previous cases, the sugar production is fixed at 7.2 kg/s as in the base case scenario and the various mass streams are adjusted accordingly (38% of juice and 20% of syrup are diverted to ethanol production).

The new, material integrated BPC, leads to an increase of ethanol production which passes from 4.32 kg/s of the base case up to 5.6 kg/s.

Operating parameters (pressures and solid content increases of the 5 evaporation effects and stripping column pressure) of the new BPC are optimized in order to minimize the overall process heat demand. In Figure 3.36 the grand composite curve of this latter optimized configuration is shown. The total process heat demand is around 75 MW when operating the stripper column around 4.2 bar.

The increase in total site heat demand compared to the previous case (Case CSE2) is due to the fact that more than 60 % of juice is diverted to the multi-effect evaporator. Again, the pressure of the stripper appears to be a critical decision variable for the reduction of the process MER. In more detail, optimization results show that the process thermal requirement increases almost proportional to the decrease in stripper operating pressure due to the progressive reduction of condenser heat that can be used to cover the heat demand of the first evaporation effect. In Figure 3.37, it is possible to notice that the reduction in thermal demand achievable by adopting a pressurized stripper column is rather low (maximum 2 MW) for values of operating pressure ranging between 4.2 and 3.9 bar. The case with environmental distillation compete in terms of total thermal demand with the cases at higher pressures (leading to only 2-3 MW increase in process thermal demand with respect to the case of a stripper at 4.2 bar). Conversely, in a quite large range of stripper pressures (between 3.5 bar and the environment pressure), distillation thermal profiles overlap the first evaporation effect profiles too much, leading to a dramatic increase in process thermal demand.
Figure 3.36: Grand composite curve of case CSE3 - total heat integration of the combined sugar and ethanol production plant with recirculation of molasses for ethanol production and stripping column operating at 4.2 bar

Figure 3.37: Optimal trade-off between Stripper operating pressure and process thermal requirement: Front of optimized solutions
3.4 Conclusions

The objective of the present chapter was to discuss the conceptual design of a sugarcane conversion process, by focusing on the minimization of the process thermal demand being this a paradigmatic example of energy intensive industrial process. Different process configurations were explored for the conversion of 138.9 kg/s of sugarcane. In particular starting from the definition of three base case scenarios (sugar production, ethanol production and sugar and ethanol production) different Basic Plant Configurations (BPCs) were generated and subsequently modified according to an organized procedure consisting in three steps: component staging, addition of new connections between components, addition or substitution of components. According to the so-called HEATSEP method presented in Section 2.3.5, a BPC consists in all the components that are responsible for mechanical and chemical conversions of the raw materials while all the heating and cooling processes are considered as half heat exchangers. The information about temperatures and heat loads is then used to evaluate the potential for heat integration by means of Pinch Analysis rules. The methodology considered here should start in general from the heuristic definition of a base case BPC. For the case of the sugarcane conversion process, the process concept based on ethanol production was derived from the sugar production BPC by substituting some of the subprocesses. In particular the multi-effect evaporator and sugar crystallization were substituted with yeast fermentation and ethanol distillation. Accordingly, the combined sugar and ethanol process was also derived from the first two cases in which the two products were obtained separately.

Design parameters of different process components influencing the production rate of the different products were fixed according to some data found in the literature (mainly presented in [28, 27]). Conversely, those design parameters influencing the process thermal demand were considered among the set of decision variables to be optimized following the objective of the minimum process thermal demand.

In order to select these parameters the HEATSEP method suggests to discard all the previous cooling and heating processes and the possible thermal matching by means of a predefined heat exchangers network, and to virtually cut all the thermal links between subsequent components of the BPC. All the independent end-temperatures and mass flow-rates are then included in the whole set of decision variables along with other parameters. As discussed in Section 2.3.5, this method is in particular well suited when the majority of these end-temperatures and mass flow rates can be adjusted. When dealing with a productive process, a large number of the end-temperatures and mass flow rates are instead dictated by production requirements. The application of the HEATSEP method was shown not to significantly help identify additional decision variables.

In order to interpret the results of the parameter optimization, the grand composite curve was built for each optimized BPC. This graphical tool provided by the Pinch Analysis gives important information about the heat pockets in the process heat cascade. The entity of these heat pockets (in terms of heat load and of extent of the temperature interval) can suggest which are the temperature intervals (i.e. the subprocesses) that can be further optimized for minimizing the process thermal demand. In particular, when looking at a better heat integrated process, components staging is a way to generate a greater number of heat sinks and heat sources to be matched in the process heat cascade. Conversely, the effects of changing the material connections between existing components and the substitution or the addition of new components are less easy to identify in the process grand composite curve. Thus, the organized procedure for the modification of the BPC was revealed to be the only way to systematically investigate all the opportunities for better process energy efficiency.

While component staging and the changes in connections between components do not alter substantially the original idea behind the BPC (sugar production, ethanol production, etc.), the further addition of components (or subprocesses) leads to substantially new BPCs.

The different configurations of the sugarcane conversion process explored in the present chapter showed different opportunities for heat integration as a consequence of the intrinsic thermal behavior of the productive subprocesses. Both the sugar and the ethanol are obtained by water separation. While sugar is obtained basically by evaporating the water from the juice extracted from the sugarcane, the ethanol is produced by biochemical conversion of the sugar (exothermic process) and by subsequent removal of water from the wine by means of distillation. Both subprocesses are highly energy intensive so they are the parts of the process that were mainly subject to modifications in order to minimize the
process thermal demand.

It was in fact possible to interpret the different opportunities for heat integration of the different BPCs (i.e. the different minimum thermal demand of the optimized configurations) by looking at the specific contribution of the multi-effect evaporator and distillation subprocesses to the process heat cascade. This was relatively simple in case of separate production of sugar and ethanol. In case of the combined production of sugar and ethanol, the integrated grand composite curves of local subprocesses was instead used for this purpose. This graphical tool, which is built as a grand composite curve, brings to light additional information about local thermal contributions to the process thermal cascade (for instance that of a specific subprocess) by highlighting the shape of the local grand composite curve and the way it integrates with the grand composite curve of remaining parts of the process. Examples of integrated grand composite curves are given on page 96.

The conversion of 138.9 kg/s of sugarcane in 14.4 kg/s of sugar was firstly considered. In this case the base case minimum thermal requirement resulted of 100 MW and was subsequently reduced to 62 MW mainly by intervening on the number of effects, the concentration and the pressure profiles of the multi-effect evaporator. For the case of only ethanol production, 9.8 kg/s of motor fuel ethanol or 8.3 kg/s of high grade ethanol were considered. The minimum thermal requirement of the base case (motor fuel ethanol production) resulted of 86 MW and was subsequently reduced to 48 MW by carrying out the motor fuel ethanol distillation into two stripping-rectifying columns. When aiming at the production of high grade ethanol instead, the stripper and the rectifier columns must be placed in sequence. As a result of higher desired purity of the product, the thermal demand of the high grade ethanol production process is greater than in case of motor fuel ethanol even in the case one of the two columns is operated under pressurized conditions (a minimum thermal demand of 93 MW of the optimized process configuration was evaluated here).

It is possible to conclude that yeast fermentation and ethanol distillation leads in general to less heat integration potentials in comparison with evaporation and sugar crystallization. This can be explained by observing that the heat source and the heat sinks in the ethanol distillation subprocess are separated by a greater temperature interval (the boiler of a distillation column operates around the evaporation temperature of the water while the condenser operates at the azeotropic temperature of the ethanol-water mixture) resulting in less potential for heat integration also in the case ethanol distillation is further split in more than two columns. On the contrary heat sinks and heat sources of the multi-effect evaporator are generated at the same temperatures (the juice boils more or less at the same temperature of saturated steam) thus leading to a greater potential for process heat integration.

When dealing with combined sugar and ethanol production, the potential for process thermal integration introduced by the multi-effect evaporator for syrup production is mitigated by the high thermal demand of the ethanol distillation. The base case scenario of combined sugar and ethanol production was defined such that sugar and high grade ethanol production rates are equal to half of the production rates obtained in the case of separate production. A minimum thermal requirement of 92 MW of this base case scenario was evaluated by setting the parameters of the multi-effect evaporators as in the optimized condition of the sugar production configuration (case S1) and by using environmental distillation. Further modifications of the structure of the process and subsequent parameter optimizations led to a reduction of the process thermal demand. In particular, the major reduction in process thermal demand was once again obtained by operating one of the two distillation columns under pressurized conditions. However, the potential for thermal integration was shown to be limited by the high thermal demand of high grade ethanol distillation.

Particularly interesting is the case in which a greater sucrose concentration of the must for ethanol production was considered and molasses were also recycled for ethanol production. In this case a greater yield of high grade ethanol is obtained for a unit of juice. In the present work an increased from 4.3 to 5.6 kg/s of ethanol output was considered (almost 30% increase in ethanol yield for the same sugar production rate). In so doing an increase of the process thermal demand from 62 MW to 75 MW was estimated (around 21% increase) which confirms the fact that it is less energy intensive to separate the water by means of a multi-effect evaporator than by means of ethanol distillation. Accordingly, it would be convenient to further increase the sucrose concentration of the must at the inlet of the fermentor for instance by diverting more syrup. Nevertheless the yeast cannot stand high sucrose and ethanol
concentration in the substrate thus the potential benefit of separating the water in advance can only be partially exploited.

A summary of results obtained in Chapter 3 is presented in Table 3.4.

It is apparent that the real convenience of choosing a specific configuration among all that were generated and modified throughout the discussion in the present chapter, cannot be based on the only objective of reducing the process thermal demand (which is the goal in this work), but should consider all the economical aspects related to process modifications. Nonetheless, the results presented here give important indications about the benefits derived from more integrated processes. For instance, in the case of ethanol production, bigger investment costs are introduced by pressurized distillation columns which on the other hand is a key point for the reduction of the energy bill.

Table 3.4: Summary of results of Chapter 3 - (1: Heat Demand; 2: Power Demand; 3: Total Heat Integration of base case BPC; 4: Motor Fuel Ethanol; 5: High Grade Ethanol)

<table>
<thead>
<tr>
<th>Figure</th>
<th>Sugar Production</th>
<th>Ethanol Production</th>
<th>Combined Sugar and Ethanol Production</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>H.D.(^\d)</td>
<td>P.D.(^\d)</td>
<td>Sug.</td>
</tr>
<tr>
<td>Base</td>
<td>3.9</td>
<td>179</td>
<td>17</td>
</tr>
<tr>
<td>T.H.I.(^\d)</td>
<td>3.15</td>
<td>100</td>
<td>&quot;</td>
</tr>
<tr>
<td>S1</td>
<td>3.16</td>
<td>62</td>
<td>&quot;</td>
</tr>
<tr>
<td>Base</td>
<td>3.20</td>
<td>149</td>
<td>12</td>
</tr>
<tr>
<td>T.H.I.(^\d)</td>
<td>3.22</td>
<td>86</td>
<td>&quot;</td>
</tr>
<tr>
<td>E1</td>
<td>3.24</td>
<td>48</td>
<td>&quot;</td>
</tr>
<tr>
<td>E2</td>
<td>3.26</td>
<td>93</td>
<td>&quot;</td>
</tr>
<tr>
<td>Base</td>
<td>3.27</td>
<td>164</td>
<td>14</td>
</tr>
<tr>
<td>T.H.I.(^\d)</td>
<td>3.28</td>
<td>92</td>
<td>&quot;</td>
</tr>
<tr>
<td>CSE1</td>
<td>3.29</td>
<td>69</td>
<td>&quot;</td>
</tr>
<tr>
<td>CSE2</td>
<td>3.32</td>
<td>62</td>
<td>&quot;</td>
</tr>
<tr>
<td>CSE3</td>
<td>3.36</td>
<td>75</td>
<td>(+)</td>
</tr>
</tbody>
</table>

A further increase in plant profitability can be obtained by exploiting the Bagasse by-product for combined heat and power generation which can be sold to the market in addition to sugar and ethanol. The synthesis of a plant for combined production of sugar, ethanol, heat and power is discussed in the next chapter where the synthesis of the total industrial site including a bagasse fueled CHP plant is analyzed.
Chapter 4

Total site synthesis problem: sugarcane process and CHP systems

4.1 Introduction

In the previous chapter an organized procedure for the generation of process Basic Plant Configurations (BPCs) following the objective of a minimum process thermal demand, was applied to the case of the sugarcane conversion into sugar and ethanol. Following the idea of progressively adding process options, a first base case BPC of the sugarcane conversion process including only the sugar production was subsequently modified in order to accommodate the production of ethanol with different quality resulting in different total process thermal demands. If the reduction of the process energy demand is not the unique criterion for the definition of the ultimate process configuration, the development of tools for the effective synthesis of process configurations with minimum energy demand remains of primary importance especially for the cases in which the cost of energy consumption has a great impact in plant economy.

The synthesis approach for the minimization of the process energy consumption shown in the previous chapter is mostly based on exploiting an increased number of process integration opportunities while changing the process structure and parameters towards more complex scenarios. Pinch Analysis tools are chosen for the evaluation of the potential for heat recovery within the process. The combined sugar and ethanol production process from sugarcane is in fact a paradigmatic application for energy integration strategies because of the high number of hot and cold streams involved, the external hot utility requirement at different temperature levels (basically for juice evaporation and ethanol distillation), and the electricity demand for juice extraction by milling.

A further improvement in terms of process productivity is explored here by observing the presence of a significant amount of residue (bagasse) from the juice extraction subprocess. It could then be possible for instance to subsequently generate additional BPCs including both the combined sugar and ethanol production process and the bagasse conversion process for instance converting the biomass into synthetic natural gas (SNG) or additional ethanol by means of cellulosic fermentation.

Among different concepts of conversion of bagasse into useful products, the production of heat and electricity is considered here, all the remaining process alternatives being not explored for reasons of brevity. This allows to finally consider within the synthesis problem also the utility subsystems that is the set of devices entitled to cover the heat and power demands of the process. In fact, a considerable amount of bagasse makes on-site electricity production to be a rather obvious choice when designing modern sugarcane mills.

This latter problem is addressed as the total site synthesis, that is the problem of the definition of the type, number of components of the process plus the utility systems and their connections.

While in the previous chapter the objective followed was the minimum process thermal demand, the so-called total site synthesis problem is solved here following the objective of maximum net electrical
Total site synthesis problem: sugarcane process and CHP systems

power (while heat is produced only for supporting the sugar and ethanol production process) under the hypothesis of constant sugar and ethanol production, considering the thermal streams of the process and those of the CHP system as a whole set of streams to be integrated.

The results of optimizations presented in Chapter 3 have already provided a general indication about the amount of heat the CHP system has to supply to the process. On the other hand, the several solutions that were found to minimize process hot utility requirement are no longer equivalent in this new set of optimization problems.

In particular when the electricity production is found to compete with the sugar and ethanol production, it becomes crucial to maximize heat and power integration not only among the ethanol and sugar production sub-processes but also between the productive processes and the CHP system. In other words the attention is now on the way exergy (that is the potential of work generation) is exploited throughout the whole total site heat cascade while in the previous chapter the issue was how to recover heat within the process. Compared to the results presented so far, the results of the new optimization problems are therefore expected to suggest process modifications that maximize the total site integration and not necessarily minimize heat demand of the productive sub-processes.

In Chapter 2, and in particular in Sections 2.1.3 and 2.3, two basic different methods for structural and design parameters optimization were discussed. In the general case of a power system in which material streams are recirculated between components, the whole set of decision variables must be optimized simultaneously (see the algorithm in Figure 2.32 at page 53).

Conversely, when it is possible to express the objective function (in the following sections the total site net power) as a linear combination of some of the process mass flow rates, the optimization can be performed following a two-level procedure (see Figure 2.33). In this case in fact, for given performances of the independent sub-processes the heat and power integration can be expressed as a linear programming problem in which mass flow rates are the decision variables. In an outer step, at each iteration of the optimization procedure, it is possible to optimize performance parameters (pressures, temperatures, etc.) which have a non-linear relation with the total site net power.

While the minimization of the demand for external energy of the sugarcane process was shown to be related to the adjustment of pressure and temperatures for which a two-level optimization strategy was not of help, the maximization of the total site net power is a paradigmatic case in which this approach can reduce the computational effort. In fact, a material separation is observed between subsystems. The mathematical representation of the total site can be at least separated into three sub-systems which participate in the net power generation and in the heat cascade proportionally to their material streams: 1. the combined ethanol and sugar production process for which the main material is the sucrose-rich juice, 2. the bagasse conversion plant for which the material stream can be identified with the chemical constituents of the bagasse, 3. the steam network which delivers heat to the process and generates power through the expansion of steam between headers.

Accordingly, the total site synthesis of the sugarcane mill is proposed in terms of structural and parameter optimization problem as follows:

1. The BPC of the productive process consisting of the recirculation of molasses for ethanol production as in Case CSE3 (see Section 3.3.2) is taken as a reference, being this the process configuration previously analyzed which gives the best trade-off between maximization of sugar and ethanol production and minimization of process heat and power demands. Number of units, operating pressures, concentration profiles of the multi-effect evaporator plus the pressure of the ethanol distillation stripper are considered among the whole set of the upper-level decision variables. As mentioned before, the production process is fixed in terms of mass flow rates so, for each optimization iteration the process participate with constant power demand and thermal streams in the total site heat and power integration problem.

2. Two BPCs are considered for the Bagasse conversion sub-system: bagasse combustion (case CHP1) and bagasse gasification and gas turbine fueled with syngas (case CHP2). Modeling and simulation of basic processes for the conversion of the bagasse was done in Belsim Vali flow-sheeting environment [132]. As a result of the simulation specific power and heat loads of this sub-system are evaluated. While it could be possible to consider some of the parameters of components involved
in bagasse conversion among the set of the decision variables (non-linear variables of the upper level optimization step), the analysis is limited here to fixed values of performance parameters of the bagasse conversion sub-system. Conversely, the bagasse mass flow rate is considered as a sensitivity parameter or as a decision variable of the inner level optimization step (along with all the other mass flow rates of the system according to the MILP formulation of the heat and power integration problem).

3. A steam network superstructure is defined in terms of possible steam and condensates headers and expansion stages between headers. When from the interpretation of the grand composite curve of the productive process it is not possible to draw indications about optimal pressure levels or temperatures of steam headers, these parameters are included in the whole set of upper-level decision variables in order to explore different steam superstructure. Conversely, for a given steam network superstructure, optimal values of steam mass flow rate and optimal selection of steam headers are left to be evaluated as a result of the heat and power integration problem (solving a MILP optimization problem).

The reader is referred to the Appendix for a better description of all the computational tools used for modeling, simulating and optimizing the plant configurations analyzed in this chapter.
4.2 Bagasse properties

As shown in Figure 3.3 on page 65, after the juice is extracted from the sugarcane the remaining part of the cane is removed as by-product. This relatively dry-residue is called bagasse, which has still a 50% moisture content and consists basically of cellulose, hemicellulose and lignin.

Bagasse is extensively used as an internal energy source in sugar cane industry. In particular, after a drying process, combustion or gasification are the common ways of converting this sub-product into heat and electricity [108, 112, 123]. Production of Synthetic Natural Gas (SNG) based on methanation of biomass, among which bagasse can be a possible candidate, is also a particularly interesting pathway [43]. The integration of the ethanol production and the bagasse conversion processes shows that the interest of converting bagasse into natural gas largely competes with electricity production [142]. Additional ethanol production via enzymatic hydrolysis of bagasse is another promising alternative. Different studies in the literature focused on the possible improvements of technologies for the ethanol production from bagasse [17, 63, 87].

The content of bagasse that is extracted from a unit of sugarcane can range between 25% to 30% in mass of which 50% is in average water. The portion of extracted bagasse is here fixed to 28% by mass of the total sugarcane input (138.9 kg/s), in agreement with the reference work from which main plant data were obtained [27].

According to Hugot [62], the average weight dry basis composition of bagasse is: Carbon [47%], Hydrogen [6.5%], Oxygen [44%], Ash [2.5%] (as reported in Figure 3.2). Different empirical formulas have been proposed in the past for the evaluation of heating values of different type of biomass as a function of the ultimate analysis of the feedstock and of the ash and water content. Among others, the Channiwala correlation was chosen for this work as it was already implemented in the Vali flow-sheet simulation software [18]. Accordingly, a higher heating value of 19513 kJ/kg dry basis is evaluated, corresponding to a lower heating value of 7834 kJ/kg at humidity of 50% weight basis (the status of the bagasse at the outlet of the extraction sub-system). Another empirical correlation for the calculation of the lower heating value of the bagasse was provided by Hugot [62] and is here reported in Equation (4.1), where $P_{Bag}$ is the remaining sucrose content of the bagasse (the sucrose mass percentage in the bagasse) and $\phi_{Bag}$ is the relative humidity (in percentage). Under the additional assumption there is no sugar left in the bagasse, he Hugot correlation gives a value of 7640 kJ/kg. So the Channiwala correlation
Bagasse properties

Bagasse properties

... gives a 2.5% greater estimate of the bagasse Lower Heating Value with respect to the Hugot correlation. Other correlations found in the literature, like the well-known Boie correlation, give instead intermediate estimates.

\[ LHV_{Bag} = 17790 - 50.23 \cdot P_{Bag} - 203 \cdot \phi_{Bag} \]  

(4.1)

Being the sugarcane input fixed at 138.9 kg/s as an assumption of the present analysis, the actual mass flow rate of bagasse discarded by the juice extraction sub-system is 38.9 kg/s leaving 100 kg/s of raw juice to be processed for sugar and ethanol production. As a consequence, the resulting thermal power theoretically available from the total combustion of the bagasse mass flow rate is of 304742.6 kW (based on LHV at 50% humidity).
4.3 Bagasse combustion and steam cycle (CHP 1)

4.3.1 Modeling bagasse combustion

A flow-sheet of the bagasse conversion sub-system is given in Figure 4.2 as appearing in the Vali simulation environment [132]. As a modeling assumption, the bagasse conversion sub-system is separated from the steam network sub-system. In this way the mass flow rate of bagasse is considered independent of the mass flow rates of the steam network and can be evaluated as a result of the heat and power integration problem. Accordingly, the boiler is conceptually separated into two parts: at the hot side the thermal streams associated with the radiative and convective heats of combustion (included in the bagasse conversion sub-system) and at the cold side the thermal streams associated with the counter-current steam flow (included in the steam network sub-system).

The bagasse released by the extraction sub-system has an high content of water (50% weight basis). Since the presence of moisture lowers the performance of the thermal conversion of the biomass due to evaporation and desorption of water, a drying process is needed to reduce the wood moisture content at least to 30% [121].

A zero-dimensional, steady state formulation for the air-drier found in an article by Gassner et al. is used to model the drying process [43]. The driving force is the difference of vapor partial pressure between the hot air stream and the surface of the wood.

The humidity at the wood surface $\phi_{\text{wood}}$ can be expressed locally as a function of the relative humidity $\phi_{\text{air}}$ and the temperature $t_{\text{air}}$ (in $^\circ$C) of the air in contact with the wood surface. An empiric correlation found in the same article is used for this purpose:

$$
\phi_{\text{wood}} = A \cdot \sqrt{\phi_{\text{air}}} + B \cdot \phi_{\text{air}} + C \cdot \phi_{\text{air}}^2 + D \cdot \phi_{\text{air}}^3
$$

$$
A = 2.865 \cdot 10^{-2}
B = 2.307 \cdot 10^{-1} - 1.273 \cdot 10^{-3} \cdot (t_{\text{air}})
C = -2.519 \cdot 10^{-1}
D = 2.199 \cdot 10^{-1} + 8.630 \cdot 10^{-4} \cdot (t_{\text{air}})
$$

In particular, along the air-drier, the steam partial pressure at the wood surface decreases and the steam partial pressure in the air increases. Under the assumption that no steam is exchanged along the directions of the mass streams but only in the direction normal to the virtual plane dividing the two streams, the mass transfer can be expressed as a function of the partial pressures at the inlet and outlet sections of the air-drier.

Following a formulation similar to that of the heat transfer between counter-current material streams, the total steam mass flow rate $m_{\text{steam}}$ that passes from the wood to the air can be expressed as a product between the total mass flow of air $m_{\text{air}}$, an overall mass transfer coefficient $U_p$ and a counter-current log-mean difference of partial pressures:

$$
\Delta \dot{m}_{\text{steam}} = \dot{m}_{\text{air}} \cdot U_p \cdot \frac{\Delta p_1 - \Delta p_2}{\ln \frac{\Delta p_1}{\Delta p_2}} \tag{4.3}
$$

where $\Delta p_1$ and $\Delta p_2$ are the differences of partial pressures respectively at the air-outlet and at the air inlet. In the same reference work by Gassner et al. a value of $11.16 \cdot 10^{-3}$ bar$^{-1}$ for $U_p$ is given as a result from an interpolation of data about performance of rotary drum air-drier found in [31].

For stand alone drying systems, environmental air is normally used as drying agent. In order to increase the driving force of the process, the inlet air is normally heated up to 200$^\circ$C. In this way great humidity gradient is obtained at the air inlet thus reducing the residence time of the bagasse in the drier for a given value of desired humidity at the outlet. When available, hot gases can be used in place of environmental air leading to lower capital and operating costs. This is the case of bagasse combustion and gasification plants. Accordingly combustion gases, after being used for steam generation are further used for bagasse drying.
Bagasse combustion is modeled as total oxidation of the elementary chemical constituents. In real combustion processes a part of the input solid fuel behaves as inert compound and is removed as ashes. This part is usually specified through the so-called proximate analysis (along with fixed carbon and water content) of a solid fuel. Values of ashes in bagasse are reported to range between 1 to 2.5 % in mass [62]. Here no ashes are considered in the bagasse and an equivalent amount is mass of nitrogen is considered instead. This assumption actually leads to a slight overestimation of the flue gases mass flow rate but does not affect the energy balance being nitrogen considered as an inert compound during combustion and no NO formation is modeled. Even if, in actual biomass combustion part of the nitrogen in the air is oxidized leading to the formation of NO, the contribution of these set of reactions to the energy balance can be neglected with respect to the bigger contribution of the oxidation of fixed carbon and hydrogen.

Biomass is virtually decomposed in its chemical constituents in gaseous phase and graphite \((N_2, O_2, H_2, C_{solid})\) in a preliminary reactor (DE Vol) where only mass and energy balances are accounted for given quantities of input and output species. The difference in chemical energy rate between input of solid biomass and the output of gaseous compounds, represented as heat \(q_{201}\), is then included in the energy balance of the actual combustion reactor (COMBUST) where total conversion of fuel in combustion products (water and carbon dioxide) is modeled specifying the combustion stoichiometry.

In the combustion reactor, complete oxidations of graphite and hydrogen take place. In agreement with actual operation of industrial fixed-grate boilers, an excess of air of 0.3 is considered. Inside the boiler, the heat is transferred between combustion products and steam by means of both radiation and convection. Here we assume that radiation occurs over 1000\(\, ^\circ\, C\) boiler, the heat is transferred between combustion products and steam by means of both radiation and convection. Here we assume that radiation occurs over 1000\(\, ^\circ\, C\) and this part of the total heat transfer is modeled with a thermal stream \((q_{r,202})\) at constant temperature of 1000\(\, ^\circ\, C\). The remaining convective part of the heat of combustion is that of the flue gases cooling \((q_{c,201})\).

Environmental air is used for combustion and is injected into the combustion chamber by fans (isentropic efficiency = 0.78) in order to overcome pressure drops in the boiler and air dryer (total power \(w_{e,201}\)). In order to increase the thermal output at higher temperatures, air is preheated up to 600\(\, ^\circ\, C\). This thermal stream is then included in the whole set of thermal streams to be integrated along with all the thermal streams of the bagasse energy conversion sub-system.

Flue gases at temperature of 200\(\, ^\circ\, C\) are used for bagasse drying and are injected counter-currently with respect to the biomass. As a result of the drying process the water content of the biomass is reduced from 50\% to 35\% in mass while the flue gases exit the air-drier at around 70\(\, ^\circ\, C\) with a relative humidity of 74\%. In order to prevent condensation of flue gases, a further cooling process that would allow to recover additional low-grade heat is not considered. 4.71 \(kJ/kg_{bagasse}\) of flue gases are produced from the bagasse drying and combustion with the following mass fractions: 60.67\% N2, 4.23\% O2, 16.80\% H2O and 18.30\% CO2.

Energy and mass balances were evaluated for 1 \(kg/s\) of bagasse input, under the hypothesis that no heat losses occur in the system. Simulation results are reported in Figure 4.2. An error of energy balance of 100 kW was obtained (about 1.3\% of the LHV) which was verified to be related to the way the calculation of biomass LHV is implemented in the flow-sheet simulation software. In the light of the possible overestimation of the bagasse heating value, of the energy balance error and in order to take into account actual heat losses from the boiler, a combustion efficiency of 85\% is assumed. The 25\% of heat losses (1175 kW of the total heat duty obtained from the aforementioned simulation which is not exploited within the total site heat cascade) is charged to the radiative part of the total heat duty \((q_{r,202})\).

As a consequence the following heat and power loads are evaluated for the bagasse conversion sub-system:

- Radiative heat load (hot stream): 3376 \(kJ/kg_{bagasse}\) at 1000\(\, ^\circ\, C\).
- Convective heat load (hot stream): 4586 \(kJ/kg_{bagasse}\) between 1000\(\, ^\circ\, C\) and 200\(\, ^\circ\, C\).
- Air-preheating heat load (cold stream): 1380 \(kJ/kg_{bagasse}\) between 45\(\, ^\circ\, C\) and 400\(\, ^\circ\, C\).
- Fan electricity consumption: of 75.5 \(kJ/kg_{bagasse}\). Additional 50 \(kJ/kg_{bagasse}\) are included for accounting the electricity absorbed by bagasse conveyors so that a total 125.5 \(kJ/kg_{bagasse}\) of
Figure 4.2: Flowsheet of bagasse drying and combustion in Vali Belsim [132]
electricity consumption of the bagasse conversion subsystem is considered.

4.3.2 Definition of the steam network superstructure

The steam network subsystem is entitled for the production of electric power by means of steam expansions and for the distribution of heat throughout the productive process. A steam network can also be used to exploit hot thermal streams at low temperature level. In fact, as total site heat integration is considered, this low-grade heat might be used for preheating water to be used for steam generation.

The optimization of the optimal steam network structure starts from the definition of a network superstructure which must include all the steam and condensate headers (defined by pressure and temperature of the steam or water) among which the optimal subset of headers is to be found through a MILP optimization as described in Section 2.2.3.

In agreement with the optimization strategy based on the so-called two-level optimization procedure (see Section 2.2.2), the optimization of the structure and design parameters of the steam network is subdivided into two parts. The parameters that have a non-linear relation with the power output are optimized in an outer level along with all the other non-linear decision variables of the total site, while the structure and the steam mass flow rates are optimized in the inner step according to the MILP formulation of the steam network synthesis. At the inner optimization level, for a given pressures and temperatures of steam headers of the steam network superstructure inherited from a the outer optimization level, a deterministic algorithm is used to find the optimal combination of headers to be activated and the respective steam mass flow rates that maximize the total site heat integration that is power generation.

For a better description of the different tools employed for performing all the calculations reported in the following section the reader is referred to the Appendix.

A way to increase the heat integration options is to set a high number of steam network superstructure headers. This is in agreement with the idea of increasing number of component stages, being in this way possible to better exploit the so-called process heat pockets. As shown in Figure 4.3 a heat pocket is a portion (temperature interval) of the heat cascade in which the heat demand of thermal streams at the lowest temperature level is covered by the excess of heat available at the highest temperatures within that interval. This corresponds to the situation in which heat is cascaded through a wide temperature range. For instance this is what happens in the multi-effect evaporator where the heat provided to the first effect is exploited in the whole heat cascade of the process by means of subsequent evaporations and condensations.

When a heat pocket extends in a large temperature interval there is the interest in exploiting the temperature difference between the hot and cold streams for power generation, otherwise letting the correspondent exergy rate to be destroyed as a consequence of the finite temperature differences between streams. Thus the pressures of the steam headers might be arranged in such a way that a part of water heating and steam evaporation is performed by using the process heat instead of using the heat from fuel combustion.

In Figure 4.4, for a given process grand composite curve (in red), the increase in steam network headers is shown to increase heat integration. In so doing a greater amount of exergy is supposed to be transferred to the steam network thus increasing the power output. In reality, the increase in steam network complexity is beneficial until the capital investment is counterbalanced by the increase in power generation efficiency. This in fact leads to quite simple steam network configurations in the case of CHP systems which in general cannot benefit from economy of scale factors like big steam power plants.

In the following paragraphs a steam network superstructure with one production header and two steam condensation headers is considered, being necessary at least to provide heat to the productive process (draw-off) and being profitable to expand part of the steam till the cold utility temperature level (condensing turbine).

It is apparent that the analysis of the shape of the grand composite curve of the productive process could facilitate the choice of the optimum pressure levels and number of steam and condensate headers. If, in theory, it could be possible to optimize the non-linear decision variables of the steam network without a preliminary interpretation of the process grand composite curve, an accurate analysis of the heat integration opportunities between the process and the steam network can reduce the optimization
Figure 4.3: Heat pockets in a process heat cascade

Figure 4.4: Heat pockets and integration opportunity for a steam network: a) with one steam production header and one condensation header c) with one steam production header and two condensation headers
effort by simply neglecting those values of decision variables that certainly lead to sub-optimal solutions.

With reference to the specific case of the combined sugar and ethanol production plant (case CSE3), the optimization of pressures and concentration profiles of the multi-effect evaporator and of the stripper operating pressure may lead to important variations of the process grand composite curve, as shown in the Section 3.3.2. When a steam network is considered at least one steam utilization/condensation header (draw-off) has to operate at the highest temperature at which the process requires heat. In the case of the combined sugar and ethanol production process this corresponds to the temperature level of the stripper reboiler when this operates at pressures higher than the environmental pressure and to the temperature level of the first evaporation effect when the stripper operates at environmental pressure.

In addition, it is apparent that a way to maximize power production is to reduce exergy losses in the boiler by increasing the steam evaporation pressure and the super-heating final temperature. Since the objective here is to maximize power output (thermodynamic objective) it is apparent that these parameters are not decision variables being otherwise maximized up to their upper bounds. Accordingly they are fixed to maximum technically feasible values.

To sum up, the parameters of the steam network superstructure are set as follows:

- one steam production header at 80 bar, super-heating final temperature equal to 800 K (527°C)
- one steam draw-off at $p_{\text{stripper}} + 2$ bar (this latter pressure difference allows to set the temperature of the steam draw-off slightly higher than the first evaporation effect which results the locus of process thermal demand at the highest temperature when environmental distillation is adopted)
- one steam condensation header at 305 K (32°C)
- steam expansion isentropic efficiency equal to 0.8

### 4.3.3 Total site optimization problem and results

Here we discuss the results of the following total site optimization problem involving a CHP system based on total bagasse combustion and a steam cycle (which structure and mass flow rates are assessed as an inner optimization of the steam network superstructure presented in the previous section):

$$\text{max } P_{\text{net}} = P_{\text{CHP}} - P_{\text{process}}$$

considering the following (upper level) decision variables with their respective lower and upper bounds in square brackets:

- n number of evaporation effects [3,5,7]
- $p_i$ operating pressure of the i-effect [$p_{i-1} \div 0.1 \text{bar}$] (the first effect operating temperature is fixed at 115°C)
- $B_i$ solid concentration at the outlet of the i-effect (the outlet concentration of the last effect is fixed at 65%)
- $p_{\text{stripper}}$ operating pressure of the stripper for ethanol distillation [1.013 ÷ 5] bar

And the following decision variables of the inner MILP problem

- $i_l$ binary variable for the activation of the l-steam/condensate header
- $m_l$ steam mass flow rate of the l-steam/condensate header

The sugar and ethanol production rates are kept at the same values of case CSE3 (7.2 kg/s and 5.6 kg/s respectively).

Optimization results show that best total site heat integration is obtained when the stripper operates at environmental pressure. In spite of a slight reduction in process heat demand when pressurized distillation is used (see Figure 3.37 on page 99), net power generation decreases for higher pressures of
the steam draw-off. On the contrary, solutions with the stripper operating at environmental pressure result in greater power outputs. Distillation of ethanol extends over a quite a big temperature interval so that it is not possible to divide the multi-effect evaporator in many stages. For this reason, three evaporation effects are enough to minimize the process thermal requirement at low temperature levels and to let the water pre-heating from the condensation temperature up to the temperature of the steam draw-off be carried out with process thermal streams.

In Figure 4.5 the heat integration for one of the near optimal solutions with three evaporation effects is given. The total power output of the steam cycle is 76190 kW (25% cycle thermal efficiency) of which 13575 kW are consumed by the process and 5835 kW are used for running bagasse conveyor and air fans of the boiler, leading to a net power output of 56780 kW. This value was obtained for the following pressures and concentration profile of the 3-effect evaporator:

1. 1st effect: $B_1 = 23.1\%$; ($T_1$ fixed at 115°C)
2. 2nd effect: $B_2 = 32.3\%$; $T_2 = 70°C$ ($p = 0.30$ bar);
3. 3rd effect: ($B_3$ fixed at 65%); $T_3 = 62°C$ ($p = 0.17$ bar);

![Integrated composite Curve of Unit RNK from model sugar_cane](image)

Figure 4.5: Case CHP1: integrated grand composite curve (blue: steam network thermal streams, red: bagasse combustion and process thermal streams)

In Figure 4.5 it is also possible to notice that the thermal profile of the optimized multi-effect evaporator allows to perform the first part of the water-heating by using process hot streams. This solution can increase power generation with respect to less heat integrated solutions, however can also lead to a dramatic increase in heat-exchanger network complexity. This part of water heating is carried out by using several hot streams of the process and in particular the heat of condensation of steam produced by the evaporation effects and distillation. However, heat exchanger network capital costs may compete with those of the CHP system. In fact, a CHP system designed for the combustion of all the bagasse mass flow rate could represent the largest share of total site capital costs.

While only a detailed thermo-economic analysis could help clarifying this point, it is interesting to consider the situation in which only the bagasse that is necessary to cover the process hot utility
requirement (which has to be minimized) is burnt and some power is still produced. In order to assess this quantity is therefore necessary to perform another optimization. It is apparent in fact that for a given quota of bagasse to be burnt, values of decision variables must be optimized in order to maximize total site heat integration (i.e. power generation).

Figure 4.5 shows that for total combustion of bagasse, power generation is maximized when using a condensation turbine thus letting the major part of the steam to be expanded down to the temperature of the cooling water. When reducing the mass flow rate of bagasse to be burnt, the share of total heat produced by the CHP system and used by the process regularly increases until only a back-pressure turbine configuration is needed. It is also possible to notice that no other significant heat pockets appear in the process heat cascade to justify an additional steam header providing heat to an intermediate temperature level. For total bagasse combustion, the choice of only one back pressure and one condensing turbine results to be good enough for exploiting all the heat of bagasse combustion while obtaining a significant power output and still providing the heat to the productive process.

Conversely, when looking for the CHP system using the minimum share of bagasse to be burnt sufficient to cover the process heat demand, the use of a condensation turbine is not more justified, while it becomes interesting to explore steam network configurations with a steam draw off at an intermediate temperature level. Since it is not clear the pressure of this second steam header, this variable must be included within the set of the decision variables.

A two-objectives optimization problem is considered in order to explore a wide range of system configurations leading to maximum net power production at progressively lower portions of bagasse to be burnt. This problem has the following mathematical representation:

\[
\begin{align*}
\text{max} & \quad P_{\text{net}} = P_{\text{CHP}} - P_{\text{process}} \\
\text{min} & \quad \dot{m}_{\text{Bagasse}} 
\end{align*}
\]

considering the following (upper level) decision variables with their respective lower and upper bounds in square brackets:

- \( n \) number of evaporation effects \([3, 5, 7]\)
- \( p_i \) operating pressure of the \( i \)-effect \([p_{i-1} \div 0.1\text{bar}]\) (the first effect operating temperature is fixed at \(105^\circ\text{C}\))
- \( B_i \) solid concentration at the outlet of the \( i \)-effect (the outlet concentration of the last effect is fixed at 65%)
- \( p_{\text{stripper}} \) stripper operating pressure \([1.013 \div 5]\text{bar}\)
- \( p_{\text{v2}} \) steam back pressure \([0.05 \div 2.5]\text{bar}\)

And the following decision variables of the inner MILP problem

- \( i_l \) binary variable for the activation of the \( l \)-steam/condensate header
- \( m_l \) steam mass flow rate of the \( l \)-steam/condensate header

Figure 4.6 shows the front of optimal total site configurations leading to maximum power generation for different bagasse quota used for combustion. As a result of the optimization, the minimum quantity of bagasse necessary to cover the process thermal demand is found to be around 35% of the total mass flow rate \((13.7 \text{ kg/s})\) which however leaves around \(10 \text{ MW}\) of electricity to be bought from the network. In reality, the formulation of the optimization problem leads to investigate only those CHP configurations in which the heat for the process is totally covered by the steam at the outlet of a back pressure turbine. Only the CHP back pressure turbines with maximum performance are investigated and all the configurations in which only part of the heat is provided by the back pressure turbine and the remaining part with a separate steam boiler are neglected. In fact the case in which only a boiler is used to cover the process heat demand (case CSE3 in Figure 3.36 on page 99) and no power is produced requires 30% of the total amount of available bagasse. Accordingly, from 30% to 35% of bagasse quota,
Total site synthesis problem: sugarcane process and CHP systems

Figure 4.6: Maximum total site net power for different bagasse quota fueling a CHP plant with $T_{\text{max}}=527^\circ C$ and $p_{\text{max}}=80$ bar

Figure 4.7: Combustion of the minimum part of bagasse needed to cover process thermal requirement: integrated grand composite curve (blue: steam network thermal streams, red: bagasse combustion and process thermal streams)
it is possible to produce power but only a part of the heat demand of the process can be covered using the steam from the back-pressure turbine, the remaining part to be covered with a separate steam boiler.

Particularly interesting is the configuration in which both process heat and power demands are balanced by the combined heat and power production. This solution, of which the grand composite curve is shown in Figure 4.7, was obtained with stripper operating at environmental pressure and the following values of a 3-effects evaporator:

1. 1st effect: \( B_1 = 20.1\% ; \) \( T_1 \) fixed at 115\(^\circ\)C
2. 2nd effect: \( B_2 = 27.8\% ; T_2 = 70\^\circ\)C \( (p = 0.30 \text{ bar}) \);
3. 3rd effect: \( B_3 \) fixed at 65\%; \( T_3 = 60\^\circ\)C \( (p = 0.15 \text{ bar}) \);

The optimal configuration of the CHP system corresponds in this case only to a back-pressure turbine. Conversely, optimization results show that for higher bagasse quota maximum power generation is obtained with progressively lower values of back pressure (until the condition in which it is convenient to use a condensing turbine) and one steam draw off to cover the stripper reboiler thermal requirement. Rankine cycle thermal efficiency is around 14\%, with a decrease of about 11 points with respect to the case in which the total amount of bagasse is burnt (Figure 4.5).
4.4 Overview on biomass gasification

Different biomass conversion pathways have been proposed in the literature, depending on the end-use technology (combustion for heating purposes, transportation, power production) and on the quality of feedstock (concentration of lignin, cellulose and hemicellulose and moisture content).

Among others, a short and complete overview on biomass energy conversion technologies can be found in [65] from which the diagram in Figure 4.8 was taken. Biomass pyrolysis for liquid fuel production, biomass digestion or fermentation for gaseous fuels and biomass gasification for high grade syngas production are particularly promising pathways when dealing with woody biomass.

Research on biomass gasifiers increased in the last two decades due to the new interest on clean and efficient energy conversion technologies. The development of coal gasification facilities was fostered in the past decades by progressively higher prices of more conventional fossil fuels [55, 135]. Conversely commercial biomass fired gasifiers were built in the past basically for low-grade gas production and only few for power generation [3, 126]. A detailed report on the technical and economical aspects of biomass gasification power generating system was published in the middle nineties [13].

Since the availability of biomass feedstock varies among seasons, an important volume of woody biomass is today used in co-combustion or co-gasification plants which allow great flexibility in fuel supply and are less subject to techno-economical issues occurring with pure biomass fired power systems [47, 61].

In parallel different research groups are focusing on the production of hydrogen-rich syngas from biomass to be used as fuel in advanced energy conversion plants like fuel cells [5, 15, 138]. Although hydrogen is still expensive to produce, the production of hydrogen by upgrading the syngas obtained from gasifiers with subsequent reforming reactors and membranes, allows to couple biomass gasification technologies with different advanced power generating technologies [53, 66].

As the purpose of the present chapter is to describe possible scenarios of bagasse utilization in large CHP systems, the attention in the following pages is drawn towards the use of biomass-derived syngas for power production in gas turbines possibly in combined cycle mode.

4.4.1 Biomass gasification

A good review on gas production technologies covering both theoretical and technical aspects can be found in [117], while a techno-economic comparison between biomass pyrolysis and biomass gasification can be found in [14].

Gasification is a thermal decomposition (pyrolysis) of solid fuel into volatile matter (gas, TAR, oil and phenolic compounds) followed by a set of reactions between the solid residue of the pyrolysis (called fixed carbon or CHAR) with reactive gases (steam, hydrogen, carbon dioxide, air or oxygen), a part of which are generated by the pyrolysis while another part are added as additional oxidizing agent. It is common to call gasification just this second subset of reactions taking place between 700°C and 1500°C. Pyrolysis generally occurs between 300°C and 600°C. At lower temperatures usually only a drying process takes place. Depending on the type of gasifier and on the type of biomass, different can be the sequence of the afore-mentioned reactions leading to different quality of the syngas.

When dealing with biomass gasification it is particularly difficult to describe in detail the pyrolysis phase for which instead the following condensed expression are commonly given (for the average wood formula $CH_{1.4}O_{0.6}$):

$$CH_{1.4} + O_{0.6} \rightarrow 0.6CO + 0.7H_2 + 0.4C$$

$$CH_{1.4} + O_{0.6} \rightarrow 0.6CO + 0.35H_2 + 0.225C + 0.175CH_4 \tag{4.4}$$

In reality not all the biomass follows the same decomposition chemistry and part of the substrate is converted into compounds that are heavier than the products in Equation (4.4). Compared to thermal decomposition of coal, biomass pyrolysis is much more affected by low kinetics due to the presence of high moisture content and to the complexity of the starting material (cellulose, hemicellulose, lignin, etc.).
Figure 4.8: Biomass conversion pathways for heat and power production (adapted from [65])
Conversely, a less number of reactions take place at higher temperatures between the fixed carbon and the reactive gases. These reactions can be grouped into two main subsets.

**Oxidations:**

- Partial Oxidation: 
  \[ C + \frac{1}{2}O_2 \rightarrow CO \quad \Delta H = -111\text{kJ/kmol} \]
- Combustion: 
  - Carbon: \[ C + O_2 \rightarrow CO_2 \quad \Delta H = -197\text{kJ/kmol} \]
  - CO: \[ CO + \frac{1}{2}O_2 \rightarrow CO_2 \quad \Delta H = -283\text{kJ/kmol} \] (4.5)
- Hydrogen: \[ H_2 + \frac{1}{2}O_2 \rightarrow H_2O \quad \Delta H = -242\text{kJ/kmol} \]
- Methane: \[ CH_4 + 2O_2 \rightarrow CO_2 + 2H_2O \quad \Delta H = -802\text{kJ/kmol} \]

**Reductions:**

- Boudouard: \[ C + CO_2 \rightarrow 2CO \quad \Delta H = 173\text{kJ/kmol} \]
- Carbon Water: \[ C + H_2O \rightarrow CO + H_2 \quad \Delta H = 131\text{kJ/kmol} \] (4.6)
- Methanation: \[ C + 2H_2 \rightarrow CH_4 \quad \Delta H = -87\text{kJ/kmol} \]

While oxidations are exothermic, reductions are mainly endothermic except for methane production reaction. The conversion of reactants is limited by the thermodynamic equilibrium that is by the temperature and the pressure at which the reactions take place. In particular at high temperature the endothermic reactions are favored (Le Chantelier’s principle) while reactions leading to less gaseous volumes are favored by high pressures.

In addition, endothermic reforming reactions of hydrocarbons (methane, ethane and other heavy compounds) can take place between 500°C and 850 °C.

As a consequence thermodynamic analysis based on the aforementioned stoichiometry allows to estimate the quality range of the gas that can be obtained with gasifier operating at given temperature and pressure and with a given oxidizing agent. For given thermodynamic conditions, some of the reactions are favored more than others, so the actual heat rate of the gasifier for a given input of biomass can be evaluated. However thermodynamic analysis can provide only rough indications about the composition of the product gas since in reality kinetics does not let the reactions to reach the equilibrium thus leading usually to lower quality gas.

### 4.4.1.1 Classification of biomass gasification technologies

Gasifiers are classified in the literature following different criteria. It is a consolidated approach to distinguish gasifiers on the base of the method the solid fuel come in contact with the oxidizing agent. Accordingly the following types of gasifiers are identified: moving/fixed bed (updraft or downdraft), fluidized bed (stationary or circulating bed), entrained flow and molten bath.

Entrained flow gasifiers are particularly promising because of high operating temperatures (between 1200 °C and 1500°C) which favor the production of hydrogen-rich and low TAR-laden syngas. Even though some research programs are focusing in new biomass entrained flow gasifiers, fuel size must be under some millimeters [56]. This limits this technology to be used essentially for coal gasification.

Molten bath gasifiers exhibits more flexibility on fuel quality since very high temperature of the bath (more than 1500°C) allows complete thermal degradation of the fuel leading to a gas complete free of TARs. Conversely high heat losses and problems of bath entrainment on the product gas prevents the adoption of this technology for power production.

The research in biomass gasification focused primarily on the remaining designs which are schematically represented in Figure 4.9.

Gasification performance is commonly assessed using the following quantities:

- Cold Gas Efficiency:
  \[ \text{Cold Gas Efficiency} = \frac{\dot{m} \cdot HHV_{\text{Product Gas}}}{\dot{m} \cdot HHV_{\text{Solid Feedstock}}} \] (4.7)

- Gasification Efficiency:
  \[ \text{Gasification Efficiency} = \frac{\dot{m} \cdot HHV_{\text{Product Gas + Byproducts + Recoverable Heat Content}}}{\dot{m} \cdot HHV_{\text{Solid Feedstock}}} \] (4.8)
Biomass gasification in fixed bed gasifiers was performed since the last World War. A short review on european technologies can be found in [9]. Fixed bed gasifiers are quite reliable technologies even though some internal moving parts have a complicated design. High residence time of biomass in the reactor and counter-current flows of biomass and oxidizing agent leads to high thermal efficiency and high solid carbon conversion. Non-homogeneous gasification leads to high content of TAR and phenolic compounds.

The most common commercial technologies is the updraft Lurgi Dry Ash Gasifier. For biomass gasification however the downdraft configuration allows TAR produced in the pyrolysis zone to be cracked in the oxidizing zone thus leading to very small TAR content in the product gas. We call here product gas the gas exiting the gasifier which may be still quite rich in particles and other undesired compounds while we call syngas the same gas downstream of the gas cleaning section [41].

Fixed bed gasifiers are auto-thermal since partial combustion of the substrate occurs in presence of air, thus often leading to low cold gas efficiency. In addition they have smaller capacity than fluidized bed gasifiers.

Greater flexibility in particle size of feedstock is allowed in fluidized bed gasifier. This, along with better product-gas quality compared to fixed bed reactors, is the main reason behind the use of this technology for biomass gasification. TAR compounds and other originated pyrolysis products are efficiently converted in lighter products because of uniform bed at high temperatures. Fluidized bed gasifiers feature no moving parts and bigger amounts of biomass input than fixed bed gasifiers, thus leading to take more advantage of economy of scale factors. Reduced residence time of the substrate in gasification zone limits some of the conversion of solid carbon which partially leaves the reaction zone with ashes. However high cold gas efficiency and low TAR-laden product gas make this technology the most interesting for advanced energy conversion systems. In addition due to higher homogeneous temperatures of the bed it is possible to inject greater steam quantity which increases hydrogen content in the product gas.

4.4.1.2 Recent research in biomass gasification

Some new developments in biomass gasification technologies concern the use of steam and CO₂ as oxidizing agent, both of the procedures resulting highly endothermic. Heat from a separate combustion can be transfered to the gasification zone by means of advanced high temperature heat transfer equipment. Even though heat pipes have reached recently a high level of interest especially in the case of integrated gasification fuel cell systems, most common technologies are circulating bed gasifiers also known as twin...
A group of research centers are lately investigating the feasibility of biomass gasification by means of multi-stages gasifiers with interesting results about TAR and hydrogen yields in the product gas. Among different original concepts we recall here the Fast Internally Circulating Fluidized Bed Gasifier and the Dual Fluidized Bed Gasifier which combine a steam-gasification reactor with an air-combustion reactor, along with other designs based on two fixed bed reactors in which pyrolysis and gasification (plus TAR cracking) take place separately.

Status of the research regarding the development of steam gasification by means of fast internally circulated fluidized bed gasifiers (FICFB) is reported in [58]. The heat for the steam gasification is provided by the circulation of bed material that is heated up to high temperatures by means of combustion of the solid carbon and part of the product gas in a separate combustion zone (see Figure 4.10a). A 100 kWt pilot scale gasifier was run for 1600 hr with wood chips as a fuel and natural catalyst addition in the bed. TAR load between 0.5 to 1.5 g/Nm³, particles load of 10 to 20 g/Nm³, ammonia load of 500 to 1000 ppm and hydrogen sulfide load of 20 to 50 ppm were found in the product gas. A 500 kWt and another 8 MWt pilot scale gasifiers were therefore built to investigate the possible coupling with a MCFC and a gas engine. In particular for the 8 MWt test case combustion temperature were kept around 1000° to 1100° C, gasification zone at 900° C showing a good recirculation rate and low temperature gradients. Pressure drops in the gasification zone are around 80 to 100 mbar. Steam to fuel ratio was changed between 0.5 to 1.

A very similar design is the so-called Dual Fluidized bed reactor in which the bed material is moved by a pneumatic system [100] (see Figure 4.10b). Other twin fluidized bed gasifier concepts for biomass gasification are proposed in [32, 51].

Recently at the Technical University of Denmark a test facility consisting in a two-stages biomass gasifier, the so-called Viking gasifier (see Figure 4.11a) was built and coupled with a gas engine [57, 46]. Biomass pyrolysis is let to occur inside the feeding device of the biomass (updraft). The biomass is pyrolyzed before entering the gasification reactor by means of a gas stream that bring the biomass up to 600° C. In the first top section partial oxidation takes place raising the temperature up to 1100-1200° C and then the gas passes through the bottom of the gasifier in which other gasification processes occur (around 800° C). This configuration allows to reach very low TAR content in the product gas (around 0.015 g/Nm³).

The BioHPR is a biomass gasification technology developed and patented by the Technical University
of Münch en (see Figure 4.11b) [95]. The gasifier developed within this project aims at solving the problem of the heat transfer by using a liquid-metal heat pipes heat exchanger. The resulting product gas is rich in hydrogen and with TAR load around 3 to 7 g/Nm$^3$. Some methane and ethane are also produced.

4.4.1.3 Modeling Gasification

Mathematical models of gasifiers are useful for estimating gas composition, utility consumption of the gasifier (steam / air / thermal energy) and efficiency. There are basically three types of modeling:

**Black Box** Empirical Correlation are built by means of experimental data.

**Equilibrium Model** Thermodynamic equilibrium is used to estimate limit of conversion of the substrate into products. One possibility is to consider a set of defined reactions (stoichiometric model) and express the equilibrium constant of each reaction as a function of operating temperature and pressure. Another possibility is to specify the possible chemical species in the product gas and evaluate their respective yields by minimization of the Gibbs free Energy function (which depends on temperature and pressure).

**Kinetic Model** A complex set of equation involving chemical reactions and heat and mass transfer is implemented. Detailed calculation about gas composition and temperature profile within gasifiers can be obtained.

Only Kinetic Models provide good estimation of a large variety of gasification technology, though requiring a high number of parameters which apply in each case only for a specific design. Black box model are simple but can lose accuracy when the simulated conditions are far from experimental conditions. Equilibrium models are the most used for preliminary analysis of gasification. In presence of high temperature conditions (entrained bed gasifiers) they exhibit higher accuracy than in case of biomass gasification in fixed bed reactors or low-temperature fluidized bed gasifiers.

A recent dissertation on equilibrium thermodynamics of biomass gasification can be found in [6]. According to this study the gasification product is considered as a mixture of solid carbon and a gas phase (mixture of 60 organic species). Theoretical composition of the product gas of pyrolysis of several biomass feedstock is evaluated by the minimization of Gibbs free energy at different values of temperature, pressure, equivalence ratio and steam to carbon ratio. In addition, theoretical sulfur and
nitrogen species composition and solid characterization are given. Methane yields evaluated by equilibrium thermodynamic approach are always less than those resulting from actual gasification processes and suggested explanation is that methane can be more a product of TAR decomposition rather than an actual decomposition of the biomass.

A non-stoichiometric thermodynamic equilibrium model of circulating fluidized bed gasification is discussed in [83]. The same paper presents the result of gasification of six different types of woody biomass. Experimental data show that there are significant deviations between the equilibrium model predictions and the actual products compositions especially concerning the carbon conversion and methane yields, the latter claimed as a product of incomplete cracking of pyrolysis products. In conclusion a semi-equilibrium model is proposed. For this purpose the first equilibrium model is adjusted by assuming given yields of methane and solid carbon according to experimental results and applying the equilibrium calculation for the other species (TAR excluded). Good accordance with the experimental data is found in this latter case.

A parametric simulation of biomass gasification for hydrogen production based on chemical equilibrium is reported in [88] in which results are also compared to some experimental data. Again, methane, char, and TAR yields are shown to be highly unpredictable. Optimal values of temperatures in actual gasifiers are usually higher than those estimated with equilibrium models.

In fixed bed gasifiers the velocity of the solid fuel flow through fixed bed gasifiers is much lower compared to the case of fluidized bed gasifiers, so that gasification cannot be modeled without considering transport phenomena [101, 139] or without considering some experimental data [33]. An alternative although not accurate modeling approach is to distinguish between zones at different temperatures corresponding to different preponderant processes. Fluidized bed reactors allow the reactions to occur homogeneously inside the bed (i.e. the bed is more or less at the same temperature in every place) so that they can be considered as perfectly mixed reactors. This is particularly true for the case of coal gasification for which a thermodynamic equilibrium model is sufficient for preliminary design considerations. Conversely lower reactivity of biomass with respect to coal, limits the accuracy of thermodynamic equilibrium methods in estimating gas composition also in case of fluidized bed gasifiers [115]. Even a detailed stoichiometric model usually underestimates the presence of methane and ethane in the product gas [83].

4.4.2 TAR

The product gas of biomass gasification (at the outlet of gasifier) consists mainly in CO, CO$_2$ and H$_2$, water and some amount of other hydrocarbons including light hydrocarbons or heavy condensible hydrocarbons which are usually addressed as TAR. The definition, the formation and the conversion of TAR are discussed in a detailed report produced in the late nineties by the American NREL [96].

The report is the result of an extensive literature survey made on almost 400 papers on the field of the conversion of biomass and biomass derived gas treatment. The following definition of TAR is given: “The organics, produced under thermal or partial-oxidation regimes (gasification) of any organic material [...] generally assumed to be largely aromatic”. This definition reflects the problem of a conventional approach in defining and measuring TAR. It is broadly accepted however to define TAR as follows: “material in the product stream that is condensible in the gasifier or in downstream processing steps or conversion devices and especially heavier than benzene”. In more general sense TAR is the material that can be highly detrimental for final energy conversion processes like boilers, gas turbines and fuel cells. Accordingly, it is possible then that some non-condensible hydrocarbons (i.e. not rigorously TAR) like ethylene, cyclopentadiene and benzene are also included among TAR.

TAR formation is particularly difficult to model via rigorous chemistry since it depends mainly on kinetic effects which highly depend on the particular geometry of reactors. However, a classification of gasification technologies on the basis of TAR formation is possible since operating temperatures and residence times of biomass inside the gasification zone are generally sufficient to estimate the order of magnitudes of TAR yield.

TAR compounds are generally grouped according to the degree of decomposition of the organic substrate which is mainly related to the residence time of the substrate and to the operating temperature
Overview on biomass gasification

of the reactor:

- primary products (cellulose-derived products such as levoglucosan, hydroxyacetaldehyde, and furfurals plus analogous hemicellulose-derived products and lignin-derived)
- secondary products (phenolics and olefins)
- alkyl tertiary products (methyl derivatives of aromatics, such as methyl acenaphthylene, methyl-naphthalene, toluene, and indene)
- condensed tertiary products (benzene, naphthalene, acenaphthylene, anthracene or phenanthrene, pyrene and methoxyphenols)

According to a general correlation between TAR types in the syngas and the temperature at which biomass conversion reactions take place, primary products at are found primarily at 500°C, secondary products at 750°C and tertiary (especially alkyl) products at 1000°C.

The same report provides a review on gasification technologies which shows a dependency between type of gasifier (pyrolyzer, updraft, downdraft and fluidized bed) and TAR yields on the product gas. As a general indication TAR load in product gas is around 100 g/Nm³ for updraft gasifiers (the dirtiest technology) and around 1 g/Nm³ for downdraft gasifiers (the cleanest technology) and around 10 g/Nm³ for fluidized bed gasifiers (intermediate TAR laden syngas). Reasons for so different loads are to be found on the kinetics and on the actual geometry. A critical aspect is the possibility for the oxidant to be in direct contact with the bare biomass or with the charcoal. In updraft gasifiers biomass is injected from the top and the combustion between charcoal and air takes place on the grate, while primary TAR compounds are produced in the intermediate gasification zone. In downdraft gasifiers biomass is injected from the bottom and heat for the gasification is provided by the combustion of biomass and TAR in the first zone. Only 10% of primary compounds are converted in secondary TAR compounds leading to very light TAR laden gas. The fluidized bed gasifiers operate usually with partial combustion of charcoal and this leads to a slight TAR content on the product gas.

Even though the most promising method for TAR reduction is to reduce TAR formation in the gasifier (e.g. by using some catalysts in the gasifier), more common are the downstream methods like thermal cracking, physical removal, catalytic cracking.

4.4.3 Gas cleaning technologies

A detailed review on gas cleaning technologies can be found in [117, 120].

The product gas obtained from biomass gasification is more or less rich in fine particles, alkali metals, sulfur species and heavy hydrocarbons (commonly addressed as TARs) which may lead to degradation of downstream technologies. The design of the gas cleaning section is therefore crucial in order to up-grade the product gas to the final quality requisites of the syngas without high thermal losses.

Gas cleaning technologies are commonly classified into two groups: cold and hot technologies. Cold gas cleaning is based on gas quenching and removal of undesired compounds. Hot gas cleaning is based instead on removal of fine particles and alkali around 500°C and subsequent TAR cracking in partial oxidation or steam reforming when TAR need to be converted into lighter compounds.

Even though cold technologies allow to avoid the problem of high temperature heat transfer since the cooling of the gas is done mainly by water scrubbing (quenching), the heat losses are quite high leading to low system thermal efficiency. In addition water scrubbers and wet electrostatic precipitators, these latter used for removal of metallic particles, are quite expensive. TAR are removed as condensate and sent to the waste treatment section. In addition to the difficulties in handling such pollutants in condensate form, TAR can represent an important part of the chemical energy content of the product gas which is in this case lost. As a consequence of the TAR removal the total gasification efficiency (including gasification and gas cleaning) is lower than in the case hot technologies are employed.

Hot technologies are particularly suited in case of power generating devices operate at high temperatures. Even though at the outlet of the gasifier most of the particles are removed by cyclones, alkali compounds remains in vapor phase at temperature higher than 500°C. Under this temperature they
condensate around fine particles which can be removed by a rigid filter like for instance a ceramic filter (or candle filter). Depending on the tolerance of downstream components towards TAR, the gas may undergo a subsequent upgrading process in reformers. In case of high temperature fuel cell systems for instance, TAR must be totally reformed with steam reforming, partial oxidation or auto-thermal reforming [59]. In addition, even though sulfur species are more rare in biomass compared to coal, they are highly poisoning for fuel cells so that an effective desulfurization must be considered [122]. Since these latter processes occur at temperature between 500°C and 850°C system efficiency can be increased by pre-heating the gas up to reforming temperature for instance by recovering part of the heat of the upstream cooling processes.

The major advantage introduced by hot gas cleaning is the possibility to maintain the syngas at high temperatures. However high temperature cleaning technologies are in general more expensive or less reliable than cold gas cleaning due to the critical operating conditions. Additional technical issues can raise in case of pressurized gas cleaning.

In both cold and hot gas cleaning several hot and cold thermal streams appear in the system, thus heat integration techniques, like Pinch Analysis, are important design tools for reaching high system efficiency.

4.4.4 Biomass integrated gasification combined cycles

Combined cycles are the large scale power production technology with the highest thermal efficiency. The integration of gasification systems with combined cycles was technically explored in the Seventies. Since then many commercial plants were built employing different type of gasifiers [118, 94]. Nowadays the state of the art of coal based IGCC is represented by the NETL - FutureGen project [25].

In parallel, biomass integrated gasification combined cycles (BIGCC) were also explored however showing the aforementioned limitation on scale due to biomass availability (< 100 MWe) over a year time. A detailed report commissioned by DOE-NREL on cost and performance of BIGCC was published in the nineties [20] and similar data can be found in [13, 137].

BIGCC show system thermal efficiencies between 40 to 45 % between 30 and 100 MWe and specific costs between 3000 and 2000 $/kWe in the same range of installed power.

Biomass gasification can be carried out either in a pressurized or in atmospheric environment. Pressurized equipment is in average three of four times more expensive than atmospheric pressure even if pressurized gas requires less volume.

In case of atmospheric gasification, the injection of the syngas in gas turbine combustor requires the compression of high volume of gas which can lower the system efficiency. In addition gas cooling is required before compression. As a consequence, in this case, cold gas cleaning must be considered in which TAR are removed and high heat losses occur.

In case of pressurized gasification and hot gas cleaning, the syngas is injected in the combustor at relative high temperature and also with high TAR content which are in fact burnt together with the other lighter substances in the gas turbine [85]. No TAR control is in this case needed thus reducing system complexity. Efficiencies are usually higher than other biomass fueled power systems especially for high installed power. This fact counterbalance in the long run the extra cost of pressurized technologies, which can be 4 to 5 times bigger than the cost of atmospheric technologies for equal biomass input.

Technical issues and potential for commercial scale applications of biomass integrated gasification combined cycle based on pressurized circulating fluidized bed gasifier are discussed in [19].

Steam injection at the level of the gas turbine combustor (like in case of the STIG cycle [113]) can increase gas turbine efficiency. For the same reasons a way to increase efficiency of biomass integrated gasification power system is to use pressurized steam gasification which also partially increase the hydrogen yield in the syngas [130].
4.5 Bagasse integrated gasification combined cycle (CHP 2)

In the present section we discuss the problem of identifying the components and their parameters that maximize the net power production of the total sugarcane conversion industrial including a CHP system based on bagasse gasification. In comparison with the CHP system analyzed in the previous pages based on bagasse combustion, the intention here is to explore the potential of power generation with a quite advanced CHP system consisting in a pressurized Fast Internally Circulated Fluidized Bed gasifier and a combined cycle.

While different studies on bagasse gasification have been reported in the literature \[21, 29, 52, 74, 98, 108\], large power plants based on bagasse gasification has not been shown yet to be an economically viable solution. Some technical investigations by the Sugarcane Technology Center in collaboration with TBS-Termiska Processer AB seem to leave open the possibility of future developments of this type of technology.

In agreement with the methodology discussed in the previous chapters and summarized in Section 4.1, the bagasse based IGCC is separated into two subsystems which participate separately in the heat and power integration problem (along with the sugarcane conversion process for the combined production of sugar and ethanol): the bagasse conversion subsystem (here including bagasse drying, gasification and gas turbines) and the steam network subsystem.

In this way, for fixed values of intensive parameters of components (some of which are optimized in an outer optimization step according to the two-level optimization procedure described in Section 2.2.4), the heat and power integration problem can be formulated as a linear programming problem in which decision variables are the mass flow rates. In addition we assume total conversion of juice in ethanol and sugar and total conversion of bagasse into syngas. Accordingly only steam mass flow rates are optimized in the inner optimization step in order to maximize heat recovery for power generation.

4.5.1 Modeling bagasse gasification and gas turbine

Bagasse is gasified in a fast internally circulated fluidized bed gasifier (FICFB). Steam is injected in the gasification reactor while part of the gas and part of the fixed carbon is burnt in a second reactor in presence of air. Heat of combustion is transfered to support the endothermic gasification reactions by recirculating bed material from the combustor to the gasification zone.

An overview of the bagasse conversion sub-system is shown in Figure 4.12. Bagasse is firstly dried (DRIER), then gasified in the pressurized FICFB gasifier at 850°C in presence of steam. The hot product gas passes through a cyclone which removes the bed particles and fixed carbon. These substances are sent to the external combustor (COMB2) where they are burnt with part of the product gas. The combustion occur in pressurized environment and exhaust gases are subsequently expanded. The remaining part of the product gas is cooled down to 500°C and then pass through a candle filter where fine particles (along with condensate alkali metals) are removed. Finally the syngas is burnt in a gas turbine.

As done for the CHP system based on direct bagasse combustion discussed in Section 4.3, some of the hot exhaust gases can be used for bagasse drying before being vented thus avoiding the costs and inefficiencies of heat transfer between hot gases ad air for drying. In particular exhaust gases are cooled down to 200°C before entering the drier. Bagasse drying was modeled as in Section 4.3.

A black-box model of FICFB gasifier developed by Gassner et al. was implemented \[44\]. Due to the difficulties of simple thermodynamic equilibrium models in estimating methane and TAR concentration in syngas produced by actual biomass gasification, a semi-stoichiometric model was adjusted in order to reproduce some experimental data of a small scale FICFB gasifier \[58\]. Accordingly, the carbon conversion rate and the concentrations of ethane and TAR in the product gas are specified and the concentration of lighter compounds (H₂, CO, CH₄, H₂O and N₂) is estimated by correcting the equilibrium of some reactions (i.e. the specified stoichiometry does not represent at all the physical model but it is just a mathematical expedient). This latter procedure is done by introducing a virtual temperature difference (\(\Delta T\)) for each reactions (see Equation (4.10) where \(K_p\) is the adjusted equilibrium constant) from the specified reaction temperature (\(T_p = 850°C\)).
Figure 4.12: Flowsheet of bagasse drying, gasification and gas turbines in Vali [132]
In order to close the system of equations at the gasifier boundaries (which is solved simultaneously by the flow-sheet simulator Vali [132]), three reactions were considered:

\[
\begin{align*}
\text{Methanation} & : \quad C + 2H_2 \rightleftharpoons CH_4 \quad \Delta H = -87 \text{kJ/kmol} \\
\text{Boudouard} & : \quad C + CO_2 \rightleftharpoons 2CO \quad \Delta H = 173 \text{kJ/kmol} \\
\text{Water-gas shift} & : \quad CO + H_2O \rightleftharpoons CO_2 + H_2 \quad \Delta H = -41 \text{kJ/kmol}
\end{align*}
\] (4.11)

The three virtual temperature differences were adjusted by Gassner in order to reproduce experimental data of FICFB gasifier found in [58].

TAR production is fixed at 10 g/Nm\(^3\) in agreement with average values of TAR production in fluidized bed gasifiers. However, since no detailed analysis about TAR composition resulting from the FICFB were found, four TAR compounds are considered in order to fairly represent major species (mostly tertiary TAR compounds since the gasification temperature is quite high):

<table>
<thead>
<tr>
<th>Compound</th>
<th>represented TAR specie</th>
<th>Concentration (%mass)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Toluene (C(_6)H(_5)CH(_3))</td>
<td>1-ring compounds</td>
<td>65</td>
</tr>
<tr>
<td>Naphthalene (C(_{10})H(_8))</td>
<td>2-rings compounds</td>
<td>20</td>
</tr>
<tr>
<td>Phenol (C(_6)H(_5)OH)</td>
<td>phenolic and heterocyclic compounds</td>
<td>10</td>
</tr>
<tr>
<td>Pyrene (C(<em>{16})H(</em>{10}))</td>
<td>3-rings and others</td>
<td>5</td>
</tr>
</tbody>
</table>

Table 4.1: TAR species and their respective quantity considered in modeling FICFB gasifier output

Steam is injected in the gasifier at 400\(^\circ\)C in quantity necessary to obtain a Steam to Carbon ratio of 0.2 in the gasifier as specified in [58].

The heat for gasification is provided by the combustion of the remaining solid carbon in the product gas which is removed by high temperature cyclone along with the bed material. Since the combustion of this solid carbon is not sufficient to support the gasification thermal demand, partial combustion of the product gas is considered. The right quantity of by-passed gas is evaluated as a result of the thermal balance between this combustion and the gasifier heat rate.

The cyclone and the rigid barrier filter were modeled as pressure drops (50 mbar) since this components do not involve any macroscopic thermodynamic transformation or change in chemical composition of the gas.

Pressurized gasification is considered. The combustion reactor used for heating the fluidized bed is at the same pressure of the gasifier. This allows the use of hot gas cleaning technologies, being possible in this way to inject the syngas directly into the gas turbine combustor without intermediate compression of the syngas which would imply the use of cold technologies instead. Temperatures of both gas turbine combustor and of the exhaust gases of the gasifier combustion are fixed at 1200\(^\circ\)C.

Isentropic efficiencies of turbo-machinery were fixed to 0.85.

In technical practice, maximum pressure for the fluidized bed gasifier and the gas cleaning chain for a BIGCC plant can range 20 to 30 bar [20]. Accordingly, the pressure at the gas turbine combustor was fixed at 20 bar. The pressure of the remaining components are evaluated by the flow-sheet simulator, (for fixed pressure drops of 50 mbar in each component, half heat exchangers included). As a result the gasifier operating pressure is 20.2 bar.

Some heat losses were considered in the system:

- At the gasifier the heat loss is fixed to 10% of the chemical power input of the biomass.
- At the two combustors the heat losses are fixed to 5% of the chemical energy rate input of the syngas.
- 15% heat loss of the total heat obtained from gas cooling is considered.
In addition exhaust-gases temperature is fixed to $100^\circ C$. Since at the hot outlet of the bagasse drier, the exhaust gases are at $60^\circ C$ and 70% of relative humidity (as a consequence of the wood drying process), the other exhaust gas stream coming from the combustion reactor can be cooled down until $200^\circ C$ so that the mixed stream reach the desired exhaust gas temperature.

System simulation was performed for 1 kg/s of biomass input. This allows to evaluate specific heat and power loads and the actual heat loads an power resulting from total bagasse conversion are evaluated by multiplying the specific values by the mass flow rate of bagasse.

As a result around 3500 $Nm^3/h$ of product gas are produced (see composition in Table 4.2), of which around 35% is burnt in the gasifier-combustor and then expanded producing 1195 kW. The remaining 65% is sent to the gas turbine for a gross power production of 4195 kW of which 2765 kW are used to run the air-compressor. By assuming an additional power requirement of 75 kW for some auxiliary devices like bagasse conveyors and additional milling, the net power production of the gasification and gas turbine subsystem is around 2555 kW which corresponds already to 32% thermal efficiency.

<table>
<thead>
<tr>
<th>Compound</th>
<th>Moles (%)</th>
<th>Mass (%)</th>
</tr>
</thead>
<tbody>
<tr>
<td>$N_2$</td>
<td>1.0277</td>
<td>1.3444</td>
</tr>
<tr>
<td>$CO_2$</td>
<td>17.3541</td>
<td>35.6680</td>
</tr>
<tr>
<td>$CO$</td>
<td>2.3458</td>
<td>3.0686</td>
</tr>
<tr>
<td>$H_2O$</td>
<td>49.5295</td>
<td>41.6710</td>
</tr>
<tr>
<td>$CH_4$</td>
<td>13.7041</td>
<td>10.2674</td>
</tr>
<tr>
<td>$H_2$</td>
<td>8.6515</td>
<td>0.8145</td>
</tr>
<tr>
<td>C(s)</td>
<td>4.3618</td>
<td>2.4467</td>
</tr>
<tr>
<td>Toluene</td>
<td>0.1581</td>
<td>0.6804</td>
</tr>
<tr>
<td>Pyrene</td>
<td>0.0055</td>
<td>0.0223</td>
</tr>
<tr>
<td>Phenol</td>
<td>0.0238</td>
<td>0.1047</td>
</tr>
<tr>
<td>Naphtalene</td>
<td>0.0350</td>
<td>0.2093</td>
</tr>
<tr>
<td>Ethane</td>
<td>2.8031</td>
<td>3.6725</td>
</tr>
</tbody>
</table>

Table 4.2: Evaluated gas composition at the outlet of the FICFB gasifier

The resulting higher heating value of the gas produced by the gasification is 10270 $kJ/kg$ while the HHV of the syngas at the inlet of the gas turbine is 9700 $kJ/kg$. Accordingly a Cold Gas Efficiency (Equation (4.7)) of 0.67 is evaluated. Around 20790 $Nm^3/h$ of exhaust gases are produced (see composition in Table 4.3).

<table>
<thead>
<tr>
<th>Compound</th>
<th>Moles (%)</th>
<th>Mass (%)</th>
</tr>
</thead>
<tbody>
<tr>
<td>$CO_2$</td>
<td>7.5941</td>
<td>12.1683</td>
</tr>
<tr>
<td>$H_2O$</td>
<td>21.3387</td>
<td>13.9964</td>
</tr>
<tr>
<td>$N_2$</td>
<td>61.7529</td>
<td>62.9836</td>
</tr>
<tr>
<td>$O_2$</td>
<td>9.3145</td>
<td>10.8517</td>
</tr>
</tbody>
</table>

Table 4.3: Composition of the exhaust gases at the vent of the gasification and gas turbine subsystem

In the light of the total site heat integration problem, all the thermal streams of the gasification and gas turbine subsystem are not matched a priori, except for the case of the combustion and the gasification units, being the two reactors in reality thermally integrated by the circulating bed.

This corresponds to consider all the cooling or heating processes as half heat exchangers as done in Section 4.3 for the first CHP system. For the case of the gasification and gas turbine subsystem (see Figure 4.12), the thermal streams in Table 4.4 are identified.

### 4.5.2 Definition of the steam network superstructure

The steam network is the subsystem entitled for part of the power production, being the major part of the electricity produced by the gas turbine, and for distributing the heat through-out the total industrial plant. In fact the steam network not only allows to distribute the steam from the HRSG to the process thus heating the productive process, but also operates as a way to exploit the possible heat pockets of
the heat cascade thus increasing the heat recovery (i.e. the power production) as already discussed in Section 4.3.2.

The maximum number of headers of the steam network superstructure can be envisioned by interpreting the shape of the grand composite curve of the productive process. In the present chapter we assume that the productive process is the case CSE3 presented in Section 3.3.2 for which the definition of the steam network superstructure was already discussed in Section 4.3.2. This is based on one steam production line, one steam draw-off for process heating and one condensing turbine.

In the case of the combined cycle configuration it is quite frequent that more than one steam production headers are considered leading to a configuration of the bottoming steam cycle with two or three pressure levels. This can be interpreted as the consequence of the optimal heat integration between the exhaust gases coming from the gas turbine and the steam production thermal profiles. In case of steam power plants in fact, thermal efficiency is increased by introducing more steam draw-offs exploiting the lower temperature intervals (heat recovery) and possibly by increasing the pressure of the steam line above the critical point (supercritical cycles) as represented in Figure 4.13. Conversely, in case of combined cycles, the hot thermal profile available for the bottoming steam cycle shows less space for heat recovery at lower levels and thermal efficiency is normally increased by adding steam pressure lines thus activating more than one pinch-points (see Figure 4.14).

Accordingly the adoption of a second pressure steam line to enhance the power generation within the steam bottoming cycles is also considered here as possible advanced plant option after the heat integration opportunities of the standard case with just one steam pressure level is discussed.

### 4.5.3 Total site optimization problem and results

The optimization problem is set as follows:

\[
\text{max } P_{\text{net}} = P_{\text{CHP}} - P_{\text{process}}
\]

considering the following (upper level) decision variables with their respective lower and upper bounds in square brackets:

- \(n\): number of evaporation effects \([3,5,7]\)
- \(p_i\): operating pressure of the \(i\)-effect \([p_{i-1} ÷ 0.1\text{bar}]\) (the first effect operating temperature is fixed at \(115\°C\))
- \(B_i\): solid concentration at the outlet of the \(i\)-effect (the outlet concentration of the last effect is fixed at \(65\%\))
- \(p_{\text{strippler}}\): stripper operating pressure \([1.0135\text{bar}]\)

And the following decision variables of the inner MILP problem

<table>
<thead>
<tr>
<th>Thermal stream</th>
<th>(T_{in} [\degree C])</th>
<th>(T_{out} [\degree C])</th>
<th>Heat load [kW]</th>
</tr>
</thead>
<tbody>
<tr>
<td>Cold Streams</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Water pre-heating</td>
<td>25</td>
<td>214</td>
<td>-160</td>
</tr>
<tr>
<td>Evaporation</td>
<td>214</td>
<td>214</td>
<td>-378</td>
</tr>
<tr>
<td>Superheating</td>
<td>214</td>
<td>400</td>
<td>-88</td>
</tr>
<tr>
<td>Hot Streams</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Syngas cooling</td>
<td>850</td>
<td>500</td>
<td>394</td>
</tr>
<tr>
<td>GT(^1) exhaust gas cooling</td>
<td>593</td>
<td>200</td>
<td>2475</td>
</tr>
<tr>
<td>EXP(^2) exhaust gas cooling</td>
<td>621</td>
<td>204</td>
<td>776</td>
</tr>
</tbody>
</table>

Table 4.4: Hot and cold thermal streams of the gasification and gas turbine subsystem (1: GT = Gas Turbine; 2: EXP = gasifier combustion exhaust gas expander)
Figure 4.13: Example of integrated grand composite curve showing the thermal integration between heat of solid fuel combustion (red) and the steam network (blue) in large steam power plants.

Figure 4.14: Example of integrated grand composite curve showing the thermal integration between topping (red) and bottoming (blue) cycles in large combined cycle power plants.
i: binary variable for the activation of the l-steam/condensate header

m: steam mass flow rate of the l-steam/condensate header

The power generated by the CHP system is evaluated as the summation of the net power production of the gasification and gas turbine subsystem (gas turbine plus expansion of exhaust gases from the FICFB gasifier minus power demand of the auxiliary devices like water pump and biomass milling and conveyor) plus the power generated by means of the steam cycle, which is evaluated as a result of the heat and power integration problem (inner optimization level) at each step of the outer level optimization.

A total gross power of around 126.3 MWe is produced, corresponding to an electrical efficiency of 41.5%. Almost 99.3 MWe result from the operation of the gasification and gas-turbine sub-system (2555 kWc/kgbagasse multiplied by the total bagasse mass flow rate of 38.9 kg/s). The remaining 27 MWe are instead generated by the steam cycle consisting in a back pressure turbine delivering the steam to the first evaporator effect (this heat subsequently cascades through the various process streams), and in a condensing turbine. As a consequence of a process electrical consumption of 14.5 MWe the total site net power production is 111.7 MWe consisting in net electricity to be sold to the grid, which revenues add to those of selling sugar and ethanol.

Optimization results show again that the are many near-optimal sets of values of multi-effect decision variables. Conversely low distillation pressure favors always bigger production of electricity, being in this way possible to lower the pressure of the steam draw-off (at maximum down to the temperature level of the first evaporation effect) thus leading to greater expansion ratios.

In particular in Figure 4.15, one of these near-optimal solutions is presented in terms of integrated grand composite curve of the steam network within the total site heat cascade, which was obtained with 5 effects and the following values of decision variables:

1. 1\textsuperscript{st} effect: \(B_1 = 21.7\%\); \((T_1 \text{ fixed at } 115^\circ\text{C})\)
2. 2\textsuperscript{nd} effect: \(B_2 = 22.2\%\); \(T_2 = 103^\circ\text{C} \) \((p = 1.12 \text{ bar})\);
3. 3\textsuperscript{rd} effect: \(B_3 = 28.7\%\); \(T_3 = 64^\circ\text{C} \) \((p = 0.23 \text{ bar})\);
4. 4\textsuperscript{th} effect: \(B_4 = 61.9\%\); \(T_3 = 56^\circ\text{C} \) \((p = 0.14 \text{ bar})\);
5. 5\textsuperscript{th} effect: \((B_3 \text{ fixed at } 65\%\)); \(T_3 = 56^\circ\text{C} \) \((p = 0.13 \text{ bar})\);

The integrated grand composite curve of the steam network is in fact the graphical tool that gives a better overview of the heat integration between the hot thermal streams (syngas cooling and gas turbine exhaust gas), the steam network and the sugar production process, this latter appearing on the right-down side of the red grand composite curve.

In the same picture it is also possible to notice that temperature difference between hot thermal streams and the thermal profiles of the high pressure steam line is enough to ensure effective heat transfer within the HRSG without investing in large heat transfer surface.

The gas turbine pressure ratio is in fact a crucial decision variable for obtaining optimal thermal profiles at the HRSG. This parameter has a high influence not only on the gas turbine power output (favored by high pressure ratios) but also on the gas turbine outlet temperature and the amount of heat available from the exhaust gas cooling which govern the HRSG (favored by low pressure ratios). As a result the optimal value of the pressure ratio of a gas turbine working in combined cycle mode is usually half of the optimal pressure ratio when the same turbine is operated in open cycle mode.

In principle it could be possible to investigate the influence of this design parameter also for this case. However, as an assumption, the pressure of the gas turbine was fixed a 20 bar in order to comply with the constraints in maximum operating pressure of the hydro-gasification plant, so that the feasibility of the heat transfer for given pressure levels and temperature of steam production is checked afterwards. As shown in Figure 4.15 this was in fact verified for fixed values of the intensive parameters as in Section 4.3 (80 bar and \(T_{\text{max}} \text{ at } 527^\circ\text{C})).\)

It is however possible to increase the power output by exploring more advanced steam network configurations. According to the aforementioned directions for improvements in large steam cycles and
in combined cycles (see Figures 4.13 and 4.14), the following additional structural options for the steam network are considered:

- Addition of steam draw-offs for increasing internal heat recovery (in particular we notice in Figure 4.15 the presence of two heat pockets at the left-end corner of the grand composite curve between the hot gas and the temperature level of the first evaporation effect).

- Addition of steam production lines at progressively higher pressure (> 80 bar) which should increase the exergy recovery at higher temperatures.

For the same design parameters of the productive process (same multi-effect evaporator and same environmental distillation) and of the gasification and gas turbine sub-systems, an advanced steam network configuration is proposed in Figure 4.16. In particular this latter configuration was obtained with additional steam draw-offs at 25 bar and at 13 bar and other two steam pressure lines at 200 bar and 140 bar resulting in a quite complex IGCC configuration (three pressure steam generation lines, three draw-offs and one condensing turbine). In so doing the steam cycle power generation increases up to 30.3 MWₑ which corresponds to an increase of 3 MWₑ in total site net power generation (115 MWₑ) and of almost 1 absolute point in thermal efficiency (42.5%). However, the heat transfer between hot gases and the thermal profiles of different portions of the steam network is in this case particularly critical and can be obtained only by means of large heat transfer surfaces.

Figure 4.15: Case CHP2 - integrated grand composite curve (blue: steam network thermal streams, red: bagasse gasification, gas turbines and process thermal streams)
In Chapter 3 different concepts of sugarcane conversion process were proposed. Each of these concepts was translated into a basic plant configuration (BPC) which was subsequently modified following the organized procedure presented in Section 2.4 (components staging, change in connections between components, addition or substitution of components), and optimized following the objective of minimum process thermal requirement for fixed production of useful products. Accordingly, two BPCs were proposed for the separate production of sugar and ethanol and a third BPC involving the combined production of the two products was also studied.

Starting from this latter process configuration in which 5.6 kg/s of ethanol and 7.2 kg/s of sugar are produced, the further conversion of the bagasse by-product was studied in this chapter. Among different possible pathways for bagasse conversion, the plant options for the combined heat and power generation was investigated here.

The considerable amount of this by-product (38.9 kg/s) and its chemical energy content (7834 kJ/kg at humidity of 50% weight basis) allow in fact not only to produce enough power and heat for covering the process needs but also to generate and extra amount of electricity to be sold to the market. A set of BPCs for combined sugar, ethanol and electricity production is considered in this chapter. Among all possible concept of bagasse fueled CHP plants, only two BPCs were studied here, the first one based on bagasse fueled steam cycle (CHP1) and the second one based on bagasse integrated gasification combined cycle (CHP2).

Total site synthesis could have been performed following the same organized procedure used in Chapter 3 for the synthesis of the sugarcane conversion process. This was applied here by proposing two BPCs for the bagasse conversion subprocess, a bagasse fueled steam boiler and a bagasse fueled gasifier, which however were not modified throughout the analysis. In front of the variety of the sub-processes involved in the production of goods, sugar and ethanol in the specific case, which makes it difficult to codify process

Figure 4.16: Case CHP2 (advanced configuration): integrated grand composite curve (blue: steam network thermal streams, red: bagasse gasification, gas turbines and process thermal streams)

4.6 Conclusions

In Chapter 3 different concepts of sugarcane conversion process were proposed. Each of these concepts was translated into a basic plant configuration (BPC) which was subsequently modified following the organized procedure presented in Section 2.4 (components staging, change in connections between components, addition or substitution of components), and optimized following the objective of minimum process thermal requirement for fixed production of useful products. Accordingly, two BPCs were proposed for the separate production of sugar and ethanol and a third BPC involving the combined production of the two products was also studied.

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alternatives, the methodology adopted for the synthesis of the sugarcane conversion process in Chapter 3 basically organizes these process alternatives in a limited number of categories (component staging, addition of new material connections between components, addition or substitution of components).

In Chapter 2 a methodology for the synthesis of CHP system was presented in detail. According to this methodology the synthesis of CHP plants can be partially tackled by means of tools that allow to solve systematically some local linear problems with relative low effort (using a deterministic algorithm for structural and parameter optimization). This is particularly true for the steam networks considered here (which embed steam cycles), which topology can be generated and evaluated without dealing with heuristics guidelines which are instead necessary when dealing with more general material and energy conversion systems like the sugarcane conversion process. In reality, these guidelines for the systematic generation of different system configurations were conceived in the introductory chapters following methodologies that were proposed in the literature for the synthesis of power systems [80, 91, 106]. We observe in fact that some of the modification to the system BPC, when sub-systems exhibit linearity, can be to some extent systematically generated and their impact in heat and power demand/generation evaluated.

Accordingly, the definition of the structure and the design parameters of the two CHP systems considered in this chapter were partially solved in a systematic way by solving the MILP optimization problem for the selection of the optimal steam network configuration described in Section 2.2.3. According to the two-level optimization strategy that was introduced in Section 2.2.4, this latter problem is solved within the inner optimization step in which the heat and power integration problem is solved, and for a given steam network superstructure the set of steam and condensate headers leading to maximum heat recovery for power generation is evaluated.

Although the organized procedure for process synthesis (which was followed in the Chapter 3 for the synthesis of the sugarcane conversion process) substantially differ from the methodology discussed in Chapter 2 which implements some systematic solution of local linear problems according to a super-structure formulation, we observe that it is possible to draw a parallel between the two strategies.

**Addition of stages of components** This synthesis approach, which was extensively applied to the case of the multi-effect evaporator and to the distillation sub-system, is at the basis of the definition of a steam network with multiple steam-headers, and leads to several stages of steam expansion. The same approach can be further extended to the multiplication of compression and expansion stages in any thermodynamic cycle. Component staging appears in reality as a way which increases the number of thermal stream within a systems thus increasing the degree of freedom in process design making it easier to minimize the system thermal requirement.

**Addition of splitter and mixers, new connections between components** This approach was used to describe the synthesis steps leading to the combined ethanol and sugar production and to the definition of distillation of high grade ethanol in sequence of distillation columns and motor fuel ethanol in a parallel of stripping-rectifying columns. The same approach is implemented in the systematic synthesis of steam networks. In particular, it was shown in Section 2.2.3.1 that depending on the way the steam network is adapted to an already defined process thermal cascade, different steam expansions can depart from the same headers and subsequently join in other headers at lower pressures.

**Addition of new components** This approach lets new process concepts to be implemented in the original BPC either by substituting some of the existing components or by adding completely new material conversion streams, therefore increasing process complexity and possibly production flexibility. This is the step in process synthesis in which new BPCs are generated.

Most of the works in the literature about the systematic synthesis of chemical or power plants were in fact based on a preliminary definition of a system superstructure [42, 49], in which the presence of each component is mathematically associated with a binary variable. Accordingly, the optimal system configuration is found as an optimization of a mixed integer non linear model of the system, for solution of which several deterministic algorithms were developed in the past [34]. However, the formulation of
Conclusions

the synthesis problem of whatever system starts from a more or less limited number of components. Thus the effort in the present work was to show an organized way to generate new system concepts (new BPCs). This procedure partially relies on the technical experience (which may suggest new process components), and partially on the capacity of the engineer to suggest new possible layouts using the same components.

Still, when possible, the systematic solution of synthesis sub-problems, like for instance the heat and power integration problem, may help effectively solve the overall synthesis problem.

The application of the two-level optimization strategy is however possible until these three sub-systems do not interact with each other by means of material recirculating streams.

For instance, this is not the case of the molasses generated within the crystallization sub-systems, that are recycled into the yeast fermentation sub-process leading to a non-linear relation between power and heat contributions of the different sub-processes and the splitting fractions at the juice splitter. As it was already mentioned in Section 3.3, the ethanol and sugar production ratio can be either included in the high-level non linear decision variable set (non-linear) or used as a sensitivity parameter as shown in Figure 3.35 at page 98.

According to the two-level optimization strategy, at each step of the outer level optimization (in which parameters governing the performance of components are chosen), the heat and power integration problem is solved as an inner optimization step, the objective of which can be one among several criteria. For instance the objective function used in Section 2.1.3 is the minimum operating costs.

As it was already shown by means of a graphical representation of the linear optimization problem (see Figure 2.17 on page 30) the outcome of the optimization problem based on the minimum operating costs target, depends on the purchasing price of fuel and electricity (when imported from the network as an utility) and the selling price of electricity (when sold to the market). It would have been necessary to assume prices for electricity, sugarcane and additional fuel depending on real values of the market in order to investigate the actual convenience of the various configurations of the system.

However the objective here was limited to the maximization of net power production. Yet, the previous formulation of the problem in terms of minimum operating costs target was adopted. It is apparent in fact, that for high prices of electricity (both selling and purchasing) and for high prices of extra fuel consumption (for instance Natural Gas) and in presence of the bagasse by-product with no cost, the minimum operating cost target optimization leads to configuration with maximum power generation (see Figure 2.20 on page 37). Accordingly, prices of electricity and fuels were set to virtual values which were only functional to drive the MILP optimization step (the inner step of the two-level optimization strategy in which the heat and power integration problem is solved and the steam network design established) towards the total site configuration leading to maximum net power. In other words, from the mathematical point of view, prices were used as weights in order to favor the solution corresponding to maximum power generation.

The conversion of the bagasse into heat and electricity is an interesting option that can further increase process profitability. In particular, 37% of bagasse is necessary for covering the heat and power demands of the sugar and ethanol production process considered in this work. Conversely, for total bagasse conversion corresponding to a total chemical energy rate input of almost 304 MW, a net electric power generation of 57 MWe was obtained in case of a bagasse fueled steam cycle. In case of a bagasse gasification combined cycle (with total site heat integration) almost double the amount of power was obtained (111-115 MWe).

These total site configurations were obtained by optimizing simultaneously the productive process and the steam network of the CHP system. Again the shape of the grand composite curve was used to investigate the total site heat integration. This Pinch Analysis tool is in fact particularly useful for the definition of the optimal pressure levels of the steam network which is used to distribute the heat to the process and to generate electrical power (about this topic the reader is referred to [90]). According to the MILP formulation of the steam network synthesis problem, all the possible pressure levels must be considered in advanced in a steam network superstructure (as discussed in Section 2.2.3) and the optimum steam network structure and steam mass flow rates are evaluated as a result of the MILP optimization. The process grand composite curve gives a straightforward indication about which is the
minimum temperature level (or more than one) at which the heat must be delivered to the productive process thus giving the indication of optimal pressure levels of the steam network. The maximum pressure level of steam condensation was here linked to the pressure level of the stripping column (which was included among the set of decision variables). The thermal demand of this component appears in fact at the highest temperature level of the process heat cascade (or at almost the same temperature of the first evaporation effect in case of environmental distillation). The results of optimization almost always confirm that it is convenient to perform distillation at the environmental pressure. This means that with the increase of the distillation pressure, the total site heat integration is not sufficiently enhanced to compensate the effect of the reduction of the steam expansion ratio as a consequence of the increase of the pressure (temperature) at which the steam must be used for process heating. The optimal pressure levels of other steam draw offs at lower temperature levels were necessarily treated as decision variables since the purpose of the optimization was indeed to investigate different configurations of the process (i.e. of its heat cascade) in order to find the one maximizing the net power production, and being therefore not clear in advance which are the optimal intermediate temperature levels where the heat must be delivered to the process by steam condensation. In general, in order to exploit all the thermal exergy along the heat cascade, it would be necessary to install a steam network with a high number of steam/condensate headers which are able to thermally balance the process heat cascade at all the temperature levels (i.e. reducing to zero all the heat pockets of the total site heat cascade).

Here only one back-pressure turbine and one condensing turbine were considered. Thus, when burning all of the bagasse, the optimal pressure levels of the steam network superstructure are rather obvious: the back pressure must be fixed according to the maximum temperature level of process thermal demand and the condensing turbine outlet pressure is the minimum pressure that can be obtained by using the cold utility (here environmental water was considered so that the condensation pressure was fixed at 0.05 bar). In fact, when a small number of steam draw offs is considered, greater power production is obtained by optimizing the process heat cascade so that the excess heat from the process can be used for pre-heating the water of the steam network at lower temperature intervals (see Figure 4.6). As a consequence there was no reason to include any steam pressure levels among the set of decision variables to be optimized at the outer optimization level. On the contrary, for lower amount of bagasse to be burnt in the steam boiler, the heat loads of the process heat cascade become larger so that a condensing turbine could only produce a little power and it is more interesting to investigate the contribution steam expansions at intermediate pressure levels.

A particular attention has been given to the case in which the CHP system produces exactly the same quantity of heat and power required by the process (see Figure 4.7). In this case it is sufficient to install one back pressure turbine at the exit of which all the steam is used for process heating. This appears also to be the most common case in technical practice since all the demand of the productive process for external utilities can be satisfied internally so that the process economy becomes completely independent on the trends of the energy market. Steam turbines with moderate performances are for this reason economically interesting for industrial cogeneration already above some MW of electrical power output. However, when dealing with very large steam power plant like the case discussed in Section 4.3, the additional power production must compete with other power production plants (that is with the electricity market) and therefore higher performances must be achieved to justify such capital investments. In this work the maximum pressure of the steam cycle was fixed at 80 bar which is quite conservative value compared to modern steam cycles for only power generation.

Conversely for the second CHP plant presented here (see Section 4.5) higher components performances were considered. Investment costs of biomass integrated gasification combined cycles are in fact considerably higher than more traditional steam cycle power plants therefore such plants are profitable only if efficiency is high enough to guarantee high revenues from electricity sale. Here pressurized fluidized bed gasifier, hot gas cleaning technologies were considered. While for the first CHP configuration with total bagasse combustion, most of the power is obtained by a steam condensing turbine, in the second CHP configuration, a great part of the power is produced by means of gas turbines (almost 100 MW out of 126 MW of gross power generation). The fluidized bed gasifier considered in Section 4.5 is designed to separate the hydrogen and carbon monoxide rich gas obtained from biomass gasification (which fuels a gas turbine), from the combustion gases obtained from char combustion (which is expanded...
in a gas expander). The steam for the bottoming steam cycle is then generated by recovering heat from the exhaust gases at the outlet of the two gas turbines (available from a maximum temperature of 620 °C) and from syngas cooling (from 850°C to 500°C). The amount of heat available from these exhaust gases is comparable to the process thermal demand. Thus the optimization of the process parameters and of the steam network pressure levels result particularly useful for maximizing power production.

A maximum thermal efficiency of 42.5% was obtained with a three level combined cycle power plant which shows that with the integrated gasification of bagasse and with maximum total site heat integration a high amount of power can be potentially produced with high thermal efficiency. In particular, the benefit in terms of efficiency introduced by total site heat and power integration can be estimated by comparing the cascade of efficiencies of the same fluidized bed gasifier (67% of Cold Gas Efficiency) and of a commercial combined cycle (55% of thermal efficiency) if considered as thermally separated subsystems. This would result in 37.5% efficient combined cycle fueled with bagasse syngas which is around 5 absolute points less efficient than the case studied in Section 4.5. This difference can be attributed to the high total site thermal integration. The major benefit is indeed obtained by recovering the heat from the hot syngas at the outlet of the gasifier for steam generation which is a common plant solution of commercial integrated gasification combined cycles. Compared to more conventional plant based on cold gas cleaning, hot gas cleaning allows to convert a greater part of the syngas thermal energy directly in the gas turbine, therefore additional exergy losses caused by transferring the same thermal energy to the steam cycle can be avoided. On the other hand the present analysis showed that total site heat integration can counterbalance the possible loss in power generation for covering the thermal demand of the process.

A summary of results of Chapter 4 is reported in Table 4.5.

Table 4.5: Summary of results of Chapter 4 (1: CHP electrical efficiency accounts for the CHP electric output after power demand of CHP auxiliaries devices is also satisfied; 2: Steam production pressure level; 3: Back Pressure Turbine; 4: Steam Draw-off; 5: Condensing Turbine)

<table>
<thead>
<tr>
<th>Steam Net. Conf.</th>
<th>Figure</th>
<th>Bag. Quota [%]</th>
<th>CHP Power [MWe]</th>
<th>CHP El.Eff.</th>
<th>Net Power [MWe]</th>
</tr>
</thead>
<tbody>
<tr>
<td>Boiler (Steam at 6 bar)</td>
<td>3.36</td>
<td>30</td>
<td>0</td>
<td>/</td>
<td>-13.5</td>
</tr>
</tbody>
</table>

CHP1: bagasse combustion in steam boiler for combined Heat and Power

| 1 PR.L.² , B.P.T.³ (5 bar) | 4.7 | 34 | 3.5 | 3.4 | - 10 |
| 1 PR.L. , B.P.T. (3 bar) | 4.5 | 100 | 70.4 | 23 | 56.8 |

CHP2: bagasse integrated gasification combined cycle

| 1 PR.L. , 1 D.O. , C.T. | 4.15 | 100 | 126.3 | 41.5 | 111.7 |
| 3 PR.L. , 3 D.O. , C.T. | 4.16 | 100 | 129.3 | 42.5 | 115.0 |

Among the different process options explored in Chapters 3 and 4, the case of combined production of sugar ethanol and electricity appears to be the most interesting one from the energy efficiency point of view. The actual interest in such an advanced industrial scenario can be estimated only by considering these results together with economical aspects. In addition to investment costs, other critical aspects are the availability of sugarcane over the year, the storage capability and the prices of ethanol sugar and electricity.

A large bagasse-fueled power plant implies that the total site economy highly depends on the price of the electricity and it was shown in Chapter 2 how this value can dramatically affect the profitability of power generation especially in case of advanced power plants for which long pay-back times are usually expected. In case of small CHP plants designed for supporting the sugar and ethanol production the cost of sugarcane can be allocated to the sugar and ethanol products only, the bagasse being in this
case considered as a by-product. In case of the combined production of sugar ethanol and electricity, the cost of the sugarcane must instead be allocated to all the three products, the bagasse resulting a value-product of the sugarcane conversion equivalent to the sucrose-rich juice. Among possible criteria, in case of multi-product energy intensive industrial processes the criterion suggested by the exergoeconomic analysis may be of great help. For this topic the reader is referred to [35, 40, 129].
Chapter 5

Conclusions

The present work aimed at discussing methodologies already documented in the literature and at proposing a new procedure for the synthesis of industrial processes with high heat and power requirements.

In Chapter 2 main methodological aspects are presented. These comprise an overview of Pinch Analysis tools, a discussion about the synthesis of steam networks, a general overview on methodologies on synthesis of power generating plants and finally the description of an organized procedure for the generation and modification of system structural alternatives. In this first chapter two optimization procedures are basically presented and compared: the HEATSEP method (based on the definition of system basic plant configurations) and the 2-level optimization procedure (based on the definition of system superstructures).

In Chapter 3 and 4, the synthesis of the sugarcane conversion plant is discussed. In particular in Chapter 3 the organized procedure for the generation and modification of plant configuration is used for the synthesis of the sugarcane conversion plant for sugar, ethanol and combined production. In this chapter the HEATSEP method is used for the optimization of process parameters following the objective of minimum process energy demand. In Chapter 4 the synthesis of the total site configuration including the bagasse conversion subsystem is presented considering two alternatives: bagasse combustion and bagasse gasification. In this chapter the two-level optimization procedure is considered for the optimization of the design parameters and for the selection of an optimal steam network structure.

Conclusions are drawn in Chapter 5 with particular reference to methodological aspects and to possible further directions of future research.

In agreement with a top-down approach for the synthesis of a generic industrial process, the objective of the synthesis is to define the process configuration leading to the more profitable production of useful product starting from a given amount of raw material. Accordingly the procedure proposed here is based on the organized generation and modification of plant configurations which have in common the same input of raw material. For each plant configuration the attention is drawn to the optimal selection of components of the productive process and of the utility system and their optimal parameters that allow to reduce the process energy consumption while keeping constant the production rates of desired products. For this purpose Pinch Analysis tools are used to evaluate minimum process demand of external energy and also to estimate opportunities for further modifications of plant configurations.

The proposed synthesis procedure was applied to a case study of a sugarcane conversion plant with 138.9 kg/s of cane input. The plant configurations that are explored in this work and in particular in Chapter 3 are those for sugar production, for ethanol production and for combined production of sugar and ethanol. For each plant configuration those design parameters that allow to keep constant the production rate of product(s) are considered constant while those parameters that are related to the process thermal requirement are optimized in order to minimize the process energy demand. For this purpose the HEATSEP method proposed by Lazzaretto and Toffolo was used [80]. Most of the modifications in structure and parameters that were found responsible for great reduction in process thermal demand were located in particular in the multi-effect evaporator and the ethanol distillation subprocesses. For the case of sugar production only, major reductions in process thermal requirement were obtained by
increasing the number of the evaporation effects, while, for the case of ethanol production only, pressurized distillation allows a better process heat integration. In these two first cases the reduction of process thermal requirement is obtained mainly by observing the effect of component staging in the shape of the process grand composite curve. In the case of combined and sugar ethanol production, as a consequence of the simultaneous presence of water evaporation and ethanol distillation, a proper computer-aided optimization procedure was instead necessary to evaluate the optimal parameters of the multi-effect evaporator and of the distillation subsystems. A summary of results of was reported in Table 3.4 on page 102.

The conversion of bagasse for combined heat and power production was taken into consideration in Chapter 4. However, instead of following the organized procedure for the generation and modification of the process alternatives, only two options for the bagasse conversion were considered: bagasse combustion and bagasse gasification. In particular, the structure and the production rates of the productive process were considered fixed to those of the combined sugar and ethanol production plant configuration. The number of evaporation effect is the only structural parameter related to a process component that was subject to modification. In addition the optimal steam network structure is assessed by means of a selection of the optimal structural alternatives included in a superstructure a formulation of which was discussed in Section 2.2.3. The system subject to the optimization comprises therefore three subsystems: the productive process, the bagasse conversion subsystem and the steam network. The three subsystems participate in the heat and power integration problem with heat and power loads that are proportional to the mass flow rates of the main material streams flowing through each single subsystem. Accordingly, a two-level optimization procedure proposed by Marechál et al. was used [42, 90].

**METHODOLOGICAL CONTRIBUTION TO THE SOLUTION OF THE SYNTHESIS PROBLEM**

Looking at the final aim in the synthesis of complex energy systems, consisting in the formulation of a systematic algorithm for BPC generation/modification of a generic complex energy system, in the present work an organized procedure for the synthesis of energy intensive industrial plant was proposed and applied to the case study of the sugarcane conversion plant.

According to this procedure, a Basic Plant Configuration (BPC) is defined according to an original idea of the plant. A BPC comprises all the main productive components while all the thermal streams that are identified by virtually cutting the thermal links between subsequent components are considered among the whole set of thermal streams to be integrated. In reality only a subset of all the possible thermal streams in this way identified are also real heating and cooling processes required by the productive process. Accordingly, the heat recovery potential deriving from the maximum heat integration between thermal streams is evaluated by means of Pinch Analysis rules (in particular by solving the so-called problem table which gives also the shape of the process grand composite curve), while the synthesis of the HENs entitled to physically realized the heat integration is left a separate problem to be solved in future works.

The procedure proposed for the modification of a BPC consists in the three following main steps (to be applied in sequence) for the modification of the BPC:

1. staging of components
2. new material connections between components
3. change components or addition of new components

The first two steps do not significantly alter the nature of the process. In particular, this is strictly true only when staging components (for instance staging of the multi-effect evaporator or distillation). The addition or the change in material connections between components actually do not affect the original idea behind the BPC but can alter the quantity and the quality of the product. For the case study of the sugarcane conversion process, different connections were explored between distillation columns (which lead to different quality of ethanol) and molasses recirculation towards ethanol production was
also considered (which lead to increase ethanol production). The final step leads to the generation of new BPCs. In reality one could suggest a BPC that is completely different from the original one (base case). While in general it is possible to conceive completely different processes converting the same raw material into different products, it is more common, when adopting a top-down design approach of the process (looking at the different production alternatives from the same amount of raw material) that a set of basic plant configurations share the same subset of sub-processes (components) responsible for the basic transformations of the raw material. For the case of the sugarcane conversion plant, these are the juice extractions and the juice treatment sub-processes.

As stated in the Introduction, it was worth pointing out that the suggested procedure responds to the need of generating/modifying process alternatives in order to explore further potential for heat and power integration (by multiplying the number of heat sources and heat sinks in the process). Thus, the general problem of the definition of the most profitable set of components and their connections (the ultimate objective of process synthesis) still remains partially to be solved. However, the methodology presented here could be used also for this larger purpose by looking for the values of all the operating parameters that maximize the overall process profitability for each new BPC.

Indeed one of the major aspects to be taken into account when dealing with energy intensive industrial processes is the process energy efficiency which is considered as the objective in the present work. Accordingly, for each new BPC only those parameters affecting the thermal demand of the process were optimized here. These parameters were selected using the so-called HEATSEP method [80] which, in addition to the aforementioned idea of separating the problem of the HEN synthesis from the problem of the BPC synthesis by virtually cutting thermal links between subsequent components, suggests to include all the independent end-temperatures and mass flow rates resulting from these cuts into the set of decision variables. This approach was shown to be particularly effective for the synthesis of power generating plants (the reader is referred to the following examples in the literature [79, 128]). In this work the same approach was applied to the design optimization of the sugarcane conversion plant where, however, most of the temperatures are imposed by productive requirements.

CRITICAL REMARKS AND IDEAS FOR FUTURE RESEARCH

An important part of the present work was spent for the discussion of different methodologies for the synthesis of CHP systems and power generating plants. This arose spontaneously from the nature of the energy intensive industrial processes which in most cases require a CHP system to support the high thermal and power demand of the productive process. In addition, for the case of the sugarcane process, a great amount of by-product (bagasse) with high energy content can be used to fuel a CHP plant and possibly for additional power generation leading to the forth process concept that was analyzed here, consisting in combined sugar, ethanol and electricity production. On the other hand, CHP systems (considered as stand-alone facilities) or power generating systems can be seen as a subset of industrial processes (in terms of energy consumption, internal heat transfer processes and generation of goods) so that the same methodology of generation/modification of basic plant configurations may apply. In this case, it is worth observing that the aforementioned dichotomy between the problem of the synthesis of the BPC leading to maximum quality and quantity of products and the problem of maximum primary energy saving does not apply anymore, the ultimate objective of the synthesis coinciding in general with maximum energy efficiency (or plant profitability including capital costs and revenues from electricity sale). For the synthesis of power generating plants, of which CHP plants can be considered as a particular case with the additional constraint of satisfying a process thermal requirement, different approaches were proposed in the literature. Among others, the discussion in the present work focused on those methodologies based on the usual separation between the synthesis and design of BPC components and the HEN synthesis responsible for the system internal heat recovery.

Again, the issue is how to generate/modify the system BPC. Accordingly, we observed in this work that when looking at process energy efficiency the strategies that are used for the synthesis of a general industrial process do not differ from those that can be used for the synthesis of power generating plants.

In particular, two strategies were considered here. One consists in the definition of a superstructure
embracing since the beginning all the possible system alternatives (about this topic the reader is referred for instance to the following works in the literature [42, 90, 91, 105]). The other one consists in letting the generation of the system BPC to be an open issue in the synthesis problem itself and trying to adopt systematic procedure for modifying the BPC. This latter strategy was already partially introduced in the literature as an extension of the HEATSEP method [79, 76]. In the author point of view, after having carried out research periods in different laboratories which employ these two different strategies (at the Industrial Energy System Laboratory at EPFL in Lausanne and at the Department of Mechanical Engineering at University of Padova), the two strategies show different potentials.

When it is possible to identify parts of a system that participate linearly (for instance through their main material mass flow rates) in the objective function(s), the definition of a superstructure seems particularly helpful since it can be combined with a two-level structural and parametric optimization procedure. In a first level the intensive parameters responsible for non-linearities in the objective function are optimized while in a inner second level the mass flow rates and the structure (active parts of the superstructure) are optimized by means of (mixed integer) linear programming techniques. This was shown for the case of the synthesis of CHP systems based on steam networks (see figure 2.22 on page 2.22) a linear mathematical model of which (already introduced in the literature in [105]) was presented in Section 2.2.3.

The formulation of a superstructure is in fact particularly useful when there is a high number of process combinations (i.e. integer variables) that can be described with a relatively simple model. On the other hand, the formulation of the superstructure requires defining the system structural alternatives in advance. In this case the major effort in solving the synthesis problem is shifted towards the need of robust MI(N)LP solvers.

The second synthesis strategy, based on the systematic modification of process structures, can potentially overcome this drawback. When dealing with a large number of system structural alternatives (and when their formulation in terms of superstructure becomes too large) the generation of system BPCs is left as an open issue. Starting from a given base case BPC, this strategy aims then at systematically modifying this BPC by introducing in sequence: component staging, new connections between components, new components. This strategy was applied in Chapter 3 for the modification of the base case BPCs converting sugarcane into sugar and ethanol, while in Chapter 4 two BPCs for the bagasse conversion subsystem were proposed and for each case a superstructure formulation of the steam network was preferred instead. For each structural alternative it is necessary to perform a parameter optimization. As a result of large process structures, the number of design parameters to be optimized can be quite large.

This is a general issue in the synthesis of complex energy systems that can be faced by reducing the total system optimization problem in a sequence of subproblems. The two-level optimization procedure based on a superstructure indeed reduces the overall optimization problem into the two subproblems associated with the two levels. When instead the second synthesis strategy is applied, the parameter optimization involves the overall system structure. In this case decomposition strategies suggested in the literature, like those discussed in Section 2.3.4, are quite promising, especially when it is easy to identify a physical separation between subsystems. The idea of decomposing the system into subsystems (i.e. the overall optimization problem into subproblems) is, however, particularly challenging when the system benefits from a high degree of heat and power integration. In fact, being the HEN synthesis considered as a separate problem, it is in any case necessary to verify the feasibility of the heat transfer between thermal streams (by means of Pinch Analysis rules). In particular the main difficulties arose when the set of thermal streams includes thermal streams belonging to different subsystems, so that the set of constraints to be considered in each optimization subproblem must account for the response of the other sub-systems to the change of heat loads and temperatures of the thermal streams belonging to the subsystem in hand.

The final aim of the research, which is left to further investigation in future works, consists in developing an algorithm (to be translated into a computer code) that automatically modifies a given base case BPC. The major problem to overcome is the mathematical description of the criteria for BPC modification which must rely on intrinsic process properties. For instance, in case of steam networks, instead of defining the superstructure including all options about steam and condensate headers (as in
Section 2.2.3), a possible direction of work consists in starting from the concept of an elementary steam cycle and then let the algorithm modify components (like steam turbines) by introducing staging and new connections between components so that new steam and condensate headers are generated throughout the optimization and not defined \textit{a priori}. 
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Appendix A

Computational tools

In the present work a set of computational tools, some of which developed at the Industrial Energy System Laboratory at EPFL, was used to carried out simulations and optimizations of the different process alternatives of the sugarcane plant considered in Chapter 3 and 4.

The different tools that were used for different purposes are:

- Matlab Simulink 7 for sugarcane process modeling and simulation [124].
- Aspen Plus 11 for detailed modeling and simulation of distillation columns [4].
- Belsim Vali 4.4 for detailed modeling and simulation of bagasse combustion and gasification and of gas turbines [132].
- Easy 2.0 for solving heat and power integration problems (and for generating all the Composite Curves in the present work) [26].
- MOO for multi-objective optimization based on a genetic algorithm [82].

In order to systematically handle the data recollection from the simulation environment and to pass the information to the heat and power integration software and to the multi-objective optimizer (when performing optimizations), the communication and computation platform OSMOSE developed at LENI was used [103]. This platform is coded in the Matlab environment [93]. It consists in a structure of Matlab files which activate different computation plug-ins, some being third-party softwares, and share, recollect and store information by means of a structure variable o. For a better description of OSMOSE the reader is referred to [42].

A.1 Programming a computation with OSMOSE platform

The computation procedure is handled systematically by OSMOSE provided that some fields of the so-called frontend file, which is the main OSMOSE user interface, are properly filled with the information about the specific model and the type of computation that must be performed. In Figure A.1 an example of frontend is shown where it is possible to recognize the structure variable o which eventually contains the information about the model, type of computation and results. In the first instance the type of computation must be declared. This is done through activating given computation subroutines with binary (logic) variables (e.g. DoOneRun=1 for enabling a single calculation iteration, DoSensi=1 for enabling a sensitivity analysis, DoMoo=1 for enabling the genetic algorithm based optimizer, etc.). Detailed information is then given in corresponding subroutines that follow the model definition (e.g. if DoOneRun=1 then the field DefineOneRun must be properly filled in). The subroutine DefineModel is instead the part of the frontend in which the information about the model must be provided. This part includes the actual model of the system in its simulation environment (which in general can be different than Matlab) and the definition of the heat and power integration problem if this latter problem is left to be solved as a MILP optimization problem by means of a separate software.
function o = frontend

% DoOneRun = 1; % Perform a single evaluation of your model % 1: yes, 0: no
% DoSensi = 0; % Perform a sensitivity analysis % 1: yes, 0: no
% DoMoo = 0; % Perform an optimisation with moo % 1: yes, 0: no
% DoRestartMoo = 0; % Restart an optimisation with moo % 1: yes, 0: no
% DoPushPareto = 0; % Optimizes each point of the pareto front %
% DoRecompute = 0; % Recompute the points on the Pareto front to get the
% DoParetoAnalysis = 0; % Plot figures for analysis of the Pareto results
% DoAutoReport = 0; % Generate an automatic report of the computation %
% DoCustomReport = 0; % Generate a custom report of the computation % 1:
% o = launch_osmose(o);

Figure A.1: Snapshot of OSMOSE frontend
A.1.1 Definition of the model

The model definition starts with some classification entries which are useful for a subsequent identification of the model within a database. The fields within the “Direct access” paragraph are used to point to the actual system model file which can be a process flow-sheet diagram built with a third party software (e.g. Aspen Plus, Belsim Vali, etc.) or simply other Matlab code, expressing the relation between given input and output variables (model Tags ). Accordingly, all the variables that are defined as constant (Status = \{'CST'\} ) are the input variables also called model parameters, while all the output variables are defined as dependent (Status = \{'OFF'\} ). In this work Matlab Simulink is used as the main modeling environment. The modeling of the sugarcane process in Matlab Simulink is discussed in more detail in Section A.3.

One of the potentials of the OSMOSE platform, which however was only partially exploited in this work, is that the information exchange between the frontend and different third party environments is handled through already built communication handlers. Thus, as soon as one of these third party simulation environments are recognized within the field model.software, a proper handler is activated which allows to set values of input variables, run the simulation of the model by means of the third-party utility in batch mode, recollect output variables and store all the simulation details within the structure variable o.

The definition of the input variables is done within the “Model Parameters” paragraph. Each input variable (model parameter) is defined by assigning several attributes among which the most important are the unique name of the variable (TagName ), its status as constant or dependent variable (Status ), its default numerical value (DefaultValue ) and the variable unit (this attribute is critical for the third party simulation environment where values of variables are always associated to a given unit system).

In order to use the Simulink environment, for which a pre-defined communication handler has not yet been embedded in OSMOSE, a simple external function for each Simulink model (e.g. cane_sugar2.m in Figure A.2) was programmed. A snapshot of the Simulink communication handler for the Simulink file smlk_cane_sugar02containing the process model is shown in Figure A.3. In this separate function, model parameters (model Tags with Status = \{'CST'\} ) as defined in the frontend, are recollected and evaluated in the current Matlab working space so that they can be accessed by the Simulink Environment. Subsequently, the simulation is activated. As soon the simulation is performed all the model dependent variables that were saved automatically in the Matlab working space throughout the simulation are stored in the structure variable o to be accessible for subsequent calculations.

A.2 Definition of the heat and power integration problem

The heat integration problem of a set of stream can be solved within the OSMOSE environment as a linear programming optimization problem in which the heat cascade problem is set as a linear constraint according to the Pinch Analysis rules (see Equation (2.2)). This optimization is performed by means of a separate software called Easy [26] which is run by OSMOSE provided that the problem is defined with a specific formalism. This external software is basically an optimization environment for MILP problems. Accordingly, several problems in the field of energy systems can be solved using Easy. Among others, the most common problem is to evaluate the MER (Minimum Energy Requirement) hot utility and cold utility demands of a given process (with a given set of thermal streams). Another common problem to be solved within Easy involves the definition of the structure and mass flow rates of a system starting from a system superstructure in which each subsystem’s contribution to the system heat integration and to the system power generation or demand can be expressed as a linear function of the mass flow rate of a material stream. This synthesis procedure is part of the two-level optimization strategy described in Section 2.2.4 (see Figure 2.22) and in Section 2.3.5 (see Figure 2.33).

In the light of this latter problem, which involves the definition of a system superstructure with several subsystems, the definition of the set of thermal streams to be integrated is done following a grouping strategy. The suggested formalism in OSMOSE consists in Groups containing Units which contain Streams. An example of a definition of such a superstructure is given in Figure A.4.

A thermal Stream is properly identified by its unique TagName, its parental Unit (Parent) and by
% Classification by grouping
model GROUP = ('Chemical process');
model TYPE = ('Sugar cane conversion plant');
model SUBTYPE = ('Sugar production');

% model detail level
model PHYSICAL_REPRESENTATION = ('0d');

% Direct access
model FILENAME = ('cane_sugar_02.m');
model MAINFILE = ('cane_sugar_02.m');
model LOCATION = ('$\.working_folder\sugar\_cane\sugar\');
model SOFTWARE = ('Matlab');

% User tagging
model TAGNAME = ('sugar cane');
model DISPLAYNAME = ('sugar cane');
model DESCRIPTION = ('conversion of sugarcane into sugar only');

% Model parameters
nc = 0;
nc = nc + 1;
model TAGS(nc).DISPLAYNAME = ('\\_EVAP');
model TAGS(nc).TAGNAME = ('\\_EVAP');
model TAGS(nc).DESCRIPTION = ('\texttt{switch for multi-effect evaporator}');
model TAGS(nc).DEFAULTVALUE = 3;
model TAGS(nc).UNIT = {'\'};
model TAGS(nc).STATUS = ('CST');
model TAGS(nc).isVIT = 10;
%
nc = nc + 1;

Figure A.2: Snapshot of the subroutine DefineModel in OSMOSE frontend
Definition of the heat and power integration problem

Figure A.3: Snapshot of the OSMOSE code for systematic exchange of simulation variables between OSMOSE and Simulink

```matlab
function o = conc_sugar_02(s)
    % calling the 'o' structure to get the model parameters
    id = find(strncmp('CST',o.Model.Tags.Status,1)) ;
    n_par = length(id);
    for i=1:n_par
        eval(sprintf('s%d = %s;',id(i)),char(o.Model.Tags(id{i}).TagNames{1}));
    end
    % Simulation environment parameters
    options = simset('hurricane') ; % get simulation parameters from another file
    options = simset(options,'SrcWorkspace','current'); % set the model workspace
    % Model simulation
    load var_vec; % loading tables of constant parameters
    fprintf('Running Simulink ...
')
    sim('smil_conc_sugar_03',1,options);
    fprintf('OK \n')
    % Tags assignment (Model outputs)
    s = who;
    n_var = length(s);
    nt = 0;
    for i=1:n_var
        s(i).name = cellstr(s(i).name);
        id_tag = strmatch('tag',s(i).name);
        if id_tag == 1
            nt=nt+1;
            Tags(nt).TagName = s(i).name;
            Tags(nt).DisplayName = s(i).name;
            Tags(nt).Status = {'OFF'};
            value = eval(char(s(i).name));
            Tags(nt).Value = value.signals.values;
        end
    end
    o = update_model_tags(o,Tags);
end
```
%% Groups
ng = 0; ng = ng+1;
model.EI.Groups(ng).TagName = ('sugar_cane');
model.EI.Groups(ng).DisplayName = ('sugar_cane');
model.EI.Groups(ng).Description = ('sugar cane total process');
model.EI.Groups(ng).AddToProblem = 1;
ng = ng+1; ...

%% Units
nu = 0; nu = nu+1;
model.EI.Units(nu).Type = ('process');
model.EI.Units(nu).TagName = ('pro1');
model.EI.Units(nu).DisplayName = ('pro1');
model.EI.Units(nu).Parent = ('sugar_cane');
model.EI.Units(nu).AddToProblem = 1;
model.EI.Units(nu).ITY = ('O');
model.EI.Units(nu).Flin = ('O');
model.EI.Units(nu).Fmax = ('1000');
model.EI.Units(nu).Cost1 = ('O');
model.EI.Units(nu).Cost2 = ('O');
model.EI.Units(nu).Conv1 = ('O');
model.EI.Units(nu).Conv2 = ('O');
model.EI.Units(nu).Power1 = ('O');
model.EI.Units(nu).Power2 = ('O');
nu = nu+1; ...

%% Streams
ns = 0; ns = ns+1;
model.EI.Streams(ns).Type = ('q');
model.EI.Streams(ns).Parent = ('pro1');
model.EI.Streams(ns).TagName = ('H_L01');% Inlet flow enthalpy [kJ/kg]
model.EI.Streams(ns).Tin = ('Tag_Tin_L_1');% Inlet temperature [K]
model.EI.Streams(ns).Min = ('Tag_O_L_1');% Outlet flow enthalpy [kJ/kg]
model.EI.Streams(ns).Tout = ('Tag_Tout_L_1');% Outlet temperature [K]
model.EI.Streams(ns).Hout = (0);% Outlet flow enthalpy [kJ/kg]
model.EI.Streams(ns).Dmin_2 = (2);% Minimum temperature approach [K]
ns = ns+1; ...

Figure A.4: Snapshot of OSMOSE code for the definition of a set of constant thermal streams
declaring its type. This latter field is used to distinguish between thermal Streams \{\textit{\textquoteleft}qt\textquoteright\} and other types of Streams (e.g. material). Numerical values must be assigned to its inlet and outlet temperatures and its heat load (defined as the difference between inlet and outlet enthalpy rates). These values are recollected from the structure variable \textit{o} in which simulation results have been previously stored.

Furthermore a value must be assigned to the minimum temperature difference contribution (\textit{DTmin,2}) of the Stream. This is in fact used to set the so-called problem table according to the Pinch Analysis rules of which an example is given in Section 2.1.1.1. A common way to account for the minimum temperature difference \(\Delta T_{\text{min}}\) between hot and cold thermal streams is in fact to shift up (in terms of temperatures) the whole Cold Composite Curve by \(\Delta T_{\text{min}}/2\) and shift down the whole Hot Composite Curve by the same quantity so that the activation of the heat transfer feasibility constraint is graphically represented by the point in which the two curves touch each other. An alternative way is to assign different values of such minimum temperature difference contributions to different thermal streams depending on their heat transfer properties. In technical practice it is common to consider greater values of minimum temperature difference when the heat transfer involves material streams with poor heat transfer properties (e.g. low convective heat transfer coefficients). For a detailed discussion about this alternative method for accounting the minimum temperature difference between thermal streams the reader is referred to \cite{84}.

Similar fields are then used to define Units and Groups. In particular, depending on the way the heat and power loads of a Unit are acting in the optimization, different types of Units can be considered. In case heat loads must be considered constant a Unit is addressed to be of the \textit{process} type, whereas in case the heat loads must be adjusted through the optimization (by adjusting the mass flow rate of the main material stream) a Unit is considered of the \textit{utility} type.

If a synthesis problem is formulated as a MILP optimization problem in which mass flow rates are the linear decision variables and binary variables are used to enable subsystems (Unit), a system superstructure must be defined with the aforementioned formalism in OSMOSE. In this case at least one \textit{process} Unit (which fixes the size of the heat and power loads) and one \textit{utility} Unit. A \textit{utility} Unit is associated with a binary variable and a real variable which are adjusted in order to meet the objective of the MILP optimization (e.g. minimum operating costs, minimum annual costs, maximum power, etc.). As an example, we recall here the problem of minimum operating costs of an industrial site in which a given productive process participate in the total heat and power integration with constant loads and a CHP system is used to cover part or total the process heat and power requirements. The CHP system plays the role of the \textit{utility} Unit, which size can be adjusted in order to minimize the total site operating costs. Additional hot and cold utility Streams (grouped in separate Units) are also to be considered since in general it is also possible that the CHP system is used only to partially cover the process thermal requirements, the remaining part being instead covered by a hot utility (e.g. combustion) and by an environmental cold utility (e.g. water or air). An example of OSMOSE code for the definition of such a heat and power integration problem is shown in Figure A.5 in which the detailed definition of Groups, Units and Streams was omitted since they have already been shown in Figure A.4.

The MILP formulation of \textit{utility} Units, which are the parts of the system superstructure that are subject to adjustments through the optimization, is done by filling in given fields of the unit variable (\textit{\textquoteleft}utility\textquoteright)). The general MILP problem involves the assignment of binary variables for enabling given units. When instead all the Units are considered to appear also in the final structure, the problem is reduced to a LP problem where only mass flow rates are adjusted. Different problem formulations are then activated by means of the field \textit{ITY} : set \textit{ITY}=\textquoteleft0\textquoteright for \textit{process} Units, set \textit{ITY}=\textquoteleft1\textquoteright for LP problems, set \textit{ITY}=\textquoteleft2\textquoteright for MILP problem.

The real variables of the MILP problem are not referring to the same mass flow rates of the model simulation environment. In fact the heat and power integration problem is solved after the actual system model is simulated. The idea is to evaluate mass and energy balances of each of the subsystems (Units) by means of an external modeling and simulation tool (e.g. Aspen, Vali, Simulink, etc.). Then the optimal combination of Units and their optimal mass flow rates are found as a result of the subsequent MILP optimization which accounts for the heat and power integration of the Units. Thus the adjustment of the mass flow rate of a \textit{utility} Unit is done by simply considering an additional variable \textit{F} used as a multiplication factor of all the heat loads of thermal streams and powers belonging to the Unit.
%% Groups
ng = 0;
ng = ng+1; model.EI.Groups(ng).TagName = ('sugar_cane');
...
ng = ng+1; model.EI.Groups(ng).TagName = ('Bag_COMB');
...
ng = ng+1; model.EI.Groups(ng).TagName = ('SNR');
...

%% Units
nu = 0;
uu = nu+1; model.EI.Units(uu).Type = ('process');
model.EI.Units(uu).TagName = ('pro1');
model.EI.Units(uu).Parent = ('sugar_cane');
...
uu = nu+1; model.EI.Units(uu).Type = ('process');
model.EI.Units(uu).TagName = ('pro2');
model.EI.Units(uu).Parent = ('sugar_cane');
...
%------------------------------------- bagasse combustions -------------------------------------
uu = nu+1; model.EI.Units(uu).Type = ('utility');
model.EI.Units(uu).TagName = ('pro9');
model.EI.Units(uu).Parent = ('Bag_COMB');
...
%------------------------------------- steam cycle -------------------------------------
uu = nu+1; model.EI.Units(uu).Type = ('utility');
model.EI.Units(uu).TagName = ('steam');
model.EI.Units(uu).Parent = ('SNR');
...
% ------------------------------------- other utilities -------------------------------------
uu = nu+1; model.EI.Units(uu).Type = ('utility');
model.EI.Units(uu).TagName = ('cold');
model.EI.Units(uu).Parent = ('main');
...

%% Streams
...

Figure A.5: Snapshot of OSMOSE code for the MILP formulation of a heat and power integration problem
Definition of the heat and power integration problem

particular a linear expression of the power load of a Unit can be given by means of a linear combination of the coefficients Power1(constant coefficient) and Power2(which is multiplied with the multiplication factor $F$). Ideally the energy and mass balances are previously evaluated for 1 kg/s of mass flow rate of each system Unit, so that the values of the variable $F$ of a Unit corresponds to the actual optimal mass flow rate.

Accordingly, boundary conditions for the additional variable $F$ are given with the Fmin and Fmax fields. Cost functions are to be given as linear functions of the multiplication factor. The values of the coefficients for the operating cost function are given with the Cost1 and Cost2 fields, while values of the coefficients for the capital cost function are given with the Cinv1 and Cinv2 fields.

The solution of the heat and power integration problem is activated in the frontend file as one of the last commands (o.ComputeEI=1) of the “model definition” section as shown in Figure A.6. The objective function must be declared according to the different types of problem to be solved. A post computation is also possible provided that it is properly programmed in a separate file which path and name has to be specified in the model.PostEIMFunction field.

A.2.1 Modeling steam network superstructures in OSMOSE

The formulation of steam network superstructures can be done in OSMOSE by describing the thermal streams that are related to the operation of elementary structural components of a steam network. According to the MILP formulation of the steam networks synthesis problem discussed in Section 2.2.3 a steam network can be built by assembling steam headers, condensate headers connected by steam production headers and steam condensation headers. While steam and condensate headers correspond to given thermodynamic states of the water (which intensive thermodynamic variables are given as model parameters to be optimized in an outer optimization level), steam production headers and steam condensation headers are thermodynamic transformations (thermal processes) which generate a given number of thermal Streams. The formulation of such elementary structural components of steam network superstructures is implemented in OSMOSE through a specific formalism, of which an example is given in Figure A.7. This consists in the definition of Units generating thermal streams which explicit definition is avoided in OSMOSE since it is done automatically (as a result of the definition of thermodynamic states of steam and condensate headers) in the Easy environment.

The Units to be defined are: SYNHEAV for steam production headers (in which the end-steam header is defined), SYNHEAC for steam condensation headers (in which the end-condensate header is defined). In order to specify the thermodynamic state of the steam at the turbine outlet the Unit SYNHEAVU is
Figure A.7: Snapshot of OSMOSE code for the formulation of a steam network superstructure

```plaintext
%-------- Definition of Steam Network Units -----------------------------
nu = nu+1;
technology.EL.Units[nu].Type=('SYNHEAV'); %Steam Production Header
technology.EL.Units[nu].TagName = ('SYNHEAV');
technology.EL.Units[nu].Parent = ('ENK');
technology.EL.Units[nu].Pressure=('SU');
technology.EL.Units[nu].Temperature=('SU0');
technology.EL.Units[nu].SuperheatingDT=('1');
technology.EL.Units[nu].Vapf=('1');
technology.EL.Units[nu].DTmin_2=('5');
...
uu = nu+1;
technology.EL.Units[nu].Type=('SYNHEAV'); %Steam Header
technology.EL.Units[nu].TagName = ('SYNHEAV1');
technology.EL.Units[nu].Parent = ('ENK');
technology.EL.Units[nu].Pressure=('@backpressure');
technology.EL.Units[nu].Temperature=('1');
technology.EL.Units[nu].SuperheatingDT=('20');
technology.EL.Units[nu].Vapf=('1');
technology.EL.Units[nu].DTmin_2=('5');
...
uu = nu+1;
technology.EL.Units[nu].Type=('SYNHEAC'); %Condensate Header
technology.EL.Units[nu].TagName = ('SYNHEAC1');
technology.EL.Units[nu].Parent = ('ENK');
technology.EL.Units[nu].Pressure=('@backpressure');
technology.EL.Units[nu].Temperature=('1');
technology.EL.Units[nu].SuperheatingDT=('0');
technology.EL.Units[nu].Vapf=('0');
technology.EL.Units[nu].DTmin_2=('5');
...```
introduced and its pressure is set at the same level of the SYNHEAC Unit. This let to produce steam to be used at that pressure level for heating purposes only.

Thermodynamic states of steam and condensate headers are specified by means of the pressure, temperature, vapf and SuperheatingDT fields.

A.3 Modeling the sugarcane process in Matlab Simulink

Simulink is a Matlab software package for modeling, simulating and analyzing dynamical systems. In the present work all of the systems were considered in steady state condition therefore in principle there is not the need for such modeling and simulation environment. Simulink solves Ordinary Differential Equations (differential equations containing functions and derivatives of the time only) numerically. In the general case of a dynamical system, the system behavior within a given time span is in fact described in terms of such differential equations. In Simulink the model is described in terms of algebraic equations of the Laplace operator $s$ by using simple algebraic operators. Due to the recurrence of the same types of differential equations in several physical domains, a library of pre-defined functions (blocks) is available in Simulink.

Such a modeling method is well suited to be represented by a graphical interface available in Simulink in which blocks are connected to each other by input and output signals (arrays of variables which are in general functions of the time).

While the general purpose of such an environment is to simulate dynamical systems, Simulink can also be used for other purposes for instance to numerically solve non-linear equations and to evaluate simple mathematical expressions. In this case used is as graphical interface of the Matlab environment thus allowing to access a large set of computation utilities. This motivates the use of Simulink also for modeling steady state systems although its full capability is not exploited in this latter case.

Accordingly, Simulink models of the sugarcane conversion plant for sugar and ethanol production were built to perform all the analysis in the present work and were properly embedded in the OSMOSE environment as described in Section A.1.

As an example, the overview of the model of the sugarcane process for combined sugar and ethanol production is presented in Figure A.8 where physical subprocesses (e.g. juice extraction, treatment, multi-effect evaporator, etc.) are shown in green. In the same graphical representation of the process, thermal streams data are displayed in red (hot) and blue (cold) and electrical or mechanical energy demands in black. Different subprocesses are linked to each other by signals passing on the values of the main variables characterizing the material streams (e.g. mass flow rate, temperature, pressure, solid concentration, juice purity, etc.).

Each subprocess contains other Simulink subsystems in which component characteristics are modeled with a set of elementary transfer functions. This modeling strategy is translated into an equivalent hierarchical representation of the system in terms of Simulink graphical (and computational) objects as shown in Figure A.9. While most of the material transformations (splitting or mixing of material streams) are described in terms of simple algebraic expressions between input signals or programmed in separate Matlab routines which are automatically called by the Simulink environment.

The model is simulated by numerically solving the subsystem sequentially (from output signals for given values of the input signals). Accordingly, if a system (subprocess, component or elementary transfer function) characteristic is modeled by means of any sort of signal loop (when transfer function are given in implicit form), the state of the model (at a given time if the model is dynamical, or the steady state) is eventually assessed by means of several convergence loops. Such loops were avoided while modeling the sugarcane conversion plant thus leading to a pure fixed-state evaluation of a sequence of algebraic functions.

A.4 Optimizing model parameters with MOO

The optimization of model parameters is done by activating the MOO computation in the frontend as described in Figure A.1. The optimization parameters are set in the DefineMooOptim subrou-
Figure A.8: Overview of the Simulink model of the sugarcane plant for the combined sugar and ethanol production (case CSE3 in Section 3.3.2)
Figure A.9: Hierarchical process flow-sheeting using Simulink
The MOO optimizer is based on a genetic algorithm. Some of the most critical parameters of this type of algorithms are the size of initial population (InitialPopulationSize) and the stopping criterion based on the maximum number of iterations (max_evaluations). Other parameters regarding the type of crossover, mutation or selection functions are currently not accessible via OSMOSE. The default criteria used by MOO are documented in [82]. The optimization problem is correctly set up once the objective function(s) and the decision variable(s) are specified. While the genetic algorithm of the MOO optimizer is not able to implement any type of constraints, it is however necessary to set proper boundaries of the search space by assigning the Limits of the possible range of variation of each decision variable. Integer decision variables can also be considered in the optimization. Such variables are distinguished from the real variables by means of the Is_integer field.

```matlab
function o = DefineMooOptim(o)

% Definition of the optimization problem

% Number of objectives [required]

% Number of maximal iterations [required]

% Size of the initial population, i.e. m

% Objectives definition

% Define the decision variables [required]

% ModelTagName = {'sugar_cane'};

% TagName = {'p_net'};

% MinOrMax = {'max'};

% DisplayName = {'Net Power'};

% Define the decision variables [required]

% ModelTagName = {'sugar_cane'};

% DisplayName = {'p stripper'};

% TagName = {'p stripper'};

% Unit = {''};

% Limits = [1 5];

% Is_integer = 0;
```

Figure A.10: Snapshot of OSMOSE code for setting the MOO optimization
Bibliography


# SYNTHESIS OF ENERGY INTENSIVE INDUSTRIAL PROCESSES: METHODOLOGICAL ASPECTS AND A CASE STUDY OF A SUGARCANE CONVERSION PLANT

## Errata

Matteo Morandin  
September 6, 2010

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Chapter 3

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Chapter 4

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Chapter 5

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